

The clique density theorem

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Abstract

Turán's theorem is a cornerstone of extremal graph theory. It asserts that for any integer $r \geq 2$, every graph on n vertices with more than $\frac{r-2}{2(r-1)} \cdot n^2$ edges contains a clique of size r , i.e., r mutually adjacent vertices. The corresponding extremal graphs are balanced $(r-1)$ -partite graphs.

The question as to how many such r -cliques appear at least in any n -vertex graph with γn^2 edges has been intensively studied in the literature. In particular, Lovász and Simonovits conjectured in the 1970's that asymptotically the best possible lower bound is given by the complete multipartite graph with γn^2 edges in which all but one vertex class is of the same size while the remaining one may be smaller.

Their conjecture was recently resolved for $r = 3$ by Razborov and for $r = 4$ by Nikiforov. In this article, we prove the conjecture for all values of r .

1. Introduction

Extremal graph theory was initiated as a separate subarea of combinatorics by P. Turán in 1941. In his famous article [14] the following problem is solved: Given integers $n \geq r \geq 3$, what is the maximum number of edges that an n -vertex graph may have without containing a clique of size r , i.e., r vertices any two of which are connected by an edge. It turns out that there is a unique extremal graph for this problem, which is the complete $(r-1)$ -partite graph with the property that the sizes of any two of its vertex classes differ by at most one. In particular, if a graph with n vertices has more than $\frac{r-2}{2(r-1)} \cdot n^2$ edges, then it needs to contain an r -clique, and for fixed r , the constant $\frac{r-2}{2(r-1)}$ appearing in this statement is sharp.

Given this result, one may ask how many r -cliques are guaranteed to exist in graphs having more edges. That is, given an integer $r \geq 3$ and a real number number $\gamma > \frac{r-2}{2(r-1)}$ we want to know: what is the minimum number of r -cliques appearing in an n -vertex graph with at least γn^2 edges? Following the work [5], [8], [10], and [6], a general conjecture was formulated by Lovász and Simonovits in [7]. The guiding idea behind their conjecture is that, up to

some “rounding errors,” there should be for each such case an extremal graph that is again complete and multipartite. Moreover, all its vertex classes should be of the same size, except for one that may be smaller.

Now consider such an $(s+1)$ -partite graph, s of whose vertex classes have size $\frac{n(1+\alpha)}{s+1}$, so that the remaining class contains just $\frac{n(1-s\alpha)}{s+1}$ vertices, where $\alpha \in [0, \frac{1}{s}]$. A short calculation discloses that for $\gamma = \frac{s}{2(s+1)}(1-\alpha^2)$, this graph has γn^2 edges and that the number of its r -cliques is

$$\frac{1}{(s+1)^r} \binom{s+1}{r} (1+\alpha)^{r-1} (1-(r-1)\alpha) \cdot n^r.$$

We thus arrive at the following clique density conjecture due to Lovász and Simonovits.

CONJECTURE 1.1. *If $r \geq 3$ and $\gamma \in [0, \frac{1}{2})$, then every graph on n vertices with at least γn^2 edges contains at least*

$$\frac{1}{(s+1)^r} \binom{s+1}{r} (1+\alpha)^{r-1} (1-(r-1)\alpha) \cdot n^r$$

cliques of size r , where $s \geq 1$ is an integer with $\gamma \in [\frac{s-1}{2s}, \frac{s}{2(s+1)}]$ and $\alpha \in [0, \frac{1}{s}]$ is implicitly defined by $\gamma = \frac{s}{2(s+1)}(1-\alpha^2)$.

The aim of this article is to prove this conjecture.

Remark 1.2. (1) If $s \leq r-2$, then the binomial coefficient $\binom{s+1}{r}$ vanishes, which means that, in accordance with Turán’s construction, the clique density conjecture does not predict the existence of any r -cliques for $\gamma \leq \frac{r-2}{2(r-1)}$.

(2) If $r \geq 3$ and $\gamma > \frac{r-2}{2(r-1)}$ are fixed while n tends to infinity, the clique density conjecture guarantees, in particular, $\Omega_\gamma(n^r)$ many r -cliques. This phenomenon is known as “supersaturation” in the literature. Due to the above discussion it should be clear that the precise factor occurring in the clique density conjecture is optimal for fixed r and γ .

(3) If $\gamma \in [0, \frac{1}{2})$ is not of the form $\gamma = \frac{t}{2(t+1)}$ for some positive integer t , then there is a unique way of choosing the pair (s, α) as above. On the other hand, if $\gamma = \frac{t}{2(t+1)}$ has this form, there are two legitimate choices for this pair, namely $(t, 0)$ and $(t+1, \frac{1}{t+1})$. Yet it is not hard to verify that both of them lead to the same lower bound of

$$\frac{1}{(t+1)^r} \binom{t+1}{r} \cdot n^r$$

on the number of r -cliques.

We would like to conclude this introduction with some historical comments: Let G be any n -vertex graph with at least γn^2 edges. Goodman [5]

proved that G contains at least $\frac{1}{3}\gamma(4\gamma - 1)n^3$ triangles. This fact was also obtained by Nordhaus and Stewart [10]. Moon and Moser [8] proved that if $\gamma \geq \frac{1}{3}$, then G also contains at least

$$\frac{1}{12}\gamma(4\gamma - 1)(6\gamma - 2)n^4$$

cliques of size four and stated without proof that similarly, if $\gamma \geq \frac{r-2}{2(r-1)}$, then G contains at least

$$(1.1) \quad \frac{1}{r!} \cdot 2\gamma(4\gamma - 1)(6\gamma - 2) \cdot \dots \cdot (2(r-1)\gamma - (r-2)) \cdot n^r$$

cliques of size r . This estimate was subsequently shown by Kadziivanov and Nikiforov [6]. It may be observed that the factor appearing in front of n^r in (1.1) is a convex function of γ for $\gamma \geq \frac{r-2}{2(r-1)}$. We will return to this “convex bound” in Section 3. It is not hard to check that if $\gamma = \frac{t}{2(t+1)}$ with $t \geq r-2$ is one of the “critical” values from Remark 1.2(3), then the convex bound is optimal and yields the same prediction on the number of r -cliques in G as the clique density conjecture does. Between these critical values, however, the optimal bound is piecewise concave. (We will check this in Section 4.) Thus the piecewise linear function interpolating between these critical values should also be a lower bound on the number of r -cliques in G , and this has in fact been shown by Bollobás [1]. For an alternative proof of a more general result, we refer to [13].

The case $r = 3$ and $\gamma \in [\frac{1}{4}, \frac{1}{3}]$ of the clique density conjecture was studied by Fisher [3] (see also [4] and [2, Rem. 3.3]). An altogether different approach to this case has later been given by Razborov in the fifth section of [11]. The proof described there is based on what one might call the “differential calculus of flag algebra homomorphisms,” which in turn constitutes an important part of Razborov’s flag algebraic investigations. Shortly afterwards, Razborov [12] used this calculus for resolving the case $r = 3$ of Conjecture 1.1 for all γ .

The next important step is due to Nikiforov [9], who found an independent proof for the case $r = 3$ and settled the case $r = 4$ as well. In [9] Nikiforov suggests to study the clique density problem in the setting of “weighted graphs,” and we will follow this idea in the sequel. The problem thus translates into a question about polynomial forms, and we follow Nikiforov in applying differential techniques to these forms. Moreover, we use some of Razborov’s ideas in this framework.

2. Weighted graphs

Given a set X and a positive integer r , we use $X^{(r)}$ to denote the collection of all r -element subsets of X . Also, if n refers to a positive integer, then $[n]$ is, by definition, shorthand for $\{1, 2, \dots, n\}$. By a *weighted graph of order n* , we mean a pair consisting of a sequence (x_1, x_2, \dots, x_n) of n nonnegative real

numbers the sum of which is equal to 1 and a function $a: [n]^{(2)} \rightarrow [0, 1]$. In such situations, if $e = \{i, j\} \in [n]^{(2)}$, we will often write a_e or a_{ij} in place of $a(e)$.

Whenever \mathcal{G} is such a weighted graph of order n and r is a positive integer, we define the r -clique density of \mathcal{G} to be

$$\mathcal{G}(K_r) = \sum_{M \in [n]^{(r)}} \prod_{e \in M^{(2)}} a_e \prod_{i \in M} x_i.$$

Notice, for instance, that

$$\mathcal{G}(K_1) = x_1 + x_2 + \dots + x_n = 1.$$

The following weighted variant of Conjecture 1.1 is, as we are soon going to see, equivalent to it. To the best of our knowledge, it has for the first time been formulated explicitly by Nikiforov [9].

