ARTICLE IN PRESS
Discrete Applied Mathematics xxx (xxxx) xxx

Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

Lower bounds and properties for the average number of colors in the non-equivalent colorings of a graph

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ARTICLE INFO

Article history:
Received 15 July 2021
Received in revised form 16 June 2022
Accepted 23 August 2022
Available online xxxx

Keywords:
Graph coloring
Average number of colors
Graphical Bell numbers

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. We study the average number $\mathcal{A}(G)$ of colors in the non-equivalent colorings of a graph G. We conjecture several lower bounds on $\mathcal{A}(G)$, determine the value of this graph invariant for some classes of graphs and give general properties of $\mathcal{A}(G)$ which we will use for proving the validity of the conjectures for specific families of graphs, namely chordal graphs and graphs with maximum degree at most 2.

1. Introduction

A coloring of a graph G is an assignment of colors to its vertices such that adjacent vertices have different colors. The chromatic number $\chi(G)$ is the minimum number of colors in a coloring of G. 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 [1,7–9,11,12] under the name of (graphical) Bell number.

Recently, Hertz et al. [10] have defined a new graph invariant $\mathcal{A}(G)$ which is equal to the average number of colors in the non-equivalent colorings of a graph G. It can be seen as a generalization of a concept linked to Bell numbers. More precisely, the Bell numbers $(\mathsf{B}_n)_{n\geq 0}$ count the number of different ways to partition a set that has exactly n elements. The 2-Bell numbers $(\mathsf{T}_n)_{n\geq 0}$ count the total number of blocks in all partitions of a set of n elements. Odlyzko and Richmond [14] 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 graph invariant $\mathcal{A}(G)$ that we study in this paper generalizes A_n. Indeed, 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. Hence, for a graph of order n, $\mathcal{A}(G) = \mathsf{A}_n$ if G is the empty graph of order n.

The close link between Bell numbers and graph colorings indicates that it is possible to use graph theory to discover nontrivial inequalities for the Bell numbers. For example, as shown in [10], $\mathcal{A}(\mathsf{P}_n) = \frac{\mathsf{B}_n}{\mathsf{B}_{n-1}}$ and $\mathcal{A}(\mathsf{P}_n) < \mathcal{A}(\mathsf{P}_{n+1})$ for $n \geq 1$, where P_n is the path on n vertices. This immediately implies $\mathsf{B}_n^2 < \mathsf{B}_{n-1}\mathsf{B}_{n+1}$, which means that the sequence $(\mathsf{B}_n)_{n\geq 0}$ is strictly log-convex. This result has also been proved recently by Alzer [2] using numerical arguments.

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https://doi.org/10.1016/j.dam.2022.08.011
0166-218X/

Please cite this article as: A. Hertz, H. Mélot, S. Bonte et al., Lower bounds and properties for the average number of colors in the non-equivalent colorings of a graph, Discrete Applied Mathematics (2022), https://doi.org/10.1016/j.dam.2022.08.011.

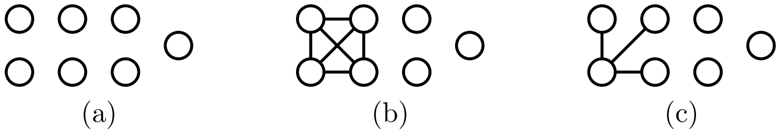

Fig. 1. Three graphs that reach the lower bounds of Conjectures 1, 2 and 3.

Very little is known about $\mathcal{A}(G)$ and there is to date no study concerning extremal properties of this graph invariant. The best possible upper bound for $\mathcal{A}(G)$ is clearly the order n of G since all colorings of G use at most n colors and $\mathcal{A}(\mathsf{K}_n) = n$ for the clique K_n of order n. It seems however much more complex to define a lower bound for $\mathcal{A}(G)$, as a function of n, which is reached by at least one graph of order n. We think that the best possible lower bound is reached by the empty graph $\overline{\mathsf{K}}_n$ of order n (i.e., the graph of order n with no edges).

Conjecture 1. *Let G be a graph of order n. Then,*

$$\mathcal{A}(G) \geq \mathcal{A}(\overline{\mathsf{K}}_n)$$

with equality if and only if G is isomorphic to $\overline{\mathsf{K}}_n$.

Note that despite the apparent simplicity of Conjecture 1, its validity cannot be proven by simple intuitive means such as sequential edge removal. Indeed, there are graphs G for which the removal of any edge strictly increases $\mathcal{A}(G)$. This is the case, for example, for the complete bipartite graph with two vertices in one set of the bipartition and four vertices in the other set.

The next two conjectures are stronger in the sense that, as shown in Section 5, it suffices to show that one of them is true to prove the validity of Conjecture 1. Let $G \cup p\mathsf{K}_1$ be the graph obtained from G by adding p isolated vertices, let K_n be the clique of order n, and let $\mathsf{K}_{1,n-1}$ be the star of order n (i.e. the graph with one vertex of degree $n-1$ and $n-1$ vertices of degree 1).

Conjecture 2. *Let G be a graph of order n. Then,*

$$\mathcal{A}(G) \geq \mathcal{A}(\mathsf{K}_{\chi(G)} \cup (n-\chi(G))\mathsf{K}_1)$$

with equality if and only if G isomorphic to $\mathsf{K}_{\chi(G)} \cup (n-\chi(G))\mathsf{K}_1$.

Conjecture 3. *Let G be a graph of order n. Then*

$$\mathcal{A}(G) \geq \mathcal{A}(\mathsf{K}_{1,\Delta(G)} \cup (n-\Delta(G)-1)\mathsf{K}_1)$$

with equality if and only if G is isomorphic to $\mathsf{K}_{1,\Delta(G)} \cup (n-\Delta(G)-1)\mathsf{K}_1$, where $\Delta(G)$ is the maximum degree of G.

The three conjectures come from the discovery systems *GraPHedron* [13] and *PHOEG* [3]. For illustration, by exhaustive enumeration, we have checked that:

- the graph of Fig. 1(a) minimizes $\mathcal{A}(G)$ among all graphs G of order 7;
- the graph of Fig. 1(b) minimizes $\mathcal{A}(G)$ among all graphs G of order 7 and chromatic number $\chi(G) = 4$;
- the graph of Fig. 1(c) minimizes $\mathcal{A}(G)$ among all graphs G of order 7 and maximum degree $\Delta(G) = 3$.

In the next section we fix some notations, while Section 3 is devoted to basic properties of $\mathcal{A}(G)$. In Section 4, we give values of $\mathcal{A}(G)$ for some particular graphs G. We then explain in Section 5 the links between the three conjectures and we establish their validity for chordal graphs and for graphs G with maximum degree $\Delta(G) \leq 2$.

2. Notation

For basic notions of graph theory that are not defined here, we refer to Diestel [4]. Let $G = (V, E)$ be a simple undirected graph. The *order* $n = |V|$ of G is its number of vertices and the *size* $m = |E|$ of G is its number of edges. We write $G \simeq H$ if G and H are two isomorphic graphs, and $\overline{G}$ is the complement of G. 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. We write $\mathsf{K}_{a,b}$ for the complete bipartite graph where a and b are the cardinalities of the two sets of vertices of the bipartition. Hence, as already mentioned, $\mathsf{K}_{1,n-1}$ is the *star* of order n. For a subset S of vertices in a graph G, we write $G[S]$ for the subgraph of G induced by S.

Let $N(v)$ be the set of neighbors of a vertex v in G. A vertex v is *isolated* if $|N(v)| = 0$ and is *dominant* if $|N(v)| = n-1$ (where n is the order of G). 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. A graph is *chordal* if each of its induced subgraphs contains a simplicial vertex.

