Maximizing proper colorings on graphs

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\begin{abstract}

The number of proper \( q \)-colorings of a graph \( G \), denoted by \( P_G(q) \), is an important graph parameter that plays fundamental role in graph theory, computational complexity theory and other related fields. We study an old problem of Linial and Wilf to find the graphs with \( n \) vertices and \( m \) edges which maximize this parameter. This problem has attracted much research interest in recent years, however little is known for general \( m, n, q \). Using analytic and combinatorial methods, we characterize the asymptotic structure of extremal graphs for fixed edge density and \( q \). Moreover, we disprove a conjecture of Lazebnik, which states that the Turán graph \( T_s(n) \) has more \( q \)-colorings than any other graph with the same number of vertices and edges. Indeed, we show that there are infinite many counterexamples in the range \( q = O(s^2/\log s) \). On the other hand, when \( q \) is larger than some constant times \( s^2/\log s \), we confirm that the Turán graph \( T_s(n) \) asymptotically is the extremal graph achieving the maximum number of \( q \)-colorings. Furthermore, other (new and old) results on various instances of the Linial–Wilf problem are also established.

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\end{abstract}
1. Introduction

A proper $q$-coloring of a graph $G$ is an assignment mapping every vertex to one of the $q$ colors in such a way that no two adjacent vertices receive the same color. Let $P_G(q)$ denote the number of proper $q$-colorings in a graph $G$. Introduced by Birkhoff [2] in 1912, who proved that $P_G(q)$ is always a polynomial in $q$, this important graph parameter, as now commonly referred to as chromatic polynomial of $G$, has been extensively investigated over the past century. As it is already NP-hard to determine whether this number $P_G(q)$ is nonzero (even for $q = 3$ and planar graph $G$), the focus of substantial research has been to obtain good bounds for $P_G(q)$ over various families of graphs.

The original motive for Birkhoff [2] to consider the chromatic polynomial was the famous four-color conjecture (now a theorem), which equivalently asserts that the minimum $P_G(4)$ over all planar graphs is at least one. For every $q \geq 5$, it was obtained by Birkhoff in [3] that $P_G(q) \geq q(q - 1)(q - 2)(q - 3)^{n-3}$ for every planar graph $G$ with $n$ vertices, which is also sharp. Motivated from computational complexity, Linial [11] arrived at the problem of minimizing the number of acyclic orientations of graph $G$, which equals $|P_G(-1)|$ by a result of Stanley [18], over the family $\mathcal{F}_{n,m}$ of graphs with $n$ vertices and $m$ edges. He gave a surprising answer that for any $n, m$, there exists a universal graph minimizing $|P_G(q)|$ over the family $\mathcal{F}_{n,m}$ for every integer $q$. This graph is obtained from a clique $K_k$ by adding $n - k - 1$ isolated vertices and an extra vertex adjacent to $l$ vertices of the clique $K_k$, where $k > l \geq 0$ are the unique integers satisfying $\binom{k}{2} + l = m$.

Linial [11] then asked for the counterpart of his result, that is, to maximize $|P_G(q)|$ over all graphs with $n$ vertices and $m$ edges for integers $q$. Wilf (see [1,20]) independently raised the same maximization problem from a different point of view, the backtracking algorithm for finding a proper $q$-coloring. Since then, this problem has been the subject of extensive research, and many upper bounds on $P_G(q)$ over the family $\mathcal{F}_{n,m}$ have been obtained (see, for instance, [5–7,12,15]). The case $q = 2$ (for all $n, m$) was solved by Lazebnik in [6] completely. In the same paper, Lazebnik conjectured that in the range $m \leq n^2/4$, the graphs with $n$ vertices and $m$ edges maximizing the number of $3$-colorings must be complete bipartite graphs $K_{a,b}$ minus the edges of some star, plus isolated vertices. This was confirmed in a breakthrough paper [13] of Loh, Pikhurko and Sudakov, who further determined the asymptotic values of $a, b$. For $q \geq 4$, they also showed that the same graphs achieve the maximum number of $q$-colorings, for all sufficiently large $m < \kappa_q n^2$ where $\kappa_q \approx 1/(q \log q)$. In fact, Loh et al. [13] provided a general approach which enables to find the asymptotic solution of the Linial–Wilf problem by reducing it to a quadratically constrained linear problem, which we shall introduce in Section 2. Despite the efforts by various researchers, still very little was known for general $m, n, q$. “Perhaps part of the difficulty for general $m, n, q$ stems from the fact that the maximal graphs are substantially more complicated than the minimal graphs that Linial found” (quoted from [13]).
The first contribution of our paper is a structural theorem that allows us to substantially simplify the quadratically constrained linear problem for general instances. Here we state it in a graph theoretic fashion and direct readers to Theorem 3.1 for the specific statement linking to the optimization problem. This structural theorem asserts that extremal graphs must be asymptotically “close” to the ones in some family $G_k$, where $k > 1$ is an integer only depending on the edge density of graphs. To be precise, for fixed $q$, the family $G_k$ consists of complete multipartite graphs with at least $k$ and at most $q$ parts as well as graphs obtained from a complete $k$-partite graph by adding some additional vertices each of which adjacent to the vertices of all but two fixed parts. To measure the “closeness”, we define the edit distance of two graphs with the same number of vertices to be the minimum number of edges that need to be added or deleted from one graph to make it isomorphic to the other. We say $G$ is $d$-close to $H$, if the edit distance between graphs $G$ and $H$ is at most $d$.

**Theorem 1.1.** For any real $s > 1$, the following holds for all sufficiently large $n$. Let $G$ be an $n$-vertex graph with $\frac{s-1}{2s}n^2 + o(n^2)$ edges which maximizes the number of $q$-colorings over graphs with the same number of vertices and edges. Then there exists an $n$-vertex graph in $G_{[s]}$ which is $o(n^2)$-close to $G$.

We point out that the proofs of the following results will heavily rely on the structure given by Theorem 3.1, and we expect that it will also provide useful insights to other unsolved ranges of the Linial–Wilf problem.

Let $T_s(n)$ denote the complete $s$-partite $n$-vertex graph with nearly-equal parts, i.e., the balanced Turán graph with $n$ vertices and $s$ parts. Unlike the complicated situation in the general case, Lazebnik conjectured (see [9]) that the Turán graphs $T_s(n)$ are always extremal whenever $q \geq s$. More specifically,

**Conjecture 1.2 (Lazebnik).** For integers $q \geq s > 1$ and $n$ divisible by $s$, the Turán graph $T_s(n)$ has more proper $q$-colorings than any other graph with the same number of vertices and edges.

The case when $q = s$ immediately follows from the well-known Turán’s theorem. Lazebnik [8] confirmed this when $q = \Omega(n^6)$, and proved with Pikhurko and Woldar [9] that $T_2(2n)$ is extremal when $q = 3$ and is asymptotically extremal when $q = 4$. Loh, Pikhurko and Sudakov [13] showed that when $q = s + 1 \geq 4$, $T_s(n)$ is the unique extremal graph for sufficiently large $n$, which was improved to all $n$ by Lazebnik and Tofts in [10]. And Norine [15] partially confirmed this conjecture for sufficiently large $n$, provided that $s$ divides $q$. Very recently, Tofts [19] proved that when $q = 4$ and $s = 2$, $T_2(n)$ is the unique extremal graph for all $n$. Surprisingly, despite these positive results, we disprove Conjecture 1.2 by the following.
Theorem 1.3. For all integers \( s \geq 50000 \) and \( q_0 \) such that \( 20s \leq q_0 \leq \frac{s^2}{200 \log s} \), there exists an integer \( q \), within distance at most \( s \) from \( q_0 \), such that Conjecture 1.2 is false for \((s,q)\).

On the other hand, we show that Conjecture 1.2 asymptotically holds for all large \( s \) and \( q \geq \frac{100s^2}{\log s} \).

Theorem 1.4. For sufficiently large integers \( s \) and \( q \) such that \( q \geq \frac{100s^2}{\log s} \), the following holds for all sufficiently large \( n \). Every extremal graph which maximizes the number of proper \( q \)-colorings over graphs with \( n \) vertices and \( \frac{\Delta - 1}{2\sqrt{s}} n^2 + o(n^2) \) edges is \( o(n^2) \)-close to the Turán graph \( T_s(n) \).

The above two results together show that for fixed integer \( s \), the order of magnitude \( \frac{s^2}{\log s} \) is the threshold for the number of colors \( q \) (up to a constant factor): there are many counterexamples to Conjecture 1.2 when \( q \) is smaller than \( \frac{s^2}{200 \log s} \), while the Turán graph \( T_s(n) \) asymptotically becomes optimal once \( q \) exceeds \( \frac{100s^2}{\log s} \). We will discuss related issues about the precise structure of extremal graphs in Section 7.

In the next result, we consider Conjecture 1.2 for integers \( s \), where \( q \) is not far from \( s \).

Theorem 1.5. (i) If \( s \leq q \leq s + 2 \), then for all integers \( s > 1 \) and sufficiently large integers \( n \), every extremal graph which maximizes the number of \( q \)-colorings over graphs with \( n \) vertices and \( \frac{\Delta - 1}{2\sqrt{s}} n^2 + o(n^2) \) edges is \( o(n^2) \)-close to the Turán graph \( T_s(n) \).

(ii) If \( s + 3 \leq q \leq 2s - 7 \), where \( s \geq 10 \) is an integer, then Conjecture 1.2 is false for \((s,q)\).

1.1. Notation

A graph \( G = (V,E) \) is given by a pair of its (finite) vertex set \( V(G) \) and edge set \( E(G) \), which does not contain loops or multi-edges. For a subset \( X \) of vertices, we use \( G[X] \) to denote the subgraph of \( G \) induced by \( X \), and write \( e_G(X) \) to denote the number of edges in \( G[X] \) (when it is clear from the context, we will drop the subscript for brevity). We will make the convention that the set of colors used in a proper \( q \)-coloring is \([q] := \{1,2,\ldots,q\}\), and for the remainder of the paper, we consider \( q \) as a fixed integer parameter. We also adopt the typographic convention for representing a vector using boldface type, as in \( \mathbf{v} \) for a vector whose coordinates are \( v_i \). To simplify the presentation, we often omit floor and ceiling signs whenever these are not crucial and make no attempts to optimize the absolute constants involved. All our asymptotic notation symbols (\( O, o, \Omega, \omega, \Theta \)) are relative to the number of vertices \( n \), unless otherwise specified with a subscript. Finally, the function \( \log \) refers to the natural logarithm.
1.2. Organization

In Section 2 we introduce the optimization problem of [13], which asymptotically reduces the Linial–Wilf question to a quadratically constrained linear problem, some tools used in mathematical optimization, and some related results concerning the stability. We then study the structure of solutions to the optimization problem for general instances and finish the proof of Theorem 1.1 in Section 3. In Section 4, we present some prompt applications of the structural result obtained in the previous section, and we find the solutions for certain instances including Theorem 1.5 (i). The counterexamples to Conjecture 1.2 will be given in Section 5, which prove Theorem 1.3 and Theorem 1.5 (ii). In Section 6 we work on the optimization for integers s by considering certain continuous relaxation, which leads to a complete proof of Theorem 1.4. The final section contains some concluding remarks and open problems.

2. The optimization problem

The problem of maximizing the number of proper $q$-colorings can be asymptotically reduced to a quadratically constrained linear program, as shown by Loh et al. in [13]. In this section, we describe this optimization problem. Following the notation of [13], we define the objective and constraint functions

$$\text{OBJ}_q(\alpha) := \sum_{A \neq \emptyset} \alpha_A \log |A|, \quad V_q(\alpha) := \sum_{A \neq \emptyset} \alpha_A, \quad \text{and} \quad E_q(\alpha) := \sum_{A \cap B = \emptyset} \alpha_A \alpha_B,$$

where the vector $\alpha$ has $2^q - 1$ coordinates $\alpha_A \in \mathbb{R}$ indexed by nonempty subsets $A \subset [q]$ of colors, and the sum in $E_q(\alpha)$ runs over all unordered pairs of disjoint nonempty sets $\{A, B\}$. We shall sometimes write $\sum_A$ in place of $\sum_{A \neq \emptyset}$, when it is clear from the context that the empty set is excluded. Let $\text{FEAS}_q(s)$ be the feasible set of vectors defined by the constraints $\alpha \geq 0$, $V_q(\alpha) = 1$, and $E_q(\alpha) \geq \frac{s-1}{2s}$, where $1 < s \leq q$ is a real parameter (not necessarily integer).

**Main Optimization Problem.** Determine $\text{OPT}_q(s) := \max_{\alpha \in \text{FEAS}_q(s)} \text{OBJ}_q(\alpha)$.

The maximum value $\text{OPT}_q(s)$ exists since $\text{FEAS}_q(s)$ is compact. We remark that our notation is slightly different from the notation in [13], as we replaced the parameter $\gamma$ used in [13] (corresponding to the edge density of the target graph) with the $\frac{s-1}{2s}$ instead. Our choice of parameter was motivated by fact that the balanced Turán graph $T_s(n)$ has approximately $\frac{s-1}{2s} \cdot n^2$ edges, where $1 < s \leq q$ is an integer number.

We are ready to state the main theorem from [13], which asymptotically reduces the original problem of maximizing $q$-colorings to the previous optimization problem.

**Theorem 2.1.** For any $\varepsilon > 0$, the following holds for any sufficiently large $n$, and any $1 < s \leq q$. 
(i) Every $n$-vertex graph with at least $\frac{s-1}{2s} n^2$ edges has fewer than $e^{(\text{OPT}_q(s)+\varepsilon)n}$ proper $q$-colorings.

(ii) Any $\alpha$ which solves $\text{OPT}_q(s)$ yields a graph $G_\alpha(n)$ which has at least $\frac{s-1}{2s} n^2 - 2^q n$ edges and more than $e^{(\text{OPT}_q(s)-\varepsilon)n}$ proper $q$-colorings.

The construction of $G_\alpha(n)$ in [13] is as follows. Partition the vertex set of $G_\alpha(n)$ into clusters $V_A$ such that $|V_A|$ differs from $\alpha_A n$ by less than 1, and for every disjoint pair $A, B \subseteq [q]$, join every vertex in $V_A$ to every vertex of $V_B$ by an edge. Assume that $\alpha$ solves $\text{OPT}_q(s)$, it is easy to show that the number of proper $q$-colorings of $G_\alpha(n)$ is roughly $e^{(\text{OPT}_q(s)+o(1))n}$, and if $m$ denotes the number of edges of $G_\alpha(n)$ then $|m - \frac{s-1}{2s} n^2| \leq 2^q n$.

To prove the stability of our results, we need to following statement from [13].

**Theorem 2.2.** For any real $\varepsilon > 0$ and $s > 1$, the following holds for all sufficiently large $n$. Let $G$ be an $n$-vertex graph with $m \leq \frac{s-1}{2s} n^2$ edges which maximizes the number of $q$-colorings. Then $G$ is $\varepsilon n^2$-close to $G_\alpha(n)$, for an $\alpha$ which solves $\text{OPT}_q(s')$ for some $\frac{s'-1}{2s'} - \frac{m}{n^2} < \varepsilon$ with $s' \leq s$.

Using **Theorem 2.2** together with the continuity of $\text{OBJ}_q$, $V_q$, $E_q$ and $\text{OPT}_q$ (for the continuity of $\text{OPT}_q$ we refer the interested reader to [13, Claim 5, p. 661]), one can derive a more convenient statement whose proof we defer to Appendix A.

**Corollary 2.3.** For any real $s > 1$, the following holds for all sufficiently large $n$. Let $G$ be an $n$-vertex graph with $m = \frac{s-1}{2s} n^2 + o(n^2)$ edges which maximizes the number of $q$-colorings. Then $G$ is $o(n^2)$-close to $G_\alpha(n)$ for some $\alpha$ which solves $\text{OPT}_q(s)$.

### 2.1. Some preliminaries about mathematical optimization

One commonly used tool in mathematical optimization is the method of *Lagrange multipliers*, which is used to find the extrema of a multivariate function $f(x)$ subject to the constraints $g_i(x) = 0$ for $i = 1, \ldots, m$, where the objective function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ and constraint functions $g_i : \mathbb{R}^n \rightarrow \mathbb{R}$ are continuously differentiable. This method asserts that if $x_0$ is a regular local extremum for $f$, then there exist constants $\lambda_i$ (the *Lagrange multipliers*) such that

$$
\nabla f(x_0) = \sum_{i=1}^{m} \lambda_i \nabla g_i(x_0),
$$

where a point $x_0 \in \mathbb{R}^n$ is called regular if the gradients $\nabla g_1(x_0), \nabla g_2(x_0), \ldots, \nabla g_m(x_0)$ are linearly independent over $\mathbb{R}$.