CLAIM 2.1. *Let $r \geq 3$ denote an integer, and let \mathcal{G} be a weighted graph. Suppose that a positive integer s and a real number $\alpha \in [0, \frac{1}{s}]$ are chosen in such a way that $\mathcal{G}(K_2) = \frac{s}{2(s+1)}(1 - \alpha^2)$. Then*

$$\mathcal{G}(K_r) \geq \frac{1}{(s+1)^r} \binom{s+1}{r} (1 + \alpha)^{r-1} (1 - (r-1)\alpha).$$

To see that this indeed entails Conjecture 1.1, take a graph G and an integer $r \geq 3$, label the vertices of G arbitrarily as $\{v_1, v_2, \dots, v_n\}$, and construct a weighted graph \mathcal{G} of order n by the stipulations $x_1 = x_2 = \dots = x_n = \frac{1}{n}$ and

$$a_{ij} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are joined by an edge of } G, \\ 0 & \text{otherwise} \end{cases}$$

for all $\{i, j\} \in [n]^{(2)}$. Plainly G has exactly $\mathcal{G}(K_2) \cdot n^2$ edges and $\mathcal{G}(K_r) \cdot n^r$ cliques of size r , which proves the desired estimate.

As we shall not need the converse direction, we only give a sketch of its proof. Let a weighted graph \mathcal{G} of order n specified by the sequence (x_1, \dots, x_n) of n real numbers and by the function $a: [n]^{(2)} \rightarrow [0, 1]$ be given. Consider a large integer k and form a graph H whose vertices fall into n independent classes V_1, V_2, \dots, V_n whose sizes are approximately kx_1, kx_2, \dots, kx_n respectively, and in which for each unordered pair $\{i, j\} \in [n]^{(2)}$, roughly a proportion of a_{ij} among all possible edges from V_i to V_j is present in a sufficiently random way. Such a graph H can, in particular, be arranged to have k vertices, $\mathcal{G}(K_2) \cdot k^2 \pm O(k)$ edges and $\mathcal{G}(K_r) \cdot k^r \pm O(k^{r-1})$ cliques of size r , so letting k tend to infinity we may in fact derive Claim 2.1 from Conjecture 1.1.

Throughout the rest of this article, we follow Nikiforov’s suggestion [9] to think about the clique density problem in terms of weighted graphs.

3. The convex lower bound

In this section we discuss an analogue of the convex bound (1.1) adapted to the setting of weighted graphs. The proof we describe is essentially the same as that given by Kadžiivanov and Nikiforov in [6]. Nevertheless it might be helpful to include full details here, because the second step of the proof of the clique density theorem to be given in Section 5 will involve some similar calculations.

Moreover, our proof of the clique density theorem uses the convex bound in two quite different ways. First, it implies that the clique density theorem holds for the critical values $\gamma = \frac{t}{2(t+1)}$, where t is some positive integer, while our approach to Claim 2.1 cannot deal with these values due to nondifferentiability issues. Second, it is going to be helpful later on to have some “approximate version” of the clique density theorem available.

PROPOSITION 3.1. *Given a weighted graph \mathcal{G} and an integer $r \geq 2$ such that the quantity $\gamma = \mathcal{G}(K_2)$ is not smaller than $\frac{r-2}{2(r-1)}$, we have*

$$\mathcal{G}(K_r) \geq \frac{1}{r!} \cdot 2\gamma(4\gamma - 1)(6\gamma - 2) \cdot \dots \cdot (2(r - 1)\gamma - (r - 2)).$$

Proof. Clearly this follows by means of an easy induction on r from the following statement:

(*) *If a weighted graph \mathcal{G} satisfies $\gamma = \mathcal{G}(K_2) \geq \frac{r-2}{2(r-1)}$ for some $r \geq 2$, then*

$$\mathcal{G}(K_r) \geq \frac{2(r - 1)\gamma - (r - 2)}{r} \cdot \mathcal{G}(K_{r-1}) \quad \text{and} \quad \mathcal{G}(K_{r-1}) > 0.$$

Thus it suffices to verify (*) instead, and this will again be done by induction on r . The base case $r = 2$ is obvious in view of $\mathcal{G}(K_1) = 1$. So suppose now that \mathcal{G} is a weighted graph satisfying $\gamma = \mathcal{G}(K_2) \geq \frac{r-1}{2r} > \frac{r-2}{2(r-1)}$ for some $r \geq 2$ and that

$$r \cdot \mathcal{G}(K_r) \geq (2(r - 1)\gamma - (r - 2)) \cdot \mathcal{G}(K_{r-1}) \quad \text{as well as} \quad \mathcal{G}(K_{r-1}) > 0$$

hold. For the induction step, we remark that these assumptions trivially entail $\mathcal{G}(K_r) > 0$, so that it only remains to estimate $\mathcal{G}(K_{r+1})$ from below. Let n denote the order of \mathcal{G} , and suppose that \mathcal{G} is given by the sequence (x_1, x_2, \dots, x_n) of n real numbers and by the function $a: [n]^{(2)} \rightarrow [0, 1]$.

For each $M \subseteq [n]$, we write

$$A_M = \prod_{e \in M^{(2)}} a_e \quad \text{and} \quad X_M = \prod_{i \in M} x_i.$$

Now consider any $M \in [n]^{(r+1)}$, and define

$$B_M = \sum_{e \in M^{(2)}} \prod_{f \in M^{(2)} - \{e\}} a_f$$

as well as

$$C_M = \sum_{N \in M^{(r)}} A_N.$$

We claim that these expressions satisfy

$$(3.1) \quad 2B_M - C_M \leq (r^2 - 1)A_M.$$

To see this, we note that this inequality is linear in each of its variables a_e with $e \in M^{(2)}$, which entails that we only need to look at the case where $a_e \in \{0, 1\}$ holds for all $e \in M^{(2)}$. Now if additionally the number

$$K = \# \{e \in M^{(2)} \mid a_e = 0\}$$

is at least 2, then $A_M = B_M = 0$, and $C_M \geq 0$; if $K = 1$, then $A_M = 0$, $B_M = 1$, $C_M = 2$; and finally if $K = 0$, then $A_M = 1$, $B_M = \frac{1}{2}r(r + 1)$, and $C_M = r + 1$. This completes the proof of (3.1).

Multiplying this estimate by X_M and summing over all possibilities for M , we infer

$$(3.2) \quad \sum_{M \in [n]^{(r+1)}} (2B_M - C_M)X_M \leq (r^2 - 1)\mathcal{G}(K_{r+1}).$$

Setting

$$\eta_L = \sum_{i \in [n] - L} x_i \prod_{\ell \in L} a_{i\ell}$$

for all $L \in [n]^{(r-1)}$, we shall now investigate the sum

$$\Omega = \sum_{L \in [n]^{(r-1)}} A_L X_L \eta_L^2.$$

Expanding the squares, we get several “quadratic terms” in which some x_i^2 appears as a factor and some “mixed terms” for which this is not the case. Let Ω_{sq} and Ω_{mix} denote the corresponding sums. In view of the inequality $a_e^2 \leq a_e$, which is valid for all $e \in [n]^{(2)}$, we may estimate

$$\begin{aligned} \Omega_{\text{sq}} &\leq \sum_{L \in [n]^{(r-1)}} A_L X_L \sum_{i \in [n] - L} x_i^2 \prod_{\ell \in L} a_{i\ell} = \sum_{Q \in [n]^{(r)}} A_Q X_Q \sum_{i \in Q} x_i \\ &= \sum_{Q \in [n]^{(r)}} A_Q X_Q \left(1 - \sum_{i \in [n] - Q} x_i\right) = \mathcal{G}(K_r) - \sum_{M \in [n]^{(r+1)}} C_M X_M. \end{aligned}$$

Moreover, we have

$$\Omega_{\text{mix}} = 2 \sum_{M \in [n]^{(r+1)}} B_M X_M,$$

whence

$$\Omega = \Omega_{\text{sq}} + \Omega_{\text{mix}} \leq \mathcal{G}(K_r) + \sum_{M \in [n]^{\binom{r+1}{2}}} (2B_M - C_M)X_M.$$

