The number of cliques in graphs of given order and size

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Abstract

Let $k_r(n,m)$ denote the minimum number of r-cliques in graphs with n vertices and m edges. We give a lower bound on $k_r(n,m)$ that approximates $k_r(n,m)$ with an error smaller than $n^r/\left(n^2-2m\right)$. This essentially solves a sixty year old problem.

The solution is based on a constraint minimization of certain multilinear forms. In our proof, a combinatorial strategy is coupled with extensive analytical arguments.

Keywords: *number of cliques; mulitilinear forms; Turán graph.*

1 Introduction

Our graph theoretic notation follows [3]; in particular, an r-clique is a complete subgraph on r vertices.

What is the minimum number $k_r(n,m)$ of r-cliques in graphs with n vertices and m edges? This problem originated with the famous graph-theoretical theorem of Turán more than sixty years ago, but despite numerous attempts, never got a satisfactory solution, see [2], [4], [5], [6], [7], and [9] for some highlights of its long history. Most recently, the problem was discussed in detail in [1].

The best result so far is due to Razborov [9]. Applying tools developed in [8], he achieved a remarkable progress for $r=3$. This method, however, failed for $r>3$, and Razborov challenged the mathematical community to extend his result.

The aim of this paper is to answer this challenge. We introduce a class of multilinear forms and find their minima subject to certain constraints. As a consequence, we obtain a lower bound on $k_r(n,m)$, approximating $k_r(n,m)$ with an error smaller than $n^r/\left(n^2-2m\right)$.

Our proof is build on combinatorial main strategy, complemented with analytical arguments using Taylor's expansion, Lagrange's multipliers, compactness, continuity, and connectedness. We believe that such cooperation can be developed further and applied to other problems in extremal combinatorics.

2 Main results

Suppose $1 \leq r \leq n$, let $[n] = \{1, \ldots, n\}$, and write $\binom{[n]}{r}$ for the set of r-subsets of $[n]$. For a symmetric $n \times n$ matrix $A = (a_{ij})$ and a vector $\mathbf{x} = (x_1, \ldots, x_n)$, set

$$L_r(A, \mathbf{x}) = \sum_{X \in \binom{[n]}{r}} \prod_{i,j \in X,\ i<j} a_{ij} \prod_{i \in X} x_i. \tag{1}$$

Define the set $\mathcal{A}(n)$ of symmetric $n \times n$ matrices $A = (a_{ij})$ by

$$\mathcal{A}(n) = \{A : \ a_{ii} = 0 \text{ and } 0 \leq a_{ij} = a_{ji} \leq 1 \text{ for all } i, j \in [n]\}.$$

Our main goal is to find $\min L_r(A, \mathbf{x})$ subject to the constraints

$$A \in \mathcal{A}(n), \ \mathbf{x} \geq 0, \ L_1(A, \mathbf{x}) = b, \text{ and } L_2(A, \mathbf{x}) = c,$$

where b and c are fixed positive numbers. Since every $L_s(A, \mathbf{x})$ is homogenous of first degree in each x_i, for simplicity we assume that $b = 1$ and study

$$\min \{L_r(A, \mathbf{x}) : (A, \mathbf{x}) \in \mathcal{S}_n(c)\}, \tag{2}$$

where $\mathcal{S}_n(c)$ is the set of pairs $(A, \mathbf{x})$ defined as

$$\mathcal{S}_n(c) = \{(A, \mathbf{x}) : \ A \in \mathcal{A}(n), \ \mathbf{x} \geq 0, \ L_1(A, \mathbf{x}) = 1, \text{ and } L_2(A, \mathbf{x}) = c\}.$$

Note that $\mathcal{S}_n(c)$ is compact since the functions $L_s(A, \mathbf{x})$ are continuous; hence (2) is defined whenever $\mathcal{S}_n(c)$ is nonempty. The following proposition, proved in 2.2.3, describes when $\mathcal{S}_n(c) \neq \varnothing$.

Proposition 2.1 *$\mathcal{S}_n(c)$ is nonempty if and only if $c < 1/2$ and $n \geq \lceil 1/(1 - 2c) \rceil$.*

Hereafter we assume that $0 < c < 1/2$ and set $\xi(c) = \lceil 1/(1 - 2c) \rceil$.

To find (2), we solve a seemingly more general problem: for all $c \in (0, 1/2)$, $n \geq \xi(c)$, and $3 \leq r \leq n$, find

$$\varphi_r(n, c) = \min \{L_r(A, \mathbf{x}) : \ r \leq k \leq n, \ \ (A, \mathbf{x}) \in \mathcal{S}_k(c)\}.$$

We obtain the solution of (2) by showing that, in fact, $\varphi_r(n, c)$ is independent of n.

To state $\varphi_r(n, c)$ precisely, we need some preparation. Set $s = \xi(c)$ and note that the system

$$\binom{s-1}{2} x^2 + (s - 1) xy = c, \tag{3}$$

$$(s - 1) x + y = 1, \tag{4}$$

$$x \geq y$$

has a unique solution

$$x = \frac{1}{s} + \frac{1}{s}\sqrt{1 - \frac{2s}{s-1}c}, \qquad y = \frac{1}{s} - \frac{s-1}{s}\sqrt{1 - \frac{2s}{s-1}c}. \tag{5}$$

Write $\mathbf{x}_c$ for the s-vector $(x, \ldots, x, y)$ and let $A_s \in \mathcal{A}(s)$ be the matrix with all off-diagonal entries equal to 1. Note that equations (3) and (4) give $(A_s, \mathbf{x}_c) \in \mathcal{S}_s(c)$.

Setting $\varphi_r(c) = L_r(A_s, \mathbf{x}_c)$, we arrive at the main result in this section.

Theorem 2.2 *If $c \in (0, 1/2)$ and $3 \leq r \leq \xi(c) \leq n$, then $\varphi_r(n, c) = \varphi_r(c)$.*

Note first that the premise $r \leq \xi(c)$ is not restrictive, for, $\varphi_r(n, c) = 0$ whenever $r > \xi(c)$. Indeed, assume that $r > \xi(c)$ and write $\mathbf{y}$ for the r-vector $(x, \ldots, x, y, 0, \ldots, 0)$ whose last $r - s$ entries are zero. Writing B for the $r \times r$ matrix with A_s as a principal submatrix in the first s rows and with all other entries being zero, we see that $(B, \mathbf{y}) \in \mathcal{S}_r(c)$ and $L_r(B, \mathbf{y}) = 0$; hence $\varphi_r(n, c) = 0$, as claimed.