An extension of the method of Lagrange multipliers is the *method of Karush–Kuhn–Tucker* (see, e.g., [4]), or KKT for short. Consider the following optimization problem:
Maximize \( f(x) \), subject to \( g_i(x) \leq 0 \) and \( h_j(x) = 0 \),

\[
(2)
\]

where \( f \) is the objective function, \( g_i \) \( (i = 1, 2, \ldots, m) \) are the inequality constraint functions and \( h_j \) \( (j = 1, 2, \ldots, l) \) are the equality constraint functions. If \( f : \mathbb{R}^n \rightarrow \mathbb{R} \), \( g_i : \mathbb{R}^n \rightarrow \mathbb{R} \), \( h_j : \mathbb{R}^n \rightarrow \mathbb{R} \) are continuously differentiable at a point \( x_0 \), and \( x_0 \) is a local extremum for \( f \) that satisfies some regularity conditions (see below), then there exist constants \( \mu_i \) \( (i = 1, \ldots, m) \) and \( \lambda_j \) \( (j = 1, \ldots, l) \), named KKT multipliers, such that the following hold:

\[
\begin{align*}
\nabla f(x_0) &= \sum_{i=1}^{m} \mu_i \nabla g_i(x_0) + \sum_{j=1}^{l} \lambda_j \nabla h_j(x_0) \\
\mu_i g_i(x_0) &= 0 \text{ for } i = 1, 2, \ldots, m \\
\mu_i &\geq 0 \text{ for } i = 1, 2, \ldots, m.
\end{align*}
\]

(3)

A point \( x_0 \) is regular for the KKT optimization if it satisfies some constraint qualifications, such as:

- Linear independence constraint qualification (LICQ): the gradients of the active inequality constraints (the set of all constraints \( g_i(x_0) \leq 0 \) for which the equality holds) and the gradients of the equality constraint functions are linearly independent at \( x_0 \);
- Slater’s condition: If the equality constraints are given by linear functions \( h_j \), and the inequality constraints are given by convex functions \( g_i \), and there exists a point \( x_1 \) such that \( h_j(x_1) = 0 \) for all \( j \) and \( g_i(x_1) < 0 \) for all \( i \), then any point \( x_0 \) is regular.

### 2.2. Basic properties of the solutions

In this section we prove some basic results that will be used later in the paper. We begin with a proposition asserting that \( E_q(\alpha) \) should be least possible for the optimal feasible \( \alpha \). We remark that the next statement appears implicitly in [13].

**Proposition 2.4.** Let \( \alpha \in \text{FEAS}_q(s) \) be a local maximum point for \( \text{OBJ}_q \). Then \( E_q(\alpha) = \frac{s-1}{2s} \).

**Proof.** Assume, towards contradiction, that there exists a local maximum point \( \alpha \) to \( \text{OBJ}_q \) such that \( E_q(\alpha) > \frac{s-1}{2s} \). Since \( E_q(\alpha) > 0 \), there exists a nonempty set \( A \subseteq \{q\} \) such that \( \alpha_A \cdot \sum_{B \cap A = \emptyset} \alpha_B > 0 \). In particular \( A \neq \{q\} \) and \( \alpha_A > 0 \). Let \( \alpha' \) be obtained from \( \alpha \) by setting \( \alpha'_A := \alpha_A - \varepsilon \), \( \alpha'_{[q]} := \alpha_{[q]} + \varepsilon \) and keeping all the other entries unchanged, where \( \varepsilon > 0 \) is small. We have \( V_q(\alpha') = V_q(\alpha) = 1 \),

\[
E_q(\alpha') = E_q(\alpha) - \sum_{B \cap A = \emptyset} \varepsilon \cdot \alpha_B \quad \text{and} \quad \text{OBJ}_q(\alpha') = \text{OBJ}_q(\alpha) + \varepsilon \cdot \log \frac{q}{|A|},
\]

where \( A \subseteq \{q\} \).
and by taking $\varepsilon$ sufficiently small, we can obtain $\alpha' \in \text{FEAS}_q(s)$ such that $\text{OBJ}_q(\alpha') > \text{OBJ}_q(\alpha)$, which contradicts the local maximality of $\alpha$, concluding the proof of this proposition. \qed

Since $\text{FEAS}_q(s')$ is always a subset of $\text{FEAS}_q(s)$ for $s' \geq s$, we have

**Observation 2.5.** $\text{OPT}_q(s)$ is strictly decreasing with respect to the parameter $s$.

We finish the section with two fairly straightforward propositions about the sets in the support of a solution. The first one is as follows.

**Proposition 2.6.** For any solution $\alpha$ of $\text{OPT}_q(s)$, we have $\bigcup \{A : \alpha_A > 0\} = [q]$.

**Proof.** Assume, for contradiction, that $\bigcup \{A : \alpha_A > 0\} \neq [q]$ and let $B = [q] \setminus \bigcup \{A : \alpha_A > 0\}$. Let $A$ be any set in the support of $\alpha$. If we "replace" $A$ by $A \cup B$, i.e., if we let $\alpha'$ be the vector obtained from $\alpha$ such that $\alpha'_{A \cup B} = \alpha_A$, $\alpha'_A = 0$ and $\alpha'_X = \alpha_X$ for all $X \notin \{A \cup B, A\}$, then $V_q(\alpha') = V_q(\alpha)$, $E_q(\alpha') = E_q(\alpha)$ and $\text{OBJ}_q(\alpha') > \text{OBJ}_q(\alpha)$, a contradiction. \qed

The last proposition gives us some information about the support whenever it contains an intersecting pair.

**Proposition 2.7.** Let $\alpha$ be a solution to $\text{OPT}_q(s)$, and suppose there exist two sets $A, B \subseteq [q]$ in the support of $\alpha$ such that $A \cap B \neq \emptyset$. Then either $A \subseteq B$ or for every $c \in A \setminus B$ there exists a set $C$ in the support of $\alpha$ which is disjoint from $B$ and contains $c$.

**Proof.** Suppose, towards contradiction, that there exists $c \in A \setminus B$ such that no set $C$ in the support of $\alpha$ is disjoint from $B$ and contains $c$. Let $\alpha'$ be the vector obtained from $\alpha$ by replacing $B$ with $B \cup \{c\}$, i.e., $\alpha'_B := 0$, $\alpha'_{B \cup \{c\}} = \alpha_{B \cup \{c\}} + \alpha_B$, and $\alpha'_X = \alpha_X$ for all $X \notin \{B, B \cup \{c\}\}$. Clearly $V_q(\alpha') = V_q(\alpha) = 1$. Moreover $E_q(\alpha') = E_q(\alpha)$, as every set in the support of $\alpha$ that intersects $B \cup \{c\}$ must also intersect $B$. But $\text{OBJ}_q(\alpha') = \text{OBJ}_q(\alpha) + \alpha_B \log \frac{|B| + 1}{|B|} > \text{OBJ}_q(\alpha)$, a contradiction. \qed

### 3. The structure of the support graph

Let $\alpha \in \text{FEAS}_q(s)$. The support graph of $\alpha$, denoted by $\text{SUPP}_q(\alpha)$, is the graph defined over the support of $\alpha$ (that is, those sets $A$ for which $\alpha_A > 0$) whose edges are formed by connecting pairs of disjoint sets. We will investigate the structure of $\text{SUPP}_q(\alpha)$ for all solutions $\alpha$ to $\text{OPT}_q(s)$ in this section.

We define two classes of support graphs as follows. Let $P_k$ be the class of all $\text{SUPP}_q(\alpha)$ for which the support of $\alpha$ forms a $k$-partition of $[q]$. Let $Q_k$ be the class of all $\text{SUPP}_q(\alpha)$ for which the support of $\alpha$ consists of a $k$-partition $A_1, \ldots, A_{k-1}, A_k$ of $[q]$ together with the set $A_1 \cup A_2$. We write $\mathcal{P} := \cup_k P_k$ and $\mathcal{Q} := \cup_k Q_k$. Loosely speaking, $P_k$ corresponds
to solutions whose support graph is a clique of size $k$, and $Q_k$ corresponds to solutions whose support graph is obtained from a clique on $k+1$ vertices by removing two adjacent edges. In this section, we show

**Theorem 3.1.** For integer $q$ and real $1 < s \leq q$, all solutions $\alpha$ to $\text{OPT}_q(s)$ are such that $\text{SUPP}_q(\alpha)$ is in either $\cup_{[s] \leq k \leq q} P_k$ or $Q_{[s]}$. And when $[s] < q$, we have $\text{SUPP}_q(\alpha) \notin P_q$.

This result tells us about the structure of the support graph for a solution to $\text{OPT}_q(s)$ and will play critical role in solving the relevant instances of $\text{OPT}_q(s)$. One can check that Theorem 3.1 together with Corollary 2.3 readily implies our main structural result Theorem 1.1. The proof of Theorem 3.1 will be divided into seven steps, outlined below.

**Step 1:** There exists a solution $\alpha$ to $\text{OPT}_q(s)$ such that none of the graphs $3K_1, C_4$ and $C_5$ appear as induced subgraphs of $\text{SUPP}_q(\alpha)$ (see Fig. 1);

**Step 2:** For any solution $\alpha$ to $\text{OPT}_q(s)$, if $\text{SUPP}_q(\alpha)$ does not contain an induced copy of $3K_1$, then it also does not contain an induced matching of size 2;

**Step 3:** For any solution $\alpha$ to $\text{OPT}_q(s)$, there exist no four subsets $A, B, C$ and $D$ in the support of $\alpha$ such that they induce a path $A - B - C - D$ in $\text{SUPP}_q(\alpha)$ and $|A| > |C|, |D| > |B|$;

**Step 4:** For any solution $\alpha$ to $\text{OPT}_q(s)$, if $\text{SUPP}_q(\alpha)$ can be obtained from a clique by removing a star (a collection of edges sharing a common endpoint), then the star must have exactly two edges, and $\text{SUPP}_q(\alpha) \in Q$;

**Step 5:** For any solution $\alpha$ to $\text{OPT}_q(s)$, if $\text{SUPP}_q(\alpha) \in Q$ then in fact $\text{SUPP}_q(\alpha) \in Q_{[s]}$;

**Step 6:** For any $\alpha$ from Step 1, it is true that $\text{SUPP}_q(\alpha) \in (\cup_{k \geq [s]} P_k) \cup Q_{[s]}$.

**Step 7:** All solutions to $\text{OPT}_q(s)$ are such that $\text{SUPP}_q(\alpha)$ is in either $\cup_{[s] \leq k \leq q} P_k$ or $Q_{[s]}$.

We will show the proofs of the above steps in the forthcoming subsections.

### 3.1. Step 1: excluding graphs with 3 nonnegative eigenvalues

We first prove the following proposition which shall be frequently used throughout the section.
Proposition 3.2. Let \( \alpha \) be a solution to \( \text{OPT}_q(s) \) and let \( A_1, A_2, \ldots, A_k \subseteq \{q\} \) be vertices in \( \text{SUPP}_q(\alpha) \). Let \( 1, g, \beta \in \mathbb{R}^k \) be defined as \( 1_i := 1, \beta_i := \sum_{x \cap A_i \neq \emptyset} \alpha_x, \) and \( g_i := \log |A_i|, \) for \( i = 1, 2, \ldots, k \). Then the vectors \( 1, g, \beta \) are linearly dependent over \( \mathbb{R} \).

Proof. Suppose, towards contradiction, that \( 1, g, \beta \) are linearly independent over \( \mathbb{R} \). Then there exists a vector \( \gamma \in \mathbb{R}^k \) such that \( 1 \cdot \gamma = 0 \), while \( g \cdot \gamma = \beta \cdot \gamma = 1 \), where \( (\cdot) \) denotes the standard inner product in \( \mathbb{R}^k \). Let \( \alpha' \) be obtained from \( \alpha \) by replacing \( \alpha'_{A_i} := \alpha_{A_i} + \varepsilon \cdot \gamma_i \) for \( i = 1, \ldots, k \), where \( \varepsilon > 0 \) is sufficiently small. Clearly \( \alpha' \geq 0 \) when \( \varepsilon \) is sufficiently small and \( V_q(\alpha') = 1 \), as \( 1 \cdot \gamma = 0 \). We also have

\[
E_q(\alpha') = E_q(\alpha) + \varepsilon + O(\varepsilon^2) \quad \text{and} \quad \text{OBJ}_q(\alpha') = \text{OBJ}_q(\alpha) + \varepsilon,
\]

therefore when \( \varepsilon \) is sufficiently small, \( \alpha' \in \text{FEAS}_q(s) \) and \( \text{OBJ}_q(\alpha') > \text{OBJ}_q(\alpha) \), a contradiction that establishes the proposition. \( \square \)

We say \( \lambda \) is an eigenvalue of a graph \( G \) when \( \lambda \) is an eigenvalue of its adjacency matrix. The following proposition is the main ingredient in the proof of Step 1.

Proposition 3.3. Let \( \alpha \) be a solution to \( \text{OPT}_q(s) \), let \( A_1, A_2, \ldots, A_k \subseteq \{q\} \) be vertices in \( \text{SUPP}_q(\alpha) \), and let \( H \) be the subgraph of \( \text{SUPP}_q(\alpha) \) induced by these vertices. Then \( H \) has at most two positive eigenvalues. Moreover, if \( H \) has at least three nonnegative eigenvalues, then there exists another solution \( \alpha' \) to \( \text{OPT}_q(s) \) such that \( \text{SUPP}_q(\alpha') \) is a strictly smaller induced subgraph of \( \text{SUPP}_q(\alpha) \). Furthermore \( \alpha \) and \( \alpha' \) differ only in the coordinates \( A_1, A_2, \ldots, A_k \) and the segment that joins \( \alpha \) and \( \alpha' \) is entirely contained in \( \text{FEAS}_q(s) \).

Proof. Let \( 1, g, \) and \( \beta \) be as such as in Proposition 3.2 for the vertices \( A_1, \ldots, A_k \). Because \( 1, g, \) and \( \beta \) are linearly dependent, we have \( \dim(\text{span}\{1, g, \beta\}) \leq 2 \). Let \( M \) denote the \( k \times k \) adjacency matrix of \( H \). Let \( W \subseteq \mathbb{R}^k \) be the subspace spanned by the eigenvectors of \( M \) associated with nonnegative eigenvalues. Because \( M \) is symmetric, if \( H \) has at least 3 nonnegative eigenvalues, then \( \dim(W) \geq 3 \), so there exists a vector \( \gamma \in W \) perpendicular to the vectors \( 1, g, \) and \( \beta \). Since \( \gamma \in W \), we must have \( \gamma^T \cdot M \cdot \gamma \geq 0 \). Let \( \alpha' \) be obtained from \( \alpha \) by replacing \( \alpha'_{A_i} := \alpha_{A_i} + \varepsilon \cdot \gamma_i \), where \( \varepsilon > 0 \) will be chosen later. If \( \varepsilon \) is sufficiently small, we have \( \alpha' \geq 0 \). Moreover, \( V(\alpha') = 1 \), and

\[
E_q(\alpha') = E_q(\alpha) + \varepsilon^2 \gamma^T \cdot M \cdot \gamma \geq E_q(\alpha) \quad \text{and} \quad \text{OBJ}_q(\alpha') = \text{OBJ}_q(\alpha).
\]

Thus we must conclude that \( \gamma^T \cdot M \cdot \gamma = 0 \), otherwise we would get a solution \( \alpha' \) to \( \text{OPT}_q(s) \) with \( E_q(\alpha') > \varepsilon^2 \gamma^T \cdot M \cdot \gamma \), contradicting Proposition 2.4. In particular, \( H \) does not have 3 positive eigenvalues (we could just repeat the same argument replacing \( W \) with the subspace spanned by the eigenvectors of \( M \) associated with the 3 positive eigenvalues). Clearly the segment joining \( \alpha \) and \( \alpha' \) is entirely contained in \( \text{FEAS}_q(s) \), and by choosing
\[\varepsilon\] appropriately, we can make one extra coordinate of \(\alpha'\) to be zero, thereby reducing the size of the support of the solution, and concluding the proof. \(\Box\)

From the proof of Proposition 3.3, we remark the following.

**Observation 3.4.** Let \(H, 1, g, \) and \(\beta\) be such as in Proposition 3.3 and its proof. If \(H\) has at least three nonnegative eigenvalues, then there exists a vector \(\gamma\) in the kernel of the adjacency matrix of \(H\) such that \(\gamma\) is perpendicular to the vectors \(1, g, \) and \(\beta\).

Let \(C_5^+\) be the 5-vertex graph obtained from \(C_5\) by adding an edge. It is easy to verify that the eigenvalues of \(3K_1\) are 0, 0, and 0; the eigenvalues of \(C_4\) are 2, 0, 0, and -2; the eigenvalues of \(C_5\) are 2, \(2\cos \frac{2\pi}{5}\), \(2\cos \frac{4\pi}{5}\), \(2\cos \frac{4\pi}{5}\); and the eigenvalues of \(C_5^+\) are \(\lambda_1, \lambda_2, 0, \lambda_3,\) and -2, where \(\lambda_1 \approx 2.48, \lambda_2 \approx 0.69, \lambda_3 \approx -1.17\) are the roots to the equation \(\lambda^3 - 2\lambda^2 - 2\lambda + 2 = 0\). We remark that these graphs have three nonnegative eigenvalues each, and that \(C_5^+\) contains \(C_4\) as an induced subgraph. The following proposition finishes the proof of Step 1.

**Proposition 3.5.** No solution \(\alpha\) to \(\text{OPT}_q(s)\) has \(C_5\) as induced subgraph of \(\text{SUPP}_q(\alpha)\). Furthermore, there exists a solution \(\alpha\) to \(\text{OPT}_q(s)\) such that \(\text{SUPP}_q(\alpha)\) does not contain induced copies of \(3K_1, C_5^+\) and \(C_4\).

**Proof.** Let \(\alpha\) be an arbitrary solution to \(\text{OPT}_q(s)\). Proposition 3.3 asserts that \(\text{SUPP}_q(\alpha)\) does not contain induced copies of \(C_5\), since \(C_5\) has three positive eigenvalues.

If \(\text{SUPP}_q(\alpha)\) contains either \(3K_1, C_5^+\) or \(C_4\) as induced subgraphs, we just repeatedly apply Proposition 3.3 (with \(H = 3K_1, C_5^+\) or \(C_4\)) to find a new solution \(\alpha'\) with strictly smaller support, until there are no more induced copies of these graphs in \(\text{SUPP}_q(\alpha')\). This is possible because each of \(3K_1, C_5^+, C_4\) has three nonnegative eigenvalues. It is important to remark here that

(i) whenever there are copies of \(3K_1\) appearing as induced subgraphs of \(\text{SUPP}_q(\alpha)\), we always choose to apply Proposition 3.3 to remove induced copies of \(3K_1\) first, and

(ii) when \(3K_1\) do not appear but there is a copy of \(C_5^+\) in \(\text{SUPP}_q(\alpha)\), we apply Proposition 3.3 to remove the induced copies of \(C_5^+\) (rather than removing induced copies of \(C_4\));

(iii) finally, when there are no induced copies of \(3K_1\) or \(C_5^+\), we apply Proposition 3.3 to remove the remaining induced copies of \(C_4\).