In combination with (3.2) this yields

$$\Omega \leq \mathcal{G}(K_r) + (r^2 - 1)\mathcal{G}(K_{r+1}).$$

On the other hand, we get a lower bound on Ω from the Cauchy-Schwarz inequality,

$$\left(\sum_{L \in [n]^{\binom{r-1}{2}}} A_L X_L \eta_L \right)^2 \leq \sum_{L \in [n]^{\binom{r-1}{2}}} A_L X_L \cdot \sum_{L \in [n]^{\binom{r-1}{2}}} A_L X_L \eta_L^2,$$

where

$$\sum_{L \in [n]^{\binom{r-1}{2}}} A_L X_L \eta_L = r \sum_{Q \in [n]^{\binom{r}{2}}} A_Q X_Q = r \cdot \mathcal{G}(K_r)$$

and

$$\sum_{L \in [n]^{\binom{r-1}{2}}} A_L X_L = \mathcal{G}(K_{r-1}).$$

So altogether we have

$$r^2 \mathcal{G}(K_r)^2 \leq \mathcal{G}(K_{r-1}) (\mathcal{G}(K_r) + (r^2 - 1)\mathcal{G}(K_{r+1})).$$

Invoking now the induction hypothesis, we obtain, after a permissible cancellation of $\mathcal{G}(K_{r-1})$, that

$$(2(r - 1)r\gamma - r(r - 2))\mathcal{G}(K_r) \leq \mathcal{G}(K_r) + (r^2 - 1)\mathcal{G}(K_{r+1}),$$

and hence indeed

$$(2r\gamma - (r - 1))\mathcal{G}(K_r) \leq (r + 1)\mathcal{G}(K_{r+1}),$$

which completes the induction step. This finally proves (*) and thus the proposition. □

We would now like to make those consequences of Proposition 3.1 explicit that we shall really utilise in the sequel. The following corollary is a slight modification of inequality (25) from [6].

COROLLARY 3.2. *Suppose that r and s are integers satisfying $r \geq 2$ and $s \geq r - 1$. Then for every weighted graph \mathcal{G} satisfying $\gamma = \mathcal{G}(K_2) > \frac{s-1}{2s}$, one has*

$$\mathcal{G}(K_r) > \frac{1}{s} \cdot \binom{s}{r} \cdot \left(\frac{2\gamma}{s-1} \right)^{r-1}.$$

Proof. Clearly $\frac{s-1}{2s} \geq \frac{r-2}{2(r-1)}$, wherefore Proposition 3.1 tells us

$$\mathcal{G}(K_r) \geq \frac{1}{r!} \cdot 2\gamma(4\gamma - 1)(6\gamma - 2) \cdot \dots \cdot (2(r - 1)\gamma - (r - 2)).$$

Now for each $i \in \{1, 2, \dots, r - 1\}$, we have

$$2i\gamma - (i - 1) > 2\gamma \left(i - \frac{s(i - 1)}{s - 1} \right) = \frac{2\gamma(s - i)}{s - 1} \geq 0$$

and hence

$$\mathcal{G}(K_r) > \left(\frac{2\gamma}{s - 1} \right)^{r-1} \cdot \frac{(s - 1) \cdot \dots \cdot (s - r + 1)}{r!} = \frac{1}{s} \cdot \binom{s}{r} \cdot \left(\frac{2\gamma}{s - 1} \right)^{r-1}. \quad \square$$

COROLLARY 3.3. *Under the additional assumption $\alpha \in \{0, \frac{1}{s}\}$, Claim 2.1 holds.*

Proof. We have already seen in the introduction that we have $\gamma = \frac{t}{2(t+1)}$ for some nonnegative integer t in these cases. If $t \leq r - 2$, then our claim is obvious, so we may suppose $t \geq r - 1$ from now on. Now γ is large enough for Proposition 3.1 to be applicable, and the desired result follows. \square

4. Some analytical preparations

This section provides a thorough analysis of the function occurring in Claim 2.1. It also includes some further technical results that we will need in the next section for the proof of the clique density theorem.

Throughout the present section, we fix two integers $r \geq 3$ and $s \geq r - 1$ as well as a real number $M \geq 1$ satisfying

$$(4.1) \quad \left(\frac{s - 1}{s} \right)^{r-2} > \frac{s - r + 1}{s - 1} \cdot M^{r-2}.$$

Define the function $F_r: [0, \frac{1}{2}] \rightarrow [0, \frac{1}{r!}]$ as follows: given $\gamma \in [0, \frac{1}{2}]$, choose the unique positive integer t for which $\gamma \in [\frac{t-1}{2t}, \frac{t}{2(t+1)})$ is true, determine the real number $\alpha \in (0, \frac{1}{t}]$ solving the equation $\gamma = \frac{t}{2(t+1)}(1 - \alpha^2)$, and set

$$F_r(\gamma) = \frac{1}{(t + 1)^r} \binom{t + 1}{r} (1 + \alpha)^{r-1} (1 - (r - 1)\alpha).$$

In particular, we have

$$(4.2) \quad F_r \left(\frac{t - 1}{2t} \right) = \frac{1}{t^r} \binom{t}{r}$$

for every positive integer t .

In terms of this function, the statement of Claim 2.1 can be shortened to the inequality $\mathcal{G}(K_r) \geq F_r(\mathcal{G}(K_2))$, which is allegedly valid for all weighted graphs \mathcal{G} . We have more or less already seen earlier that F_r is continuous and

clearly it is piecewise differentiable as well. Moreover, F_r vanishes identically on the interval $[0, \frac{r-2}{2(r-1)}]$. If $\gamma \in (\frac{t-1}{2t}, \frac{t}{2(t+1)})$ holds for some integer $t \geq r-1$, then differentiating the equation locally defining $F_r(\gamma)$ with respect to α , we infer

$$-\frac{t\alpha}{t+1} \cdot F'_r(\gamma) = -\frac{(r-1)r}{(t+1)^r} \binom{t+1}{r} \alpha(1+\alpha)^{r-2}.$$

As $\alpha > 0$, it follows that

$$(4.3) \quad F'_r(\gamma) = \frac{(r-1)r}{t(t+1)^{r-1}} \binom{t+1}{r} (1+\alpha)^{r-2} > 0.$$

Thus F_r is strictly increasing on the interval $[\frac{r-2}{2(r-1)}, \frac{1}{2})$ and, as

$$\lim_{\gamma \rightarrow 1/2} F_r(\gamma) = \lim_{t \rightarrow \infty} \frac{1}{(t+1)^r} \binom{t+1}{r} = \frac{1}{r!},$$

it possesses an inverse

$$F_r^{-1}: [0, \frac{1}{r!}) \longrightarrow [\frac{r-2}{2(r-1)}, \frac{1}{2}).$$

Moreover, the above expression for $F'_r(\gamma)$ decreases as α decreases, whence F_r is in an obvious sense piecewise concave. Notice that the identity function F_2 on $[0, \frac{1}{2})$ has essentially the same properties as F_r . This concludes our discussion of the most elementary properties of these functions.

Next we propose to look at the function

$$H: [\frac{r-2}{r-1} \cdot M, M] \longrightarrow \mathbb{R}_0^+$$

given by

$$\eta \longmapsto \frac{1}{s^{r-1}} \binom{s}{r-1} \cdot \frac{(r-1)\eta - (r-2)M}{\eta^{r-1}}.$$

CLAIM 4.1. *The function H is strictly increasing and satisfies*

$$F_{r-1} \left(\frac{s-2}{2(s-1)} \right) < H(M) \leq F_{r-1} \left(\frac{s-1}{2s} \right).$$

Proof. If $\eta \in [\frac{r-2}{r-1} \cdot M, M)$, then

$$H'(\eta) = \frac{(r-2)(r-1)}{s^{r-1}} \binom{s}{r-1} \cdot \frac{M-\eta}{\eta^r} > 0,$$

which entails the first part of our claim. Furthermore, by (4.1) we have

$$H(M) = \frac{1}{s^{r-1}} \binom{s}{r-1} \cdot \frac{1}{M^{r-2}} > \frac{s-r+1}{s(s-1)^{r-1}} \binom{s}{r-1} = \frac{1}{(s-1)^{r-1}} \binom{s-1}{r-1},$$

i.e.,

$$H(M) > F_{r-1} \left(\frac{s-2}{2(s-1)} \right).$$

Finally, using $M \geq 1$, we get

$$H(M) = \frac{1}{s^{r-1}} \binom{s}{r-1} \cdot \frac{1}{M^{r-2}} \leq \frac{1}{s^{r-1}} \binom{s}{r-1} = F_{r-1} \left(\frac{s-1}{2s} \right). \quad \square$$

Notice, in particular, that the composition $F_{r-1}^{-1} \circ H$ is defined everywhere on the interval $\left[\frac{r-2}{r-1} \cdot M, M \right]$ and that its range is contained in $\left[\frac{r-3}{2(r-2)}, \frac{s-1}{2s} \right]$, which in turn is included in $\left[0, \frac{1}{2} \right]$. For $t \in \{r-2, r-1, \dots, s-1\}$, there exists a unique real number $\vartheta_t \in \left[\frac{r-2}{r-1} \cdot M, M \right]$ satisfying $H(\vartheta_t) = F_{r-1} \left(\frac{t-1}{2t} \right)$. The number ϑ_{s-1} will play a special role later, and sometimes it will just be denoted by ϑ . Evidently one has

$$\frac{r-2}{r-1} \cdot M = \vartheta_{r-2} < \vartheta_{r-1} < \dots < \vartheta_{s-1} = \vartheta < M.$$

Furthermore, (4.2) leads to

$$(4.4) \quad H(\vartheta_t) = \frac{1}{t^{r-1}} \binom{t}{r-1}$$

for any $t \in \{r-2, r-1, \dots, s-1\}$. In particular, for $t = s-1$, we get

$$(4.5) \quad \vartheta^{r-1} = \left(\frac{s-1}{s} \right)^{r-1} \cdot \frac{s}{s-r+1} \cdot ((r-1)\vartheta - (r-2)M)$$

due to the definition of H .