Next, note an explicit form of $\varphi_r(c)$:

$$\begin{aligned}\varphi_r(c) &= \binom{s-1}{r} x^r + \binom{s-1}{r-1} x^{r-1} y \\ &= \binom{s}{r} \frac{1}{s^r} \left(1 - (r-1)\sqrt{1 - \frac{2s}{s-1}c}\right)\left(1 + \sqrt{1 - \frac{2s}{s-1}c}\right)^{r-1}.\end{aligned}$$

Since $\varphi_r(c)$ is defined via the discontinuous step function $\xi(c)$, the following properties of $\varphi_r(c)$ are worth stating:

- $\varphi_r(c)$ is continuous for $c \in (0, 1/2)$;
- $\varphi_r(c) = 0$ for $c \in (0, 1/4]$ and is increasing for $c \in (1/4, 1/2)$;
- $\varphi_r(c)$ is differentiable and concave in any interval $((s-1)/2s, s/2(s+1))$.

2.1 The number of cliques

Write $k_r(G)$ for the number of r-cliques of a graph G and let us outline the connection of Theorem 2.2 to $k_r(G)$. Let

$$k_r(n, m) = \min\{k_r(G) : \ G \text{ has } n \text{ vertices and } m \text{ edges}\},$$

and suppose that $k_r(n, m)$ is attained on a graph G with adjacency matrix $A = (a_{ij})$. Clearly, for every $X \in \binom{[n]}{r}$,

$$\prod_{i,j \in X, \ i<j} a_{ij} = \begin{cases} 1, & \text{if } X \text{ induces an } r\text{-clique in } G, \\ 0, & \text{otherwise.} \end{cases}.$$

Hence, letting $\mathbf{x} = (1/n, \ldots, 1/n)$, we see that

$$L_1(A, \mathbf{x}) = 1, \ L_2(A, \mathbf{x}) = m/n^2, \text{ and } L_r(A, \mathbf{x}) = k_r(G)/n^r;$$

thus Theorem 2.2 gives

$$k_r(n, m) \geq \varphi_r\left(n, m/n^2\right) n^r = \varphi_r\left(m/n^2\right) n^r.$$

Setting $s = \xi(m/n^2) = \lceil 1/(1 - 2m/n^2) \rceil$, we obtain an explicit form of this inequality

$$k_r(n, m) \geq \binom{s}{r} \frac{1}{s^r} \left(n - (r-1)\sqrt{n^2 - \frac{2sm}{s-1}}\right)\left(n + \sqrt{n^2 - \frac{2sm}{s-1}}\right)^{r-1}. \qquad (6)$$

Inequality (6) turns out to be rather tight, as stated below and proved in Section 2.3.

Theorem 2.3

$$k_r(n,m) < \varphi_r\left(\frac{m}{n^2}\right)n^r + \frac{n^r}{n^2-2m}.$$

Note, in particular, that if $m < (1/2-\varepsilon)\,n^2$, then

$$k_r(n,m) < \varphi_r\left(m/n^2\right)n^r + n^{r-2}/2\varepsilon,$$

so the order of the error is lower than expected.

Known previous results

For $n^2/4 \leq m \leq n^2/3$ inequality (6) was first proved by Fisher [6]. He showed that

$$k_3(n,m) \geq \frac{9nm - 2n^3 - 2\left(n^2-3m\right)^{3/2}}{27} = \varphi_3\left(m/n^2\right)n^3,$$

but did not discuss how close the two sides of this inequality are.

Recently Razborov [9] showed that for every fixed $c \in (0,1/2)$,

$$k_3\left(n,\lceil cn^2\rceil\right) = \varphi_3(c)\,n^3 + o\left(n^3\right).$$

Unfortunately, his approach, based on [8], provides no clues whatsoever how large the $o(n^3)$ term is; in particular, in his approach this term is not uniformly bounded when c approaches 1/2. In [9] Razborov challenged the mathematical community to prove that $k_r\left(n,\lceil cn^2\rceil\right) = \varphi_r(c)\,n^r + o(n^r)$ for $r > 3$. Our Theorem 2.2 responds to this challenge.

2.2 Proof of Theorem 2.2

We first show that $\varphi_r(n,c)$ increases in c whenever $\varphi_r(n,c) > 0$.

Proposition 2.4 *Let $c \in (0,1/2)$ and $3 \leq r \leq \xi(c) \leq n$. If $\varphi_r(n,c) > 0$ and $0 < c_0 < c$, then $\varphi_r(n,c) > \varphi_r(n,c_0)$.*

Proof Suppose that

$$\xi(c) \leq k \leq n, \ \ (A,\mathbf{x}) \in \mathcal{S}_k(c), \text{ and } \ \varphi_r(n,c) = L_r(A,\mathbf{x}).$$

Setting $\alpha = c_0/c$, we see that $\alpha A \in \mathcal{A}(k)$ and

$$L_2(\alpha A,\mathbf{x}) = \alpha L_r(A,\mathbf{x}) = c_0;$$

thus $(\alpha A,\mathbf{x}) \in \mathcal{S}_k(c_0)$. Hence we obtain

$$\varphi_r(n,c) = L_r(A,\mathbf{x}) = \alpha^{-\binom{r}{2}}L_r(\alpha A,\mathbf{x}) > L_r(\alpha A,\mathbf{x}) \geq \varphi_r(n,c_0),$$

completing the proof of Proposition 2.4. □

Proof of Theorem 2.2

Let us first define a set of n-vectors $\mathcal{X}(n)$ by

$$\mathcal{X}(n) = \{(x_1, \ldots, x_n) : x_1 + \cdots + x_n = 1 \text{ and } x_i \geq 0,\ 1 \leq i \leq n\}.$$

Now the two conditions $\mathbf{x} \geq 0$ and $L_1(A, \mathbf{x}) = 1$ can be combined into one: $\mathbf{x} \in \mathcal{X}(n)$.

Assume for a contradiction that the theorem fails: let

$$c \in (0, 1/2),\ 3 \leq r \leq \xi(c) \leq n,\ A = (a_{ij}),\ \mathbf{x} = (x_1, \ldots, x_n),\ \text{and } (A, \mathbf{x}) \in \mathcal{S}_n(c) \tag{7}$$

be such that

$$\varphi_r(n, c) = L_r(A, \mathbf{x}) < \varphi_r(c). \tag{8}$$

Assume that n is the minimum integer with this property for all $c \in (0, 1/2)$. Hereafter we shall refer to this assumption as the "main assumption". An immediate consequence of the main assumption is the following

Claim 2.5 *If $(A, \mathbf{y}) \in \mathcal{S}_n(c)$ and $\varphi_r(n, c) = L_r(A, \mathbf{y})$, then $\mathbf{y} > 0$.* □

We introduce now some notation and conventions simplifying the presentation of analytical calculations. For short, for every $i, j, \ldots, k \in [n]$, set

$$C_i = \frac{\partial L_2(A, \mathbf{x})}{\partial x_i}, \quad C_{ij} = \frac{\partial L_2(A, \mathbf{x})}{\partial x_i \partial x_j}, \quad D_{ij\ldots k} = \frac{\partial L_r(A, \mathbf{x})}{\partial x_i \partial x_j \cdots \partial x_k},$$

and note that

$$C_{ij} = a_{ij}, \quad \text{and} \quad \frac{\partial L_r(A, \mathbf{x})}{\partial a_{ij}} a_{ij} = D_{ij} x_i x_j. \tag{9}$$