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

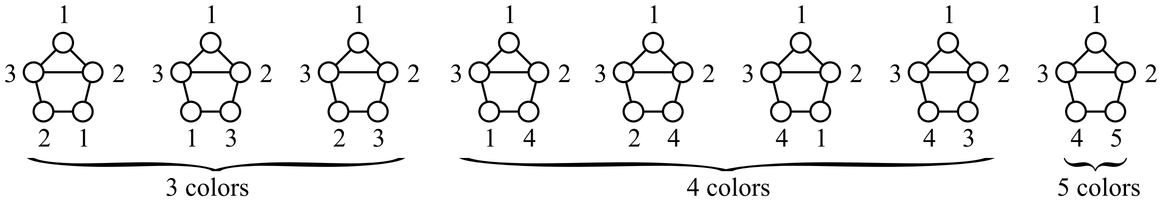

Fig. 2. The non-equivalent colorings of $\overline{\mathrm{P}}_5$.

- $G_{|uv}$ is the graph (of order $n-1$) obtained from G 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.

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, while the *join* G_1+G_2 of G_1 and G_2 is the graph obtained from $G_1 \cup G_2$ by adding all possible edges between the vertices of G_1 and those of G_2. Also, as already mentioned, $G \cup p\mathrm{K}_1$ is the graph obtained from G by adding p isolated vertices.

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* $\chi(G)$ of 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

$$\mathcal{B}(G)=\sum_{k=1}^{n} S(G,k)=\sum_{k=\chi(G)}^{n} S(G,k),$$

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

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

The average number $\mathcal{A}(G)$ of colors in the non-equivalent colorings of a graph G can therefore be defined as

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

Note that $\mathcal{B}(\overline{\mathrm{K}}_n)=\mathrm{B}_n$, $\mathcal{T}(\overline{\mathrm{K}}_n)=\mathrm{T}_n$, and $\mathcal{A}(\overline{\mathrm{K}}_n)=\mathrm{A}_n$. As another example, consider the complement $\overline{\mathrm{P}}_5$ of a path on 5 vertices. As shown in Fig. 2, there are three non-equivalent colorings of $\overline{\mathrm{P}}_5$ with 3 colors, four with 4 colors, and one with 5 colors, which gives $\mathcal{B}(\overline{\mathrm{P}}_5)=8$, $\mathcal{T}(\overline{\mathrm{P}}_5)=30$ and $\mathcal{A}(\overline{\mathrm{P}}_5)=\frac{30}{8}=3.75$.

3. Basic properties of $\mathcal{A}(G)$

As for several other invariants in graph coloring, the *deletion–contraction* rule (also often called the *Fundamental Reduction Theorem* [6]) 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 [8,12], 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

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

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

Property 4. *Given any two graphs G_1 and G_2, we have*

$$\mathcal{A}(G_1+G_2)=\mathcal{A}(G_1)+\mathcal{A}(G_2).$$

Proof. As observed in [1], given any coloring of $G_1 + G_2$, none of the vertices of G_1 can share a color with a vertex of G_2, which immediately gives $\mathcal{B}(G_1 + G_2) = \mathcal{B}(G_1)\mathcal{B}(G_2)$. For $\mathcal{T}(G_1 + G_2)$, assuming that G_1 and G_2 are of order n_1 and n_2, respectively, we get

$$\begin{aligned}\mathcal{T}(G_1 + G_2) &= \sum_{k=1}^{n_1}\sum_{k'=1}^{n_2}(k+k')S(G_1,k)S(G_2,k') = \sum_{k=1}^{n_1}S(G_1,k)\sum_{k'=1}^{n_2}(k+k')S(G_2,k')\\ &= \sum_{k=1}^{n_1}S(G_1,k)\left(k\sum_{k'=1}^{n_2}S(G_2,k') + \sum_{k'=1}^{n_2}k'S(G_2,k')\right)\\ &= \sum_{k=1}^{n_1}kS(G_1,k)\sum_{k'=1}^{n_2}S(G_2,k') + \sum_{k=1}^{n_1}S(G_1,k)\sum_{k'=1}^{n_2}k'S(G_2,k')\\ &= \mathcal{T}(G_1)\mathcal{B}(G_2) + \mathcal{B}(G_1)\mathcal{T}(G_2).\end{aligned}$$

Hence,

$$\begin{aligned}\mathcal{A}(G_1 + G_2) &= \frac{\mathcal{T}(G_1 + G_2)}{\mathcal{B}(G_1 + G_2)} = \frac{\mathcal{T}(G_1)\mathcal{B}(G_2) + \mathcal{B}(G_1)\mathcal{T}(G_2)}{\mathcal{B}(G_1)\mathcal{B}(G_2)}\\ &= \frac{\mathcal{T}(G_1)}{\mathcal{B}(G_1)} + \frac{\mathcal{T}(G_2)}{\mathcal{B}(G_2)} = \mathcal{A}(G_1) + \mathcal{A}(G_2). \quad \square\end{aligned}$$

The following Corollary is also proved in [10].

Corollary 5. *If v is a dominant vertex of a graph G, then,*

$$\mathcal{A}(G) = \mathcal{A}(G - v) + 1.$$

Proof. If v is a dominant vertex of a graph G, then $G \simeq (G - v) + \mathsf{K}_1$, and since $\mathcal{A}(\mathsf{K}_1) = 1$, Property 4 gives $\mathcal{A}(G) = \mathcal{A}(G - v) + 1$. $\square$

We think that $\mathcal{A}(G') < \mathcal{A}(G)$ for all proper induced subgraphs G' of a graph G, which is equivalent to state that $\mathcal{A}(G - v) < \mathcal{A}(G)$ for any G and for any vertex v in G. While we failed to prove it, the following lemma is the key ingredient in the proof of Property 7 and its two corollaries, which shows that $\mathcal{A}(G - v)$ is indeed strictly smaller than $\mathcal{A}(G)$ in some special cases. In the following, given a subset W of vertices in a graph G, we denote by $S_{W,i}(G, k)$ the number of non-equivalent colorings of G that use exactly k colors, and where exactly i of them appear on W. Hence, $S(G, k) = \sum_{i=0}^{|W|} S_{W,i}(G, k)$.

Lemma 6. *Let v be a vertex in a graph G of order n and let $N(v)$ be its set of neighbors in G. Then*

- $\mathcal{B}(G) = \mathcal{B}(G - v) + \displaystyle\sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|}(k - i)S_{N(v),i}(G - v, k)$, *and*
- $\mathcal{T}(G) = \mathcal{T}(G - v) + \displaystyle\sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|}(k(k - i) + 1)S_{N(v),i}(G - v, k)$.