Later on we shall need some estimates concerning these numbers ϑ_t .

CLAIM 4.2. *If the integer t belongs to the interval $[r-2, s-2]$, then $\vartheta_t \leq \frac{t}{t+1} \cdot M$. In addition, we have $\vartheta \geq \frac{s-1}{s} \cdot M$.*

Proof. Whenever $t \in [r-2, s-2]$ is an integer, we have $H(\vartheta_{t+1}) \leq H(M)$. Owing to (4.4) and the definition of H this yields

$$\frac{1}{(t+1)^{r-1}} \binom{t+1}{r-1} \leq \frac{1}{s^{r-1}} \binom{s}{r-1} \frac{1}{M^{r-2}}.$$

Multiplying this by $(t-r+2)(t+1)^{r-2}/t^{r-1}$ we infer $H(\vartheta_t) \leq H\left(\frac{t}{t+1} \cdot M\right)$, thus proving the first part of our claim. Similarly but more easily, we deduce from $M \geq 1$ that $H\left(\frac{s-1}{s} \cdot M\right) \leq H(\vartheta)$, which leads to the second part of the claim. □

CLAIM 4.3. *If $\eta \in \left[\frac{r-2}{r-1} \cdot M, M \right]$ and $\nu = (F_{r-1}^{-1} \circ H)(\eta)$, then the function*

$$Q: [0, \nu] \longrightarrow \mathbb{R}$$

defined by

$$\delta \longmapsto (r-1) \binom{s}{r-1} \delta - s^{r-1} \eta^{r-2} F_r(\delta)$$

attains its global maximum at $\delta = \nu$.

Proof. Choose an integer $t \in [r-2, s-1]$ as well as a real number $\beta \in [0, \frac{1}{t}]$ such that $\nu = \frac{t}{2(t+1)}(1 - \beta^2)$. Since Q is piecewise convex and convex functions attain their global maxima at boundary values, it suffices to establish the following two statements:

- (A) the function Q is increasing on $[\frac{t-1}{2t}, \nu]$;
- (B) if $d \in [t-1]$, then $Q(\frac{d-1}{2d}) \leq Q(\frac{t-1}{2t})$.

For the proofs of both of these subclaims, we use

$$(C) M^{r-2} \cdot \frac{1}{t^{r-1}} \binom{t}{r-1} \leq \frac{1}{s^{r-1}} \binom{s}{r-1},$$

which is an obvious consequence of $H(\vartheta_t) \leq H(M)$.

Now, to verify (A), take any $\delta \in (\frac{t-1}{2t}, \nu)$ and write $\delta = \frac{t}{2(t+1)}(1 - \alpha^2)$, where $\alpha \in (\beta, \frac{1}{t})$. Multiplying (C) by $(r-1)s^{r-1}$ one obtains

$$s^{r-1} M^{r-2} \frac{(r-1)r}{t(t+1)^{r-1}} \binom{t+1}{r} \left(\frac{t+1}{t}\right)^{r-2} \leq (r-1) \binom{s}{r-1}.$$

In view of $\eta \leq M$ and $\alpha \leq \frac{1}{t}$ this implies

$$s^{r-1} \eta^{r-2} F'_r(\delta) \leq (r-1) \binom{s}{r-1},$$

whence $Q'(\delta) \geq 0$. Thereby we have proved assertion (A).

Let us now turn our attention to (B). If $t \leq r-1$, then F_r vanishes at all relevant numbers and our claim is obvious. So henceforth we may suppose $t \geq r$ and for similar reasons $d \geq r-1$ as well. The function

$$\Phi: \left[\frac{1}{t}, \frac{1}{r-1}\right] \longrightarrow [0, 1]$$

defined by

$$x \longmapsto (1-x)(1-2x) \cdots (1-(r-1)x)$$

is obviously convex, wherefore

$$\frac{\Phi\left(\frac{1}{t}\right) - \Phi\left(\frac{1}{d}\right)}{\frac{1}{d} - \frac{1}{t}} \leq -\Phi'\left(\frac{1}{t}\right).$$

Since

$$-\Phi'\left(\frac{1}{t}\right) = \left\{ \frac{t}{t-1} + \frac{2t}{t-2} + \cdots + \frac{(r-1)t}{t-r+1} \right\} \Phi\left(\frac{1}{t}\right) \leq \frac{(r-1)rt}{2(t-r+1)} \Phi\left(\frac{1}{t}\right),$$

it follows that

$$\begin{aligned} \frac{1}{t^r} \binom{t}{r} - \frac{1}{d^r} \binom{d}{r} &\leq \left(\frac{1}{d} - \frac{1}{t}\right) \frac{(r-1)r}{2(t-r+1)} \cdot \frac{1}{t^{r-1}} \binom{t}{r} \\ &= (r-1) \left(\frac{t-1}{2t} - \frac{d-1}{2d}\right) \cdot \frac{1}{t^{r-1}} \binom{t}{r-1}. \end{aligned}$$

Multiplying this by

$$s^{r-1}\eta^{r-2} \cdot \frac{1}{t^{r-1}} \binom{t}{r-1} \leq \binom{s}{r-1},$$

which in view of $\eta \leq M$ is a consequence of (C), we deduce

$$s^{r-1}\eta^{r-2} \left\{ \frac{1}{t^r} \binom{t}{r} - \frac{1}{d^r} \binom{d}{r} \right\} \leq (r-1) \binom{s}{r-1} \left(\frac{t-1}{2t} - \frac{d-1}{2d} \right),$$

which is easily seen to be equivalent to (B). □

The following result will only be used for $k = 2$ and $k = r$, but the general case is not really harder.

CLAIM 4.4. *For each integer $k \geq 2$, the function*

$$J_k : \left[\frac{r-2}{r-1} \cdot M, M \right] \rightarrow \mathbb{R}$$

defined by

$$\eta \mapsto \eta^k (F_k \circ F_{r-1}^{-1} \circ H)(\eta)$$

is concave or convex on the intervals $[\vartheta_t, \vartheta_{t+1}]$, where $t \in \{r-2, r-1, \dots, s-2\}$, and $[\vartheta, M]$, depending on whether $k \geq r-1$ or $k \leq r-1$.

Proof. Treating both cases for k at the same time, we select any $t \in \{r-2, r-1, \dots, s-1\}$ and intend to verify that the second derivative of J_k has the expected sign on $(\vartheta_t, \vartheta_{t+1})$, where for convenience $\vartheta_s = M$. Utilising that $x \mapsto \frac{2x-1}{x^2}$ is strictly increasing on $(0, 1)$ we may define a function

$$S : (\vartheta_t, \vartheta_{t+1}) \rightarrow \left(\frac{t}{t+1}, 1 \right)$$

such that

$$(F_{r-1}^{-1} \circ H)(\eta) = \frac{t}{2(t+1)} \cdot \frac{2S(\eta) - 1}{S(\eta)^2}$$

holds for all $\eta \in (\vartheta_t, \vartheta_{t+1})$. Since the right-hand side may be rewritten as

$$\frac{t}{2(t+1)} \times \left\{ 1 - \left(\frac{1}{S(\eta)} - 1 \right)^2 \right\},$$

we have

$$\frac{1}{s^{r-1}} \binom{s}{r-1} \frac{(r-1)\eta - (r-2)M}{\eta^{r-1}} = \frac{1}{(t+1)^{r-1}} \binom{t+1}{r-1} \frac{(r-1)S(\eta) - (r-2)}{S(\eta)^{r-1}}.$$