Next we spell out the Taylor's expansion for the functions $L_2(A, \mathbf{x})$ and $L_r(A, \mathbf{x})$. Letting $\mathbf{y} = (x_1 + \Delta_1, \ldots, x_n + \Delta_n)$, Taylor's formula gives

$$L_2(A, \mathbf{y}) - L_2(A, \mathbf{x}) = \sum_{i=1}^{n} C_i \Delta_i + \sum_{1 \leq i < j \leq n} C_{ij} \Delta_i \Delta_j \tag{10}$$

and

$$L_r(A, \mathbf{y}) - L_r(A, \mathbf{x}) = \sum_{s=1}^{r} \sum_{1 \leq i_1 < \cdots < i_s \leq n} D_{i_1 \ldots i_s} \Delta_{i_1} \cdots\ \Delta_{i_s}. \tag{11}$$

We also use extensively Lagrange multipliers. Since $\mathbf{x} > 0$, by Lagrange's method, there exist λ and μ such that

$$D_i = \lambda C_i + \mu \tag{12}$$

for all $i \in [n]$. Likewise, if $0 < a_{ij} < 1$, we have

$$\frac{\partial L_r(A, \mathbf{x})}{\partial a_{ij}} = \lambda \frac{\partial L_2(A, \mathbf{x})}{\partial a_{ij}} = \lambda x_i x_j,$$

and so, in view of (9),

$$D_{ij} = \lambda a_{ij} \quad \text{whenever} \quad 0 < a_{ij} < 1. \tag{13}$$

The rest of the proof is presented in a sequence of formal claims. First we show that $\varphi_r(n, c)$ is attained on a $(0, 1)$-matrix A.

Claim 2.6 *Let $(A,\mathbf{x}) \in \mathcal{S}_n(c)$ satisfy (7) and (8), and suppose that A has the smallest number of entries a_{ij} such that $0 < a_{ij} < 1$. Then A is a $(0,1)$-matrix.*

Proof Assume for a contradiction that $i,j \in [n]$ and $0 < a_{ij} < 1$. By symmetry we assume that $C_i \geq C_j$.

Let

$$f(\alpha) = \frac{a_{ij}\alpha^2 - (C_i - C_j)\alpha}{(x_i+\alpha)(x_j-\alpha)}, \tag{14}$$

and suppose that α satisfies

$$0 < \alpha < x_j \text{ and } 0 \leq a_{ij} + f(\alpha) \leq 1. \tag{15}$$

Let $\mathbf{y}_\alpha = (x_1 + \Delta_1, \ldots, x_n + \Delta_n)$, where

$$\Delta_i = \alpha, \quad \Delta_j = -\alpha, \quad \text{and} \quad \Delta_l = 0 \text{ for } l \in [n] \setminus \{i,j\}, \tag{16}$$

and define the $n \times n$ matrix $B_\alpha = (b_{ij})$ by

$$b_{ij} = b_{ji} = a_{ij} + f(\alpha) \quad \text{and} \quad b_{pq} = a_{pq} \text{ for } \{p,q\} \neq \{i,j\}. \tag{17}$$

Note that $B_\alpha \in \mathcal{A}(n)$, $\mathbf{y}_\alpha \in \mathcal{X}(n)$, and

$$L_2(B_\alpha, \mathbf{y}_\alpha) - L_2(A, \mathbf{y}_\alpha) = f(\alpha)\frac{\partial L_2(A,\mathbf{y}_\alpha)}{\partial a_{ij}} = f(\alpha)(x_i+\alpha)(x_j-\alpha).$$

Hence, Taylor's expansion (10) and equation (14) give

$$\begin{aligned} L_2(B_\alpha, \mathbf{y}_\alpha) - L_2(A,\mathbf{x}) &= L_2(A,\mathbf{y}_\alpha) - L_2(A,\mathbf{x}) + f(\alpha)(x_i+\alpha)(x_j-\alpha) \\ &= (C_i - C_j)\alpha - a_{ij}\alpha^2 + f(\alpha)(x_i+\alpha)(x_j-\alpha) = 0; \end{aligned}$$

thus $(B_\alpha, \mathbf{y}_\alpha) \in \mathcal{S}_n(c)$.

Note also that, in view of (9),

$$\begin{aligned} L_r(B_\alpha, \mathbf{y}_\alpha) - L_r(A, \mathbf{y}_\alpha) &= \frac{\partial L_r(A,\mathbf{y}_\alpha)}{\partial a_{ij}} f(\alpha) = f(\alpha) y_i y_j \frac{D_{ij}}{a_{ij}} \\ &= f(\alpha)(x_i+\alpha)(x_j-\alpha)\frac{D_{ij}}{a_{ij}}. \end{aligned}$$

Hence Taylor's expansion (11), Lagrange's conditions (12) and (13), and equation (14) give

$$\begin{aligned} L_r(B_\alpha, \mathbf{y}_\alpha) - L_r(A,\mathbf{x}) &= L_r(A,\mathbf{y}_\alpha) - L_r(A,\mathbf{x}) + f(\alpha)(x_i+\alpha)(x_j-\alpha)\frac{D_{ij}}{a_{ij}} \\ &= (D_i - D_j)\alpha - D_{ij}\alpha^2 + f(\alpha)(x_i+\alpha)(x_j-\alpha)\frac{D_{ij}}{a_{ij}} \\ &= \lambda(C_i - C_j)\alpha - D_{ij}\alpha^2 + f(\alpha)(x_i+\alpha)(x_j-\alpha)\frac{D_{ij}}{a_{ij}} \\ &= \frac{D_{ij}}{a_{ij}}\big((C_i - C_j)a_{ij}\alpha - a_{ij}\alpha^2 + f(\alpha)(x_i+\alpha)(x_j-\alpha)\big) \\ &= \frac{D_{ij}}{a_{ij}}(C_i - C_j)(a_{ij}-1)\alpha \leq 0. \end{aligned}$$

If there exists $\alpha \in (0, x_j)$ such that either $a_{ij} + f(\alpha) = 0$ or $a_{ij} + f(\alpha) = 1$, we see that the matrix B_α has fewer entries belonging to $(0,1)$ than A, contradicting the hypothesis and completing the proof. Assume therefore that $0 < a_{ij} + f(\alpha) < 1$ for all $\alpha \in (0, x_j)$. This implies that

$$a_{ij} x_j = C_i - C_j,$$

for, otherwise $\lim_{\alpha \to x_j} |f(\alpha)| = \infty$, and so, either $a_{ij} + f(\alpha) = 0$ or $a_{ij} + f(\alpha) = 1$ for some $\alpha \in (0, x_j)$.