This priority (namely \(3K_1 > C_5^+ > C_4\)) will play an important role in the proof of Step 7.

The process described above has to end eventually, because the support always reduces in size at each application of Proposition 3.3. At the end, we obtain a solution \(\alpha'\) to
OPT_q(s) such that SUPP_q(α') has no induced copies of 3K_1, C_5^+ and C_4, and α and α' are connected in FEAS_q(s) by a piecewise linear path. □

At last, we state a useful observation that will be needed in the subsequent steps.

**Observation 3.6.** For any α, if SUPP_q(α) does not contain an induced copy of 3K_1 then any color i ∈ [q] is contained in at most two subsets of the support of α.

3.2. Step 2: excluding matchings of size two

**Proposition 3.7.** Let α be a solution of OPT_q(s) such that SUPP_q(α) does not contain induced copies of 3K_1. Then SUPP_q(α) does not contain induced matchings of size two.

**Proof.** Suppose for a contradiction that some α violates the proposition. We know there exist four vertices A, B, C, D of SUPP_q(α) such that A ∩ C = B ∩ D = ∅ and all other intersections A ∩ B, B ∩ C, C ∩ D, D ∩ A are nonempty.

Without losing generality, we assume that the intersection A ∩ B is of the smallest size among all pairwise nonempty intersections of the sets in \{A, B, C, D\}. There exists a subset S of C ∩ D such that |S| = |A ∩ B|. Clearly A ∩ S = B ∩ S = ∅. We define B' = (B \ (A ∩ B)) ∪ S, and D' = (D \ S) ∪ (A ∩ B). By Observation 3.6, if X is in the support of α and X ∩ (A ∩ B) ≠ ∅ then either X = A or X = B. Similarly, if X ∩ S ≠ ∅, then either X = C or X = D. In particular, α'B' = αD' = 0. Let α' be a vector obtained from α by defining α'B' = αB, αD' = αD, α'B = 0, α'D = 0, and letting α'X = αX for all X ∈ \{B, B', D, D'\}. It is easy to see that |B'| = |B| and |D'| = |D|, therefore OBJ_q(α') = OBJ_q(α) = OPT_q(s).

The edges between B', D' and another subset X ∈ \{A, B, B', C, D, D'\} in SUPP_q(α') are the same as the edges between B, D and X in SUPP_q(α), as this color-swapping does not affect those adjacencies. We also have B' ∩ D' = ∅, while A ∩ B' = ∅ = A ∩ B. Therefore, E_q(α') ≥ E_q(α) + α'Aα'B' > E_q(α). Note that OBJ_q(α') = OBJ_q(α) = OPT_q(s), so α' and α are both global maximum points for OBJ_q and by Proposition 2.4, E_q(α') = E_q(α) = s^{-1}, a contradiction. This completes the proof of this proposition, thereby proving Step 2. □

3.3. Step 3: excluding paths with four vertices

**Proposition 3.8.** For any solution α to OPT_q(s), there exist no four subsets A, B, C and D in the support of α such that they induce a path A − B − C − D in SUPP_q(α) and |A| > |C|, |D| > |B|.

**Proof.** Suppose that for some solution α to OPT_q(s) there exist four subsets A, B, C and D in the support of α such that they induce a path A − B − C − D in SUPP_q(α) and |A| > |C|, |D| > |B|. By symmetry, we assume that |D| ≥ |A|. Let
be the adjacency matrix of the induced path $A - B - C - D$, where its rows/columns are arranged according to the order $B, D, A, C$. Let $\lambda = \sqrt{\frac{\kappa + 1}{2}}$. It can be verified that $M$ has four eigenvalues $\lambda, -\lambda, \lambda - 1, -\lambda + 1$ and their corresponding eigenvectors

$$M = \begin{bmatrix}
0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 \\
\end{bmatrix}$$

Note that the above four eigenvectors are orthogonal. Let $1$, $g$, and $\beta$ be such as in Proposition 3.2 for the vertices $B, D, A, C$. We have $g = (x_1, x_2, x_3, x_4)^T$, where $x_1 = \log |B|$, $x_2 = \log |D|$, $x_3 = \log |A|$ and $x_4 = \log |C|$. We remark that $x_2 > x_1$, $x_3 > x_4$ and $x_2 \geq x_3$.

We claim that there exists a vector $v := a v_1 + b v_2 + c v_3 + d v_4$ such that $v \cdot 1 = 0$, $v \cdot g = 0$ and $v^T M v = 2(\lambda^2 + 1) \cdot [\lambda(a^2 - b^2) + (\lambda - 1)(c^2 - d^2)] > 0$. We first rewrite $v \cdot 1 = 0$ as $a(1 + \lambda) + d(1 - \lambda) = 0$, which together with $\lambda^2 = \lambda + 1$ implies that $d = \frac{\lambda + 1}{\lambda - 1} \cdot a = \lambda^3 a$. Substituting $d = \lambda^3 a$, the second equation $v \cdot g = 0$ becomes

$$a(1 + 3\lambda)(x_1 - x_2 - x_3 + x_4) + b(-\lambda x_1 - x_2 + x_3 + \lambda x_4) + c(x_1 - \lambda x_2 + \lambda x_3 - x_4)$$

$$= 0.$$ 

If $x_1 - \lambda x_2 + \lambda x_3 - x_4 = 0$, then we may choose $a, b$ such that $a(1 + 3\lambda)(x_1 - x_2 - x_3 + x_4) + b(-\lambda x_1 - x_2 + x_3 + \lambda x_4) = 0$ and choose $c$ sufficiently large such that $v^T M v > 0$, thereby the claim follows. If $x_1 - \lambda x_2 + \lambda x_3 - x_4 \neq 0$, then we choose $a = b = 1$, $d = \lambda^3$ and

$$c = \frac{(3\lambda + 2)x_2 + 3\lambda x_3 - (2\lambda + 1)x_1 - (4\lambda + 1)x_4}{x_1 - \lambda x_2 + \lambda x_3 - x_4}$$

such that the second equation $v \cdot g = 0$ is satisfied. We will show $|c| > \lambda^3$, which implies $v^T M v > 0$ and hence the claim. Note that $x_2 > x_1, x_3 > x_4$ and $x_2 \geq x_3$, so $(3\lambda + 2)x_2 + 3\lambda x_3 - (2\lambda + 1)x_1 - (4\lambda + 1)x_4 > 0$, thus it suffices to show that

$$(3\lambda + 2)x_2 + 3\lambda x_3 - (2\lambda + 1)x_1 - (4\lambda + 1)x_4 > \lambda^3(x_1 - \lambda x_2 + \lambda x_3 - x_4)$$

and

$$(3\lambda + 2)x_2 + 3\lambda x_3 - (2\lambda + 1)x_1 - (4\lambda + 1)x_4 > -\lambda^3(x_1 - \lambda x_2 + \lambda x_3 - x_4).$$

To see this, using $\lambda^3 = 2\lambda + 1$ and $\lambda^4 = 3\lambda + 2$, the above two inequalities can be simplified as $(6\lambda + 4)x_2 > 2x_3 + (4\lambda + 2)x_1 + 2\lambda x_4$ and $x_3 > x_4$, which are obviously true, thereby establishing the claim.
Proof. To well.

Now \( \gamma = \) of SUPP Proposition 2.6 implies this Proposition 2.7 implies are a star clique Proposition 3.4.

While keeping the other entries unchanged, where \( \varepsilon > 0 \) is sufficiently small. We have \( \alpha' \geq 0, V_q(\alpha') = 1, \) and OBJ\(_q(\alpha') = \) OBJ\(_q(\alpha)\); because \( 1, g \) and \( \beta \) are linearly dependent (this implies \( v \cdot \beta = 0 \)), we also have

\[
E_q(\alpha') = E_q(\alpha) + \varepsilon^2 v^T M v > E_q(\alpha),
\]

which contradicts Proposition 2.4. This finishes the proof. \( \square \)

3.4. Step 4: the star has two petals

**Proposition 3.9.** For any solution \( \alpha \) to OPT\(_q(s)\), if SUPP\(_q(\alpha)\) can be obtained from a clique by removing a star (a collection of edges sharing a common endpoint), then the star must have exactly two edges and SUPP\(_q(\alpha) \in Q\).

**Proof.** Let \( \alpha \) be a solution to OPT\(_q(s)\) such that SUPP\(_q(\alpha)\) is a graph obtained from a clique by removing the edges of a star. Assume that the support of \( \alpha \) consists of sets \( B_1, \ldots, B_t, A_1, \ldots, A_k, C \) for some \( t \geq 0 \) and \( k \geq 1 \) such that sets \( B_1, \ldots, B_t, A_1, \ldots, A_k \) are disjoint, \( C \cap B_i = \emptyset \) and \( C \cap A_j \neq \emptyset \) for all \( i, j \). Since \( \alpha \) is a solution to OPT\(_q(s)\), Proposition 2.7 implies that every color in \( C \cup A_1 \cup \ldots \cup A_k \) is covered at least twice by this union. This is only possible when \( C = A_1 \cup A_2 \ldots \cup A_k \), and thus \( k \geq 2 \). Moreover, Proposition 2.6 implies that \( B_1, \ldots, B_t, A_1, \ldots, A_k \) form a partition of \([q]\). To prove that SUPP\(_q(\alpha) \in Q\), we need to show that \( k = 2 \). Assume, towards contradiction, that \( k \geq 3 \).

Without loss of generality, we assume that \( C = [p] \) for some integer \( p < q \). Instead of working on \([q]\) and its OPT\(_q(s)\), we will turn to the study of the smaller ground set \([p]\) and a new optimization which can be viewed as a restriction of OPT on \([p]\). Let \( \gamma = \sum_{i=1}^{k} \alpha_{A_i} + \alpha_C \) and \( \tilde{\alpha} \) be the vector with \( 2^p - 1 \) coordinates such that its support consists of \( A_1, \ldots, A_k, C \) and \( \tilde{\alpha}_{A_i} = \frac{\alpha_{A_i}}{\gamma}, \tilde{\alpha}_C = \frac{\alpha_C}{\gamma} \). Choose real \( s' \) so that \( \frac{s'-1}{2s'} = E_p(\tilde{\alpha}) \).

Now we consider the new optimization problem OPT\(_p(s')\) restricted to the ground set \([p]\). Since \( \alpha \) solves OPT\(_q(s)\), by our definitions, it is clear that \( \tilde{\alpha} \) solves OPT\(_p(s')\) as well.

We have seen that \( \tilde{\alpha} \) maximizes OBJ\(_p(\tilde{\alpha})\) subject to \( \alpha_A \geq 0 \) for all nonempty \( A \subseteq [p] \), \( E_p(\alpha) - \frac{s'-1}{2s'} \geq 0 \) and \( V_p(\alpha) = 1 \). We will apply the method of Karush–Kuhn–Tucker to \( \tilde{\alpha} \) and OBJ\(_p\) (recall the Section 2.1). Before proceeding, we point out that \( \tilde{\alpha} \) is a regular point for OBJ\(_p\), as one can easily verify that \( \tilde{\alpha} \) satisfies the LICQ conditions. For convenience, write \( \tilde{\alpha}_i := \tilde{\alpha}_{A_i}, T := \sum_{i=1}^{k} \tilde{\alpha}_i \) and \( P := \prod_{i=1}^{k} |A_i| \). Let \( \pi_A \) denote the
projection on the coordinate $A$, i.e., $\pi_A(\alpha) = \alpha_A$. By (3), there exist constants $\mu_A \leq 0, \mu$ and $\lambda \leq 0$ such that

$$\nabla \text{OBJ}_p(\tilde{\alpha}) = \left( \sum_{A \subseteq \rho} \mu_A \cdot \nabla \pi_A \right) + \mu \cdot \nabla V_p(\tilde{\alpha}) + \lambda \cdot \nabla E_p(\tilde{\alpha}).$$

For subset $A$ with $\tilde{\alpha}_A = 0$, we have

$$\log |A| = \mu_A + \mu + \lambda \cdot \sum_{B \cap A = \emptyset} \tilde{\alpha}_B \leq \mu + \lambda \cdot \sum_{B \cap A = \emptyset} \tilde{\alpha}_B. \quad (4)$$

For $C$ and $A_i$, we have $\mu_C = \mu_{A_i} = 0$, so

$$\log |C| = \mu \quad \text{and} \quad \log |A_i| = \mu + \lambda \cdot (T - \tilde{\alpha}_i). \quad (5)$$

By (5) and summing $\log |A_i|$ from $i = 1$ to $k$, we get that $\lambda \cdot T = \frac{1}{k-1} \log \frac{P}{|C|}$ and thereby

$$\frac{1}{k-1} \log \left( \frac{P}{|A_i|^{k-1}|C|} \right).$$

As $k \geq 3$, by substituting $A := C \setminus A_i$ in (4), we obtain $\log(|C| - |A_i|) \leq \log |C| + \lambda \cdot \tilde{\alpha}_i$, thus

$$|A_i|^{k-1} \cdot (|C| - |A_i|)^{k-1} \leq P \cdot |C|^{k-2}$$

for all $i = 1, 2, \ldots, k$. Let $x_i := |A_i|/|C|$ and assume $x := x_1 \geq x_2 \geq \ldots \geq x_k > 0$, then $1 > x \geq \frac{1}{k}$ as $\sum_{i=1}^{k} x_i = 1$. In addition, the previous inequality implies that

$$x^{k-1}(1-x)^{k-1} \leq x \cdot \prod_{j=2}^{k} x_j. \quad (6)$$

For $k \geq 3$, one can check that $x^{k-2} \geq (\frac{1}{k})^{k-2} > (\frac{1}{k-1})^{k-1}$. This inequality, together with the AM–GM inequality, implies

$$x^{k-1}(1-x)^{k-1} > x \cdot \frac{(1-x)^{k-1}}{(k-1)^{k-1}} \geq x \cdot \prod_{j=2}^{k} x_j,$$

contradicting (6) and finishing the proof of Step 4. \Box
3.5. Step 5: computing the size of the support when the solution is in $Q$

We introduce restricted versions of the MAIN OPTIMIZATION PROBLEM. Fix an integer $k \geq 1$ and a collection $\{A_1, \ldots, A_{k-1}, A_k, A_1 \cup A_2\}$ of $[q]$ such that $A_1, \ldots, A_k$ form a $k$-partition of $[q]$. We consider the following optimization:

\[
\text{Maximize } \sum_{i=1}^{k} \alpha_i \log |A_i| + \beta \log(|A_1| + |A_2|) \\
\text{Subject to } \sum_{i=1}^{k} \alpha_i + \beta = 1, \\
\sum_{i=1}^{k} \alpha_i^2 + \beta^2 + 2\beta(\alpha_1 + \alpha_2) \leq \frac{1}{s}, \\
\alpha_i \geq 0, \beta \geq 0 \text{ for } i = 1, \ldots, k.
\]

(7)

The conditions of (7) are consistent with the conditions of the MAIN OPTIMIZATION PROBLEM, when restricted to vectors with support in $P_k \cup Q_k$. By compactness, the maximum of (7) exists, which is achieved either in the boundary or interior of its domain, where the vectors in the interior have strict positive coordinates. By Cauchy–Schwarz, we have

\[
\frac{1}{s} \geq \beta^2 + 2\beta(\alpha_1 + \alpha_2) + \sum_{i=1}^{k} \alpha_i^2 \geq (\beta + \alpha_1)^2 + \sum_{i=2}^{k} \alpha_i^2 \geq \frac{1}{k} \left( \beta + \sum_{i=1}^{k} \alpha_i \right)^2 = \frac{1}{k},
\]

which implies $k \geq s$, and since $k$ is an integer we must also have $k \geq \lceil s \rceil$. We also remark that if $\alpha_1 + \alpha_2, \beta > 0$ then the inequality is strict, i.e. $k > s$. We derive a necessary condition for the maximum to be attained in the interior of the domain of (7). Let

\[
S_1 := \frac{1}{k-1} \left[ \log(|A_1| + |A_2|) + \sum_{i=3}^{k} \log |A_i| \right], \text{ and} \\
S_2 := \frac{1}{k-1} \left[ -\log^2 \left( \frac{|A_1| \cdot |A_2|}{|A_1| + |A_2|} \right) + \sum_{i=1}^{k} \log^2 |A_i| \right].
\]

Lemma 3.10. If $\alpha = (\alpha_1, \ldots, \alpha_k, \beta) > 0$ is a local maximum point for (7), then

\[
\alpha_1 = \frac{1}{\lambda} \log \left( \frac{|A_1| + |A_2|}{|A_2|} \right), \ \alpha_2 = \frac{1}{\lambda} \log \left( \frac{|A_1| + |A_2|}{|A_1|} \right), \ \beta = \frac{1}{\lambda} \log \left( \frac{|A_1| \cdot |A_2|}{|A_1| + |A_2|} \right) - \frac{\mu}{\lambda},
\]

for each $i = 3, \ldots, k$, we have $\alpha_i = \frac{\log |A_i| - \mu}{\lambda}$, and the value of the objective function of (7) is

\[
\beta \log(|A_1| + |A_2|) + \sum_{i=1}^{k} \alpha_i \log |A_i| = \mu + \frac{\lambda}{s},
\]
where \( \lambda = (k - 1) \sqrt{\frac{s}{k-1} (S_2 - S'_1^2)} > 0 \) and \( \mu = S_1 - \frac{\lambda}{k-1} \). In particular, we have \( k \neq s + 1, \log \left( \frac{|A_1| + |A_2|}{|A_1| + |A_2|} \right) > \mu, \) and \( \log |A_i| > \mu \) for each \( i \geq 3 \).