Proof. Since $S_{N(v),i}(G, k) = S_{N(v),i}(G - v, k - 1) + (k - i)S_{N(v),i}(G - v, k)$, we have

$$\begin{aligned}\mathcal{B}(G) &= \sum_{k=1}^{n}S(G,k) = \sum_{k=1}^{n}\sum_{i=0}^{|N(v)|}S_{N(v),i}(G,k)\\ &= \sum_{k=1}^{n}\sum_{i=0}^{|N(v)|}S_{N(v),i}(G-v,k-1) + \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|}(k-i)S_{N(v),i}(G-v,k)\\ &= \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|}S_{N(v),i}(G-v,k) + \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|}(k-i)S_{N(v),i}(G-v,k)\\ &= \mathcal{B}(G-v) + \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|}(k-i)S_{N(v),i}(G-v,k)\end{aligned}$$

and

$$\begin{aligned}
\mathcal{T}(G) &= \sum_{k=1}^{n} kS(G,k) = \sum_{k=1}^{n}\sum_{i=0}^{|N(v)|} kS_{N(v),i}(G,k)\\
&= \sum_{k=1}^{n}\sum_{i=0}^{|N(v)|} kS_{N(v),i}(G-v,k-1) + \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} k(k-i)S_{N(v),i}(G-v,k)\\
&= \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} (k+1)S_{N(v),i}(G-v,k) + \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} k(k-i)S_{N(v),i}(G-v,k)\\
&= \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} kS_{N(v),i}(G-v,k) + \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} (k(k-i)+1)S_{N(v),i}(G-v,k)\\
&= \mathcal{T}(G-v) + \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} (k(k-i)+1)S_{N(v),i}(G-v,k). \quad \square
\end{aligned}$$

Property 7. *Let v be a vertex in a graph G. If $\chi(G[N(v)]) \geq |N(v)|-3$ then $\mathcal{A}(G) > \mathcal{A}(G-v)$.*

Proof. Let n be the order of G. We know from Lemma 6 that

$$\mathcal{A}(G) - \mathcal{A}(G-v) = \frac{\mathcal{T}(G-v)+a}{\mathcal{B}(G-v)+b} - \frac{\mathcal{T}(G-v)}{\mathcal{B}(G-v)} = \frac{a\mathcal{B}(G-v) - b\mathcal{T}(G-v)}{\mathcal{B}(G)\mathcal{B}(G-v)}$$

where

- $a = \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} (k(k-i)+1)S_{N(v),i}(G-v,k)$, and
- $b = \sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} (k-i)S_{N(v),i}(G-v,k)$.

It suffices to show that $a\mathcal{B}(G-v) - b\mathcal{T}(G-v) > 0$. Let $\mathcal{P}$ be the set of pairs (k,i) such that $S_{N(v),i}(G-v,k) > 0$. Since $\chi(G[N(v)]) \geq |N(v)|-3$, we have $k \geq i \geq |N(v)|-3$ for all $(k,i) \in \mathcal{P}$. For two pairs (k,i) and (k',i') in $\mathcal{P}$, we write $(k,i) > (k',i')$ if $k > k'$ or $k = k'$ and $i > i'$. Also, let $f(k,k',i,i') = S_{N(v),i}(G-v,k)S_{N(v),i'}(G-v,k')$. We have

$$\begin{aligned}
&a\mathcal{B}(G-v) - b\mathcal{T}(G-v)\\
=\ & a\sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} S_{N(v),i}(G-v,k) - b\sum_{k=1}^{n-1}\sum_{i=0}^{|N(v)|} kS_{N(v),i}(G-v,k)\\
=\ & \sum_{(k,i)\in\mathcal{P}} S_{N(v),i}(G-v,k)^2\Big((k(k-i)+1)-(k-i)k\Big)\\
&+ \sum_{(k,i)>(k',i')} f(k,k',i,i')\Big((k(k-i)+1)+(k'(k'-i')+1)-(k-i)k'-(k'-i')k\Big)\\
=\ & \sum_{(k,i)\in\mathcal{P}} S_{N(v),i}(G-v,k)^2 + \sum_{(k,i)>(k',i')} f(k,k',i,i')\Big((k-k')^2-(k-k')(i-i')+2\Big).
\end{aligned}$$

Note that $\mathcal{P} \neq \emptyset$ since $S_{N(v),|N(v)|}(G-v,n-1) = 1$. Hence, $\sum_{(k,i)\in\mathcal{P}} S_{N(v),i}(G-v,k)^2 > 0$, and it is sufficient to prove that $(k-k')^2-(k-k')(i-i')+2 \geq 0$ for every two pairs (k,i) and (k',i') in $\mathcal{P}$ with $(k,i) > (k',i')$. For two such pairs (k,i) and (k',i'), we have $i-i' \leq |N(v)| - (|N(v)|-3) = 3$. Hence,

- if $k = k'$, then $(k-k')^2-(k-k')(i-i')+2 = 2 > 0$;
- if $k = k'+1$, then $(k-k')^2-(k-k')(i-i')+2 = 3-(i-i') \geq 0$;
- if $k = k'+2$, then $(k-k')^2-(k-k')(i-i')+2 = 6-2(i-i') \geq 0$;
- if $k \geq k'+3$, then $(k-k')^2-(k-k')(i-i')+2 \geq 2$. $\square$

Corollary 8. *If v is a vertex of degree at most 4 in a graph G, then $\mathcal{A}(G) > \mathcal{A}(G-v)$.*

Proof. Since $|N(v)| \leq 4$, we have:

- if $N(v) = \emptyset$, then $\chi(G[N(v)]) = 0 > -3 = |N(v)|-3$;

- if $N(v) \neq \emptyset$, then $\chi(G[N(v)]) \geq 1 \geq |N(v)| - 3$.

In both cases, we conclude from Property 7 that $\mathcal{A}(G) > \mathcal{A}(G - v)$. $\square$

Corollary 9. *Let v be a simplicial vertex in a graph G. Then $\mathcal{A}(G) > \mathcal{A}(G - v)$.*

Proof. Since v is simplicial in G, we have $\chi(G[N(v)]) = |N(v)| > |N(v)| - 3$. Hence, we conclude from Property 7 that $\mathcal{A}(G) > \mathcal{A}(G - v)$. $\square$

As mentioned in Section 1, there are graphs G for which the removal of any edge strictly increases $\mathcal{A}(G)$. The next property shows that all graphs G with a simplicial vertex of degree at least 1 contain at least one edge whose removal stricly decreases $\mathcal{A}(G)$.

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

Proof. Let $H = (G - v) \cup \mathsf{K}_1$. In other words, H is obtained from $G - v$ by adding an isolated vertex. It follows from Lemma 6 that

$$\begin{aligned}\mathcal{B}(H) &= \mathcal{B}(G - v) + \sum_{k=1}^{n-1}\sum_{i=0}^{0}(k - i)S_{\emptyset,i}(G - v, k)\\ &= \mathcal{B}(G - v) + \sum_{k=1}^{n-1} kS(G - v, k)\end{aligned}$$

and

$$\begin{aligned}\mathcal{T}(H) &= \mathcal{T}(G - v) + \sum_{k=1}^{n-1}\sum_{i=0}^{0}(k(k - i) + 1)S_{\emptyset,i}(G - v, k)\\ &= \mathcal{T}(G - v) + \sum_{k=1}^{n-1}(k^2 + 1)S(G - v, k).\end{aligned}$$

Also, since $S_{N(v),i}(G-v, k)=0$ for $i \neq |N(v)|$, we have $S(G-v, k)=S_{N(v),|N(v)|}(G-v, k)$ and it follows from Lemma 6 that

$$\begin{aligned}\mathcal{B}(G) &= \mathcal{B}(G - v) + \sum_{k=1}^{n-1}(k - |N(v)|)S(G - v, k)\\ &= \Big(\mathcal{B}(G - v) + \sum_{k=1}^{n-1} kS(G - v, k)\Big) - |N(v)| \sum_{k=1}^{n-1} S(G - v, k)\\ &= \mathcal{B}(H) - |N(v)|\mathcal{B}(G - v)\end{aligned}$$

and

$$\begin{aligned}\mathcal{T}(G) &= \mathcal{T}(G - v) + \sum_{k=1}^{n-1}\Big(k(k - |N(v)|) + 1\Big)S(G - v, k)\\ &= \Big(\mathcal{T}(G - v) + \sum_{k=1}^{n-1}(k^2 + 1)S(G - v, k)\Big) - |N(v)| \sum_{k=1}^{n-1} kS(G - v, k)\\ &= \mathcal{T}(H) - |N(v)|\mathcal{T}(G - v).\end{aligned}$$

