Supersaturation for subgraph counts

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Abstract

The classic extremal problem is that of computing the maximum number of edges in an F-free graph. In the case where $F = K_{r+1}$, the extremal number was determined by Turán. Later results, known as supersaturation theorems, proved that in a graph containing more edges than the extremal number, there must also be many copies of K_{r+1}. Alon and Shikhelman introduced a broader class of problems asking for the maximum number of copies of a graph T in an F-free graph. In this paper, we determine some of these generalized extremal numbers and prove supersaturation results for them.

1 Introduction

The classic theorem of Turán [21] gives the maximum number of edges in a K_{r+1}-free graph, a number which is asymptotically $(1-\frac{1}{r})\binom{n}{2}$. It is standard to write this result as $\mathrm{ex}(n, K_{r+1}) = (1 - \frac{1}{r} + o(1))\binom{n}{2}$. Of course, if the number of edges in a graph G on n vertices exceeds $\mathrm{ex}(n, K_{r+1})$, we know that G must contain at least one K_{r+1}. One could ask about the minimum number of copies of K_{r+1} that are contained in G. Results of this type are referred to as *supersaturation* theorems. To be precise, letting $k_{r+1}(G)$ be the number of copies of K_{r+1} in a graph G, supersaturation questions ask one to determine

$$\min\{k_{r+1}(G) : G \text{ a graph with } n \text{ vertices and } \mathrm{ex}(n, K_{r+1}) + q \text{ edges}\},$$

for some $q \geq 1$. When $q = o(n^2)$, the problem was studied by Rademacher [18], Erdős [9, 6, 7], and then resolved by Lovász and Simonovits [11, 12]. For the case when $q = \Omega(n^2)$, asymptotic solutions have been found by Razborov [19] for $r = 2$, Nikiforov [15] for $r = 3$, and Reiher [20] for general r. See Pikhurko and Yilma [17] for a very informative introduction to supersaturation.

One could also ask if other structures are guaranteed to exist in graphs with more edges than the Turán number. The following theorem of Erdős and Stone [8] shows that, in a graph in which the edge count exceeds this extremal number by a constant multiple of n^2, must not only contain a K_{r+1}, but indeed a blowup of K_{r+1} with large part sizes. For a graph G, we let the blowup $G(b)$ be the graph where each vertex of G is replaced by an independent set of size b and each edge is replaced by a complete bipartite graph. We will refer to such theorems as *structural supersaturation* results.

Theorem 1.1 (Erdős-Stone)**.** *Let $r \geq 1$ be an integer and let $\varepsilon > 0$. Then there exists $n_0 = n_0(r, \varepsilon)$ such that if G is a graph on $n \geq n_0$ vertices and*

$$e(G) \geq \left(1 - \frac{1}{r} + \varepsilon\right)\binom{n}{2},$$

then G contains $K_{r+1}(b)$ for some $b \geq \varepsilon \log n/(2^{r+1}(r-1)!)$.

In more recent work, Alon and Shikhelman [2] considered generalized extremal problems involving counting copies of some fixed subgraph rather than edges. To be precise, they were interested in determining values of

$$\mathrm{ex}_T(n, F) = \max\{n_T(G) \,:\, G \text{ is an } F\text{-free graph on } n \text{ vertices}\},$$

where $n_T(G)$ is the number of copies of T in G. In particular, $\mathrm{ex}_{K_2}(n, F) = \mathrm{ex}(n, F)$. In this paper, we consider Alon-Shikhelman-type problems where T and F are either cliques or stars. We also consider supersaturation and structural supersaturation results in this vein. The following subsections will outline the history of these problems and the new results of this paper.

1.1 Cliques without cliques

The most fundamental Alon-Shikhelman-type problems involve cliques. As above, we write $k_t(G)$ for $n_{K_t}(G)$. Zykov [23], along with many others, showed that $\mathrm{ex}_{K_t}(n, K_{r+1}) = k_t(T(n, r))$, where $T(n, r)$ is the r-partite Turán graph on n vertices. Bollobás [3] discussed the general problem of minimizing the number of copies of K_s in a graph with a given number, say N, of K_ts, i.e., a supersaturation result. (Thus, if $N \leq \mathrm{ex}_{K_t}(n, K_s)$, then this minimum number is 0.) His result gives a bound of the form

$$k_s(G) \geq \psi(N),$$

where ψ is a function defined implicitly. A simpler, but slightly more transparent version is the following.