**Proof.** By the same proof of Proposition 2.4, the local maximality of (7) implies \( \sum_{i=1}^k \alpha_i^2 + \beta^2 + 2\beta(\alpha_1 + \alpha_2) = \frac{1}{\lambda} \). We can apply the KKT method as a straightforward calculation shows that the local extremum \( \alpha \) satisfies the LICQ conditions. Therefore there exist constants \( \lambda \geq 0 \) and \( \mu \) such that for each \( i \geq 3, \log |A_i| = \mu + \lambda \alpha_i, \) \( \log |A_1| = \mu + \lambda(\alpha_1 + \beta), \log |A_2| = \mu + \lambda(\alpha_2 + \beta) \) and \( \log(|A_1| + |A_2|) = \mu + \lambda(\alpha_1 + \alpha_2 + \beta) \).

If \( \lambda = 0 \), then \( \log(|A_1| + |A_2|) = \mu = \log |A_1| \), a contradiction, thus \( \lambda > 0 \).

We can rewrite the above equations as \( \alpha_i = \frac{1}{\lambda} (\log |A_i| - \mu) \) for each \( i \geq 3, \alpha_1 = \frac{1}{\lambda} \log \left( \frac{|A_1| + |A_2|}{|A_1|} \right), \alpha_2 = \frac{1}{\lambda} \log \left( \frac{|A_1| + |A_2|}{|A_2|} \right) \) and \( \beta = \frac{1}{\lambda} \left( \log \left( \frac{|A_1|}{|A_1| + |A_2|} \right) - \mu \right) \). Now solving the system \( \sum_{i=1}^k \alpha_1 + \beta = 1 \) and \( (\alpha_1 + \beta)^2 + (\alpha_2 + \beta)^2 - \beta^2 + \sum_{i=2}^k \alpha_i^2 = \frac{1}{s} \), we obtain the desired expressions of \( \lambda \) and \( \mu \). This finishes the proof. \( \Box \)

For completion, we turn to the case \( \beta = 0 \). Let \( S'_1 := \frac{1}{k} \sum_{i=1}^k \log |A_i| \) and \( S'_2 := \frac{1}{k} \sum_{i=1}^k \log^2 |A_i| \). We have the following

**Lemma 3.11.** If \( k > s \) and \( \alpha = (\alpha_1, \ldots, \alpha_k, 0) \) is a local maximum point of (7) satisfying \( \alpha_i > 0 \) for all \( i = 1, \ldots, k \), then \( \lambda' \alpha_i = \log |A_i| - \mu' \) for each \( i = 1, \ldots, k \) and the value of the objective function is

\[
\sum_{i=1}^k \alpha_i \log |A_i| = \mu' + \frac{\lambda'}{s},
\]

where \( \lambda' = k \sqrt{\frac{s}{k-s} (S'_2 - (S'_1)^2)} \geq 0 \) and \( \mu' = S'_1 - \frac{\lambda'}{k} \). In particular, \( \log |A_i| \geq \mu' \) for all \( i = 1, \ldots, k \).

**Proof.** The proof is very similar to the proof of Lemma 3.10. The only difference is that, in order to apply KKT, we use Slater’s condition instead (when \( \beta = 0 \), the nonlinear constraint becomes a convex constraint). We also remark that, when \( k = s \), we must have \( \alpha_1 = \alpha_2 = \ldots = \alpha_k = \frac{1}{k} \), and the value of the objective function is \( S'_1 \). \( \Box \)

**Remark.** In Lemma 3.11 it is possible that \( \lambda' = 0 \) (for instance, when all the \( A_i \)'s have the same size).

We now are ready to present the proof of Step 5. With slight abuse of notation, we use \( \alpha \) to express the sub-vector induced by the nonzero coordinates of vector \( \alpha \).

**Proposition 3.12.** For any solution \( \alpha \) to \( \text{OPT}_q(s) \) such that \( \text{SUPP}_q(\alpha) \in \mathcal{Q} \), we have \( \text{SUPP}_q(\alpha) \in \mathcal{Q}_{\lfloor s \rfloor} \). In particular, \( s \notin \mathbb{Z} \).
**Proof.** Let \( \alpha \) be a solution to \( \text{OPT}_q(s) \) such that \( \text{SUPP}_q(\alpha) \in Q \). We will show that in fact \( \text{SUPP}_q(\alpha) \in Q_k \). Suppose, towards contradiction, that \( \text{SUPP}_q(\alpha) \in Q_{k+1} \) for some \( k \geq |s| \). Let the support of \( \alpha \) be a collection \( \{A_1, \ldots, A_k, A_{k+1}, A_1 \cup A_2\} \) such that \( A_1, \ldots, A_{k+1} \) form a \((k+1)\)-partition of \([q]\) and rewrite \( \alpha = (\alpha_1, \ldots, \alpha_{k+1}, \beta) > 0 \).

Fixed the collection \( \{A_1, \ldots, A_{k+1}, A_1 \cup A_2\} \), we consider (7) — the restricted version of the MAIN OPTIMIZATION PROBLEM. Obviously, the vector \( \alpha \) also achieves the maximum of (7). Since \( \alpha > 0 \), we may apply Lemma 3.10. Note that \( \lambda = k \sqrt{\frac{s}{k-s}} (S_2 - S_1^2) \) and \( \mu = S_1 - \frac{\lambda}{k} \), where

\[
S_1 = \frac{1}{k} \log(|A_1| + |A_2|) + \sum_{i=3}^{k+1} \log |A_i|, \quad \text{and}
\]

\[
S_2 = \frac{1}{k} \log^2(|A_1| + |A_2|) - 2 \log \left( \frac{|A_1| + |A_2|}{|A_1|} \right) \log \left( \frac{|A_1| + |A_2|}{|A_2|} \right) + \sum_{i=3}^{k+1} \log^2 |A_i|. \]

From Lemma 3.10, we also see that \( k > s \) (because \( k+1 \neq s+1 \)), \( \log |A_i| - \mu > 0 \) for \( i \geq 3 \), \( \log \left( \frac{|A_1| + |A_2|}{|A_1| + |A_2|} \right) - \mu > 0 \) and

\[\text{OBJ}_q(\alpha) = \mu + \frac{\lambda}{s} = S_1 + \left( \frac{1}{s} - \frac{1}{k} \right) \lambda.\]

We let \( S_1' = S_1 \) and

\[
S_2' = \frac{1}{k} \log^2(|A_1| + |A_2|) + \sum_{i=3}^{k+1} \log^2 |A_i|. \]

Clearly \( S_2' > S_2 \). We construct a vector \( \alpha' \in \text{FEAS}_q(s) \) such that \( \text{SUPP}_q(\alpha') \in P_k \) and \( \text{OBJ}_q(\alpha') > \text{OBJ}_q(\alpha) \), which is a contradiction to \( \text{OBJ}_q(\alpha) = \text{OPT}_q(s) \). We let \( \alpha' = (\alpha'_1, \ldots, \alpha'_{k-1}, \alpha'_k) \) with support being the \( k \)-partition \( \{A_1 \cup A_2, A_3, \ldots, A_k, A_{k+1}\} \) of \([q]\). The coordinates of \( \alpha' \) are defined by \( \alpha'_i = \frac{\log |A_{i+1}| - \mu'}{\lambda'} \) for \( 2 \leq i \leq k \) and \( \alpha'_1 = \frac{\log (|A_1| + |A_2|) - \mu'}{\lambda'} \), where

\[\lambda' = k \sqrt{\frac{s}{k-s}} (S_2' - (S_1')^2) \quad \text{and} \quad \mu' = S_1' - \frac{\lambda'}{k}.\]

Note that \( k > s \), \( S_1' = S_1 \) and \( S_2' > S_2 \). So \( \lambda' > \lambda \) and \( \mu' < \mu \), then \( \log |A_{i+1}| - \mu' > \log |A_{i+1}| - \mu > 0 \) for \( 2 \leq i \leq k \) and \( \log(|A_1| + |A_2|) - \mu' > \log \left( \frac{|A_1| + |A_2|}{|A_{i+1}|} \right) - \mu > 0 \), which implies that \( \alpha' > 0 \). It is also not hard to verify that \( \alpha'_1 + \ldots + \alpha'_k = 1 \) and \( (\alpha'_1)^2 + \ldots + (\alpha'_k)^2 = \frac{1}{s} \), therefore indeed \( \alpha' \in \text{FEAS}_q(s) \). Simplifying the expression of \( \text{OBJ}_q(\alpha') \), we get

\[\text{OBJ}_q(\alpha') = \mu' + \frac{\lambda'}{s} = S_1' + \left( \frac{1}{s} - \frac{1}{k} \right) \lambda',\]
which is strictly larger than OBJ\(_q(\alpha)\) = OPT\(_q(s)\). This contradiction proves that \(\text{SUPP}_q(\alpha) \in Q\_{\lfloor s \rfloor}\). To complete the proof of the proposition, it remains to show that \(s \notin Z\). Since \(\alpha_1 + \alpha_2, \beta > 0\), by the remark in (8) we must have \([s] = k > s\), hence \(s\) is not an integer and we finish the proof. □

### 3.6. Step 6: establishing the structure of a solution

We quote some results in [16] that characterize graphs having at most two nonnegative eigenvalues. Let \(B_{2\ell}\) be the class of graphs \(G\) satisfying the following conditions:

- \(V(G) = X \cup Y\) with \(X \cap Y = \emptyset\), where \(X\) is a union of \(\ell\) disjoint sets \(X_1, \ldots, X_\ell\) of vertices and \(Y\) is a union of \(\ell\) disjoint sets \(Y_1, \ldots, Y_\ell\) of vertices;
- \(G[X]\) and \(G[Y]\) are two complete disjoint subgraphs of \(G\);
- for each \(i, j \geq 2\), every vertex of \(X_i\) is adjacent to every vertex of \(Y_\ell \cup \ldots \cup Y_{\ell-i+2}\) and every vertex of \(Y_j\) is adjacent to every vertex of \(X_\ell \cup \ldots \cup X_{\ell-j+2}\).

Let \(B_1\) be the class of complete graphs. For \(\ell \geq 1\), let \(B_{2\ell+1}\) be the class of graphs \(G\) for which \(V(G) = X \cup Y \cup Z, G[X \cup Y] \in B_{2\ell}\) and every vertex of \(Z\) is adjacent to all other vertices of \(G\). (See Fig. 2.)

**Lemma 3.13.** (See Lemma 4 in [16].) If a graph \(G\) does not contain any of \(3K_1, C_4, C_5\) as induced subgraphs then \(G \in \bigcup_{\ell \geq 1} B_\ell\).

We now present the proof of Step 6.

**Proposition 3.14.** For any solution \(\alpha\) to OPT\(_q(s)\) not having induced copies of \(3K_1, C_4, C_5\) in its support graph \(\text{SUPP}_q(\alpha)\), it is true that \(\text{SUPP}_q(\alpha) \in \left( \bigcup_{k \geq \lfloor s \rfloor} P_k \right) \cup Q\_{\lfloor s \rfloor}\).

**Proof.** Let \(\alpha\) be a solution to OPT\(_q(s)\) such that \(\text{SUPP}_q(\alpha)\) contains neither \(3K_1\) nor \(C_4\) as an induced subgraph. We know, by Proposition 3.5 (Step 1), that \(\text{SUPP}_q(\alpha)\) does not contain \(C_5\) as induced subgraph as well. By Lemma 3.13, \(\text{SUPP}_q(\alpha) \in \bigcup_{\ell \geq 1} B_\ell\). We will show that \(\text{SUPP}_q(\alpha) \in P \cup Q\_{\lfloor s \rfloor}\).
First we show that \( t \leq 5 \). Suppose not. Then \( \ell := \lfloor t/2 \rfloor \geq 3 \) and there exists an induced subgraph \( G \) of \( \text{SUPP}_q(\alpha) \) such that \( G \in \mathcal{B}_{2\ell} \). Recall the definition of \( \mathcal{B}_{2\ell} \). We choose four vertices \( x_1, x_2, y_1, y_2 \) of \( G \) such that \( x_1 \in X_1, x_2 \in X_2, y_1 \in Y_1, y_2 \in Y_2 \), then \( \{x_1, x_2, y_1, y_2\} \) induces a matching of size two in \( \text{SUPP}_q(\alpha) \), contradicting Proposition 3.7 (Step 2).

We claim that \( 1 \leq t \leq 3 \). Suppose not, then either \( t = 4 \) or \( t = 5 \). There exists an induced subgraph \( G \) of \( \text{SUPP}_q(\alpha) \) such that \( G \in \mathcal{B}_4 \). So \( V(G) = X_1 \cup X_2 \cup Y_1 \cup Y_2 \). If there exist two vertices \( x_1, x_2 \) in \( X_1 \), then \( \{x_1, x_2, y_1, y_2\} \) induces a matching of size two in \( \text{SUPP}_q(\alpha) \) for any \( y_1 \in Y_1, y_2 \in Y_2 \), contradicting Proposition 3.7 again. Therefore, we may assume that \( X_1 = \{A\} \) and by symmetry \( Y_1 = \{B\} \) for \( A, B \subseteq \lceil q \rceil \). Let \( X_2 = \{C_1, \ldots, C_l\} \) and \( Y_2 = \{D_1, \ldots, D_m\} \), where \( C_i, D_j \subseteq \lceil q \rceil \). Since \( X_2 \cup Y_2 \) induces a clique, the sets \( \bigcup_{i=1}^l C_i \) and \( \bigcup_{j=1}^m D_j \) are disjoint. By similar reasons, \( A \cap \left( \bigcup_{i=1}^l C_i \right) = \emptyset \) and \( B \cap \left( \bigcup_{j=1}^m D_j \right) = \emptyset \). Proposition 2.7 implies that \( A \cup C_1 \cup \ldots \cup C_l = B \cup D_1 \cup \ldots \cup D_m \).

Then clearly \( C_1 \subseteq B \setminus A \subseteq B \) and \( D_1 \subseteq A \setminus B \subseteq A \). Now, \( \{A, C_1, D_1, B\} \) induces a path \( A - C_1 - D_1 - B \) in \( \text{SUPP}_q(\alpha) \) with \( |A| > |D_1| \) and \( |B| > |C_1| \), contradicting Proposition 3.8 (Step 3).

If \( t = 1 \) then it is easy to see that \( \text{SUPP}_q(\alpha) \in \mathcal{P} \) and by \( 8 \) we must have \( \text{SUPP}_q(\alpha) \in \bigcup_{k \geq [s]} \mathcal{P}_k \). Otherwise, we may assume that \( \text{SUPP}_q(\alpha) \in \mathcal{B}_2 \cup \mathcal{B}_3 \). The support of \( \alpha \) can be expressed as a union \( X \cup Y \cup Z \) (possibly with \( Z = \emptyset \)) such that each of \( X \cup Z \) and \( Y \cup Z \) induces a clique in \( \text{SUPP}_q(\alpha) \) and there is no edge between \( X \) and \( Y \).

If \( |X| \geq 2 \) and \( |Y| \geq 2 \), then \( \text{SUPP}_q(\alpha) \) has an induced matching of size two, which cannot happen by Proposition 3.7 (Step 2). Thus, we may assume that \( |Y| = 1 \) and thereby \( \text{SUPP}_q(\alpha) \) can be viewed as a graph obtained from a clique by removing a star. Now Proposition 3.9 (Step 4) and Proposition 3.12 (Step 5) together imply that \( \text{SUPP}_q(\alpha) \in \mathcal{Q}_{[s]} \). This finishes the proof of Step 6.

**Corollary 3.15.** There exists a solution \( \alpha \) to \( \text{OPT}_q(s) \) such that \( \text{SUPP}_q(\alpha) \in \left( \bigcup_{k \geq [s]} \mathcal{P}_k \right) \cup \mathcal{Q}_{[s]} \).

### 3.7 Step 7: the structure of all solutions

In this subsection we characterize all solutions to the main optimization problem. Namely, we prove that not only we can find a solution \( \alpha \) for which \( \text{SUPP}_q(\alpha) \in \mathcal{P} \cup \mathcal{Q}_{[s]} \) as Corollary 3.15 asserts, but in fact, all solutions to \( \text{OPT}_q(s) \) necessarily satisfy \( \text{SUPP}_q(\alpha) \in \mathcal{P} \cup \mathcal{Q}_{[s]} \).

Among the first six steps in the proof of Theorem 3.1, Step 1 is the only step that fails to assert a property that all solutions necessarily enjoy, as it does not prevent the existence of a solution \( \alpha \) such that \( \text{SUPP}_q(\alpha) \) contains either \( 3K_1 \) or \( C_4 \) as induced subgraphs. To remedy this situation, we prove the following three propositions.
Proposition 3.16. If \( \alpha \) is a solution to \( \text{OPT}_q(s) \) and \( \alpha' \) is another solution to \( \text{OPT}_q(s) \) obtained from \( \alpha \) by an application of Proposition 3.3 with \( H \) being isomorphic to \( 3K_1 \), then \( \text{SUPP}_q(\alpha') \notin \mathcal{P} \cup \mathcal{Q} \).