Differentiating with respect to η and dividing by $(r-2)(r-1)$, we find

$$\frac{1}{s^{r-1}} \binom{s}{r-1} \cdot \frac{M - \eta}{\eta^r} = \frac{1}{(t+1)^{r-1}} \binom{t+1}{r-1} \cdot \frac{1 - S(\eta)}{S(\eta)^r} \cdot S'(\eta),$$

and the combination of both equations yields

$$S'(\eta) = \frac{S(\eta)(M - \eta) [(r-1)S(\eta) - (r-2)]}{\eta(1 - S(\eta)) [(r-1)\eta - (r-2)M]}.$$

Furthermore,

$$J_k(\eta) = \frac{1}{(t+1)^k} \binom{t+1}{k} \cdot \frac{kS(\eta) - (k-1)}{S(\eta)^k} \cdot \eta^k.$$

Differentiating and using the above formula for $S'(\eta)$, we get

$$J'_k(\eta) = \frac{1}{(t+1)^k} \binom{t+1}{k} \frac{k\eta^{k-1} [(r-1)S(\eta)\eta - (k-1)\eta + (k-r+1)S(\eta)M]}{S(\eta)^k [(r-1)\eta - (r-2)M]}.$$

A repetition of this argument leads to

$$J''_k(\eta) = \frac{1}{(t+1)^k} \binom{t+1}{k} \cdot \frac{k(k-1)(r-k-1)\eta^{k-2} [S(\eta)M - \eta]^2}{S(\eta)^k (1 - S(\eta)) [(r-1)\eta - (r-2)M]^2},$$

which entails the desired conclusion in view of the presence of the factor $r-k-1$ in the numerator. □

CLAIM 4.5. For each $\eta \in [\frac{r-2}{r-1} \cdot M, M]$, the difference

$$(r-1) \binom{s}{r-1} \eta^2 \nu - s^{r-1} \eta^r F_r(\nu)$$

is at most

$$\frac{r-2}{(s-1)(s+1)} \binom{s+1}{r} \cdot \left(\frac{1}{2}(r-1)s\vartheta^2 - (r-1)s\vartheta M + r(s-1)M\eta \right),$$

where $\nu = (F_{r-1}^{-1} \circ H)(\eta)$.

Proof. The difference under consideration, which we shall denote by $T(\eta)$ in the sequel, rewrites in the notation of Claim 4.4 as

$$T(\eta) = (r-1) \binom{s}{r-1} J_2(\eta) - s^{r-1} J_k(\eta).$$

In the special case $\eta = \vartheta$ we have $\nu = \frac{s-2}{2(s-1)}$ due to the definition of η , and using (4.5) and (4.2) it is not hard to check that we have equality in the inequality we seek to establish. Moreover, Claim 4.4 shows that T is piecewise convex as a function of η .

For these reasons it suffices to prove the statements

- (A) if $r-2 \leq t \leq s-2$, then $\lim_{\eta \rightarrow \vartheta_t^+} T'(\eta) \geq (r-2) \binom{s}{r-1} M$;
- (B) and $\lim_{\eta \rightarrow M^-} T'(\eta) \leq (r-2) \binom{s}{r-1} M$,

where the superscripted plus or minus signs below the limit are intended to signify that η is supposed to approach the boundary value in question from the right or from the left, respectively. Throughout the computations that follow we use the function S as well as the formulae for $J'(\eta)$ corresponding to $k = 2$ and $k = r$ from the foregoing proof.

To verify (A), we distinguish two cases.

First Case: $t = r - 2$. Note that the hypothesis of (A) yields $s \geq r$, wherefore $H(\vartheta_{r-1}) \leq H(M)$, i.e.,

$$\frac{1}{(r-1)^{r-1}} \leq \frac{1}{s^{r-1}} \binom{s}{r-1} \cdot \frac{1}{M^{r-2}}.$$

Now let $\eta \in (\vartheta_{r-2}, \vartheta_{r-1})$ be arbitrary. Then

$$\frac{(r-1)S(\eta) - (r-2)}{(r-1)^{r-1} \cdot S(\eta)^{r-1}} \leq \frac{1}{s^{r-1}} \binom{s}{r-1} \frac{(r-1)S(\eta) - (r-2)}{S(\eta)^{r-1} \cdot M^{r-2}},$$

which by the definition of S and H yields $H(\eta) \leq H(S(\eta)M)$, and thus $\eta \leq S(\eta)M$. Also, $\eta \in (\frac{r-2}{r-1} \cdot M, M)$ gives

$$\eta \geq (r-1)\eta - (r-2)M > 0,$$

which by $S(\eta) \leq 1$ may be weakened to

$$\eta \geq S(\eta)((r-1)\eta - (r-2)M).$$

Consequently

$$\eta(S(\eta)M - \eta) \geq S(\eta)(S(\eta)M - \eta)((r-1)\eta - (r-2)M),$$

i.e.,

$$\eta[(r-1)S(\eta)\eta - \eta - (r-3)S(\eta)M] \geq MS(\eta)^2[(r-1)\eta - (r-2)M].$$

Multiplying this by $(r-2)\binom{s}{r-1}S(\eta)^{-2}[(r-1)\eta - (r-2)M]^{-1}$ we infer

$$T'(\eta) \geq (r-2)\binom{s}{r-1}M,$$

as required.

Second Case: $r - 1 \leq t \leq s - 2$. Notice that Claim 4.2 entails

$$(r-2)(M - \vartheta_t)(M - \frac{t+1}{t}\vartheta_t) \geq 0,$$

whence

$$\vartheta_t \left[(r-2 - \frac{1}{t})\vartheta_t - (r-3)M \right] \geq \left(M - \frac{1}{t}\vartheta_t \right) \left[(r-1)\vartheta_t - (r-2)M \right].$$

By $t > r - 2$ the second factor on the right-hand side is positive, wherefore

$$\vartheta_t \cdot \frac{(r-2 - \frac{1}{t})\vartheta_t - (r-3)M}{(r-1)\vartheta_t - (r-2)M} \geq M - \frac{1}{t}\vartheta_t.$$

Multiplying by $(r-1)$ and subtracting $M - \frac{r-1}{t}\vartheta_t$ we obtain

$$(r-1)\vartheta_t \cdot \frac{(r-2 - \frac{1}{t})\vartheta_t - (r-3)M}{(r-1)\vartheta_t - (r-2)M} - \left(M - \frac{r-1}{t}\vartheta_t \right) \geq (r-2)M.$$

If we now multiply by $\binom{s}{r-1}$ and use

$$\lim_{\eta \rightarrow \vartheta_t^+} S(\eta) = \frac{t}{t+1}$$

as well as the definition of ϑ_t , we get indeed

$$\lim_{\eta \rightarrow \vartheta_t^+} T'(\eta) \geq (r - 2) \binom{s}{r - 1} M.$$

This completes the verification of (A).

So let us now continue with (B). From $H(M) > F_{r-1} \left(\frac{s-2}{2(s-1)} \right)$ one deduces easily that

$$S(M) > \frac{s - 1}{s} \geq \frac{r - 2}{r - 1},$$

where we have made the obvious definition

$$S(M) = \lim_{\eta \rightarrow M^-} S(\eta).$$

This entails

$$\frac{(s - r + 1)S(M)}{(r - 1)S(M) - (r - 2)} \leq s - 1,$$

which in turn implies

$$(r - 1) \left\{ \frac{(s - r + 1)S(M)}{(r - 1)S(M) - (r - 2)} - (s - 1) \right\} \left(\frac{1 - S(M)}{S(M)} \right)^2 \leq 0.$$

Adding $(r - 2)s$ and rearranging our terms, we infer

$$(r - 1)(s - 1) \frac{2S(M) - 1}{S(M)^2} - \frac{(s - r + 1)(rS(M) - (r - 1))}{S(M)((r - 1)S(M) - (r - 2))} \leq (r - 2)s.$$

Multiplying this by $\frac{M}{s} \cdot \binom{s}{r-1}$ and exploiting the equation

$$\frac{1}{M^{r-2}} = \frac{(r - 1)S(M) - (r - 2)}{S(M)^{r-1}},$$

which follows easily from the definition of S , one gets assertion (B), whereby Claim 4.5 has finally been proved. \square

5. Clique densities

We now come to the central section of this article, in which we are going to provide a proof of Claim 2.1, thus solving the clique density problem.