Theorem 1.2. *Let θ be a real number and s and t be integers with $2 \le t \le s \le \theta + 1$. If G is a graph on n vertices such that $k_t(G) \ge \binom{\theta}{t}(n/\theta)^t$, then $k_s(G) \ge \binom{\theta}{s}(n/\theta)^s$.*

This result follows from the theorem of Bollobás via Theorem 1.7′ of Section VI of [4]. A more direct approach, using the following beautiful theorem of Moon and Moser [14] and the method outlined in Lovász's Combinatorial Problems and Exercises [13, Section 10, Question 40], is also possible.

Theorem 1.3 (Moon-Moser). *For any graph G on n vertices and any $s \ge 2$,*

$$\frac{k_{s+1}(G)}{k_s(G)} \ge \frac{1}{s^2-1}\Big(s^2\frac{k_s(G)}{k_{s-1}(G)} - n\Big).$$

Nikiforov [16] shows that the conclusion of the Erdős-Stone theorem follows even from the weak hypothesis that G contains cn^{r+1} copies of K_{r+1}.

Theorem 1.4 (Nikiforov). *Let $s \ge 2$ and c and n be such that*

$$0 < c < 1/s! \quad \textit{and} \quad n \ge \exp(c^{-s}).$$

If G is a graph with n vertices and $k_s(G) \ge cn^s$, then G contains a $K_s(b)$ with $b = \lfloor c^s \log n \rfloor$.

This, together with the Bollobás result, proves a structural supersaturation extension of Zykov's result.

Theorem 1.5. *For all $\varepsilon > 0$, there is a $\delta > 0$ and an $n_0 \in \mathbb{N}$ such that if G is a graph on $n \ge n_0$ vertices and $k_t(G) \ge (1+\varepsilon)k_t(T(n,r))$, then G contains a $K_{r+1}(C \log n)$ for some $C = C(\varepsilon, r) > 0$.*

Proof. The hypothesis on $k_t(G)$ implies that, for some $\theta > r$, we have $k_t(G) \ge \binom{\theta}{t}(n/\theta)^t$. Thus, by Corollary 1.2, $k_{r+1}(G) \ge \binom{\theta}{r+1}(n/\theta)^{r+1}$, a constant multiple of n^{r+1}. Now, by Theorem 1.4, G contains a large blowup of K_{r+1}. □

1.2 Cliques without stars

If we write S_r for $K_{1,r}$, the following result due to Wood [22], and Engbers and Galvin [5] computes $\mathrm{ex}_{K_t}(n, S_{r+1})$. For $v \in V(G)$, we write $k_t(v)$ for the number of copies of K_t in G than contain vertex v. For completeness, we include the proof.

Theorem 1.6 (Wood, Engbers-Galvin). *For any $1 \le r \le n$, we have*

$$\mathrm{ex}_{K_t}(n, S_{r+1}) \le \frac{n}{t}\binom{r}{t-1} = \frac{n}{r+1}\binom{r+1}{t}.$$

Proof. Note that being S_{r+1}-free is equivalent to having maximum degree at most r. Let G be such a graph on n vertices. If we count pairs (v, S) where v is a vertex of G, S is a t-clique in G and $v \in S$ then we have

$$tk_t(G) = \sum_{v \in V(G)} k_t(v) = \sum_{v \in V(G)} k_{t-1}(G[N(v)]) \le n\binom{r}{t-1}. \qquad \square$$

Note that this result is asymptotically sharp since the graph aK_{r+1} achieves the bound whenever n is divisible by $r+1$.

In Section 2, we prove the following supersaturation result showing that if G contains too many copies of K_t then there must be many copies of S_r in G. We write $s_r(G)$ for the number of copies of S_r in G, i.e.,

$$s_r(G) = \sum_{v \in V(G)} \binom{d(v)}{r}.$$

Theorem 1.7. *Given $2 \le t \le r$, for all $\varepsilon > 0$ there exists $\delta > 0$ such that if G is a graph on n vertices having*

$$k_t(G) \ge (1+\varepsilon)\frac{n}{r+1}\binom{r+1}{t}$$

then $s_{r+1}(G) \ge \delta n$.

Note that the bound in Theorem 1.7 is asymptotically sharp. To see this, let $s > r$ and consider the graph G on $n = k(s+1)$ vertices that is the disjoint union of k copies of K_{s+1}, i.e., $G = kK_{s+1}$. Then,

$$k_t(G) = k\binom{s+1}{t} = \frac{n}{t}\binom{s}{t-1}$$

A straightforward calculation shows that, provided $s \ge r+1$,

$$\frac{\frac{n}{t}\binom{s}{t-1}}{\frac{n}{r+1}\binom{r+1}{t}} > 1,$$

and so the conditions of Theorem 1.7 are met. Further, note that

$$s_{r+1}(G) = n\binom{s}{r+1}.$$

Thus, equality is achieved in the conclusion of Theorem 1.7 with $\delta = \binom{s}{r+1}$.