Proof. Suppose, towards contradiction, that \( \text{SUPP}_q(\alpha') \in \mathcal{P} \cup \mathcal{Q} \). Let \( A, B \) and \( C \) be the vertices of \( H \). Clearly \( A, B, C \) pairwise intersect, because they induce an independent set of size three. Moreover, we have \( \text{SUPP}_q(\alpha) - \{A, B, C\} \subset \text{SUPP}_q(\alpha') \subset \text{SUPP}_q(\alpha) \). Since \( \text{SUPP}_q(\alpha') \in \mathcal{P} \cup \mathcal{Q} \), we know that some of the sets in \( \text{SUPP}_q(\alpha') \) form partition of \([q]\). Let \( \mathcal{R} \) be such a partition with maximum number of sets. Because \( \mathcal{R} \) can contain at most one element from \( \{A, B, C\} \) and \( \alpha'_A + \alpha'_B + \alpha'_C = \alpha_A + \alpha_B + \alpha_C > 0 \), we may assume, without loss of generality, that \( B, C \notin \mathcal{R} \) and \( A \) is in the support of \( \alpha' \). We remark that we do not necessarily have \( A \in \mathcal{R} \). Since \( B \cap C \neq \emptyset \), there exists a set \( A' \in \mathcal{R} \) such that \( A' \cap B \cap C \neq \emptyset \).

We claim that \( X \subseteq B \) for any subset \( X \in \mathcal{R} \) intersecting \( B \). To prove this, we use Proposition 2.7. If \( X \notin B \), then there exists a set \( Y \) in the support of \( \alpha \) which is disjoint from \( B \) and intersects \( X \). The set \( Y \) must be in the support of \( \alpha' \) as well, since \( Y \notin \{A, B, C\} \). Because \( X \cap Y \neq \emptyset \), we must have that \( \text{SUPP}_q(\alpha') \in \mathcal{Q} \), which implies \( X \subseteq Y \) (recall \( X \in \mathcal{R} \)). This is a contradiction, because \( Y \) must be disjoint from \( B \), thereby proving the claim. Therefore, there exists a subfamily \( \mathcal{R}_1 \subset \mathcal{R} \) such that \( B = \bigcup_{X \in \mathcal{R}_1} X \). By switching the roles of \( B \) and \( C \) in the previous argument, we conclude that there exists \( \mathcal{R}_2 \subset \mathcal{R} \) such that \( C = \bigcup_{X \in \mathcal{R}_2} X \). As \( B, C \notin \mathcal{R} \), we see that \( |\mathcal{R}_1| \geq 2 \) and \( |\mathcal{R}_2| \geq 2 \); as \( A' \cap B \cap C \neq \emptyset \), we must have \( A' \subseteq B \cap C \). We assume, from now on, that \( |B| \geq |C| \).

We have two cases to consider:

(i) \( C \notin B \). In this case, we have \( B - C \neq \emptyset \) and \( C - B \neq \emptyset \), so there exist two sets \( D, E \in \mathcal{R} \setminus \{A'\} \) such that \( D \subseteq B, E \subseteq C \), and \( D \cap C = E \cap B = \emptyset \); or

(ii) \( C \subseteq B \). Since \( |\mathcal{R}_2| \geq 2 \), there exists a set \( D \in \mathcal{R} \setminus \{A'\} \) such that \( D \subseteq B \cap C \).

In the first case (i), the sets \( B, C, D, E \) in the support of \( \alpha \) induce a path \( C - D - E - B \) satisfying \( |C| > |E| \) and \( |B| > |D| \). But this is forbidden by Proposition 3.8 (Step 3). In the second case (ii), if \( H' \) is the subgraph induced by the sets \( A', B, C, D \), then the adjacency matrix of \( H' \) with respect to the sets \( A', B, C, D \) (in that order) is

\[
M = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}.
\]

The matrix \( M \) has three nonnegative eigenvalues and its kernel is spanned by the vectors \((0, 1, 0, 0)\) and \((0, 0, 1, 0)\). However, there is no vector \( v \) in the kernel of \( M \) such that \( v \) is perpendicular to both \((1, 1, 1, 1)\) and \((\log |A'|, \log |B|, \log |C|, \log |D|)\).
since \( \log |B| > \log |C| \) in (ii). Hence, by Observation 3.4, \( \alpha \) cannot be an optimal solution to \( \text{OPT}_q(s) \), finishing the proof of the proposition. \( \square \)

**Proposition 3.17.** If \( \alpha \) is a solution to \( \text{OPT}_q(s) \) and \( \alpha' \) is another solution to \( \text{OPT}_q(s) \) obtained from \( \alpha \) by an application of Proposition 3.3 with \( H \) being isomorphic to \( C_5^+ \), then \( \text{SUPP}_q(\alpha') \notin \mathcal{P} \cup \mathcal{Q} \).

**Proof.** Suppose, towards contradiction, that \( \text{SUPP}_q(\alpha') \in \mathcal{P} \cup \mathcal{Q} \). Let sets \( A, B, C, D \) and \( E \) induce the subgraph \( H \) (see Fig. 3), whose adjacency matrix (with respect to the order of \( A, B, C, D, E \)) is

\[
M = \begin{pmatrix}
0 & 1 & 0 & 1 & 1 \\
1 & 0 & 1 & 0 & 1 \\
0 & 1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 & 0
\end{pmatrix}.
\]

The matrix \( M \) has three nonnegative eigenvalues and has kernel spanned by the vector \((-1, 1, 1, -1, 0)\). Therefore, the vector \( \gamma \) yielded by the proof of Proposition 3.3 for \( H \) has the form \( \gamma = (\gamma_A, \gamma_B, \gamma_C, \gamma_D, 0) \), where \( \gamma_A = \gamma_D = -\gamma_B = -\gamma_C \). Then either \( C \) or \( D \) is in the support of \( \alpha' \) (since either \( \gamma_C \geq 0 \) or \( \gamma_D \geq 0 \)); by the symmetry between \( C \) and \( D \), we may assume that \( C \in \text{SUPP}_q(\alpha') \). We point out that \( E \in \text{SUPP}_q(\alpha') \), as the coordinate \( \alpha_E \) is not changed. In addition, we have \( C \cap E \neq \emptyset \). This implies that \( \text{SUPP}_q(\alpha') \in \mathcal{Q} \); and moreover, either \( C \subset E \) or \( E \subset C \). If \( C \subset E \), together with the fact that \( A \cap E = \emptyset \), we get that \( A \cap C = \emptyset \), contradicting our definition of \( C_5^+ \). If \( E \subset C \), plus \( C \cap D = \emptyset \), we get that \( E \cap D = \emptyset \), again contradicting the definition of \( C_5^+ \). This finishes the proof. \( \square \)

**Proposition 3.18.** Let \( \alpha \) be a solution to \( \text{OPT}_q(s) \) and \( \alpha' \) be another solution to \( \text{OPT}_q(s) \) obtained from \( \alpha \) by an application of Proposition 3.3 with \( H \) being isomorphic to \( C_4 \). If \( \text{SUPP}_q(\alpha) \) does not contain an induced copy of \( 3K_1 \) or \( C_5^+ \), then \( \text{SUPP}_q(\alpha') \notin \mathcal{P} \cup \mathcal{Q} \).

**Proof.** Suppose, towards contradiction, that \( \text{SUPP}_q(\alpha') \in \mathcal{P} \cup \mathcal{Q} \). Let \( A, B, C \) and \( D \) be the vertices of \( H \), where we assume the pairs \( \{A, B\}, \{B, C\}, \{C, D\} \) and \( \{D, A\} \) induce edges in \( \text{SUPP}_q(\alpha) \), or equivalently, these are the pairs of disjoint sets. Let \( \gamma \in \mathbb{R}^4 \) be

![Fig. 3. graph $C_5^+$.](image-url)
the vector that the proof of Proposition 3.3 yields for $H$. By Observation 3.4, we have $M \cdot \gamma = 0$, where

$$M = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

is the adjacency matrix of $H$, so $\gamma_A + \gamma_C = \gamma_B + \gamma_D = 0$. As in the proof of Proposition 3.16, denote by $\mathcal{R}$ the partition of $[q]$ in $\text{SUPP}_q(\alpha')$ with maximum number of sets. We remark that among the vertices of $V(H)$, at least one but at most two belong to $\mathcal{R}$. This is because the elements of $\mathcal{R}$ induce a clique in $\text{SUPP}_q(\alpha')$. We may then assume, without loss of generality, that $A \in \mathcal{R}$ and $C, D \notin \mathcal{R}$. We claim that $B \in \mathcal{R}$. If not, then because $B \cap D \neq \emptyset$, there exists a set $B' \in \mathcal{R}$ such that $B' \cap (B \cap D) \neq \emptyset$. But if that is the case, the sets $B', B, D$ would induce a copy of $3K_1$ in $\text{SUPP}_q(\alpha)$, which is clearly a contradiction. Thus, we must have $B \in \mathcal{R}$.

We point out that there is no set $E \in \mathcal{R}$ such that $E \cap C \neq \emptyset$ and $E \cap D \neq \emptyset$, as, otherwise, the sets $A, B, E, C, D$ would induce a subgraph of $\text{SUPP}_q(\alpha)$ isomorphic to $C_5^+$, which is forbidden.

We now claim that $C \setminus A$ and $D \setminus B$ are nonempty. Assume, for contradiction, that $C \subset A$. By Proposition 2.7, since $A$ is not a subset of $C$, there exists $X$ in the support of $\alpha$ which intersects $A$ but is disjoint from $C$. Since $X \notin \{A, B, C, D\}$, $X$ must belong to $\text{SUPP}_q(\alpha')$ as well. But $X$ intersects $A$, and $A \in \mathcal{R}$, hence we conclude that $\text{SUPP}_q(\alpha') \in \mathcal{Q}$ and $A \subseteq X$. Since $X$ is disjoint from $C$, we see $A$ is also disjoint from $C$, which is a contradiction to the definition of $H$. Therefore $C$ is not a proper subset of $A$, and similarly, $D$ is not a proper subset of $B$.

The previous proved facts imply that there exist two sets $A', B' \in \mathcal{R} \setminus \{A, B\}$ such that $A, A', B, B'$ are disjoint, $A' \cap C = B' \cap D = \emptyset$, while $A' \cap D$ and $B' \cap C$ are both nonempty. For instance, take $A' \in \mathcal{R}$ which intersects $D \setminus B$ and $B' \in \mathcal{R}$ which intersects $C \setminus A$. The adjacency matrix of the subgraph of $\text{SUPP}_q(\alpha)$ induced by $A, B', A', B, C, D$ (in that order) is given by

$$M' = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

But $M'$ has three positive eigenvalues, which is forbidden by Proposition 3.3. This final contradiction establishes the proposition. \(\square\)

Propositions 3.16, 3.17, and 3.18 together with Steps 1 through 6 imply Theorem 3.1.
Proof of Theorem 3.1. Suppose towards contradiction that there exists a solution \( \beta \) to \( \text{OPT}_q(s) \) for which the support \( \text{SUPP}_q(\beta) \) belongs to neither \( P \) nor \( Q_{[s]} \). From the proof of Step 1, by repeatedly applying Proposition 3.3, we can find a solution \( \alpha' \) such that \( \text{SUPP}_q(\alpha') \) has no induced \( 3K_1 \) and \( C_4 \) and \( \beta \) and \( \alpha' \) are connected by a piecewise linear path in \( \text{FEAS}_q(s) \). From Step 6, we have \( \text{SUPP}_q(\alpha') \in P \cup Q_{[s]} \). Let \( \alpha' \) be the last node in the piecewise linear path from \( \beta \) to \( \alpha' \) before reaching the endpoint \( \alpha' \). Clearly \( \alpha' \) was obtained from \( \alpha \) by an application of Proposition 3.3 with \( H \) being isomorphic to one of \( 3K_1, C_5^+ \) or \( C_4 \). As remarked in the proof of Proposition 3.5, if \( H \) is isomorphic to \( C_4 \), we may further assume that \( \text{SUPP}_q(\alpha) \) has no induced copy of \( 3K_1 \) or \( C_5^+ \). From Propositions 3.16, 3.17 and 3.18, we conclude that \( \text{SUPP}_q(\alpha') \notin P \cup Q \), a contradiction.

If \( \text{SUPP}_q(\beta) \in P \), since the sizes of all sets in the support of \( \beta \) are at least one and add up to \( q \), it is clear that \( \text{SUPP}_q(\beta) \in \bigcup_{|s| \leq q} P_k \). In the case that \( [s] < q \), we have \( \text{SUPP}_q(\beta) \notin P_q \), as otherwise \( \text{OBJ}_q(\beta) = 0 \) which cannot be the optimal objective value. This establishes Theorem 3.1. \( \square \)

4. First applications from the structure

In this section, we provide short proofs to two results with the aid of Theorem 3.1. We first consider the structure of extremal graphs with \( n \) vertices and \( m \leq n^2/4 \) edges which maximizes the number of 3-colorings. Such extremal graphs were conjectured to be close to complete bipartite graphs plus some isolated vertices by Lazebnik [6], and this was later confirmed in [13]. Here we present an asymptotic version by a rather simple proof.

Theorem 4.1. For any \( \varepsilon > 0 \), the following holds for all sufficiently large \( n \). Let \( G \) be an \( n \)-vertex with \( m \leq n^2/4 \) edges which maximizes the number of 3-colorings. Then there exists an \( n \)-vertex graph \( G_0 \), which is a complete bipartite graph plus some isolated vertices, such that \( G \) is \( \varepsilon n^2 \)-close to \( G_0 \).

Proof. Apply Corollary 2.3 to \( G \) and \( s = \frac{n^2}{n^2 - 2m} \). Then \( G \) is \( \varepsilon n^2 \)-close to some \( G_{\alpha}(n) \), where \( \alpha \) solves \( \text{OPT}_3(s) \). By Theorem 3.1 and \( [s] = 2 \), we get \( \text{SUPP}_3(\alpha) \in Q_2 \cup P_2 \). This implies that \( G_{\alpha}(n) \) is a complete bipartite graph plus some isolated vertices, finishing the proof. \( \square \)

Next, we prove Theorem 1.5 (i). As mentioned in Section 1, the case \( q = s + 1 \) was first proved in [13] and then extended to all \( n \) in [10]. We need the following convenient definition. When \( s \geq 1 \) is integer, we define the \( s \)-balanced vector for \( q \) to be a vector \( \alpha \) such that \( \alpha_{A_i} = \frac{1}{s} \) and \( A_1, \ldots, A_s \) forms a balanced \( s \)-partition of \( [q] \).

Proof of Theorem 1.5 (i). Let us only consider when \( s + 1 \leq q \leq s + 2 \). In view of Corollary 2.3, it suffices to show that for every \( s \geq 2 \), the \( s \)-balanced vector \( \alpha \) for \( q \) is the unique solution to \( \text{OPT}_q(s) \). By Theorem 3.1 and Proposition 3.12, we see this indeed is the case for \( q = s + 1 \).
Now assume \( q = s + 2 \). It is easy to compute that \( \text{OBJ}_q(\alpha) = \frac{2}{s} \log 2 \). Suppose that there exists a solution \( \beta \) to \( \text{OPT}_q(s) \), which is not \( \alpha \). By Theorem 3.1 and Proposition 3.12, \( \text{SUPP}_q(\beta) \in \mathcal{P}_{s+1} \). Then we may assume that the sets \( A_1, A_2, \ldots, A_s \) in the support of \( \beta \) are of size 1, except \( A_{s+1} \), which is of size 2. Using Lemma 3.11, we compute that \( \lambda' = s \log 2 \) and \( \mu' = -\frac{s-1}{s+1} \log 2 \), which implies that \( \text{OBJ}_q(\beta) = \frac{2}{s+1} \log 2 < \text{OBJ}_q(\alpha) \), a contradiction. This completes the proof. \( \Box \)

5. The counterexamples to Lazebnik’s conjecture

In this section, we show various counterexamples to Conjecture 1.2. First, we prove Theorem 1.5 (ii).

**Proof of Theorem 1.5 (ii).** We first show that the 10-balanced vector \( \alpha \) for \( q = 13 \) has a smaller objective value than a vector \( \beta \in \text{FEAS}_{13}(10) \) with 11 color classes, which together with Theorem 2.1 implies that Conjecture 1.2 is false for \( (s, q) = (10, 13) \). It is easy to compute that \( \text{OBJ}_{13}(\alpha) = \frac{3}{10} \log 2 \). Let \( \beta := (\beta_1, \beta_2, \ldots, \beta_{11}) \), where \( \beta_1 = \beta_2 = \frac{1}{11} + \frac{3\sqrt{5}}{110} \) and \( \beta_3 = \ldots = \beta_{11} = \frac{1}{11} - \frac{\sqrt{5}}{105} \), and define the sizes of the color classes by \( A_1 = A_2 = 2 \) and \( A_3 = \ldots = A_{11} = 1 \). So indeed we have \( \beta \in \text{FEAS}_{13}(10) \). Now it is easy to verify that \( \text{OBJ}_{13}(\beta) = (\beta_1 + \beta_2) \log 2 = (\frac{2}{11} + \frac{3\sqrt{5}}{55}) \log 2 > \frac{3}{10} \log 2 = \text{OBJ}_{13}(\alpha) \).

We claim that Conjecture 1.2 is false for the pair \( (s, q) \), provided the \( s \)-balanced vector \( \gamma \) for \( q \) contains at least three color classes of size 2 and seven color classes of size 1. In this case, \( \gamma \) contains a subvector \( \frac{10}{s} \alpha \) formed by these 10 color classes. Define a new vector \( \gamma' \) obtained from \( \gamma \) by replacing \( \frac{10}{s} \alpha \) with \( \frac{10}{s} \beta \). It is easy to see that \( V_q(\gamma') = V_q(\gamma) = 1 \) and \( E_q(\gamma') = E_q(\gamma) = \frac{s-1}{2s} \), so \( \gamma' \in \text{FEAS}_q(s) \). Since the objective value of \( \beta \) is bigger than \( \alpha \), it holds that \( \text{OBJ}_q(\gamma') > \text{OBJ}_q(\gamma) \), proving the claim.