Now, extending $f(\alpha)$ continuously for $\alpha = x_j$ by

$$f(x_j) = \lim_{\alpha \to x_j} f(\alpha) = \lim_{\alpha \to x_j} \frac{a_{ij}\alpha(\alpha - x_j)}{(x_i + \alpha)(x_j - \alpha)} = -\frac{a_{ij} x_j}{x_i + x_j},$$

and defining $\mathbf{y}_{x_j}$ and B_{x_j} by (16) and (17), we obtain

$$L_r\left(B_{x_j}, \mathbf{y}_{x_j}\right) - \varphi_r(n, c) = L_r\left(B_{x_j}, \mathbf{y}_{x_j}\right) - L_r(A, \mathbf{x}) \le 0.$$

contradicting the main assumption since the jth entry of $\mathbf{y}_{x_j}$ is zero. This completes the proof of Claim 2.6. $\square$

Since A is a $(0,1)$-matrix with a zero main diagonal, it is the adjacency matrix of some graph G with vertex set $[n]$. Write $E(G)$ for the edge set of G, and let us restate the functions $L_r(A, \mathbf{x})$ in terms of G. We have

$$L_2(A, \mathbf{x}) = \sum_{ij \in E(G)} x_i x_j$$

and more generally,

$$L_r(A, \mathbf{x}) = \sum \{x_{i_1} \cdots x_{i_r} : \text{ the set } \{i_1, \ldots, i_r\} \text{ induces an } r\text{-clique in } G\}.$$

To complete the proof we show that (a) G is a complete graph and (b) $L_r(A, \mathbf{x}) = \varphi_r(c)$.

2.2.1 Proof that G is a complete graph

For convenience we first outline this part of the proof. Write $\overline{G}$ for the complement of G and $E\left(\overline{G}\right)$ for the edge set of $\overline{G}$. We prove that G is complete by the following sequence of steps:

- if $ij \in E\left(\overline{G}\right)$, then $C_i \neq C_j$ - Claim 2.7;
- if $ij \in E(G)$, then $D_{ij} \le \lambda$ - Claims 2.8 and 2.9;
- $\overline{G}$ is triangle-free - Claim 2.10;
- $\overline{G}$ contains no vertex of degree 3 or higher - Claims 2.11 and 2.12;
- $\overline{G}$ consists of isolated vertices - Claims 2.11 and 2.13.

Now let us give the details.

Claim 2.7 *If $ij \in E\left(\overline{G}\right)$, then $C_i \neq C_j$.*

Proof Assume for a contradiction that $ij \in E\left(\overline{G}\right)$ and $C_i = C_j$.

Let $\mathbf{y} = (x_1 + \Delta_1, \ldots, x_n + \Delta_n)$, where

$$\Delta_i = -x_i, \quad \Delta_j = x_i, \quad \text{and} \quad \Delta_l = 0 \text{ for } l \in [n] \setminus \{i, j\}.$$

We see that $\mathbf{y} \in \mathcal{X}(n)$, and Taylor's expansion (10) gives

$$L_2(A, \mathbf{y}) - L_2(A, \mathbf{x}) = C_j x_i - C_i x_i = 0;$$

thus, $(A, \mathbf{y}) \in \mathcal{S}_n(c)$.

Also, Taylor's expansion (11) and Lagrange's condition (12) give

$$L_r(A, \mathbf{y}) - L_r(A, \mathbf{x}) = D_j x_i - D_i x_i = \mu(x_i - x_i) + \lambda(C_j - C_i)x_i = 0;$$

thus $L_r(A, \mathbf{y}) = \varphi_r(n, c)$. Since the ith entry of $\mathbf{y}$ is zero, this equality contradicts Claim 2.5, completing the proof of Claim 2.7. □

In the next two claims we prove that if $ij \in E(G)$, then $D_{ij} \leq \lambda$.

Claim 2.8 *If $ij \in E(G)$, then either $D_{ij} \leq \lambda$ or $D_i = D_j$.*

Proof Select an edge $ij \in E(G)$ and assume that $D_i \neq D_j$. Then Lagrange's condition (12) gives

$$D_i - D_j = \lambda(C_i - C_j),$$

and so, $C_i \neq C_j$; by symmetry suppose that $C_i > C_j$.

Suppose that $0 < \alpha < x_j$ and let

$$f(\alpha) = \frac{\alpha^2 - (C_i - C_j)\alpha}{(x_i + \alpha)(x_j - \alpha)}. \tag{18}$$

Next, let $\mathbf{y}_\alpha = (x_1 + \Delta_1, \ldots, x_n + \Delta_n)$, where

$$\Delta_i = \alpha, \quad \Delta_j = -\alpha, \quad \text{and} \quad \Delta_l = 0 \text{ for all } l \in [n] \setminus \{i, j\},$$

and define the $n \times n$ matrix $B_\alpha = (b_{ij})$ by

$$b_{ij} = b_{ji} = 1 + f(\alpha), \quad \text{and} \quad b_{pq} = a_{pq} \text{ for } \{p, q\} \neq \{i, j\}.$$

Note that for α sufficiently small, $-1 < f(\alpha) < 0$, and so, $B_\alpha \in \mathcal{A}(n)$ and $\mathbf{y}_\alpha \in \mathcal{X}(n)$.

Taylor's expansion (10) and equation (18) give

$$L_2(B_\alpha, \mathbf{y}_\alpha) - L_2(A, \mathbf{x}) = C_i\alpha - C_j\alpha - \alpha^2 + f(\alpha)(x_i + \alpha)(x_j - \alpha) = 0;$$

thus, $(B_\alpha, \mathbf{y}_\alpha) \in \mathcal{S}_n(c)$.

Also, Taylor's expansion (11), Lagrange's condition (12), and equation (18) give

$$\begin{aligned} L_r(B_\alpha, \mathbf{y}_\alpha) - L_r(A, \mathbf{x}) &= D_i\alpha - D_j\alpha - D_{ij}\alpha^2 + D_{ij}f(\alpha)(x_i + \alpha)(x_j - \alpha) \\ &= \lambda(C_i - C_j)\alpha - D_{ij}(C_i - C_j)\alpha \\ &= \alpha(C_i - C_j)(\lambda - D_{ij}). \end{aligned}$$

Since $L_r(B_\alpha, \mathbf{y}_\alpha) \geq L_r(A, \mathbf{x})$ and $\alpha(C_i - C_j) > 0$, we see that $D_{ij} \leq \lambda$, completing the proof of Claim 2.8. □

Claim 2.9 *If $ij \in E(G)$ and $D_i = D_j$, then $D_{ij} \leq \lambda$.*

Proof Assume for a contradiction that $ij \in E(G)$, $D_i = D_j$, and $D_{ij} > \lambda$. Firts we show that $G - i - j$ is a complete graph.

Assume that this not the case and select $pq \in E\left(\overline{G}\right)$ such that $p, q \in [n] \setminus \{i, j\}$. Claim 2.7 implies that $C_p \neq C_q$; by symmetry we suppose that $C_p > C_q$.