THEOREM 5.1. *If \mathcal{G} is a weighted graph and $r \geq 2$ is an integer, then we have $\mathcal{G}(K_r) \geq F_r(\mathcal{G}(K_2))$. In other words, the estimate*

$$\mathcal{G}(K_r) \geq \frac{1}{(s + 1)^r} \cdot \binom{s + 1}{r} \cdot (1 + \alpha)^{r-1} (1 - (r - 1)\alpha)$$

holds, where s refers to a positive integer for which $\gamma = \mathcal{G}(K_2)$ belongs to the interval $\left[\frac{s-1}{2s}, \frac{s}{2(s+1)} \right]$ and $\alpha \in \left[0, \frac{1}{s} \right]$ is required to satisfy $\gamma = \frac{s}{2(s+1)}(1 - \alpha^2)$.

Before we proceed to the proof itself, we give an informal outline of the strategy we use: the proof will be by induction on r and for fixed r by induction on the order n of \mathcal{G} . Once r and n are fixed, rather than considering all possible \mathcal{G} , we will restrict our attention to a hypothetical “extremal” counterexample, where “extremal” means that the difference $F_r(\mathcal{G}(K_2)) - \mathcal{G}(K_r)$ is as large as possible. Then we already know from Corollary 3.3 that $\alpha \neq 0$ and $\alpha \neq \frac{1}{s}$. From now on, r , s , and α will be the main “global variables” describing \mathcal{G} so that we regard a quantity appearing in the proof as being “known” when we can express it in terms of them. For instance, γ , $F_r(\gamma)$, and the derivative $\lambda = F'_r(\gamma)$ that will appear shortly are “known.”

Now what remains to be done is to establish an inequality in $n + \binom{n}{2}$ variables, where n of the variables, x_1, \dots, x_n , are the “weights of the vertices” of \mathcal{G} and the remaining ones, denoted by a_{ij} , are the “weights of the edges” of \mathcal{G} . So Lagrange’s theorem on multivariate functions is applicable and yields some information per variable.

For the “vertex with number i ,” essentially we get that the density $\mathcal{G}_i(K_{r-1})$ of r -cliques it belongs to depends linearly on its weighted degree $\mathcal{G}_i(K_1)$. These terms are defined precisely below. For now it may suffice to say that the slope of this linear function is the known number $\lambda = F'_r(\gamma)$ mentioned above, while its constant term is an unknown new parameter μ .

Similarly we could get an equation for each “edge variable” $a_{ij} \in (0, 1)$, but if $a_{ij} \in \{0, 1\}$, we just get an inequality because we can vary a_{ij} in one direction only. The precise estimate we thus obtain is called (5.5) below.

There is actually a quite interesting argument due to Nikiforov [9], which would allow us to assume $a_{ij} \in \{0, 1\}$ for all $i \neq j$ here.

To gain additional information on the unknown number μ , we multiply the equation gotten for the i^{th} vertex above by the weighted degree of that vertex and sum over i . The equation thus obtained may then be weakened by a calculation inspired by Razborov’s work ([11], [12]) to the main inequality

$$(r - 1)\mathcal{G}(K_r) + (r + 1)\mathcal{G}(K_{r+1}) \leq \lambda(\gamma + 3\mathcal{G}(K_3)) - 2\gamma\mu.$$

What is a bit confusing about this estimate is that when we want to use it for learning something about r -cliques, it seems as if we should already know something about triangles and $(r + 1)$ -cliques. The way out of this difficulty is that in the graph case these are just edges and r -cliques in the neighbourhoods of vertices. This idea works in our weighted setting as well and thus allows us to bring the induction hypothesis applied to “weighted neighbourhoods” into the argument. The inequality that results relates the x_i and a_{ij} in a quite involved way, but by the results of Section 4 we can make it more well behaved with respect to them at the cost of introducing a further constant ϑ that depends on the unknown number μ . This leads to an inequality that besides r , s , and α

involves only μ and ϑ , but the original variables x_i and a_{ij} will be gone. Finally it will turn out that this inequality is wrong.

Now we proceed with the details.

Proof of Theorem 5.1. Since F_2 is the identity function confined to $[0, \frac{1}{2})$, the result is clear for $r = 2$. Arguing indirectly, let $r \geq 3$ denote the least integer for which the clique density theorem can fail,* and take n to be the least order that counterexamples can possibly have. As we have already mentioned earlier, the function

$$F_r : [0, \frac{1}{2}) \longrightarrow [0, \frac{1}{r!})$$

is continuous. Now the collection of all weighted graphs of order n may in an obvious fashion be regarded as a compact topological space, which implies that the continuous function defined on it by

$$\mathcal{G} \longmapsto \mathcal{G}(K_r) - F_r(\mathcal{G}(K_2))$$

attains an absolute minimum. Now fix a weighted graph \mathcal{G} of order n for which this minimal value occurs. This property of \mathcal{G} will be referred to as “extremality.” Choose an integer $s \geq 1$ as well as a real number $\alpha \in [0, \frac{1}{s}]$ such that the number $\gamma = \mathcal{G}(K_2)$ can be written as

$$(5.1) \quad \gamma = \frac{s}{2(s+1)}(1 - \alpha^2).$$

By the hypothesized failure of our theorem, we have

$$\mathcal{G}(K_r) < \frac{1}{(s+1)^r} \cdot \binom{s+1}{r} \cdot (1 + \alpha)^{r-1} (1 - (r-1)\alpha),$$

which clearly can only happen if $s \geq r - 1$. Also, Corollary 3.3 tells us that $\alpha \in (0, \frac{1}{s})$, and so the function F_r is differentiable at γ . As we have seen in (4.3), its derivative $\lambda = F'_r(\gamma)$ is given by

$$(5.2) \quad \lambda = \frac{(r-1)r}{s(s+1)^{r-1}} \binom{s+1}{r} (1 + \alpha)^{r-2}.$$

Let \mathcal{G} as usual be presented by the sequence (x_1, x_2, \dots, x_n) of nonnegative reals summing up to 1 and by the function $a : [n]^{(2)} \longrightarrow [0, 1]$. The remainder of the proof proceeds in five steps.

First Step: Exploiting extremality. It is clear that each of the numbers x_1, x_2, \dots, x_n has to be positive, for if one of them were to vanish, we could simply omit it, thus obtaining another counterexample whose order would be

*By the results of Razborov and Nikiforov ([12], [9]) we could assume $r \geq 5$ here, but actually there is no need for doing so.

smaller than n . Given a sequence i_1, i_2, \dots, i_m of distinct integers from $[n]$ as well as another integer $\rho \geq 1$, we set

$$\mathcal{G}_{i_1, i_2, \dots, i_m}(K_\rho) = \sum_{M \in I^{(\rho)}} \prod_{(k, j) \in [m] \times M} a_{i_k j} \prod_{e \in M^{(2)}} a_e \prod_{j \in M} x_j,$$

where $I = [n] - \{i_1, i_2, \dots, i_m\}$. Note that for $m = 0$, this coincides with our earlier notation, so no confusion can arise.

As an example, we mention that for every $i \in [n]$, we have

$$\mathcal{G}_i(K_1) = \sum_{j \in [n] - \{i\}} a_{ij} x_j,$$

which may be thought of as the weighted degree of the “vertex with index i .” These weighted degrees satisfy

$$\sum_{i \in [n]} x_i \mathcal{G}_i(K_1) = 2 \sum_{\{i, j\} \in [n]^{(2)}} x_i x_j a_{ij} = 2\mathcal{G}(K_2),$$

whence

$$(5.3) \quad \sum_{i \in [n]} x_i \mathcal{G}_i(K_1) = 2\gamma.$$

Similarly $\mathcal{G}_i(K_{r-1})$ may be regarded as the relative density of r -cliques containing “the vertex i .” It is soon going to be important for us that this quantity is also the partial derivative of $\mathcal{G}(K_r)$ with respect to x_i .

Since (x_1, x_2, \dots, x_n) is an interior point of the simplex

$$\{(\xi_1, \xi_2, \dots, \xi_n) \in [0, 1]^n \mid \xi_1 + \xi_2 + \dots + \xi_n = 1\},$$

Lagrange’s theorem concerning the extremal values of multivariate functions reveals that due to the extremality of \mathcal{G} , there exists a certain real constant μ such that

$$(5.4) \quad \mathcal{G}_i(K_{r-1}) = \lambda \mathcal{G}_i(K_1) - \mu$$

holds for all $i \in [n]$.