From the claim we obtain that Conjecture 1.2 is false for all \( (s, q) \), provided \( s + 3 \leq q \leq 2s - 7 \) and \( s \geq 10 \), finishing the proof. \( \Box \)

The next result gives us more counterexamples in a wider range, which gives rise to the proof of Theorem 1.3.

**Theorem 5.1.** If \( s, t, r \) are integers such that \( t \geq 2 \) and \( 50t \log t \leq r \leq \min\{ \frac{s}{2}, 2t^2 \log^2 t \} \), then Lazebnik’s conjecture is false for \( (s, q) \), where \( q := st + r \).

**Proof.** It is not hard to see that the objective value of the Turán solution (when \( k = s \)) is

\[
X := \frac{r}{s} \log(t + 1) + \frac{s - r}{s} \log t.
\]

We will now construct a solution \( \alpha \) with \( s + 1 \) parts which yields a larger objective value. We begin by defining the sequence of the sizes of the color classes: let \( A_1 = \ldots = A_{r-1} = t + 1 \), \( A_r = \ldots = A_s = t \) and \( A_{s+1} = 1 \). And let \( \alpha = (\alpha_1, \ldots, \alpha_{s+1}) \) such that

\[
\alpha_i := \frac{\log A_i - S_i}{(s + 1) \sqrt{s \cdot (S_2 - S_1^2)}} + \frac{1}{s + 1},
\]
where $S_1 := \frac{1}{s+1} \sum_{i=1}^{s+1} \log A_i$ and $S_2 := \frac{1}{s+1} \sum_{i=1}^{s+1} \log^2 A_i$. Observe that

$$S_2 - S_1^2 = \frac{s}{s+1} [S_2' - (S_1')^2] + \frac{s}{(s+1)^2} (S_1')^2 > 0,$$

where $S_1' := \frac{1}{s} \sum_{i=1}^{s} \log A_i$ and $S_2' := \frac{1}{s} \sum_{i=1}^{s} \log^2 A_i$, thus the $\alpha_i$'s are well-defined real numbers. Moreover

$$S_2' - (S_1')^2 = \frac{(r-1)(s-r+1)}{s^2} \log^2 \left(1 + \frac{1}{t}\right).$$

We claim that $\alpha_i \geq 0$. This is because $\log A_i \geq 0$ and $\sqrt{s \cdot (S_2 - S_1^2)} \geq \sqrt{\frac{s^2}{(s+1)^2} (S_1')^2} = S_1$. One can check that $\sum_{i=1}^{s} \alpha_i = 1$ and $\sum_{i=1}^{s+1} \alpha_i^2 = \frac{1}{s}$, hence $(\alpha, A)$ is a feasible solution, having objective value

$$Y := \sum_{i=1}^{s+1} \alpha_i \log A_i = S_1 + \sqrt{\frac{S_2 - S_1^2}{s}}.$$

To finish the proof of the theorem, we just need to show that $Y > X$. Observe that $X = S_1' + \frac{\log(1+t)}{s}$. Let $M := \frac{S_2' - (S_1')^2}{s+1}$ and $N := \frac{S_1'}{s+1}$. We have $M \leq 3N^2$, because

$$M = \frac{(r-1)(s-r+1)}{s^2(s+1)} \log^2 \left(1 + \frac{1}{t}\right) \leq \frac{r}{s^2t^2} \leq \frac{3 \log^2 t}{2s^2} \leq \frac{3(S_1')^2}{(s+1)^2} = 3N^2,$$

where we used $0 < \log \left(1 + \frac{1}{t}\right) < \frac{1}{t}$ and $r \leq \frac{3}{2} t^2 \log^2 t$. From $M \leq 3N^2$ we obtain $\sqrt{N^2 + M} \geq N + \frac{M}{3N}$, thus

$$Y = S_1 + \sqrt{N^2 + M} \geq S_1 + N + \frac{M}{3N} = S_1' + \frac{M}{3N}.$$

The only step left is to verify that $\frac{M}{3N} > \frac{\log(1+t)}{s}$, which can be done as follows

$$\frac{M}{3N} = \frac{S_2' - (S_1')^2}{3S_1'} \geq \frac{(r-1)(s-r+1)}{6s^2 \log t} \log^2 \left(1 + \frac{1}{t}\right) \geq \frac{r}{50s \log t} \cdot \frac{\log \left(1 + \frac{1}{t}\right)}{t} \geq \frac{\log \left(1 + \frac{1}{t}\right)}{s},$$

where we used $S_1 \leq \log(t+1) < 2 \log t$, $s - r + 1 \geq \frac{s}{2}$, and $\log \left(1 + \frac{1}{t}\right) \geq \frac{1}{2t}$. \qed

**Proof of Theorem 1.3.** We point out that for any integer $t$ satisfying $20 \leq t \leq \frac{8}{200 \log s}$, there always exists such an integer $r$ which satisfies $500 \log t \leq r \leq \min \left\{ \frac{s}{2}, \frac{3}{2} t^2 \log^2 t \right\}$. Therefore (provided $s \geq 50000$) for any $20s \leq q_0 \leq \frac{s^2}{200 \log s}$ there exists an integer $q$ within distance at most $s$ from $q_0$ such that Lazebnik’s conjecture is false for $(s, q)$. \qed
6. Solving $\text{OPT}_q(s)$ for integer $s$

When $s \geq 1$ is integer, recall the definition of the $s$-balanced vector for $q$ in Section 4. Because $x \mapsto \log x$ is concave, we know that, among all candidate solutions with support graph in $P_s$, the $s$-balanced vector has the largest objective value. In this section we shall show that this vector is indeed the unique solution to $\text{OPT}_q(s)$ for an integer $s$, provided that $q = \Omega \left( \frac{s^2}{\log s} \right)$.

**Theorem 6.1.** For large enough integer $s$ and for $q \geq 100 \frac{s^2}{\log s}$ the $s$-balanced vector for $q$ is the unique solution to $\text{OPT}_q(s)$.

Note that when $s$ is integer, the optimization problem $\text{OPT}_q(s)$ corresponds to the problem of maximizing the number of $q$-colorings over the family of graphs containing the Turán graph $T_s(n)$, i.e., Lazebnik’s Conjecture 1.2. In the light of Corollary 2.3, the establishment of Theorem 6.1 gives rise to Theorem 1.4.

To prove Theorem 6.1 we use the structural information from Theorem 3.1, that is, the support graph of a solution necessarily belongs to $(\bigcup_{j|s} P_j) \cup Q_s$. Additionally, we know by Proposition 3.12 that the support graph is not in $Q_s$ (since $s$ is integer), hence we shall only study candidate solutions $\alpha$ whose support forms a partition of $[q]$. So proving Theorem 6.1 amounts to showing that the solution of $\text{OPT}_q(s)$ lies in $P_s$.

With that in mind, the optimization problem (7) for $\beta = 0$ and variable $A_i$’s can be stated as follows. Fix $[s] \leq k \leq q$ and

\[
\begin{align*}
\text{Maximize} & \quad \sum_{i=1}^{k} \alpha_i \log A_i \\
\text{Subject to} & \quad \sum_{i=1}^{k} \alpha_i = 1, \sum_{i=1}^{k} \alpha_i^2 \leq 1 \frac{s}{s^2}, \sum_{i=1}^{k} A_i = q, \quad (9) \\
& \quad \alpha_i \geq 0 \text{ is real, } A_i > 0 \text{ is integer, for all } i = 1, \ldots, k.
\end{align*}
\]

It turns out that (9) becomes much simpler to analyze when we relax the conditions on the $A_i$’s and allow them to assume any nonnegative real value. By doing so, we shall obtain very good bounds for $\text{OPT}_q(s)$ in Section 6.1 for every real $s$ (not necessarily integer). Finally, in Section 6.2 we give the full proof of Theorem 6.1.

### 6.1. The continuous relaxation

Following the ideas of Norine in [15], we shall consider a continuous relaxation of (9). We relax the constraints on the variables $A_i$ by allowing them to assume any nonnegative real value. In this version of the problem, we also scale these variables by dividing each $A_i$ by $q$. The only constraint involving $q$ in (9) becomes $\sum_{i=1}^{k} A_i = 1$, which is now independent of $q$. The other effect this variable scaling has is of subtracting the value of the goal function by the constant $\log q$. In addition, it will be convenient to introduce another parameter $0 \leq \delta < \frac{1}{q}$, which represents the smallest value that one of the variables $\alpha_i$ can assume. The relaxed problem is stated as follows.
Proposition 6.2. For any solution to (10), we have $A_i = \alpha_i$ for all $i = 1, \ldots, k$.

Proof. First observe that the maximum of (10) is at least $-\log k$, since we can take $\alpha_i = A_i = \frac{1}{k}$ for all $i = 1, \ldots, k$. Moreover, if $A_i = 0$ for all $i$, then we also have $A_i = 0$ because otherwise the value of the goal function would be $-\infty$. Furthermore, if $\alpha_i = 0$ then we also have $A_i = 0$ because we could otherwise "shift the weight" of $A_i$ to another $A_j$ such that $\alpha_j > 0$ and increase the value of $F(\alpha)$. Hence, we have $\alpha_i = 0 \iff A_i = 0$.

By the method of Lagrange multipliers applied to the variables $A_i$, there exists $\lambda$ such that $A_i = \lambda A_i$ for all $i$, and the identity $\alpha_i = \lambda A_i$ is still true even if $A_i = 0$. Therefore $A_i = \alpha_i$ for all $i = 1, \ldots, k$, and the proposition.

Notice that the equivalent of Proposition 2.4 still holds in this context.

Proposition 6.3. For any solution to (10), we have $\sum_k \alpha_i = 1$.

In the succeeding proposition, we prove an upper bound for $f(\alpha)$ in (11).

\begin{equation}
\sum_{k} \alpha_i = 1, \alpha_i \geq 0, \text{ and } \alpha_i \geq \delta \text{ is real for all } i = 1, \ldots, k.
\end{equation}

We will prove a sequence of statements about the relaxation, which will lead us to a complete solution to (10). First, let us determine the values of the $A_i$'s in terms of the $\alpha_i$'s.

In above and in the rest of this subsection we do not assume that $s$ is necessarily integer, and we do allow some of the variables $A_i$ to assume the value zero. For this, we extend the range of the goal function to include $-\infty$. This is a minor technical detail and is used solely to simplify our analysis of the problem. In that case, we also extend the definition of $A_i \log B$ for $A = B = 0$.

We stress that the optimization problem (10) is well-defined, even though the goal function is discontinuous at the boundary. This is because the goal function is still upper semi-continuous and the domain is compact, so the maximum of (10) is always attained by a point in the domain.
Proposition 6.4. For any $\alpha$ in the domain of (11) we have $F(\alpha) \leq - \log s$. In particular, the maximum of (9) is at most $\log q - \log s$.

Proof. We know that the function $x \mapsto \log x$ is concave for $x > 0$, and by Jensen’s inequality we obtain

$$F(\alpha) = \sum_{i=1}^{k} \alpha_i \log \alpha_i \leq \log \left( \sum_{i=1}^{k} \alpha_i^2 \right) = - \log s,$$

thereby proving the proposition. \qed

The next proposition reveals further information about the structure of the solutions of (11).

Proposition 6.5. If $\alpha = (\alpha_1, \ldots, \alpha_k)$ is a local maximum point for (11), then the cardinality of the set $\{\alpha_1, \ldots, \alpha_k\} \setminus \{\delta\}$ is at most two.

Proof. We again use the method of Lagrange multipliers. If $\alpha_i = \frac{1}{k}$ for $i = 1, \ldots, k$, the statement of the proposition is immediately true. Otherwise, $\alpha$ is a regular point, and thus there exist two multipliers $\lambda, \mu$ such that

$$\log \alpha_i + 1 = \mu + \lambda \alpha_i$$

for all $i$ such that $\alpha_i > \delta$. But the function $f(x) := \log x - \lambda x + 1 - \mu$ is strictly concave regardless of the values of $\lambda$ and $\mu$, therefore there are at most two roots of $f(x) = 0$, which proves the proposition. \qed

It turns out that the case $k = 3$ will play vital role in the way we solve the general case. We thus derive the following two propositions for this special case. When $k = 3$ we have $\alpha_1 + \alpha_2 + \alpha_3 = 1$ and $\alpha_1^2 + \alpha_2^2 + \alpha_3^2 = \frac{1}{s}$. It will be convenient to introduce the following parametrization of the variables

$$\begin{align*}
\alpha_1 &= \frac{1}{4} + \frac{\rho}{\sqrt{6}} \cos \theta + \frac{\rho}{\sqrt{2}} \sin \theta \\
\alpha_2 &= \frac{1}{3} + \frac{\rho}{\sqrt{6}} \cos \theta - \frac{\rho}{\sqrt{2}} \sin \theta \\
\alpha_3 &= \frac{1}{3} - \frac{2\rho}{\sqrt{6}} \cos \theta,
\end{align*}$$

which clearly satisfies $\alpha_1 + \alpha_2 + \alpha_3 = 1$ and $\alpha_1^2 + \alpha_2^2 + \alpha_3^2 = \frac{1}{s}$, where $\rho := \sqrt{\frac{3-s}{3s}}$ and $\theta \in [0, 2\pi]$ is a new variable. Moreover, any triple $(\alpha_1, \alpha_2, \alpha_3)$ satisfying the constraints of (11) can be parametrized as before. By symmetry, we may even assume $\alpha_1 \geq \alpha_2 \geq \alpha_3$, or equivalently, $\theta \in [0, \frac{\pi}{3}]$. The actual range of $\theta$ is an interval of the form $[\theta_0, \frac{\pi}{3}]$, where $\theta_0 \in [0, \frac{\pi}{3}]$ is either the solution of $\alpha_3(\theta_0) = \delta$ if $\frac{1}{3} - \frac{2\rho}{\sqrt{6}} \leq \delta$, or 0 otherwise.

The parametrization (12) allows us to view $F(\alpha) = F(\alpha_1, \alpha_2, \alpha_3)$ as a function of $\theta$. With slight abuse of notation, let $F(\theta) := F(\alpha_1(\theta), \alpha_2(\theta), \alpha_3(\theta))$. 

Proposition 6.6. For any $1 < s \leq 3$, $\theta = \frac{\pi}{3}$ is a strict local minimum point for $F(\theta)$.

Proof. For $1 < s \leq 3$, we have $0 \leq \rho < \frac{\sqrt{6}}{3}$. For $\theta = \frac{\pi}{3}$, we clearly have $\alpha_1, \alpha_2, \alpha_3 > 0$. Moreover, taking derivatives with respect to $\theta$, we get

$$F'(\theta) = \alpha'_1 \log \alpha_1 + \alpha'_2 \log \alpha_2 + \alpha'_3 \log \alpha_3$$

and a straightforward computation shows that $F'(\pi/3) = 0$. Thus, in order to prove that $\frac{\pi}{3}$ is a strict local minimum point for $F(\theta)$, it is enough to show that the second derivative of $F(\theta)$ at $\theta = \frac{\pi}{3}$ is positive. Computing $F''(\theta)$ we obtain

$$F''(\theta) = \frac{(\alpha'_1)^2}{\alpha_1} + \frac{(\alpha'_2)^2}{\alpha_2} + \frac{(\alpha'_3)^2}{\alpha_3} + \alpha''_1 \log \alpha_1 + \alpha''_2 \log \alpha_2 + \alpha''_3 \log \alpha_3$$

We replace $\theta = \frac{\pi}{3}$ in the identity above and obtain

$$F''(\pi/3) = \frac{\rho^2}{3 - \frac{\rho}{\sqrt{6}}} - \frac{2\rho}{\sqrt{6}} \log \left(\frac{\frac{1}{3} + \frac{2\rho}{\sqrt{6}}}{3 - \frac{\rho}{\sqrt{6}}}\right) = \frac{\rho^2}{3 - \frac{\rho}{\sqrt{6}}} - \frac{2\rho}{\sqrt{6}} \log \left(1 + \frac{3\rho}{\sqrt{6}}\right).$$

Using the inequality $\log(1 + x) < x$ we infer that $F''(\pi/3) > 0$, proving the proposition. \qed

Proposition 6.7. If $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is a local maximum point for (11) in the case $k = 3$, and $\alpha_1 \geq \alpha_2 \geq \alpha_3 > \delta$, then $\alpha_1 = \alpha_2$. Moreover, the function $F(\theta)$ is strictly decreasing in the interval $[\theta_0, \pi/3]$.

Proof. Consider any vector $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ achieving a local maximum of $F$. By Proposition 6.5, we have $\alpha_1 = \alpha_2$ or $\alpha_2 = \alpha_3$ (since $\alpha_i > \delta$ for all $i = 1, 2, 3$). The case $\alpha_1 > \alpha_2 = \alpha_3$ corresponds to $\theta = \frac{\pi}{3}$ in the reparametrization (12), and by Proposition 6.6, $\alpha$ cannot be a maximum point for $F$. Therefore, assuming that $\alpha$ is an optimal solution to (11) we conclude that $\alpha_1 = \alpha_2$ (and thus $\theta = \theta_0 = 0$).

Using similar arguments, one can also show that in general $\theta_0$ and $\frac{\pi}{3}$ are the only two local extremum points of $F(\theta)$, and thus we have $F(\theta_0) > F(\frac{\pi}{3})$. Therefore $F(\theta)$ is strictly decreasing in $[\theta_0, \pi/3]$. \qed

Proposition 6.7 implies the next lemma, which completely solves the relaxation (11) and hence (10) as well.