Set

$$P = C_{ip} - C_{iq} - C_{jp} + C_{jq},$$

suppose that $\alpha > 0$ is sufficiently small, and let

$$f(\alpha) = \frac{\alpha^2}{C_p - C_q + P\alpha}. \tag{19}$$

Next, let $\mathbf{y}_\alpha = (x_1 + \Delta_1, \ldots, x_n + \Delta_n)$, where

$$\Delta_i = \alpha, \quad \Delta_j = -\alpha, \quad \Delta_p = f(\alpha), \quad \Delta_q = -f(\alpha), \quad \text{and} \quad \Delta_l = 0 \text{ for } l \in [n] \setminus \{i, j, p, q\}.$$

We see that $\mathbf{y}_\alpha \in \mathcal{X}(n)$.

Taylor's expansion (10) and equation (19) give

$$\begin{aligned} L_2(A, \mathbf{y}_\alpha) - L_2(A, \mathbf{x}) &= C_i\alpha - C_j\alpha - \alpha^2 + (C_p - C_q) f(\alpha) + (C_{ip} - C_{iq} - C_{jp} + C_{jq}) \alpha f(\alpha) \\ &= (C_i - C_j)\alpha - \alpha^2 + ((C_p - C_q) + P\alpha) f(\alpha) = 0; \end{aligned}$$

thus, $(A, \mathbf{y}_\alpha) \in \mathcal{S}_n(c)$.

Setting

$$Q = D_{ip} - D_{iq} - D_{jp} + D_{jq} - D_{ijp}\alpha + D_{ijq}\alpha,$$

Taylor's expansion (11), Lagrange's condition (12), and the equation $D_i = D_j$ give

$$\begin{aligned} L_r(A, \mathbf{y}_\alpha) - L_r(A, \mathbf{x}) &= (D_i - D_j)\alpha - D_{ij}\alpha^2 + (D_p - D_q) f(\alpha) \\ &\quad + (D_{ip} - D_{iq} - D_{jp} + D_{jq} - D_{ijp}\alpha + D_{ijq}\alpha)\alpha f(\alpha) \\ &= -D_{ij}\alpha^2 + \lambda (C_p - C_q) f(\alpha) + Q\alpha f(\alpha). \end{aligned}$$

Hence, recalling that $L_r(A, \mathbf{y}_\alpha) \geq L_r(A, \mathbf{x})$, we see that

$$-D_{ij}\alpha^2 + \lambda (C_p - C_q) f(\alpha) + Q\alpha f(\alpha) \geq 0,$$

and so,

$$\lambda (C_p - C_q) + Q\alpha \geq D_{ij} \frac{\alpha^2}{f(\alpha)}. \tag{20}$$

From equation (19) we have

$$\lim_{\alpha \to 0} \frac{\alpha^2}{f(\alpha)} = \lim_{\alpha \to 0} (C_p - C_q + P\alpha) = C_p - C_q,$$

and, passing to limits in (20), we obtain

$$\lambda\left(C_p - C_q\right) \geq D_{ij}\left(C_p - C_q\right),$$

contradicting the hypothesis, in view of $C_p > C_q$. Hence, $G - i - j$ is a complete graph.

There must be a vertex connected in G to both i and j. Otherwise if we remove the edge ij, the value of $L_r(A, \mathbf{x})$ will remain the same, while $L_2(A, \mathbf{x})$ will decrease, contradicting Proposition 2.4. By symmetry we suppose that the vertex n is connected to both i and j, and so, n is connected to every vertex of G other than itself.

Set $\mathbf{y} = (x_1, \ldots, x_{n-1})$ and let B be the principal submatrix of A in the first $(n-1)$ columns. Since

$$x_1 + \cdots + x_{n-1} = 1 - x_n, \tag{21}$$
$$L_2(B, \mathbf{y}) = c - x_n(1 - x_n), \tag{22}$$

and

$$L_r(A, \mathbf{x}) = x_n L_{r-1}(B, \mathbf{y}) + L_r(B, \mathbf{y}),$$

we see that $x_n L_{r-1}(B, \mathbf{y}) + L_r(B, \mathbf{y})$ is minimum subject to (21) and (22). Since $B \in \mathcal{A}(n-1)$, by the main assumption, both $L_{r-1}(B, \mathbf{z})$ and $L_r(B, \mathbf{z})$ attain a minimum on a complete graph H and for the same vector $\mathbf{z}$. Since n is joined to every vertex of H, the minimum $\varphi_r(n, c)$ is attained on a complete graph too, a contradiction completing the proof of Claim 2.9. □

Claim 2.10 *The graph $\overline{G}$ is triangle-free.*

Proof Assume for a contradiction that there exist $i, j, k \in [n]$ such that $ij, ik, jk \in E\left(\overline{G}\right)$. Let the line

$$\left(C_i - C_k\right)x + \left(C_j - C_k\right)y = 0 \tag{23}$$

intersect the triangle formed by the lines

$$x = -x_i, \quad y = -x_j, \quad x + y = x_k$$

at some point (α, β).

Let $\mathbf{y} = (x_1 + \Delta_1, \ldots, x_n + \Delta_n)$, where

$$\Delta_i = \alpha, \quad \Delta_j = \beta, \quad \Delta_k = -\alpha - \beta, \quad \text{and} \quad \Delta_l = 0 \text{ for } l \in [n] \setminus \{i, j, k\}.$$

We see that $\mathbf{y} \in \mathcal{X}(n)$, and Taylor's expansion ((10), together with equation (23), gives

$$L_2(A, \mathbf{y}) - L_2(A, \mathbf{x}) = C_i\alpha + C_j\beta - C_k(\alpha + \beta) = 0;$$

thus $(A, \mathbf{y}) \in \mathcal{S}_n(c)$.

Also, Taylor's expansion (11), Lagrange's condition (12), and equation (23) give

$$\begin{aligned} L_r(A, \mathbf{y}) - L_r(A, \mathbf{x}) &= D_i\alpha + D_j\beta - D_k(\alpha + \beta) \\ &= \mu(\alpha + \beta - \alpha - \beta) + \lambda\left(\left(C_i - C_k\right)\alpha + \left(C_j - C_k\right)\beta\right) = 0; \end{aligned}$$

thus $L_r(A, \mathbf{y}) = \varphi_r(n, c)$. Since $\mathbf{y}$ has a zero entry, this equality contradicts Claim 2.5, completing the proof of Claim 2.10. □

The following technical claim is necessary for Claims 2.12 and 2.13

Claim 2.11 *G contains no three distinct vertices i,j,k such that $ij \in E(G)$, $ik \in E(\overline{G})$, $jk \in E(\overline{G})$, and $(C_i - C_k)(C_j - C_k) > 0$.*

Proof Assume for a contradiction that i,j,k are such vertices. By Claim 2.9, $(C_i - C_k) \neq 0$ and $(C_j - C_k) \neq 0$. Consider the hyperbola defined by

$$(C_i - C_k)\,x + (C_j - C_k)\,y = xy, \tag{24}$$

and write H for its branch that contains the origin. By Jordan's theorem, H intersects the triangle formed by the lines

$$x = -x_i, \quad y = -x_j, \quad x + y = x_k$$

at some point (α, β).