Let $G' = G - vw$. Clearly, $(G' - v) \cup \mathsf{K}_1 = (G - v) \cup \mathsf{K}_1 = H$, and since v is simplicial of degree $|N(v)| - 1$ in $G - vw$, we have shown that

$$\mathcal{B}(G') = \mathcal{B}(G - vw) = \mathcal{B}(H) - (|N(v)| - 1)\mathcal{B}(G - v)$$

and

$$\mathcal{T}(G') = \mathcal{T}(G - vw) = \mathcal{T}(H) - (|N(v)| - 1)\mathcal{T}(G - v).$$

Hence,

$$\begin{aligned}\mathcal{A}(G)-\mathcal{A}(G-vw) &= \frac{\mathcal{T}(G)}{\mathcal{B}(G)}-\frac{\mathcal{T}(G-vw)}{\mathcal{B}(G-vw)}\\ &= \frac{\mathcal{T}(H)-|N(v)|\mathcal{T}(G-v)}{\mathcal{B}(H)-|N(v)|\mathcal{B}(G-v)}-\frac{\mathcal{T}(H)-(|N(v)|-1)\mathcal{T}(G-v)}{\mathcal{B}(H)-(|N(v)|-1)\mathcal{B}(G-v)}\\ &= \frac{\mathcal{T}(H)\mathcal{B}(G-v)-\mathcal{B}(H)\mathcal{T}(G-v)}{\mathcal{B}(G)\mathcal{B}(G-vw)}.\end{aligned}$$

Since v is isolated in H, it is simplicial and we know from Corollary 9 that

$$\begin{aligned}\mathcal{A}(H)>\mathcal{A}(G-v) &\iff \frac{\mathcal{T}(H)}{\mathcal{B}(H)}>\frac{\mathcal{T}(G-v)}{\mathcal{B}(G-v)}\\ &\iff \mathcal{T}(H)\mathcal{B}(G-v)-\mathcal{B}(H)\mathcal{T}(G-v)>0\end{aligned}$$

which implies $\mathcal{A}(G)-\mathcal{A}(G-vw)>0$. □

As a final property, we mention one which is proved in [10]. For the sake of completeness, as it will be useful for establishing results in Section 5, we rewrite the proof here.

Property 11 (*[10]*). *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*

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

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

Proof. Since $\mathcal{A}(F_i)<\mathcal{A}(H)$, we have $\mathcal{T}(F_i)<\frac{\mathcal{T}(H)\mathcal{B}(F_i)}{\mathcal{B}(H)}$ for $i=1,\ldots,r$. Hence,

$$\begin{aligned}\mathcal{A}(G)=\frac{\mathcal{T}(G)}{\mathcal{B}(G)} &= \frac{\mathcal{T}(H)+\sum_{i=1}^{r}\alpha_i\mathcal{T}(F_i)}{\mathcal{B}(H)+\sum_{i=1}^{r}\alpha_i\mathcal{B}(F_i)}\\ &< \frac{\mathcal{T}(H)+\sum_{i=1}^{r}\alpha_i\frac{\mathcal{T}(H)\mathcal{B}(F_i)}{\mathcal{B}(H)}}{\mathcal{B}(H)+\sum_{i=1}^{r}\alpha_i\mathcal{B}(F_i)}=\frac{\mathcal{T}(H)\left(\mathcal{B}(H)+\sum_{i=1}^{r}\alpha_i\mathcal{B}(F_i)\right)}{\mathcal{B}(H)\left(\mathcal{B}(H)+\sum_{i=1}^{r}\alpha_i\mathcal{B}(F_i)\right)}\\ &= \frac{\mathcal{T}(H)}{\mathcal{B}(H)}=\mathcal{A}(H).\quad\square\end{aligned}$$

4. Some values for $\mathcal{A}(G)$

The value $\mathcal{A}(G)$ is known for some graphs G. We mention here some of them which are proven in [10] and determine some others.

Proposition 12 (*[10]*).

- $\mathcal{A}(\overline{\mathsf{K}}_n)=\mathcal{A}(n\mathsf{K}_1)=\dfrac{\mathsf{B}_{n+1}-\mathsf{B}_n}{\mathsf{B}_n}$ *for all* $n\geq 1$;
- $\mathcal{A}(T\cup p\mathsf{K}_1)=\dfrac{\sum_{i=0}^{p}\binom{p}{i}\mathsf{B}_{n+i}}{\sum_{i=0}^{p}\binom{p}{i}\mathsf{B}_{n+i-1}}$ *for all trees T of order $n\geq 1$ and all $p\geq 0$;*
- $\mathcal{A}(\mathsf{C}_n\cup p\mathsf{K}_1)=\dfrac{\sum_{j=1}^{n-1}(-1)^{j+1}\sum_{i=0}^{p}\binom{p}{i}\mathsf{B}_{n+i-j+1}}{\sum_{j=1}^{n-1}(-1)^{j+1}\sum_{i=0}^{p}\binom{p}{i}\mathsf{B}_{n+i-j}}$ *for all $n\geq 3$ and $p\geq 0$.*

Since $S(\mathsf{K}_n, k) = 1$ for $k = n$, and $S(\mathsf{K}_n, k) = 0$ for $k < n$, we have $\mathcal{A}(\mathsf{K}_n) = n$. We prove here a stronger property which we use in the next section. Let $\left\{ {a \atop b} \right\}$ be the Stirling number of the second kind, with parameters a and b (i.e., the number of partitions of a set of a elements into b blocks).

Proposition 13. $$\mathcal{A}(\mathsf{K}_n \cup p\mathsf{K}_1) = \frac{\sum_{k=n}^{n+p} k \sum_{j=0}^{n} \binom{k-j}{n-j}\binom{n}{j}(n-j)!\left\{ {p \atop k-j} \right\}}{\sum_{k=n}^{n+p} \sum_{j=0}^{n} \binom{k-j}{n-j}\binom{n}{j}(n-j)!\left\{ {p \atop k-j} \right\}}$$ *for all $n \geq 1$ and all $p \geq 0$.*

Proof. It is proved in [11] that given two graphs G_1 and G_2, we have

$$S(G_1 \cup G_2, k) = \sum_{i=1}^{k} \sum_{j=0}^{i} \binom{i}{j}\binom{k-j}{i-j}(i-j)!S(G_1, i)S(G_2, k-j).$$

For $G_1 \simeq \mathsf{K}_n$ and $G_2 \simeq p\mathsf{K}_1$, we have $S(G_1, i) = 1$ if $i = n$, and $S(G_1, i) = 0$ otherwise. Also, $S(G_2, k-j) = \left\{ {p \atop k-j} \right\}$. Hence,

$$S(\mathsf{K}_n \cup p\mathsf{K}_1, k) = \sum_{j=0}^{n} \binom{k-j}{n-j}\binom{n}{j}(n-j)!\left\{ {p \atop k-j} \right\}.$$

The result then follows from the fact that

$$\mathcal{A}(\mathsf{K}_n \cup p\mathsf{K}_1) = \frac{\sum_{k=n}^{n+p} kS(\mathsf{K}_n \cup p\mathsf{K}_1, k)}{\sum_{k=n}^{n+p} S(\mathsf{K}_n \cup p\mathsf{K}_1, k)}. \quad \square$$

We now determine $\mathcal{A}(G)$ for G equal to the complement of a path and the complement of a cycle. In what follows, we write F_n and L_n for the nth Fibonacci number and the nth Lucas number, respectively.