Lemma 6.8. If $\alpha = (\alpha_1, \ldots, \alpha_k)$ is a local maximum point for (11) satisfying $\alpha_1 \geq \ldots \geq \alpha_k$ then there exists an integer $\ell \geq 0$ such that $k = \ell + \lfloor s^* \rfloor$, $\alpha_1 = \alpha_2 = \cdots = \alpha_{k-\ell-1} = \alpha_{k-\ell} > \delta$ and $\alpha_{k-\ell+1} = \cdots = \alpha_k = \delta$, where $s^* = s(\frac{1-\ell\delta}{1-\ell\delta^2}).$ In particular, if $\ell = 0$ then $s^* = s$ and $k = \lfloor s \rfloor$. Furthermore, we have

$$F(\alpha) \leq (1 - \ell\delta) \lfloor \log(1 - \ell\delta) - \log s^* \rfloor + \ell\delta \log \delta. \quad (13)$$
Proof. Let $\ell$ be the number of indices $i$ such that $\alpha_i = \delta$. Because we assumed $\alpha_1 \geq \alpha_2 \geq \ldots \geq \alpha_k$, we have $\alpha_{k-\ell+1} = \ldots = \alpha_k = \delta$. If we fix all but three variables $\alpha_i$ in (11) we obtain another instance of (11) with $k = 3$ (up to rescaling of the variables and parameters $s$ and $\delta$). Hence Proposition 6.7 can be applied to this sub-problem, and it implies that for any triple $1 \leq i_1 < i_2 < i_3 \leq k - \ell$ we have $\alpha_{i_1} = \alpha_{i_2} \geq \alpha_{i_3}$. From this we infer that $\alpha_1 = \ldots = \alpha_{k-\ell-1} \geq \alpha_{k-\ell}$. Let $x = \frac{\alpha_{k-\ell-1}}{1-\ell\delta}$ and $y = \frac{\alpha_{k-\ell}}{1-\ell\delta}$. We have $x \geq y > \frac{\delta}{1-\ell\delta}$, $(k - \ell - 1)x + y = 1$ and $(k - \ell - 1)x^2 + y^2 = \frac{1}{s^2}$. This system has a solution provided that $k - \ell \geq s^* > k - \ell - 1$, or equivalently $k - \ell = \lceil s^* \rceil$. To finish the proof of the lemma we use Proposition 6.4 on the sub-problem restricted to the first $k - \ell$ variables. The proposition states that $(k - \ell - 1)x \log x + y \log y \leq -\log s^*$, which combined with the identity

$$F(\alpha) = (1 - \ell\delta) [\log(1 - \ell\delta) + (k - \ell - 1)x \log x + y \log y] + \ell\delta \log \delta$$

implies (13), and we are done. \qed

6.2. Solving the optimization problem for integer $s$

We know from Proposition 6.4 that any solution of $\text{OPT}_q(s)$ has objective value at most $\log q - \log s$, whenever $s$ is an integer number. But how close to this bound is the $s$-balanced vector for $q$? The answer to this question is contained in the following proposition, which shall be used as a benchmark for comparison with other candidate solutions.

**Proposition 6.9.** For $s$ integer and $q \geq s$, if $\alpha$ is the $s$-balanced vector for $q$ then

$$\text{OBJ}_q(\alpha) \geq \log q - \log s - \frac{s^2}{2q^2}.$$  

**Proof.** We divide $q$ by $s$ (with remainder) as $q = st + r$ where $t, r$ are integers and $0 \leq r < s$. Note that $t \geq 1$ because $q \geq s$. If we denote by $\alpha$ the $s$-balanced vector for $q$ then

$$\text{OBJ}_q(\alpha) = \frac{r}{s} \log(t + 1) + \frac{s - r}{s} \log t.$$  

Let $f(x) := \log x$. If $x \in [t, t + 1]$ then \(-\frac{1}{t^2} \leq f''(x) \leq -\frac{1}{(t+1)^2}\), so the function $g(x) := \log x + \frac{2}{2t^2}$ is convex. By Jensen’s inequality, we have $g(\frac{q}{s}) \leq \frac{1}{s} \sum_{i=1}^{s} g(A_i)$ for any balanced partition $A_1, \ldots, A_s$ of $[q]$, which implies

$$\text{OBJ}_q(\alpha) \geq \log q - \log s - \frac{1}{2t^2} \cdot \frac{r(s - r)}{s^2} \geq \log q - \log s - \frac{s^2}{2q^2},$$

thereby proving the proposition. \qed
Throughout the remaining of the section, the vectors $\alpha = (\alpha_1, \ldots, \alpha_k, A_1, \ldots, A_k)$ we consider are from the domain of (9). The following list contains the proposed steps towards the proof of Theorem 6.1:

(I) If $\alpha = (\alpha_1, \ldots, \alpha_k, A_1, \ldots, A_k)$ is a solution of $\text{OPT}_q(s)$ then either $k = s$ or $k = s + 1$. Moreover if $k = s + 1$ then $\alpha_k$ is small and $A_k = 1$. This statement is a consequence of the following.

(I-1) A discrete analog of Proposition 6.2 holds, that is, $A_i \approx \alpha_i \cdot q$ for all $i$.

(I-2) By using the continuous relaxation of (9) from Section 6.1 we prove that if $k \geq s + 1$ then $\alpha_k$ is tiny. Moreover, if $k \geq s + 2$ then both $\alpha_{k-1}$ and $\alpha_k$ are small.

(I-3) If both $\alpha_{k-1}$ and $\alpha_k$ are sufficiently small, then $\alpha$ cannot be a solution of $\text{OPT}_q(s)$.

(II) If $\alpha = (\alpha_1, \ldots, \alpha_{s+1}, A_1, \ldots, A_{s+1})$ is such that $A_{s+1} = 1$, then we can estimate

$$\text{OBJ}_q(\alpha) \leq S_1 + \frac{S_2 - S_1^2}{2S_1},$$

where $S_1 = \frac{1}{s} \sum_{i=1}^{s} \log A_i$ and $S_2 = \frac{1}{s} \sum_{i=1}^{s} \log^2 A_i$. Moreover, if $\alpha_{s+1} \leq \frac{1}{\log q}$ then $S_2 - S_1^2 \leq \frac{S_1^2}{20q}$.

(III) The expression $S_1 + \frac{S_2 - S_1^2}{2S_1}$ in step (II) is maximized when $(A_1, \ldots, A_s)$ forms a balanced partition of $q - 1$.

(IV) The $s$-balanced vector is better than any candidate solution with $k = s+1$ satisfying the conditions stated in step (I).

Let us begin with discrete equivalent of Proposition 6.2 mentioned in step (I-1).

**Proposition 6.10.** Let $\alpha = (\alpha_1, \ldots, \alpha_k, A_1, \ldots, A_k) > 0$ be a solution of $\text{OPT}_q(s)$, where $s$ is any real parameter. For each $i$, we have $|A_i - \alpha_i q| < 1 + (k - 2)\alpha_i$. In particular, $\alpha_i \geq \frac{1}{2q}$ whenever $A_i \geq 2$.

**Proof.** Fix an arbitrary integer $i$. We shall prove that $\alpha_i A_j - \alpha_j A_i > -\alpha_i - \alpha_j$ for every other $j \neq i$. This inequality is trivially true when $A_i = 1$, so we may assume that $A_i \geq 2$. For each value of $j \neq i$ we have $\alpha_i \log(A_i - 1) + \alpha_j \log(A_j + 1) \leq \alpha_i \log A_i + \alpha_j \log A_j$. This is because $\alpha$ is a solution of $\text{OPT}_q(s)$ and thus $\text{OBJ}_q(\alpha) \geq \text{OBJ}_q(\alpha')$, where $\alpha'$ is obtained from $\alpha$ by replacing $A_i$ with $A_i - 1$ and $A_j$ with $A_j + 1$. Since $\log(1+x) < x$ for all $x > -1$, we have

$$0 \leq \alpha_i \log \left(1 + \frac{1}{A_i - 1}\right) + \alpha_j \log \left(1 - \frac{1}{A_j + 1}\right) < \frac{\alpha_i}{A_i - 1} - \frac{\alpha_j}{A_j + 1},$$

which implies $\alpha_i A_j - \alpha_j A_i > -\alpha_i - \alpha_j$. By switching the roles of $i$ and $j$ we also obtain $\alpha_j A_i - \alpha_i A_j > -\alpha_i - \alpha_j$, which implies $|\alpha_i A_j - \alpha_j A_i| < \alpha_i + \alpha_j$. 
Adding up these inequalities for all \( j \neq i \), we obtain \(|\alpha_i (q - A_i) - (1 - \alpha_i) A_i| < 1 + (k - 2) \alpha_i\), thereby finishing the proof of the proposition. \( \square \)

We turn to step (I-2) which is stated in the following lemma.

**Lemma 6.11.** Let \( \alpha = (\alpha_1, \ldots, \alpha_k, A_1, \ldots, A_k) > 0 \) be a solution of \( \text{OPT}_q (s) \) for large enough integer \( s \), where \( \alpha_1 \geq \alpha_2 \geq \ldots \geq \alpha_k \) and \( q \geq 100 \frac{s^2}{\log s} \). If \( k \geq s + 1 \) then \( \alpha_k < \frac{1}{50q} \).

Moreover, if \( k \geq s + 2 \) then \( \alpha_k - 1 < \frac{1}{40q} \).

Before proving Lemma 6.11, we need the following corollary of Lemma 6.8.

**Lemma 6.12.** Let \( \alpha = (\alpha_1, \ldots, \alpha_k, A_1, \ldots, A_k) > 0 \) be any element in the feasible set \( \text{FEAS}_q (s) \) for large enough \( s \) (not necessarily integer). If \( k > \lfloor s \rfloor \) and \( \alpha_1 \geq \ldots \geq \alpha_k \geq \frac{1}{50q} \) then

\[
\text{OBJ}_q (\alpha) < \log q - \log s - \frac{1}{150q} \log \left( \frac{50q}{s} \right).
\]

**Proof.** Clearly \( k \leq q \). We consider the continuous optimization problem (10) for \( s, k \), and \( \delta := \frac{1}{50q} \), and we apply Lemma 6.8 to this particular instance. Since \( k > \lfloor s \rfloor \) we have \( \ell > 0 \). Moreover, because \( \ell, s \leq q \), we have \((50q - \ell)^2 < 2500q^2 - \ell \ell \) and thus \( s^* = s \cdot \frac{(50q - \ell)^2}{2500q^2 - \ell \ell} < s \). Note that \( \alpha \) is an element of the domain of (10) for our choice of parameters, and by (13) we have

\[
\text{OBJ}_q (\alpha) \leq \log q + F (\alpha) \leq \log q - \left( 1 - \frac{\ell}{50q} \right) \log s^* - \frac{\ell \log (50q)}{50q} \\
\leq \log q - \log s + \log \left( \frac{2500q^2 - \ell \ell}{(50q - \ell)^2} \right) - \frac{\ell}{50q} \log \left( \frac{50q}{s} \right).
\]

The function \( x \mapsto \log \left( \frac{2500q^2 - sx}{(50q - x)^2} \right) - \frac{x}{50q} \log \left( \frac{50q}{s} \right) \) is decreasing for \( 1 \leq x \leq k \), since its derivative is

\[
- \frac{s}{2500q^2 - sx} + \frac{2}{50q - x} - \frac{1}{50q} \log \left( \frac{50q}{s} \right) \leq \frac{2}{49q} - \frac{\log 50}{50q} < 0,
\]

therefore we conclude that

\[
\text{OBJ}_q (\alpha) + \log s - \log q \leq \log \left( 1 + \frac{100q - s - 1}{(50q - 1)^2} \right) - \frac{1}{50q} \log \left( \frac{50q}{s} \right) \\
< \frac{100q}{(50q - 1)^2} - \frac{1}{50q} \log \left( \frac{50q}{s} \right) < - \frac{1}{150q} \log \left( \frac{50q}{s} \right)
\]

finishing the proof. \( \square \)
Equipped with Lemma 6.12 we can now prove Lemma 6.11.

**Proof of Lemma 6.11.** Let us first prove that for $k \geq s + 1$ we have $\alpha_k < \frac{1}{40q}$. Suppose, for contradiction, that $k \geq s + 1$ and $\alpha_k \geq \frac{1}{40q}$. By Lemma 6.12, we have

$$\text{OBJ}_q(\alpha) < \log q - \log s - \frac{1}{150q} \log \left(\frac{50q}{s}\right),$$

but this is a contradiction, since Proposition 6.9 implies that $\text{OBJ}_q(\alpha) = \text{OPT}_q(s) \geq \log q - \log s - \frac{s^2}{2q^2}$ and $\frac{1}{150q} \log \left(\frac{50q}{s}\right) > \frac{s^2}{2q^2}$. For the second part suppose, towards contradiction, that $k \geq s + 2$ and $\alpha_{k-1} \geq \frac{1}{40q}$. Since $\alpha_k < \frac{1}{40q}$ from Proposition 6.10 we infer that $A_k = 1$. Let $\alpha'_i := \frac{\alpha_i}{1-\alpha_k}$ for $i = 1, \ldots, k - 1$, let $\alpha' := (\alpha'_1, \ldots, \alpha'_{k-1}, A_1, \ldots, A_{k-1})$ and let $s' := s \cdot \frac{1-\alpha_k}{1-\alpha_k}$. Clearly $s' < s$, $\sum_{i=1}^{k-1} \alpha'_i = 1$ and $\sum_{i=1}^{k-1} (\alpha'_i)^2 = \frac{1}{q}$, hence $\alpha' \in \text{FEAS}_q(s')$. Moreover $\text{OBJ}_q(\alpha) = (1 - \alpha_k)\text{OBJ}_q-1(\alpha')$. Furthermore, since $\alpha'_{k-1} > \frac{1}{40q} > \frac{1}{50(q-1)}$ and $k - 1 \geq s + 1 > s' + 1$ we can apply Lemma 6.12 and deduce

$$\text{OBJ}_{q-1}(\alpha') < \log(q - 1) - \log s' - \frac{1}{150(q-1)} \log \left(\frac{50(q - 1)}{s'}\right).$$

This together with $\log s' = \log s + \log \left(1 - \frac{2\alpha_k - (s+1)\alpha_k^2}{1-s\alpha_k^2}\right) > \log s - 3\alpha_k$ implies that

$$\text{OBJ}_q(\alpha) \leq \text{OBJ}_{q-1}(\alpha') \leq \left(\log q - \frac{1}{2q}\right) - \log s + 3\alpha_k - \frac{1}{150(q-1)} \log \left(\frac{50(q - 1)}{s'}\right)$$

$$< \log q - \log s - \frac{1}{150(q-1)} \log \left(\frac{50(q - 1)}{s'}\right),$$

which gives us a contradiction as before. $\square$

The following lemma establishes step (I) by combining the steps (I-1) and (I-2) together with the proof of (I-3).

**Lemma 6.13.** Let $\alpha = (\alpha_1, \ldots, \alpha_k, A_1, \ldots, A_k) > 0$ be a solution of $\text{OPT}_q(s)$ for large enough integer $s$. If $q \geq 100\frac{s^2}{\log s}$, then we must have either $k = s$ or $k = s + 1$.

**Proof.** Suppose, towards contradiction, that $k \geq s + 2$. We assume, without loss of generality, that $\alpha_1 \geq \ldots \geq \alpha_k$. By Lemma 6.11 we must have $\alpha_k, \alpha_{k-1} < \frac{1}{40q}$, and $\frac{1}{k} \geq \frac{1}{q} \geq 4\alpha_{k-1}$. Moreover, by Proposition 6.10, we infer that $A_k = A_{k-1} = 1$, and $\frac{A_1}{4q}$. As $(\alpha_1 - \alpha_k - \alpha_{k-1})^2 \geq 4\alpha_k \alpha_{k-1}$, we may define $\zeta := \frac{(\alpha_1 - \alpha_k - \alpha_{k-1}) - \sqrt{(\alpha_1 - \alpha_k - \alpha_{k-1})^2 - 4\alpha_k \alpha_{k-1}}}{2}$ such that the following holds

$$(\alpha_1 - \zeta)^2 + (\alpha_k + \alpha_{k-1} + \zeta)^2 = \alpha_1^2 + \alpha_k^2 + \alpha_{k-1}^2.$$
We claim that $\alpha_1 \log A_1 < (\alpha_1 - \zeta) \log A_1 + (\alpha_k + \alpha_{k-1} + \zeta) \log 2$. To see this, first note that

$$
\zeta = \frac{2 \alpha_k \alpha_{k-1}}{(\alpha_1 - \alpha_k - \alpha_{k-1}) + \sqrt{(\alpha_1 - \alpha_k - \alpha_{k-1})^2 - 4 \alpha_k \alpha_{k-1}}}
\leq \frac{4 \alpha_k \alpha_{k-1}}{\alpha_1} \leq \frac{4 \alpha_k \alpha_{k-1} \cdot 4q}{A_1} \leq \frac{2}{5} \cdot \frac{\alpha_k}{A_1},
$$

hence $\zeta \log A_1 \leq \frac{2}{5} \frac{\log A_1}{A_1} \cdot \alpha_k \leq \frac{2}{5} \alpha_k < (\alpha_k + \alpha_{k-1} + \zeta) \log 2$, proving our claim. But this is a contradiction, because $\alpha' := (\alpha_1 - \zeta, \alpha_2, \ldots, \alpha_{k-1} + \alpha_k + \zeta, A_1, A_2, \ldots, A_{k-2}, 2)$ is a feasible solution to $\text{OPT}_q(s)$ yielding a better objective value than $\alpha$, therefore $k \leq s + 1$. \qed

Step (II) is a consequence of the following lemma.