Let $\mathbf{y} = (x_1 + \Delta_1, \ldots, x_n + \Delta_n)$, where

$$\Delta_i = \alpha, \quad \Delta_j = \beta, \quad \Delta_k = -\alpha - \beta, \quad \text{and} \quad \Delta_l = 0 \text{ for } l \in [n] \setminus \{i,j,k\}.$$

We see that $\mathbf{y} \in \mathcal{X}(n)$, and Taylor's expansion (10), together with equation (24), gives

$$L_2(A, \mathbf{y}) - L_2(A, \mathbf{x}) = C_i\alpha + C_j\beta - C_k(\alpha + \beta) - \alpha\beta = 0;$$

thus $(A, \mathbf{y}) \in \mathcal{S}_n(c)$.

Also, Taylor's expansion (11), Lagrange's condition (12), and equation (24) give

$$\begin{aligned} L_r(A, \mathbf{y}) - L_r(A, \mathbf{x}) &= D_i\alpha + D_j\beta - D_k(\alpha + \beta) - D_{ij}\alpha\beta \\ &= \lambda\left(C_i\alpha + C_j\beta - C_k(\alpha + \beta)\right) - D_{ij}\alpha\beta \\ &= (\lambda - D_{ij})\,\alpha\beta. \end{aligned}$$

If $D_{ij} = \lambda$, then $L_r(A, \mathbf{y}) = L_r(A, \mathbf{x})$, contradicting Claim 2.5 since $\mathbf{y}$ has a zero entry. Hence, $(\lambda - D_{ij})\,\alpha\beta > 0$. By Claims 2.8 and 2.9 we know that $D_{ij} \leq \lambda$, and so, $\alpha\beta > 0$. In view of $(C_i - C_k)(C_j - C_k) > 0$, if a point (x,y) belongs to H, then $xy < 0$; hence $\alpha\beta < 0$, a contradiction completing the proof of Claim 2.11. $\square$

Claim 2.12 *The graph $\overline{G}$ has no vertex of degree 3 or higher.*

Proof Assume for a contradiction that i,j,k,l are distinct vertices such that $ij \in E(\overline{G})$, $ik \in E(\overline{G})$, and $il \in E(\overline{G})$. Since $\overline{G}$ is triangle-free, we see that $jk \in E(G)$, $kl \in E(G)$, and $lj \in E(G)$. Claim 2.7 implies that the values $(C_i - C_j)$, $(C_i - C_k)$, and $(C_i - C_l)$ are nonzero; since two of them have the same sign, by symmetry we suppose that $(C_i - C_j)(C_i - C_k) > 0$. We see that the existence of the vertices i,j,k contradicts Claim 2.11, completing the proof of Claim 2.12. $\square$

The next claim finishes the proof that G is a complete graph.

Claim 2.13 *$\overline{G}$ consists of isolated vertices.*

Proof Claim 2.12 implies that all components of $\overline{G}$ are paths, cycles, or isolated vertices. Note first that no component of $\overline{G}$ can be an isolated edge in $\overline{G}$. Indeed, if $ij \in E\left(\overline{G}\right)$ were such an edge, then i and j have the same neighbors in G, and so, $C_i = C_j$, contradicting Claim 2.7.

Next, assume that the path $1, \ldots, k$ is a component of $\overline{G}$ for some $k \geq 3$. In G vertex 1 is joined to every neighbor of vertex 2, and so, $C_1 > C_2$; likewise we find that $C_k > C_{k-1}$. Hence $C_{i-1} > C_i < C_{i+1}$ for some $1 < i < k$. Since $(C_{i-1} - C_i)(C_{i+1} - C_i) > 0$, the vertices $i-1, i, i+1$ form a configuration contradicting Claim 2.11.

Finally, assume that a cycle $1, \ldots, k$ is a component of $\overline{G}$ for some $k \geq 3$. Since $\overline{G}$ is triangle-free, we see that $k \geq 4$ and $ij \in E(G)$ whenever $|i-j| = 2 \mod k$. By symmetry we suppose that $C_2 = \max(C_1, \ldots, C_k)$. Since $\{1,2\} \in E\left(\overline{G}\right)$ and $\{2,3\} \in E\left(\overline{G}\right)$, by Claim 2.7, $C_1 < C_2$ and $C_3 < C_2$. Thus, $(C_i - C_2)(C_3 - C_2) > 0$ and the vertices $1, 2, 3$ form a configuration contradicting Claim 2.11 and completing the proof of Claim 2.13. □

2.2.2 Proof of $L_r(A, \mathbf{x}) = \varphi_r(c)$

We know now that G is a complete graph. We have to show that $n = \xi(c)$ and $(x_1, \ldots, x_n) = (x, \ldots, x, y)$, where x and y are given by (5). Our proof is based on the following assertion.

Claim 2.14 *Let $x_3 \geq x_2 \geq x_1 > 0$ be real numbers satisfying*

$$x_1 + x_2 + x_3 = a, \tag{25}$$

$$x_1 x_2 + x_2 x_3 + x_3 x_1 = b, \tag{26}$$

and let $x_1 x_2 x_3$ be minimum subject to (25) and (26). Then $x_2 = x_3$.

Proof First note that the hypothesis implies that

$$a^2/4 < b \leq a^2/3. \tag{27}$$

Indeed, the second of these inequalities follows from Maclaurin's inequality; assume for a contradiction that the first one fails. Then, selecting a sufficiently small $\varepsilon > 0$ and setting

$$y_1 = \varepsilon,\ y_2 = \frac{a - \varepsilon - \sqrt{(a+\varepsilon)^2 - 4(b+\varepsilon^2)}}{2},\ y_3 = \frac{a - \varepsilon + \sqrt{(a+\varepsilon)^2 - 4(b+\varepsilon^2)}}{2},$$

we see that y_1, y_2, y_3 satisfy (25), (26), and

$$y_1 y_2 y_3 = \varepsilon\left(b - a\varepsilon + \varepsilon^2\right) < \varepsilon b.$$

Thus, $\min x_1 x_2 x_3$, subject to (25) and (26), cannot be attained for positive x_1, x_2, x_3, a contradiction, completing the proof of (27).