Proposition 14. $\mathcal{A}(\overline{\mathsf{P}}_n) = \dfrac{(n+1)F_{n+2} + (2n-1)F_{n+1}}{5F_{n+1}}$ *for all $n \geq 1$.*

Proof. The result is true for $n \leq 2$. Indeed,

- For $n = 1$, we have $\overline{\mathsf{P}}_1 = K_1$ which implies $\mathcal{A}(\overline{\mathsf{P}}_1) = 1 = \frac{2F_3+F_2}{5F_2}$;
- For $n = 2$, we have $\overline{\mathsf{P}}_2 = \overline{K}_2$ which implies $\mathcal{A}(\overline{\mathsf{P}}_2) = \frac{\mathsf{B}_3-\mathsf{B}_2}{\mathsf{B}_2} = \frac{3}{2} = \frac{3F_4+3F_3}{5F_3}$.

For larger values of n, we proceed by induction. It is shown in [8] that $\mathcal{B}(\overline{\mathsf{P}}_n)$=$F_{n+1}$. Also, it follows from Eqs. (4) that $\mathcal{T}(\overline{\mathsf{P}}_n) = \mathcal{T}(\overline{\mathsf{P}}_{n-1} + \mathsf{K}_1) + \mathcal{T}(\overline{\mathsf{P}}_{n-2} + \mathsf{K}_1)$. Moreover, as shown in the proof of Property 4, we have

$$\mathcal{T}(G + \mathsf{K}_1) = \mathcal{T}(G)\mathcal{B}(\mathsf{K}_1) + \mathcal{B}(G)\mathcal{T}(\mathsf{K}_1) = \mathcal{T}(G) + \mathcal{B}(G).$$

Hence,

$$\begin{aligned}
\mathcal{A}(\overline{\mathsf{P}}_n) &= \frac{\mathcal{T}(\overline{\mathsf{P}}_{n-1}) + \mathcal{B}(\overline{\mathsf{P}}_{n-1}) + \mathcal{T}(\overline{\mathsf{P}}_{n-2}) + \mathcal{B}(\overline{\mathsf{P}}_{n-2})}{F_{n+1}} \\
&= \frac{nF_{n+1} + (2n-3)F_n}{5F_{n+1}} + \frac{F_n}{F_{n+1}} + \frac{(n-1)F_n + (2n-5)F_{n-1}}{5F_{n+1}} + \frac{F_{n-1}}{F_{n+1}} \\
&= \frac{nF_{n+1} + (3n+1)F_n + 2nF_{n-1}}{5F_{n+1}} = \frac{3nF_{n+1} + (n+1)F_n}{5F_{n+1}} \\
&= \frac{(n+1)F_{n+2} + (2n-1)F_{n+1}}{5F_{n+1}}. \quad \square
\end{aligned}$$

Proposition 15. $\mathcal{A}(\overline{\mathsf{C}}_n) = \dfrac{nF_{n+1}}{L_n}$ *for all $n \geq 4$.*

Proof. It follows from Eqs. (4) that

$$\mathcal{T}(\overline{\mathsf{C}}_n) = \mathcal{T}(\overline{\mathsf{P}}_n) + \mathcal{T}(\overline{\mathsf{P}}_{n-2} + \mathsf{K}_1).$$

Moreover, it is shown in [8] that $\mathcal{B}(\overline{\mathsf{C}}_n) = L_n$. Since $\mathcal{T}(\overline{\mathsf{P}}_{n-2} + \mathsf{K}_1) = \mathcal{T}(\overline{\mathsf{P}}_{n-2}) + \mathcal{B}(\overline{\mathsf{P}}_{n-2})$, Proposition 14 implies

$$\begin{aligned}\mathcal{A}(\overline{\mathsf{C}}_n) &= \frac{\mathcal{T}(\overline{\mathsf{P}}_n) + \mathcal{T}(\overline{\mathsf{P}}_{n-2}) + \mathcal{B}(\overline{\mathsf{P}}_{n-2})}{L_n}\\ &= \frac{(n+1)F_{n+2} + (2n-1)F_{n+1}}{5L_n} + \frac{(n-1)F_n + (2n-5)F_{n-1}}{5L_n} + \frac{F_{n-1}}{L_n}\\ &= \frac{(n+1)F_{n+2} + (2n-1)F_{n+1} + (n-1)F_n + 2nF_{n-1}}{5L_n}\\ &= \frac{3nF_{n+1} + 2nF_n + 2nF_{n-1}}{5L_n} = \frac{5nF_{n+1}}{5L_n} = \frac{nF_{n+1}}{L_n}. \quad \square\end{aligned}$$

5. Lower bounds on $\mathcal{A}(G)$

In this section, we first establish links between the three conjectures of Section 1, and we then prove their validity for chordal graphs and for graphs G with maximum degree $\Delta(G) \le 2$.

5.1. Links between the conjectures

The lower bounds we are interested in depend on two parameters n and r with $1 \le r \le n$. They are equal to $\mathcal{A}(G)$ for some specific graphs G. More precisely, with the help of Propositions 12 and 13, we define

- $L_1(n) = \mathcal{A}(\overline{\mathsf{K}}_n) = \dfrac{\mathsf{B}_{n+1} - \mathsf{B}_n}{\mathsf{B}_n}$,
- $L_2(n,r) = \mathcal{A}(\mathsf{K}_r \cup (n-r)\mathsf{K}_1) = \dfrac{\displaystyle\sum_{k=r}^{n} k \sum_{i=0}^{r} \binom{k-i}{r-i}\binom{r}{i}(r-i)! \left\{ {n-r \atop k-i} \right\}}{\displaystyle\sum_{k=r}^{n} \sum_{i=0}^{r} \binom{k-i}{r-i}\binom{r}{i}(r-i)! \left\{ {n-r \atop k-i} \right\}}$,
- $L_3(n,r) = \mathcal{A}(\mathsf{K}_{1,r-1} \cup (n-r)\mathsf{K}_1) = \dfrac{\displaystyle\sum_{i=0}^{n-r} \binom{n-r}{i} \mathsf{B}_{r+i}}{\displaystyle\sum_{i=0}^{n-r} \binom{n-r}{i} \mathsf{B}_{r+i-1}}$.

Hence, for a graph G of order n,

- Conjecture 1 states that $\mathcal{A}(G) \ge L_1(n)$, with equality if and only if G is isomorphic to $\overline{\mathsf{K}}_n$;
- Conjecture 2 states that $\mathcal{A}(G) \ge L_2(n, \chi(G))$, with equality if and only if G is isomorphic to $\mathsf{K}_{\chi(G)} \cup (n-\chi(G))\mathsf{K}_1$;
- Conjecture 3 states that $\mathcal{A}(G) \ge L_3(n, \Delta(G)+1)$, with equality if and only if G is isomorphic to $\mathsf{K}_{1,\Delta(G)} \cup (n-\Delta(G)-1)\mathsf{K}_1$.

Given a graph G of order n, we are interested in the following inequalities, one of them being a conjecture, the other ones being proved here below:

$$\begin{aligned}L_1(n) &\le \min\left\{L_2(n,\ \chi(G)),\ L_3(n,\ \Delta(G)+1)\right\}\\ &\le \max\left\{L_2(n,\ \chi(G)),\ L_3(n,\ \Delta(G)+1)\right\}\\ &\le \mathcal{A}(G).\end{aligned}$$

The first inequality follows from Property 10 since $\overline{\mathsf{K}}_n$ is obtained from $\mathsf{K}_r \cup (n-r)\mathsf{K}_1$ and from $\mathsf{K}_{1,r-1} \cup (n-r)\mathsf{K}_1$ by repeatedly removing edges incident to simplicial vertices. The second inequality is trivial. The last inequality is an open problem stated in Conjectures 2 and 3. Since $L_1(n) \le \min\{L_2(n,\ \chi(G)), L_3(n,\ \Delta(G)+1)\}$, it suffices to show that one of these two conjectures is true to prove that Conjecture 1 is also true.