**Lemma 6.14.** If $\alpha = (\alpha_1, \ldots, \alpha_{s+1}, A_1, \ldots, A_{s+1})$ is a solution to $\text{OPT}_q(s)$ such that $A_{s+1} = 1$ then

$$
\text{OBJ}_q(\alpha) \leq S_1 + \frac{S_2 - S_1^2}{2S_1},
$$

where $S_1 = \frac{1}{s} \sum_{i=1}^{s} \log A_i$ and $S_2 = \frac{1}{s} \sum_{i=1}^{s} \log^2 A_i$. If, in addition, $\alpha_{s+1} \leq \frac{1}{50q}$ then $S_2 - S_1^2 \leq \frac{s^2}{20q}$.

**Proof.** We fix $A_1, \ldots, A_{s+1}$ and recall Lemma 3.11. It states that for this fixed sequence $A_1, \ldots, A_{s+1}$, we have $\alpha_i = \frac{\log A_i - \mu}{\lambda}$ for $i = 1, \ldots, s + 1$ and $\text{OBJ}_q(\alpha) = \mu + \frac{\lambda}{s}$, where

$$
\mu = S'_1 - \frac{\lambda}{s+1}, \quad \lambda = (s+1) \sqrt{s(S'_2 - (S'_1)^2)}, \quad S'_1 = \frac{1}{s+1} \sum_{i=1}^{s+1} \log A_i, \quad \text{and}
$$

$$
S'_2 = \frac{1}{s+1} \sum_{i=1}^{s+1} \log^2 A_i.
$$

We have $S'_1 = \frac{s}{s+1} S_1$ and $S'_2 = \frac{s}{s+1} S_2$, hence

$$
\lambda = (s+1) \sqrt{\frac{s^2}{s+1} (S_2 - S_1^2) + \frac{s^2}{(s+1)^2} S_1^2}.
$$

We estimate $\lambda$ in (15) using the inequality $\sqrt{a^2 + b} \leq a + \frac{b}{2a}$ for $a := \frac{s}{s+1} S_1$ and $b := \frac{s^2}{s+1} (S_2 - S_1^2)$ and obtain

$$
\lambda \leq s \cdot S_1 + \frac{s(s+1)}{2S_1} \cdot (S_2 - S_1^2).
$$
Using this bound for \( \lambda \) in the formula \( \text{OBJ}_q(\alpha) = \frac{s}{s+1} S_1 + \frac{\lambda}{s(s+1)} \) we obtain (14). To finish the proof of the lemma, we need to show that \( S_2 - (S_1)^2 \leq \frac{1}{20q} S_1^2 \) whenever \( \alpha_{s+1} \leq \frac{1}{50q} \). For that purpose, we use the identity \( \alpha_{s+1} = \frac{\log A_{s+1} - \mu}{\lambda} = \frac{\lambda - s S_1}{(s+1) \lambda} \), which, together with the inequality \( 0 \leq \alpha_{s+1} \leq \frac{1}{50q} \), implies

\[
\lambda \leq \frac{3sS_1}{2} \quad \text{and} \quad 0 \leq \lambda - s S_1 \leq \frac{s(s+1)}{30q} S_1.
\]

Multiplying the above inequality by \( \lambda + s S_1 \), we obtain \( S_2 - (S_1)^2 \leq \frac{1}{20q} S_1^2 \), which completes the proof. \( \square \)

With \( S_1 \) and \( S_2 \) as in the statement of Lemma 6.14 we have step (III).

**Lemma 6.15.** For \( s \) large enough and \( q \gg s \), the maximum of

\[
S_1 + \frac{S_2 - S_1^2}{2S_1},
\]

over all choices of \((A_1, \ldots, A_{s+1})\) satisfying both \( A_{s+1} = 1 \) and \( S_2 - S_1^2 \leq \frac{s^2}{20q} \), is attained when \((A_1, \ldots, A_s)\) forms a balanced partition of \( q - 1 \).

**Proof.** First we claim that under the conditions of the lemma, we have \( A_i = (1 + o(1)) \frac{2}{s} \) for all \( i = 1, \ldots, s \), and so \( S_1 = (1 + o(1)) \log \frac{q}{s} \), where the asymptotic notation symbol \( o(1) \) represents a function that tends to zero as \( s \) tends to infinity. This is because \( S_1 \leq \log \frac{q}{s} \) (by the concavity of \( \log \)) and the variance \( S_2 - S_1^2 \) can be bounded below by \( \frac{1}{4s} (\log A_i - \log A_j)^2 \) for any \( i \neq j \), and thus

\[
(\log A_i - \log A_j)^2 \leq 4s \cdot \frac{S_1^2}{20q} = O\left( \frac{\log^2(q/s)}{q/s} \right) = o(1).
\]

Suppose, towards contradiction, that the lemma is false, and let \( 1 \leq l, m \leq s \) be such that \( A_l \geq A_m + 2 \). Let \( \tilde{A}_l := A_l - 1, \tilde{A}_m := A_m + 1 \), and \( \tilde{A}_i := A_i \) for all \( i \notin \{l, m\} \). Moreover, let \( \tilde{S}_1 = \frac{1}{s} \sum_{i=1}^{s} \log \tilde{A}_i \) and \( \tilde{S}_2 = \frac{1}{s} \sum_{i=1}^{s} \log \tilde{A}_i \). To arrive at a contradiction, it suffices to show that \( \tilde{S}_1 + \frac{\tilde{S}_2 - S_1^2}{2S_1} > S_1 + \frac{S_2 - S_1^2}{2S_1} \). Since \( \log(1 + x) = x + O(x^2) \), we have

\[
\tilde{S}_1 - S_1 = \frac{1}{s} \log \left( 1 + \frac{A_l - A_m - 1}{A_l A_m} \right) = (1 + o(1)) \cdot \frac{A_l - A_m - 1}{sA_l A_m}. \tag{16}
\]

Moreover, if \( f(x) := \log^2(x+1) - \log^2 x \), we have \( \tilde{S}_2 - S_2 = (f(A_m) - f(A_l - 1))/s \). By the mean value theorem, there exists \( B \) such that \( A_m \leq B \leq A_l - 1 \) such that \( \tilde{S}_2 - S_2 = \frac{A_m - A_l + 1}{s} f'(B) \). However, since \( f'(B) = 2 \cdot \frac{\log(B+1) - \log B}{B+1} \), another application of
the mean value theorem yields $f'(B) = -2 \cdot \frac{\log(C/e)}{C^2}$ for some $B \leq C \leq B + 1$, hence $A_m \leq C \leq A_l$. These two identities imply

$$\tilde{S}_2 - S_2 = 2 \cdot \frac{A_l - A_m - 1}{s} \cdot \frac{\log(C/e)}{C^2} \geq 3 \cdot \frac{(A_l - A_m - 1) \log \frac{q}{s}}{2sA_lA_m}. \quad (17)$$

Combining (16) and (17) yields

$$\tilde{S}_1 + \frac{\tilde{S}_2 - S_2^2}{2S_1} \geq S_1 + \frac{S_2 - S_1^2}{2S_1} + \frac{(A_l - A_m - 1)}{2sA_lA_m},$$

which is a contradiction, thereby proving our claim that $|A_l - A_m| \leq 1$ for all $1 \leq l$, $m \leq s$. □

We are ready to prove step (IV) and hence Theorem 6.1.

**Proof of Theorem 6.1.** As mentioned in the beginning of this section, in order to prove Theorem 6.1 it suffices to show that for any solution $\alpha$ of $\mathrm{OPT}_q(s)$, the support graph $\mathrm{SUPP}_q(\alpha)$ lies in $\mathcal{P}_s$. On the other hand, we already know (by Lemma 6.13) that $\mathrm{SUPP}_q(\alpha) \in \mathcal{P}_s \cup \mathcal{P}_{s+1}$. Suppose, towards contradiction, that $\mathrm{SUPP}_q(\alpha) \in \mathcal{P}_{s+1}$, where $\alpha = (\alpha_1, \ldots, \alpha_{s+1}, A_1, \ldots, A_{s+1})$. By Lemma 6.11, we know that $\alpha_{s+1} \leq \frac{1}{50q}$ and as a consequence of Proposition 6.10 we obtain $A_{s+1} = 1$.

From Lemma 6.14 we obtain

$$\mathrm{OBJ}_q(\alpha) \leq S_1 + \frac{S_2 - S_1^2}{2S_1} \quad \text{and} \quad S_2 - S_1^2 \leq \frac{S_2^2}{20q},$$

where $S_1 = \frac{1}{s} \sum_{i=1}^s \log A_i$ and $S_2 = \frac{1}{s} \sum_{i=1}^s \log^2 A_i$. By Lemma 6.15, we infer that the maximum of $S_1 + \frac{S_2 - S_1^2}{2S_1}$ is attained when $(A_1, \ldots, A_s)$ is a balanced partition of $q - 1$. For convenience of the remaining proof, we may assume that $(A_1, \ldots, A_s)$ is a balanced partition of $q - 1$. Then we have $|A_i - A_j| \leq 1$ for all $1 \leq i, j \leq s$ and thus $|A_i - \exp(S_1)| \leq 1$. This implies that $2S_1 \geq \log \frac{q}{s}$ and $\log A_i - S_1 \leq \frac{2s}{q}$, the latter one of which in turn implies that

$$S_2 - S_1^2 \leq \frac{4s^2}{q^2}.$$

Let $S^*$ be the value of the objective function on the $s$-balanced vector for $q$. We have

$$S^* \geq S_1 + \frac{1}{s} \log \left(1 + \frac{1}{A_1}\right) \geq S_1 + \frac{1}{2q},$$

but

$$S^* \leq \mathrm{OBJ}_q(\alpha) \leq S_1 + \frac{S_2 - S_1^2}{2S_1} \leq S_1 + \frac{4s^2}{q^2} \log \frac{q}{s} \leq S_1 + \frac{1}{10q},$$

and this final contradiction finishes the proof. □
7. Concluding remarks and open problems

In Theorem 3.1 we show that for any real $s > 1$ and integer $q$, the support graph of every solution to $\OPT_q(s)$ is in either $\cup_{s \leq k \leq q} P_k$ or $Q_{[s]}$. We point out that the family $Q_{[s]}$ cannot be further reduced. This can be demonstrated by the results from [13]. The authors of [13] proved that when the edge density is smaller than $1/(q \log q)$ (so the corresponding $s$ is less than 2), the extremal graphs which maximize the number of $q$-colorings are some complete bipartite graphs plus isolated vertices, which corresponds to the family $Q_2$.

One of the reasons that we were able to solve $\OPT_q(s)$ for integers $s$ in Section 6 is that the family $Q_{[s]}$ vanishes when $s$ is integer. In general, it remains difficult to solve the $\OPT_q(s)$ for every $q$. However, we wonder if the following statement is true for any real $s > 1$: there exists a function $q(s)$ such that for any integer $q \geq q(s)$, every extremal graph with sufficiently large $n$ vertices and $m = \frac{s-1}{2s} n^2$ edges maximizing the number of $q$-colorings is $o(n^2)$-close to (or even is) a complete $[s]$-partite graph. Equivalently, it says that under the same conditions, every solution to $\OPT_q(s)$ is in $P_{[s]}$. Theorem 1.4 shows that this holds for all large integers $s$.

We can improve Theorem 1.4 to that every extremal graph is $O_{s,q}(n)$-close to the Turán graph $T_s(n)$, where the dependence in $O$ is relative to $s$ and $q$. The proof requires lengthy and tedious stability arguments and we decide to not include here. The problem of pursuing the exact structure of the extremal graphs in fact can be reduced to a universal maximum bound on $P_G(q)$ for all sparse graphs $G$ and general $q$, which we explain as follows. Let $G$ be a graph with $n$ vertices and $m = o(n^2)$ edges. A result from [13] asserts that when $q$ is fixed and $m$ is sufficiently large (so is $n$), the maximum of $P_G(q)$ is $q^n \cdot e^{((c+o(1)) \sqrt{m})}$, where $c = 2\sqrt{\log \frac{q}{q-1}} \cdot \log q$. And when $n, m$ are fixed and $q$ is sufficiently large, it is not hard to see that the maximum of $P_G(q)$ is at most $q^n \cdot \left(1 - \frac{1}{q}\right)^{c'm}$ for some absolute constant $c'$. However it is not known if the following universal upper bound $P_G(q) \leq \max \left\{ q^n \cdot e^{((-c+o(1)) \sqrt{m})}, q^n \cdot \left(1 - \frac{1}{q}\right)^{c'm} \right\}$ or similar holds for all such sparse graphs $G$ and for general $m, n, q$. If the answer is yes, this would lead to the exact structure of the extremal graphs, which are the Turán graphs. Otherwise, there exists a sparse $G$ with a larger number of $q$-colorings in some range of $q$; adding this $G$ to certain $s$-partite graph will likely give a counterexample to Conjecture 1.2 in that range of $q$.

Another related question, raised in [14] (also see [11]), was asked to find the maximum number of acyclic orientations, that is the value of $|P_G(-1)|$, over graphs $G$ with $n$ vertices and $m$ edges. An upper bound was obtained in [11] that it is at most the product of $\max\{2, d(x)\}$ over all vertices $x$, where $d(x)$ denotes the degree of $x$. It will be also interesting to find the extremal graphs in this context.

We also feel that the problem we study, maximizing the number of proper $q$-colorings over graphs with fixed number of vertices and edges, shares certain similarity with the result of Reiher [17] which finds the minimum number of cliques $K_q$ over the same family.
of graphs. Evidence suggests that the solutions to the continuous relaxation (10) are very similar to the extremal graphs Reiher found.

In [13], Loh et al. remarked that “the natural next step would be to extend the result to the range \( \frac{n}{m} \leq \frac{1}{q} \)” for general \( q \). That is the case \( 1 < s \leq 2 \). We will address this in a forthcoming paper.

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Appendix A. Stability of the main optimization problem

In this section, we prove Corollary 2.3.

Corollary 2.3. For any real \( s > 1 \), the following holds for all sufficiently large \( n \). Let \( G \) be an \( n \)-vertex graph with \( m = \frac{s-1}{2s} n^2 + o(n^2) \) edges which maximizes the number of \( q \)-colorings. Then \( G \) is \( o(n^2) \)-close to \( G_{\alpha}(n) \) for some \( \alpha \) which solves \( \text{OPT}_q(s) \).

Proof. Suppose, towards contradiction, that the corollary is false. That means that there exist \( \varepsilon > 0 \) and a sequence of graphs \( \{G_t\}_{t=1}^\infty \) such that

- \( G_t \) has \( n_t \) vertices and \( m_t \) edges;
- \( \lim_{t \to \infty} n_t = \infty \) and \( m_t = \frac{s-1}{2s} n_t^2 + o_t(n_t^2) \);
- \( G_t \) maximizes the number of \( q \)-colorings among all graphs with the same number of vertices and edges;
- \( G_t \) is not \( \varepsilon n_t^2 \)-close to \( G_{\alpha}(n_t) \) for any solution \( \alpha \) of \( \text{OPT}_q(s) \).

We may assume, by possibly passing to a subsequence of \( \{G_t\}_{t=1}^\infty \), that for all \( t \geq 1 \) we have

\[
m_t \leq \frac{(s + 1) - 1}{2(s + 1)} n_t^2
\]

and that \( n_t \) is large enough so that we can apply Theorem 2.2 to the graph \( G_t \) with \( s \) replaced by \( s + 1 \) and with \( \varepsilon \) replaced by \( \frac{\varepsilon}{2t} \). This implies that there exist \( s_t \) and \( \alpha_t \) such that the following holds:

- \( \left| \frac{s_t - 1}{2s_t} - \frac{m_t}{n_t^2} \right| < \frac{\varepsilon}{2t} \) and \( s_t \leq s + 1 \);
- \( \alpha_t \) is a solution of \( \text{OPT}_q(s_t) \);
- \( G_t \) is \( \frac{\varepsilon}{2t} n_t^2 \)-close to \( G_{\alpha_t}(n_t) \).
Note that in this case we have \( \lim_{t \to \infty} \left| \frac{s_1 - 1}{2s} - \frac{m_s}{n^2_t} \right| = 0 \), which implies \( \lim_{t \to \infty} s_t = s \).

Again, by possibly passing to a subsequence, we may assume that the sequence \( \alpha_t \) (which lives in a compact space) converges to some \( \alpha \). By the continuity of \( V_q \) and \( E_q \) we have

\[
V_q(\alpha) = \lim_{t \to \infty} V_q(\alpha_t) = 1 \quad \text{and} \quad E_q(\alpha) = \lim_{t \to \infty} E_q(\alpha_t) = \lim_{t \to \infty} \frac{s_t - 1}{2s} = \frac{s - 1}{2s},
\]

hence \( \alpha \in \text{FEAS}_q(s) \). Furthermore, by the continuity of \( \text{OPT}_q \) and \( \text{OBJ}_q \), we have

\[
\text{OPT}_q(s) = \lim_{t \to \infty} \text{OPT}_q(s_t) = \lim_{t \to \infty} \text{OBJ}_q(\alpha_t) = \text{OBJ}_q(\lim_{t \to \infty} \alpha_t) = \text{OBJ}_q(\alpha),
\]

hence \( \alpha \) is a solution to \( \text{OPT}_q(s) \). Lastly, since \( \alpha_t \to \alpha \), for \( t \) sufficiently large we have that \( G_\alpha(n_t) \) and \( G_{\alpha_t}(n_t) \) are \( \frac{\epsilon}{2} n^2_t \)-close. But because \( G_t \) is \( \frac{\epsilon}{2} n^2_t \)-close to \( G_{\alpha_t}(n_t) \), we have that \( G_t \) is \( \epsilon n^2_t \)-close to \( G_{\alpha}(n_t) \), a contradiction. This concludes the proof of the corollary. \( \square \)

References