By Lagrange's method there exist η and θ such that

$$\begin{aligned} x_1 x_2 &= \eta + \theta(x_1 + x_2) = \eta + \theta(a - x_3) \\ x_1 x_3 &= \eta + \theta(x_1 + x_3) = \eta + \theta(a - x_2) \\ x_2 x_3 &= \eta + \theta(x_2 + x_3) = \eta + \theta(a - x_1). \end{aligned}$$

If $\theta = 0$ we see that $x_1 = x_2 = x_3$, completing the proof. Suppose $\theta \neq 0$ and assume for a contradiction that $x_2 < x_3$. We find that

$$x_1 (x_3 - x_2) = \theta (x_3 - x_2),$$
$$x_2 (x_3 - x_1) = \theta (x_3 - x_1),$$

and so, $x_1 = x_2$. Solving the system (25,26) with $x_1 = x_2$, we obtain

$$x_3 = \frac{a}{3} + \frac{2}{3}\sqrt{a^2 - 3b}, \quad x_1 = x_2 = \frac{a}{3} - \frac{1}{3}\sqrt{a^2 - 3b},$$

implying that

$$x_1 x_2 x_3 = \left(\frac{a}{3} + \frac{2}{3}\sqrt{a^2 - 3b}\right)\left(\frac{a}{3} - \frac{1}{3}\sqrt{a^2 - 3b}\right)^2. \tag{28}$$

If $b = a^2/3$, we see that $x_1 = x_2 = x_3$, completing the proof, so suppose that $b < a^2/3$. We shall show that $\min x_1 x_2 x_3$, subject to (25) and (26), is smaller than the right-hand side of (28). Indeed, setting

$$y_1 = \frac{a}{3} - \frac{2}{3}\sqrt{a^2 - 3b}, \quad y_2 = y_3 = \frac{a}{3} + \frac{1}{3}\sqrt{a^2 - 3b},$$

in view of (27), we see that y_1, y_2, y_3 satisfy (25) and (26). After some algebra we obtain

$$y_1 y_2 y_3 - x_1 x_2 x_3 = -\frac{4}{27}\left(a^2 - 3b\right)^{3/2} < 0.$$

This contradiction completes the proof of Claim 2.14. $\square$

Claim 2.14 implies that, out of every three entries of $\mathbf{x}$, the two largest ones are equal; hence all but the smallest entry of $\mathbf{x}$ are equal. Writing y and x for the smallest and largest entries of $\mathbf{x}$, we see that x and y satisfy

$$\binom{n-1}{2} x^2 + nxy = c,$$
$$(n-1)\, x + y = 1,$$
$$y \leq x,$$

and so,

$$y = \frac{1}{n} - \sqrt{1 - 2\frac{n}{n-1}c}, \quad x = \frac{1}{n} + \frac{1}{n}\sqrt{1 - 2\frac{n}{n-1}c}.$$

Since the condition $1 - 2nc/(n-1) \geq 0$ gives

$$n \geq \frac{1}{1 - 2c},$$

and $y > 0$ gives

$$1 - 2c < \frac{1}{n} + \frac{1}{n^2} < \frac{1}{n-1},$$

we find that $n = \xi(c)$, completing the proof of Theorem 2.2. $\square$

2.2.3 Proof of Proposition 2.1

Suppose that $\mathcal{S}_n(c)$ is nonempty and that

$$A \in \mathcal{A}(n), \quad \mathbf{x} \geq 0, \quad L_1(A, \mathbf{x}) = 1, \quad \text{and} \quad L_2(A, \mathbf{x}) = c.$$

Then

$$c = \sum_{1 \leq i < j \leq n} a_{ij} x_i x_j \leq \sum_{1 \leq i < j \leq n} x_i x_j = \frac{1}{2} \left(\sum_i x_i \right)^2 - \frac{1}{2} \sum_i x_i^2 \leq \frac{n-1}{2n} < \frac{1}{2},$$

and so, $c < 1/2$ and $n \geq 1/(1-2c)$; thus $n \geq \lceil 1/(1-2c) \rceil$.

On the other hand, if $c < 1/2$ and $n \geq \lceil 1/(1-2c) \rceil$, let $A \in \mathcal{A}(n)$ be the matrix with all off-diagonal entries equal to 1, and let x, y satisfy

$$\binom{n-1}{2} x^2 + (n-1) xy = c,$$
$$(n-1) x + y = 1.$$

Writing $\mathbf{x}$ for the n-vector $(x, \ldots, x, y)$, we see that $L_1(A, \mathbf{x}) = 1$ and $L_2(A, \mathbf{x}) = c$; thus $\mathcal{S}_n(c)$ is nonempty, completing the proof. $\square$

2.3 Upper bounds on $k_r(n, m)$

In this section we prove Theorem 2.3. We start with some facts about Turán graphs.

The s-partite Turán graph $T_s(n)$ is a complete s-partite graph on n vertices with each vertex class of size $\lfloor n/s \rfloor$ or $\lceil n/s \rceil$. Setting $t_s(n) = e(T_s(n))$, after some algebra we obtain

$$t_s(n) = \frac{s-1}{2s} n^2 - \frac{t(s-t)}{2s},$$

where t is the remainder of n mod s; hence,

$$\frac{s-1}{2s} n^2 - \frac{s}{8} \leq t_s(n) \leq \frac{s-1}{2s} n^2. \tag{29}$$

It is known that the second one of these inequalities can be extended for all $2 \leq r \leq s$:

$$k_r(T_s(n)) \leq \binom{s}{r} \left(\frac{n}{s} \right)^r. \tag{30}$$

The Turán graphs play an exceptional role for the function $k_r(n, m)$: indeed, a result of Bollobás [2] implies that if G is a graph with n vertices and $t_s(n)$ edges, then $k_r(G) \geq k_r(T_s(n))$; hence,

Fact 2.15 $k_r(n, t_s(n)) = k_r(T_s(n))$. $\square$

Thus to simplify our presentation, we assume that $n \geq s \geq r \geq 3$ are fixed integers and m is an integer satisfying $t_{s-1}(n) < m \leq t_s(n)$.

First we define a class of graphs giving upper bounds on $k_r(n, m)$.

2.3.1 The graphs $H(n,m)$

We shall construct a graph $H(n,m)$ with n vertices and m edges, where n, s, and m satisfy $n \geq s \geq 3$ and $t_{s-1}(n) < m \leq t_s(n)$. Note that the construction of $H(n,m)$ is independent of r.

First we define a sequence of graphs $H_0, \ldots, H_{\lfloor n/s \rfloor}$ satisfying

$$t_{s-1}(n) = e(H_0) < e(H_1) < \cdots < e\left(H_{\lfloor n/s \rfloor}\right) = t_s(n), \tag{31}$$

and then we construct $H(n,m)$ using $H_0, \ldots, H_{\lfloor n/s \rfloor}$.

The graphs $H_0, \ldots, H_{\lfloor n/s \rfloor}$

For every $0 \leq i \leq \lfloor n/s \rfloor$, let H_i be the complete s-partite graph with vertex classes $I, V_1, \ldots, V_{s-1}$ such that $|I| = i$ and

$$\lfloor (n-i)/(s-1) \rfloor = |V_1| \leq \cdots \leq |V_{s-1}| = \lceil (n-i)/(s-1) \rceil.$$

Note that H_0 is the $(s-1)$-partite Turán graph $T_{s-1}(n)$, but it is convenient to consider it s-partite with an empty vertex class I. Note also that $H_{\lfloor n/s \rfloor} = T_s(n)$.

The transition from H_i to H_{i+1} can be briefly summarized as follows: select V_j with $|V_j| = \lceil (n-i)/(s-1) \rceil$ and move a vertex u from V_j to I.

In particular, we see that

$$e(H_{i+1}) - e(H_i) = \lceil (n-i)/(s-1) \rceil - i > 0,$$

implying in turn (31).