As mentioned in Section 1, the validity of Conjecture 1 cannot be proven by simple intuitive means such as sequential edge removal since there are graphs, for example $\mathsf{K}_{2,4}$, for which the removal of any edge strictly increases $\mathcal{A}(G)$. Also, we cannot proceed by induction on the number of connected components of G. Indeed, there are pairs of graphs G_1, G_2 such that $\mathcal{A}(G_1) < \mathcal{A}(G_2)$ while $\mathcal{A}(G_1 \cup \mathsf{K}_1) > \mathcal{A}(G_2 \cup \mathsf{K}_1)$. For example, for $G_1 = \mathsf{K}_{2,3}$ and $G_2 = \mathsf{K}_3 \cup 2\mathsf{K}_1$, we have

$$\mathcal{A}(G_1) = 3.5 < 3.529 = \mathcal{A}(G_2) \qquad \text{and} \qquad \mathcal{A}(G_1 \cup \mathsf{K}_1) = 3.867 > 3.831 = \mathcal{A}(G_2 \cup \mathsf{K}_1).$$

Note that proving that Conjecture 3 is true for all graphs G of order n and maximum degree $\Delta(G) = n-1$ is as difficult as proving Conjecture 1. Indeed, let v be a vertex of degree $n-1$ in a graph G of order n. Since v is a dominant vertex of G, we know from Corollary 5 that $\mathcal{A}(G) = \mathcal{A}(G-v)+1$. Hence, minimizing $\mathcal{A}(G)$ is equivalent to minimizing $\mathcal{A}(G-v)$, with no maximum degree constraint on $G-v$. We show in the next section that Conjectures 2 and 3 (and therefore 1) are true for graphs of maximum degree at most 2.

5.2. Proof of the conjectures for graphs G with $\Delta(G) \leq 2$

We start this section with a simple proof of the validity of Conjectures 2 and 3 when $\Delta(G) = 1$.

Theorem 16. *Let G be a graph of order n and maximum degree $\Delta(G) = 1$. Then,*

$$L_2(n, \chi(G)) = L_3(n, \Delta(G)+1) \leq \mathcal{A}(G),$$

with equality if and only if $G \simeq \mathsf{K}_2 \cup (n-2)\mathsf{K}_1$.

Proof. Since $\Delta(G) = 1$, we have $\chi(G) = 2$, which implies

$$\begin{aligned} L_2(n, \chi(G)) &= L_2(n, 2) \\ &= \mathcal{A}(\mathsf{K}_2 \cup (n-2)\mathsf{K}_1) \\ &= \mathcal{A}(\mathsf{K}_{1,1} \cup (n-2)\mathsf{K}_1) \\ &= L_3(n, 2) \\ &= L_3(n, \Delta(G)+1). \end{aligned}$$

Note also that $\Delta(G) = 1$ implies $G \simeq p\mathsf{K}_2 \cup (n-2p)\mathsf{K}_1$ for $p \geq 1$. Hence, all vertices in G are simplicial. We can thus sequentially remove all edges of G, except one, and it follows from Property 10 that $\mathcal{A}(G) \geq \mathcal{A}(\mathsf{K}_2 \cup (n-2)\mathsf{K}_1)$, with equality if and only $G \simeq \mathsf{K}_2 \cup (n-2)\mathsf{K}_1$. □

The proofs that Conjectures 2 and 3 are true when $\Delta(G) = 2$ are more complex. We first prove some intermediate results in the form of lemmas.

Lemma 17. *$\mathcal{A}(G \cup \mathsf{C}_n) > \mathcal{A}(G \cup \mathsf{P}_n)$ for all $n \geq 3$ and all graphs G.*

Proof. Let $H \simeq \mathsf{P}_2$ if $n = 3$ and $H \simeq \mathsf{C}_{n-1}$ if $n > 3$. We know from Eqs. (3) that $\mathcal{B}(G \cup \mathsf{C}_n) = \mathcal{B}(G \cup \mathsf{P}_n) - \mathcal{B}(G \cup H)$ and $\mathcal{T}(G \cup \mathsf{C}_n) = \mathcal{T}(G \cup \mathsf{P}_n) - \mathcal{T}(G \cup H)$. Since P_n is a proper spanning subgraph of C_n, we have $\mathcal{B}(G \cup \mathsf{C}_n) < \mathcal{B}(G \cup \mathsf{P}_n)$. Altogether, this gives

$$\begin{aligned} \mathcal{A}(G \cup \mathsf{C}_n) - \mathcal{A}(G \cup H) &= \frac{\mathcal{T}(G \cup \mathsf{C}_n)}{\mathcal{B}(G \cup \mathsf{C}_n)} - \frac{\mathcal{T}(G \cup H)}{\mathcal{B}(G \cup H)} \\ &= \frac{\mathcal{T}(G \cup \mathsf{P}_n) - \mathcal{T}(G \cup H)}{\mathcal{B}(G \cup \mathsf{P}_n) - \mathcal{B}(G \cup H)} - \frac{\mathcal{T}(G \cup H)}{\mathcal{B}(G \cup H)} \\ &= \frac{\mathcal{T}(G \cup \mathsf{P}_n)\mathcal{B}(G \cup H) - \mathcal{T}(G \cup H)\mathcal{B}(G \cup \mathsf{P}_n)}{\mathcal{B}(G \cup \mathsf{C}_n)\mathcal{B}(G \cup H)} \\ &> \frac{\mathcal{T}(G \cup \mathsf{P}_n)\mathcal{B}(G \cup H) - \mathcal{T}(G \cup H)\mathcal{B}(G \cup \mathsf{P}_n)}{\mathcal{B}(G \cup \mathsf{P}_n)\mathcal{B}(G \cup H)} \\ &= \frac{\mathcal{T}(G \cup \mathsf{P}_n)}{\mathcal{B}(G \cup \mathsf{P}_n)} - \frac{\mathcal{T}(G \cup H)}{\mathcal{B}(G \cup H)} \\ &= \mathcal{A}(G \cup \mathsf{P}_n) - \mathcal{A}(G \cup H) \\ \iff \mathcal{A}(G \cup \mathsf{C}_n) &> \mathcal{A}(G \cup \mathsf{P}_n). \quad \square \end{aligned}$$

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 18. *If $n \geq 3$, $0 \leq x \leq p$ and $1 \leq k \leq n$, then*

$$S(\mathsf{Q}_n \cup p\mathsf{K}_1, k) = \sum_{i=0}^{x} \binom{x}{i} S(\mathsf{Q}_{n+i} \cup (p-x)\mathsf{K}_1, k).$$

Proof. The result is clearly true for $p = 0$. For larger values of p, we proceed by induction. Since the result is clearly true for $x = 0$, we assume $x \geq 1$. Eqs. (2) imply

$$\begin{aligned} S(\mathsf{Q}_n \cup p\mathsf{K}_1, k) &= S(\mathsf{Q}_{n+1} \cup (p-1)\mathsf{K}_1, k) + S(\mathsf{Q}_n \cup (p-1)\mathsf{K}_1, k) \\ &= \sum_{i=0}^{x-1} \binom{x-1}{i} S(\mathsf{Q}_{n+i+1} \cup (p-x)\mathsf{K}_1, k) + \sum_{i=0}^{x-1} \binom{x-1}{i} S(\mathsf{Q}_{n+i} \cup (p-x)\mathsf{K}_1, k) \\ &= \sum_{i=1}^{x} \binom{x-1}{i-1} S(\mathsf{Q}_{n+i} \cup (p-x)\mathsf{K}_1, k) + \sum_{i=0}^{x-1} \binom{x-1}{i} S(\mathsf{Q}_{n+i} \cup (p-x)\mathsf{K}_1, k) \end{aligned}$$

$$
\begin{aligned}
&= S(\mathrm{Q}_{n+x} \cup (p-x)\mathrm{K}_1, k) + S(\mathrm{Q}_n \cup (p-x)\mathrm{K}_1, k) \\
&\quad + \sum_{i=1}^{x-1} \left(\binom{x-1}{i-1} + \binom{x-1}{i} \right) S(\mathrm{Q}_{n+i} \cup (p-x)\mathrm{K}_1, k) \\
&= \sum_{i=0}^{x} \binom{x}{i} S(\mathrm{Q}_{n+i} \cup (p-x)\mathrm{K}_1, k). \quad \square
\end{aligned}
$$