As we are now going to see, the extremality of \mathcal{G} also implies that

$$(5.5) \quad \text{for each } \{i, j\} \in [n]^{(2)}, \text{ one has } a_{ij}(\lambda - \mathcal{G}_{ij}(K_{r-2})) \geq 0.$$

This is obvious whenever a_{ij} vanishes, so let us suppose now that this number is positive. If η denotes any sufficiently small positive real number, we may construct a weighted graph \mathcal{G}^η agreeing entirely with \mathcal{G} except for having $a_{ij}^\eta = a_{ij} - \eta$. Clearly one has $\mathcal{G}^\eta(K_2) = \gamma - \eta x_i x_j$ and $\mathcal{G}^\eta(K_r) = \mathcal{G}(K_r) - \eta x_i x_j \mathcal{G}_{ij}(K_{r-2})$, wherefore

$$\mathcal{G}^\eta(K_r) - F_r(\mathcal{G}^\eta(K_2)) = \mathcal{G}(K_r) - F_r(\gamma) + \eta x_i x_j (\lambda - \mathcal{G}_{ij}(K_{r-2})) \pm O(\eta^2),$$

which in view of the assumed extremality of \mathcal{G} entails $\lambda \geq \mathcal{G}_{ij}(K_{r-2})$ and hence (5.5).

Second Step: An estimate about triangles, r -cliques, and $(r + 1)$ -cliques.
 As in the proof of Proposition 3.1, we set

$$A_M = \prod_{e \in M^{(2)}} a_e \quad \text{and} \quad X_M = \prod_{i \in M} x_i$$

for all $M \subseteq [n]$. This time, however, we need the further stipulations

$$B_M = \sum_{i \in M} \left(\sum_{j \in M - \{i\}} a_{ij} \right) A_{M - \{i\}},$$

$$C_M = \sum_{Q \in M^{(r)}} A_Q,$$

and

$$D_M = \sum_{i \in M} \sum_{\{j,k\} \in (M - \{i\})^{(2)}} (1 - a_{ij})(1 - a_{ik}) A_{M - \{i\}}$$

for all $M \in [n]^{(r+1)}$. What we shall need to know about these expressions is

$$(5.6) \quad \text{if } M \in [n]^{(r+1)}, \text{ then } B_M - (r - 1)C_M + D_M \geq (r + 1)A_M.$$

To see this, we note again that our inequality is linear in each of its variables, for which reason we may suppose $a_e \in \{0, 1\}$ for all $e \in M^{(2)}$. Form a graph H with vertex set M by putting an edge between $i, j \in M$ exactly if $a_{ij} = 1$. If H is free from cliques of size r , then $A_M = B_M = C_M = D_M = 0$. If H contains a unique such clique and i further edges, where $0 \leq i \leq r - 2$, then $A_M = 0$, $B_M = i$, $C_M = 1$, and $D_M = \binom{r-i}{2}$, wherefore indeed $B_M - (r - 1)C_M + D_M = \binom{r-i-1}{2} \geq (r + 1)A_M$. If the graph H possesses exactly two cliques of size r , then it misses precisely one edge and $A_M = 0$, $B_M = 2(r - 1)$, $C_M = 2$ as well as $D_M = 0$. Finally, if H happens to be a clique, then $A_M = 1$, $B_M = r(r + 1)$, $C_M = r + 1$ and $D_M = 0$. This analysis proves (5.6) in all possible cases.

Multiplying the inequality just obtained by X_M and summing over M , we deduce

$$(5.7) \quad \sum_{M \in [n]^{(r+1)}} (B_M - (r - 1)C_M + D_M) X_M \geq (r + 1) \mathcal{G}(K_{r+1}).$$

Next, we consider the sum

$$\Omega = \sum_{i \in [n]} x_i \mathcal{G}_i(K_1) \mathcal{G}_i(K_{r-1}).$$

Expanding the product, we get several terms involving one of the variables x_1, x_2, \dots, x_n quadratically and certain other “linear” terms. We are thus led to a decomposition

$$\Omega = \Omega_{\text{sq}} + \Omega_{\text{mix}},$$

where

$$\Omega_{\text{sq}} = \sum_{\{i,j\} \in [n]^{(2)}} (x_i^2 x_j + x_i x_j^2) a_{ij}^2 \mathcal{G}_{ij}(K_{r-2})$$

and

$$\Omega_{\text{mix}} = \sum_{M \in [n]^{(r+1)}} B_M X_M.$$

Owing to (5.5), we have

$$(5.8) \quad \Omega_{\text{sq}} \geq \sum_{\{i,j\} \in [n]^{(2)}} (x_i^2 x_j + x_i x_j^2) a_{ij} \mathcal{G}_{ij}(K_{r-2}) - \lambda \Phi,$$

where

$$\Phi = \sum_{\{i,j\} \in [n]^{(2)}} (x_i^2 x_j + x_i x_j^2) (a_{ij} - a_{ij}^2).$$

The sum on the right-hand side of (5.8) rewrites as

$$(r-1) \sum_{Q \in [n]^{(r)}} A_Q X_Q \left(1 - \sum_{q \in [n]-Q} x_q\right) = (r-1) \mathcal{G}(K_r) - (r-1) \sum_{M \in [n]^{(r+1)}} C_M X_M.$$

So altogether we have

$$\Omega \geq (r-1) \mathcal{G}(K_r) + \sum_{M \in [n]^{(r+1)}} (B_M - (r-1)C_M) X_M - \lambda \Phi,$$

which due to (5.7) may be weakened to

$$\Omega \geq (r-1) \mathcal{G}(K_r) + (r+1) \mathcal{G}(K_{r+1}) - \lambda \Phi - \sum_{M \in [n]^{(r+1)}} D_M X_M.$$

Now notice that trivially

$$\sum_{M \in [n]^{(r+1)}} D_M X_M \leq \sum_{i \in [n]} \sum_{\{j,k\} \in ([n]-\{i\})^{(2)}} a_{jk} (1 - a_{ij})(1 - a_{ik}) x_i x_j x_k \mathcal{G}_{jk}(K_{r-2}).$$

Hence, writing

$$V_{\{i,j,k\}} = a_{jk} (1 - a_{ij})(1 - a_{ik}) + a_{ik} (1 - a_{ij})(1 - a_{jk}) + a_{ij} (1 - a_{ik})(1 - a_{jk})$$

for all $\{i, j, k\} \in [n]^{(3)}$ and applying (5.5) again, we obtain

$$(5.9) \quad (r-1) \mathcal{G}(K_r) + (r+1) \mathcal{G}(K_{r+1}) - \lambda \Phi - \lambda \sum_{T \in [n]^{(3)}} V_T X_T \leq \Omega.$$

On the other hand, (5.4) and (5.3) allow us to write

$$\Omega = \lambda \sum_{i \in [n]} x_i \mathcal{G}_i(K_1)^2 - 2\gamma\mu.$$

So in view of the calculation

$$\begin{aligned}
 \sum_{i \in [n]} x_i \mathcal{G}_i(K_1)^2 &= \sum_{\{i,j\} \in [n]^{(2)}} (x_i^2 x_j + x_i x_j^2) a_{ij}^2 \\
 &\quad + 2 \sum_{\{i,j,k\} \in [n]^{(3)}} (a_{ij} a_{jk} + a_{jk} a_{ki} + a_{ki} a_{ij}) X_{\{i,j,k\}} \\
 &= -\Phi + \sum_{\{i,j\} \in [n]^{(2)}} x_i x_j a_{ij} \left(1 - \sum_{k \in [n] - \{i,j\}} x_k \right) \\
 &\quad + \sum_{\{i,j,k\} \in [n]^{(3)}} (a_{ij} + a_{jk} + a_{ki}) X_{\{i,j,k\}} \\
 &\quad - \sum_{T \in [n]^{(3)}} V_T X_T + 3\mathcal{G}(K_3) \\
 &= -\Phi - \sum_{T \in [n]^{(3)}} V_T X_T + \gamma + 3\mathcal{G}(K_3),
 \end{aligned}$$

we have

$$\Omega = \lambda(\gamma + 3\mathcal{G}(K_3)) - 2\gamma\mu - \lambda\Phi - \lambda \sum_{T \in [n]^{(3)}} V_T X_T.$$

Comparing this with (5.9) we finally arrive at the main estimate of this step, namely

$$(5.10) \quad (r - 1)\mathcal{G}(K_r) + (r + 1)\mathcal{G}(K_{r+1}) \leq \lambda(\gamma + 3\mathcal{G}(K_3)) - 2\gamma\mu.$$

Third Step: Introducing and estimating M. Let us now define a real number M such that

$$(5.11) \quad \mu = \frac{(r - 2)r}{(s + 1)^r} \binom{s + 1}{r} (1 + \alpha)^{r-1} M.$$