Constructing $H(n,m)$

Let $I, V_1, \ldots, V_{s-1}$ be the vertex classes of H_i. Select V_j with $|V_j| = \lceil (n-i)/(s-1) \rceil$, select a vertex $u \in |V_j|$, let $l = \lceil (n-i)/(s-1) \rceil - 1$, and suppose that $V_j \backslash \{u\} = \{v_1, \ldots, v_l\}$. Do the following steps:

(a) remove all edges joining u to vertices in I;

(b) move u from V_j to I, keeping all edges incident to u;

(c) for $m = e(H_i) + 1, \ldots, e(H_{i+1})$ join u to $v_{m-e(H_i)}$ and write $H(n,m)$ for the resulting graph.

Two observations are in place: first, $e(H(n,m)) = m$, and second, $H(n, e(H_i)) = H_i$ for every $i = 1, \ldots, \lfloor n/s \rfloor$.

Note also that every additional edge in step (c) increases the number of r-cliques by $k_{r-2}(H')$, where H' is the fixed graph induced by the set $[n] \backslash (I \cup V_j)$. We thus make the following

Claim 2.16 *The function $k_r(H(n,m))$ increases linearly in m for $e(H_{i-1}) \leq m \leq e(H_i)$.*

We need also the following upper bound on $k_r(H_i)$.

Claim 2.17

$$k_r(H_i) \leq \binom{s-1}{r-1}\left(\frac{n-i}{s-1}\right)^{r-1} i + \binom{s-1}{r}\left(\frac{n-i}{s-1}\right)^{r}$$

Proof Let $I, V_1, \ldots, V_{s-1}$ be the vertex classes of H_i. Since the sizes of the sets $V_1, \ldots, V_{s-1}$ differ by at most 1, we see that the set $V_1 \cup \ldots \cup V_{s-1}$ induces the Turán graph $T_{s-1}(n-i)$. Hence a straightforward counting gives

$$k_r(H_i) \leq k_{r-1}(T_{s-1}(n-i))\, i + k_r(T_{s-1}(n-i)),$$

and the claim follows from inequality (30). $\square$

2.3.2 Proof of Theorem 2.3

Assume that x is a real number satisfying

$$\frac{s-2}{2(s-1)}n^2 < x \leq \frac{s-1}{2s}n^2.$$

and define the functions $p = p(x)$ and $q = q(x)$ by

$$p \geq q, \tag{32}$$
$$(s-1)p + q = n, \tag{33}$$
$$\binom{s-1}{2}p^2 + (s-1)pq = x. \tag{34}$$

We note that

$$p(x) = \frac{1}{s}\left(n + \sqrt{n^2 - \frac{2s}{s-1}x}\right), \quad q(x) = \frac{1}{s}\left(n - (s-1)\sqrt{n^2 - \frac{2s}{s-1}x}\right).$$

Set

$$f(x) = \binom{s-1}{r}p^r + \binom{s-1}{r-1}p^{r-1}q, \tag{35}$$

and note that $f(x) = \varphi_r(x/n^2)\, n^r$; hence, to prove Theorem 2.3, it is enough to show that if

$$\frac{s-2}{2(s-1)}n^2 < m \leq \frac{s-1}{2s}n^2,$$

then

$$k_r(n, m) \leq f(m) + \frac{n^r}{n^2 - 2m}. \tag{36}$$

We first introduce the auxiliary function $\widehat{f}(x)$, defined for $x \in [t_{s-1}(n), t_s(n)]$ by

$$\widehat{f}(x) = \begin{cases} f\left(x + \frac{s-1}{8}\right), & \text{if } t_{s-1}(n) < x \leq \frac{s-1}{2s}n^2 - \frac{s-1}{8}; \\ f\left(\frac{s-1}{2s}n^2\right), & \text{if } \frac{s-1}{2s}n^2 - \frac{s-1}{8} < x \leq t_s(n). \end{cases}$$

To finish the proof of Theorem 2.3 we first show that

$$k_r(H(n,m)) \leq \widehat{f}(m), \tag{37}$$

and then derive (36) using Taylor's expansion and the fact that $k_r(n,m) \leq k_r(H(n,m))$.

Claim 2.18 *If* $m = e(H_i)$, *then*

$$k_r(H_i) \leq f\left(m - t_{s-1}(n-i) + \frac{s-2}{2(s-1)}(n-i)^2\right).$$

Proof Indeed, as mentioned above, the set $V_1 \cup \cdots \cup V_{s-1}$ induces a $T_{s-1}(n-i)$; hence,

$$i(n-i) + t_{s-1}(n-i) = m,$$

and so,

$$i(n-i) + \frac{s-1}{2s}(n-i)^2 = m - t_{s-1}(n-i) + \frac{s-1}{2s}(n-i)^2.$$

Set

$$m' = m - t_{s-1}(n-i) + \frac{s-1}{2s}(n-i)^2$$

and note that $i = q(m')$. In view of Claim 2.17, we obtain

$$k_r(H_i) \leq \binom{s-1}{r-1}\left(\frac{n-i}{s-1}\right)^{r-1} i + \binom{s-1}{r}\left(\frac{n-i}{s-1}\right)^r = f(m'),$$

completing the proof. □

Claim 2.19 $f'(x) = \binom{s-2}{r-2} p^{r-2}$.

Proof From (35) we have

$$f(x) = \binom{s-1}{r-1}\left(\frac{s-r}{r}p^r + p^{r-1}q\right),$$

and so,

$$f'(x) = \binom{s-1}{r-1}\left((s-r)p^{r-1}p' + (r-1)p^{r-2}qp' + p^{r-1}q'\right).$$

From (33) and (34) we have

$$(s-1)p' + q' = 0$$

and

$$(s-1)((s-2)pp' + p'q + pq') = (s-1)p'(q-p) = x' = 1.$$

Now the claim follows after simple algebra. □

We immediately see that $f(x)$ is increasing. Also, since $p(x)$ is decreasing, $f'(x)$ is decreasing too, implying that $f(x)$ is concave. This, in turn, implies that $\widehat{f}(x)$ is concave.

For every $i = 1, \ldots, \lfloor n/s \rfloor$, by Claim 2.18, we have

$$k_r(H_i) \leq f(m') \leq \widehat{f}(m),$$

and since, by Claim 2.16, $k_r(H(n,m))$ is linear for $m \in [e(H_i), e(H_{i+1})]$, inequality (37) follows.

To finish the proof of (36), note that by Taylor's formula, in view of the concavity of $f(x)$, we have

$$\begin{aligned}
\widehat{f}(m) &\leq f\left(m + \frac{s-1}{8}\right) \leq f(m) + \frac{s-1}{8} f'(m) = f(m) + \frac{s-1}{8}\binom{s-2}{r-2} p^{r-2} \\
&\leq f(m) + \frac{s-1}{8}\binom{s-2}{r-2}\left(\frac{n}{s-1}\right)^{r-2} < f(m) + sn^{r-2} \leq f(m) + \frac{n^r}{n^2 - 2m},
\end{aligned}$$

completing the proof of Theorem 2.3. □

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