Lemma 19. *If $n \geq 3$ is an odd number and $1 \leq k \leq n$, then*

$$S(\mathrm{C}_n \cup p\mathrm{K}_1, k) = \sum_{i=0}^{(n-3)/2} S(\mathrm{Q}_{2i+3} \cup p\mathrm{K}_1, k).$$

Proof. The result is clearly true for $n = 3$ since $\mathrm{C}_3 \simeq \mathrm{Q}_3$. For larger values of n, we proceed by induction. It follows from Eqs. (1) and (2) that

$$
\begin{aligned}
S(\mathrm{C}_n \cup p\mathrm{K}_1, k) &= S(\mathrm{P}_n \cup p\mathrm{K}_1) - S(\mathrm{C}_{n-1} \cup p\mathrm{K}_1, k) \\
&= (S(\mathrm{Q}_n \cup p\mathrm{K}_1, k) + S(\mathrm{P}_{n-1} \cup p\mathrm{K}_1, k)) - (S(\mathrm{P}_{n-1} \cup p\mathrm{K}_1, k) - S(\mathrm{C}_{n-2} \cup p\mathrm{K}_1, k)) \\
&= S(\mathrm{Q}_n \cup p\mathrm{K}_1, k) + S(\mathrm{C}_{n-2} \cup p\mathrm{K}_1, k) \\
&= S(\mathrm{Q}_n \cup p\mathrm{K}_1, k) + \sum_{i=0}^{(n-5)/2} S(\mathrm{Q}_{2i+3} \cup p\mathrm{K}_1, k) \\
&= \sum_{i=0}^{(n-3)/2} S(\mathrm{Q}_{2i+3} \cup p\mathrm{K}_1, k). \quad \square
\end{aligned}
$$

Lemma 20. *If n and x are two numbers such that $5 \leq x \leq n$ and x is odd, then*

$$S(\mathrm{C}_3 \cup (n-3)\mathrm{K}_1, k) = S(\mathrm{C}_x \cup (n-x)\mathrm{K}_1, k) + \sum_{i=0}^{x-5} \alpha_i S(\mathrm{Q}_{i+4} \cup (n-x)\mathrm{K}_1, k)$$

where

$$\alpha_i = \begin{cases} \binom{x-3}{i+1} - 1 & \text{if } i \text{ is even} \\ \binom{x-3}{i+1} & \text{if } i \text{ is odd.} \end{cases}$$

Proof. Since $\mathrm{Q}_3 \simeq \mathrm{C}_3$ we know from Lemma 18 that

$$
\begin{aligned}
S(\mathrm{Q}_3 \cup (n-3)\mathrm{K}_1, k) &= \sum_{i=0}^{x-3} \binom{x-3}{i} S(\mathrm{Q}_{i+3} \cup (n-x)\mathrm{K}_1, k) \\
&= \sum_{i=0}^{(x-3)/2} \binom{x-3}{2i} S(\mathrm{Q}_{2i+3} \cup (n-x)\mathrm{K}_1, k) \\
&\quad + \sum_{i=0}^{(x-5)/2} \binom{x-3}{2i+1} S(\mathrm{Q}_{2i+4} \cup (n-x)\mathrm{K}_1, k).
\end{aligned}
$$

It then follows from Lemma 19 that

$$
\begin{aligned}
S(\mathrm{Q}_3 \cup (n-3)\mathrm{K}_1, k) &= S(\mathrm{C}_x \cup (n-x)\mathrm{K}_1, k) + \sum_{i=1}^{(x-5)/2} \left(\binom{x-3}{2i} - 1 \right) S(\mathrm{Q}_{2i+3} \cup (n-x)\mathrm{K}_1, k) \\
&\quad + \sum_{i=0}^{(x-5)/2} \binom{x-3}{2i+1} S(\mathrm{Q}_{2i+4} \cup (n-x)\mathrm{K}_1, k) \\
&= S(\mathrm{C}_x \cup (n-x)\mathrm{K}_1, k) + \sum_{i=0}^{x-5} \alpha_i S(\mathrm{Q}_{i+4} \cup (n-x)\mathrm{K}_1, k). \quad \square
\end{aligned}
$$

Lemma 21. *If $n \geq 5$ and $3 \leq i < n$ then*

$$\mathcal{A}(\mathsf{Q}_i \cup p\mathsf{K}_1) < \mathcal{A}(\mathsf{C}_n \cup p\mathsf{K}_1)$$

Proof. Since $\mathsf{Q}_{n-1} \cup p\mathsf{K}_1$ is obtained from $\mathsf{Q}_i \cup p\mathsf{K}_1$ by iteratively adding vertices of degree 1, we know from Corollary 8 that $\mathcal{A}(\mathsf{Q}_i \cup p\mathsf{K}_1) \leq \mathcal{A}(\mathsf{Q}_{n-1} \cup p\mathsf{K}_1)$. Moreover, it is proved in [10] that $\mathcal{A}(\mathsf{Q}_{n-1} \cup p\mathsf{K}_1) < \mathcal{A}(\mathsf{P}_n \cup p\mathsf{K}_1)$ for all $n \geq 5$ and $p \geq 0$. It then follows from Lemma 17 that

$$\mathcal{A}(\mathsf{Q}_i \cup p\mathsf{K}_1) \leq \mathcal{A}(\mathsf{Q}_{n-1} \cup p\mathsf{K}_1) < \mathcal{A}(\mathsf{P}_n \cup p\mathsf{K}_1) < \mathcal{A}(\mathsf{C}_n \cup p\mathsf{K}_1). \quad \square$$

Corollary 22. *If $n \geq 5$, x is odd and $5 \leq x \leq n$, then*

$$\mathcal{A}(\mathsf{C}_3 \cup (n-3)\mathsf{K}_1) < \mathcal{A}(\mathsf{C}_x \cup (n-x)\mathsf{K}_1).$$

Proof. Lemma 20 implies

- $\mathcal{B}(\mathsf{C}_3 \cup (n-3)\mathsf{K}_1) = \mathcal{B}(\mathsf{C}_x \cup (n-x)\mathsf{K}_1) + \sum_{i=0}^{x-5} \alpha_i \mathcal{B}(\mathsf{Q}_{i+4} \cup (n-x)\mathsf{K}_1)$, and
- $\mathcal{T}(\mathsf{C}_3 \cup (n-3)\mathsf{K}_1) = \mathcal{T}(\mathsf{C}_x \cup (n-x)\mathsf{K}_1) + \sum_{i=0}^{x-5} \alpha_i \mathcal{T}(\mathsf{Q}_{i+4} \cup (n-x)\mathsf{K}_1)$,

where

- $\alpha_i = \binom{x-3}{i+1} - 1 \geq 0$ if i is even, and
- $\alpha_i = \binom{x-3}{i+1} > 0$ if i is odd.