Since (5.4) yields

$$r \cdot \mathcal{G}(K_r) = \sum_{i \in [n]} x_i \mathcal{G}_i(K_{r-1}) = \sum_{i \in [n]} x_i (\lambda \mathcal{G}_i(K_1) - \mu) = 2\gamma\lambda - \mu,$$

we have

$$(5.12) \quad \mathcal{G}(K_r) = \frac{1}{(s + 1)^r} \binom{s + 1}{r} (1 + \alpha)^{r-1} [1 - (r - 1)\alpha - (r - 2)(M - 1)]$$

owing to (5.2) and (5.11). In view of the presumed smallness of the left-hand side, this gives $M > 1$. Eventually we shall prove $M \leq 1$ as well, thereby reaching a final contradiction. Before doing that, however, we need to provide a much weaker upper bound on M , so that the results from our fourth section become available. This is our next immediate task. To achieve it, we find it convenient to introduce the abbreviations

$$A = \frac{r}{s(s + 1)^{r-1}} \binom{s + 1}{r},$$

$$B = \frac{(r-2)r}{(s+1)^r} \binom{s+1}{r},$$

and

$$C = \sqrt[r-2]{\frac{(2\gamma A)^{r-1}}{r \cdot \mathcal{G}(K_r)}}.$$

Notice that the last of these stipulations is permissible, as Proposition 3.1 entails $\mathcal{G}(K_r) > 0$ in view of $\gamma > \frac{s-1}{2s} \geq \frac{r-2}{2(r-1)}$. Applying the inequality between the arithmetic and geometric mean of $r-1$ positive real numbers, one of which is equal to $r \cdot \mathcal{G}(K_r)$ while each of the remaining $r-2$ numbers equals $C(1+\alpha)^{r-1}$, we get

$$r \cdot \mathcal{G}(K_r) + (r-2)C(1+\alpha)^{r-1} \geq 2(r-1)A\gamma(1+\alpha)^{r-2} = 2\gamma\lambda = r \cdot \mathcal{G}(K_r) + \mu$$

and hence $(r-2)C \geq BM$. Raising both sides to their $(r-2)^{\text{nd}}$ powers, after some easy simplifications we infer that

$$\left(\frac{2\gamma}{s}\right)^{r-1} \cdot \binom{s+1}{r} \geq (s+1)\mathcal{G}(K_r)M^{r-2}.$$

Using now Corollary 3.2, we obtain

$$\left(\frac{s-1}{s}\right)^{r-2} > \frac{s-r+1}{s-1} \cdot M^{r-2}.$$

As this estimate coincides with (4.1), we now have the results from Section 4 at our disposal.

Fourth Step: Induction on n . Due to (5.5), for each $i \in [n]$, we have the inequality

$$(r-1)\mathcal{G}_i(K_{r-1}) = \sum_{j \in [n] - \{i\}} x_j a_{ij} \mathcal{G}_{ij}(K_{r-2}) \leq \sum_{j \in [n] - \{i\}} \lambda x_j a_{ij} = \lambda \mathcal{G}_i(K_1).$$

Hence (5.4) yields

$$(r-1)(\lambda \mathcal{G}_i(K_1) - \mu) \leq \lambda \mathcal{G}_i(K_1),$$

i.e.,

$$\mathcal{G}_i(K_1) \leq \frac{(r-1)\mu}{(r-2)\lambda} = \frac{s}{s+1}(1+\alpha)M.$$

Thus if we define the real number η_i to obey $\mathcal{G}_i(K_1) = \frac{s}{s+1}(1+\alpha)\eta_i$, then $\eta_i \leq M$. Similarly but more easily, we have

$$0 \leq \mathcal{G}_i(K_{r-1}) = \lambda \mathcal{G}_i(K_1) - \mu,$$

whence $\mathcal{G}_i(K_1) \geq \frac{\mu}{\lambda}$, so that altogether we get $\eta_i \in \left[\frac{r-2}{r-1} \cdot M, M\right]$.

The main objective of this step is to verify that for each $i \in [n]$, one has

$$(5.13) \quad \lambda \mathcal{G}_i(K_2) - \mathcal{G}_i(K_r) \leq \frac{(r-2)s(1+\alpha)^r}{(s-1)(s+1)^{r+1}} \binom{s+1}{r} \\ \times \left(\frac{1}{2}(r-1)s\vartheta^2 - (r-1)s\vartheta M + r(s-1)\eta_i M\right).$$

Plainly it suffices to show this for $i = n$, and for brevity, we are henceforth going to write η instead of η_n . As $\mathcal{G}_n(K_1)$ is positive, we may construct a weighted graph \mathcal{G}^* of order $n - 1$ specified by the numbers $x_i^* = \frac{a_{in}x_i}{\mathcal{G}_n(K_1)}$ for $i \in [n - 1]$ and by the restriction of a to $[n - 1]^{(2)}$. Our minimal choices of r and n entail $\mathcal{G}^*(K_{r-1}) \geq F_{r-1}(\delta)$ and $\mathcal{G}^*(K_r) \geq F_r(\delta)$, where $\delta = \mathcal{G}^*(K_2)$. By our construction of \mathcal{G}^* and the case $i = n$ of (5.4), we have

$$\mathcal{G}^*(K_{r-1}) = \frac{\mathcal{G}_n(K_{r-1})}{\mathcal{G}_n(K_1)^{r-1}} = \frac{\lambda \mathcal{G}_n(K_1) - \mu}{\mathcal{G}_n(K_1)^{r-1}}.$$

Expressing the right-hand side in terms of r, s, M and η , this simplifies to $\mathcal{G}^*(K_{r-1}) = H(\eta)$, where H refers to the function defined just before Claim 4.1. Stipulating therefore $\nu = F_{r-1}^{-1}(H(\eta))$, as in the hypothesis of Claim 4.3, we have $\delta \leq \nu$. Now in view of

$$\mathcal{G}^*(K_2) = \frac{\mathcal{G}_n(K_2)}{\mathcal{G}_n(K_1)^2} \quad \text{and} \quad \mathcal{G}^*(K_r) = \frac{\mathcal{G}_n(K_r)}{\mathcal{G}_n(K_1)^r},$$

we get

$$\lambda \mathcal{G}_n(K_2) - \mathcal{G}_n(K_r) = \frac{s(1 + \alpha)^r \eta^2}{(s + 1)^r} \times \left\{ (r - 1) \binom{s}{r - 1} \delta - s^{r-1} \eta^{r-2} \mathcal{G}^*(K_r) \right\}.$$

By our bound on $\mathcal{G}^*(K_r)$, the difference in curly braces is at most $Q(\delta)$, where Q signifies the function introduced in Claim 4.3, and by that claim itself this is in turn at most $Q(\nu)$. Estimating now the product $\eta^2 Q(\nu)$ by means of Claim 4.5, we finish proving (5.13).

Fifth Step: Concluding the argument. Notice that (5.3) and (5.1) yield

$$\frac{s}{s + 1} (1 + \alpha) \sum_{i \in [n]} x_i \eta_i = \sum_{i \in [n]} x_i \mathcal{G}_i(K_1) = 2\gamma = \frac{s}{s + 1} (1 - \alpha^2),$$

wherefore

$$\sum_{i \in [n]} x_i \eta_i = 1 - \alpha.$$

Thus multiplying (5.13) by x_i and adding up the n resulting inequalities we conclude

$$\begin{aligned} 3\lambda \mathcal{G}(K_3) - (r + 1)\mathcal{G}(K_{r+1}) &\leq \frac{(r - 2)s(1 + \alpha)^r}{(s - 1)(s + 1)^{r+1}} \binom{s + 1}{r} \\ &\quad \times \left(\frac{1}{2}(r - 1)s\vartheta^2 - (r - 1)s\vartheta M + r(s - 1)(1 - \alpha)M \right). \end{aligned}$$

Combining this with (5.10) and plugging in the formulae (5.1), (5.2), (5.11), and (5.12) expressing γ, λ, μ , and $\mathcal{G}(K_r)$ in terms of r, s, α , and M we get an estimate that on first sight looks rather lengthy. After massive cancelations, however, it just reads

$$(1 - \alpha) - 2M \leq \frac{(1 + \alpha)s^2}{s^2 - 1} (\vartheta^2 - 2M\vartheta).$$

Since $\vartheta \in \left[\frac{s-1}{s}M, M\right]$ holds by Claim 4.2, we have

$$\vartheta^2 - 2M\vartheta = (M - \vartheta)^2 - M^2 \leq -\frac{s^2-1}{s^2} \cdot M^2,$$

whence

$$(1 - \alpha) - 2M \leq -(1 + \alpha)M^2,$$

i.e.,

$$(1 - M)((1 - \alpha) - (1 + \alpha)M) \leq 0.$$

But if M really was greater than 1, as suggested by our third step, then both factors of the left-hand side had to be negative. This contradiction finally proves Theorem 5.1. \square

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