Also, we know from Lemma 21 that $\mathcal{A}(\mathsf{Q}_{i+4} \cup p\mathsf{K}_1) < \mathcal{A}(\mathsf{C}_x \cup (n-x)\mathsf{K}_1)$ for $i = 0, \ldots, x-5$. Hence, it follows from Property 11 that $\mathcal{A}(\mathsf{C}_3 \cup (n-3)\mathsf{K}_1) < \mathcal{A}(\mathsf{C}_x \cup (n-x)\mathsf{K}_1)$. $\square$

We are now ready to prove the validity of Conjectures 2 and 3 when $\Delta(G) = 2$.

Theorem 23. *Let G be a graph of order n with $\Delta(G) = 2$. Then,*

$$\mathcal{A}(G) \geq L_2(n, \chi(G)),$$

with equality if and only if $G \simeq \mathsf{K}_{\chi(G)} \cup (n-\chi(G))\mathsf{K}_1$.

Proof. Since $\Delta(G) = 2$, G is the disjoint union of paths and cycles. If G does not contain any odd cycle, then $\chi(G) = 2$. It then follows from Property 10 and Lemma 17 that the edges of G can be removed sequentially, with a strict decrease of $\mathcal{A}(G)$ at each step, until we get $\mathsf{K}_2 \cup (n-2)\mathsf{K}_1$.

If $\chi(G)=3$, then at least one connected component of G is an odd cycle C_x with $x \leq n$. Again, we know from Property 10 and Lemma 17 that the edges of G can be removed sequentially, with a strict decrease of $\mathcal{A}(G)$ at each step, until we get $\mathsf{C}_x \cup (n-x)\mathsf{K}_1$. It then follows from Corollary 22 that $\mathcal{A}(G) \geq \mathcal{A}(\mathsf{C}_x \cup (n-x)\mathsf{K}_1) \geq \mathcal{A}(\mathsf{C}_3 \cup (n-3)\mathsf{K}_1)$, with equalities if and only if $G \simeq \mathsf{C}_3 \cup (n-3)\mathsf{K}_1 \simeq \mathsf{K}_3 \cup (n-3)\mathsf{K}_1$. $\square$

Theorem 24. *Let G be a graph of order n with $\Delta(G) = 2$. Then,*

$$\mathcal{A}(G) \geq L_3(n, \Delta(G) + 1),$$

with equality if and only if $G \simeq \mathsf{K}_{1,2} \cup (n-3)\mathsf{K}_1$.

Proof. Since $\Delta(G) = 2$, G is the disjoint union of paths and cycles. Also, G contains at least one vertex u of degree 2. Let v and w be two neighbors of u in G. It follows from Property 10 and Lemma 17 that the edges of G can be removed sequentially, with a strict decrease of $\mathcal{A}(G)$ at each step, until the edge set of the remaining graph H is $\{uv, uw\}$. But H is then isomorphic to $\mathsf{K}_{1,2} \cup (n-3)\mathsf{K}_1$. $\square$

5.3. Proof of the conjectures for chordal graphs

In this section, we establish the validity of the three conjectures for chordal graphs.

Theorem 25. *Conjectures 2 and 3 (and therefore 1) are true for chordal graphs.*

Proof. Let us first observe that removing an edge incident to a simplicial vertex in a chordal graph gives another chordal graph. So let G be a chordal graph. Since G is perfect, it contains a clique K of order $|K| = \chi(G)$. It is well known that chordal graphs that are not a clique contain at least two non-adjacent simplicial vertices [5]. Hence, G can be reduced to $\mathsf{K}_{\chi(G)} \cup (n-\chi(G))\mathsf{K}_1$ by repeatedly removing edges incident to simplicial vertices. We know from Property 10 that each of these edge removals strictly decreases $\mathcal{A}(G)$. We thus have $\mathcal{A}(G) \geq \mathcal{A}(\mathsf{K}_{\chi(G)} \cup (n-\chi(G))\mathsf{K}_1)$, with equality if and only if $G \simeq \mathsf{K}_{\chi(G)} \cup (n-\chi(G))\mathsf{K}_1$. Conjecture 2 is therefore true for chordal graphs.

Let us now deal with Conjecture 3. Let v be a vertex of degree $\Delta(G)$ in G. We consider the partition $(N_1(v), N_2(v))$ of the neighborhood $N(v)$ of v, where $N_1(v)$ contains all vertices of $N(v)$ of degree 1 in G (i.e., v is the only neighbor of every vertex of $N_1(v)$). Also, we consider the partition $(\overline{N}_1(v), \overline{N}_2(v))$ of the set $\overline{N}(v)$ of vertices of G that are not adjacent to v, where $\overline{N}_1(v)$ contains all vertices of $\overline{N}(v)$ of degree 0 in G. If $N_2(v) \cup \overline{N}_2(v) \neq \emptyset$ then $G[N_2(v) \cup \overline{N}_2(v) \cup \{v\}]$ contains a simplicial vertex $w \neq v$ (since it is also a chordal graph). Clearly, w is simplicial in the whole graph that includes $N_1(v)$ and $\overline{N}_1(v)$. Then:

- If $w \in N_2(v)$, we can remove all edges incident to w, except the one that links w with v. We thus get a new chordal graph in which at least one vertex has been transferred from $N_2(v)$ to $N_1(v)$, vertices of $\overline{N}_2(v)$ may have transferred to $\overline{N}_1(v)$, but no vertex has undergone the reverse transfers.
- If $w \in \overline{N}_2(v)$, we can remove all edges incident to w. We thus get a new chordal graph in which at least one vertex has been transferred from $\overline{N}_2(v)$ to $\overline{N}_1(v)$, vertices of $N_2(v)$ may have transferred to $N_1(v)$, but no vertex has undergone the reverse transfers.

Note that in both cases, no vertex has been transferred from $\overline{N}(v)$ to $N(v)$ or vice versa. Hence, by repeatedly applying the above mentioned edge removals, we get $N_2(v) = \overline{N}_2(v) = \emptyset$, which means that the resulting graph is $\mathsf{K}_{1,\Delta(G)} \cup (n-\Delta(G)-1)\mathsf{K}_1$. Again, we know from Property 10 that each of the edge removals performed strictly decreases $\mathcal{A}(G)$, which proves that $\mathcal{A}(G) \geq \mathcal{A}(\mathsf{K}_{1,\Delta(G)} \cup (n-\Delta(G)-1)\mathsf{K}_1)$, with equality if and only if $G \simeq \mathsf{K}_{1,\Delta(G)} \cup (n-\Delta(G)-1)\mathsf{K}_1$. □

6. Concluding remarks

We have established several properties for a recently defined graph invariant, namely the average number $\mathcal{A}(G)$ of colors in the non-equivalent colorings of a graph G. We then looked at bounds for $\mathcal{A}(G)$. It is easy to prove that $\mathcal{A}(G) \leq \mathcal{A}(\mathsf{K}_n) = n$ for all graphs of order n, with equality if and only if $G \simeq \mathsf{K}_n$. Hence, n is the best possible upper bound on $\mathcal{A}(G)$ for a graph G of order n. We think that the best possible lower bound on $\mathcal{A}(G)$ for a graph G of order n is $\mathcal{A}(\overline{\mathsf{K}}_n) = \frac{\mathsf{B}_{n+1}-\mathsf{B}_n}{\mathsf{B}_n}$. We have shown that despite its apparent simplicity, this conjecture cannot be proven using simple techniques like sequential edge removal. We have then refined this conjecture by proposing lower bounds related to the chromatic number $\chi(G)$ and to the maximum degree $\Delta(G)$ of G. We have thus stated three open problems. We have shown that these three conjectures are true for chordal graphs and for graphs with maximum degree at most 2.

Acknowledgments

We thank the anonymous referees for their valuable comments which helped us to restructure the original version of this article.

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