For structural supersaturation, since the star is not vertex transitive, there are different notions of a blowup of S_{r+1}; they are all of the form $K_{a,b}$. The discussion above implies that having a surplus of K_ts does not imply even the existence of a $K_{1,r+2}$. In addition, the classic construction of Füredi [10] demonstrates that it is also not possible to guarantee the existence of a $K_{2,r+1}$ (at least in the case when $t = 3$). The following theorem can be read out of his paper.

Theorem 1.8 (Füredi)**.** *For any $r \geq 1$ there exist infinitely many n so that there is a graph on n vertices which is $K_{2,r+1}$-free and contains $\Omega(n^{3/2})$ triangles. In particular, knowing that $k_3(G)$ is at least $(1+\varepsilon)\operatorname{ex}_{K_3}(n, S_{r+1})$ does not imply the existence of a $K_{2,r+1}$ in G.*

1.3 Stars without stars

Although this case is rather uninteresting, we include it for completeness.

Proposition 1.9. *If $t > 1$, then for $n \geq r+1$,*

$$\operatorname{ex}_{S_t}(n, S_{r+1}) = \begin{cases} n\binom{r}{t} & \text{if } nr \text{ is even,} \\ (n-1)\binom{r}{t} + \binom{r-1}{t} & \text{otherwise.} \end{cases}$$

Proof. Since each degree is at most r, we have that $s_t(G) = \sum \binom{d(v)}{t}$ is maximized when G is as close to r-regular as possible. If nr is even, there is an r-regular graph and otherwise there is a graph where one vertex has degree $r-1$ and all others have degree r. $\square$

One can also prove a rather uninteresting supersaturation result in this case. Since both the number of S_ts and the number of S_{r+1}s are a function of the degree sequence, it is easy to check that an excess of $\varepsilon n\binom{r}{t}$ copies of S_t yields at least $\varepsilon n(r-t+1)/t$ copies of S_{r+1}. The extremal graph is as regular as possible.

No structural supersaturation theorem for this case is true. Any $(r+1)$-regular graph has a fixed fraction more S_ts than $\operatorname{ex}_{S_t}(n, S_{r+1})$, without containing any S_{r+2}. The same Füredi example from the previous section is almost regular and hence contains at least $(1+\varepsilon)\operatorname{ex}_{S_t}(n, S_{r+1})$ copies of S_t without having a $K_{2,r+1}$.

1.4 Stars without cliques

This case is substantially more difficult than the others we've encountered up to this point. In fact, we are able only to determine $\operatorname{ex}_{S_t}(n, K_{r+1})$ asymptotically and are not able to make any progress on either the supersaturation or structural supersaturation versions of the problem. All the details can be found in Section 3.

2 Supersaturation for cliques without stars

In order to prove Theorem 1.7, we start with a lemma concerning the function $\binom{x}{s}$ where x is a postive real number.

Definition. We define, for $x \in [0, \infty)$ and $s \in \mathbb{N}_{\geq 1}$,

$$f_s(x) = \begin{cases} \dbinom{x}{s} = \dfrac{1}{s!}\, x(x-1)\cdots(x-s+1) & \text{if } x \geq s-1 \\ 0 & \text{if } 0 \leq x < s-1. \end{cases}$$

Note that, for $x > s+1$,

$$f_s'(x) = \frac{1}{s!}\sum_{i=0}^{s-1} x(x-1)\cdots\cancel{(x-i)}\cdots(x-s+1)$$

and

$$f_s''(x) = \frac{2}{s!}\sum_{0\le i<j\le s-1} x(x-1)\cdots\cancel{(x-i)}\cdots\cancel{(x-j)}\cdots(x-s+1).$$

Also, note that f_s is strictly increasing on $[s-1,\infty)$. We denote the inverse of $f_s|_{[s-1,\infty)}$ by f_s^{-1}.

Lemma 2.1. *For all $1 \le t < s$ the function $f_s \circ f_t^{-1}$ is convex on $(0,\infty)$ and strictly convex on $(\binom{s-1}{t},\infty)$.*

Proof. Note that $f_s \circ f_t^{-1}(x) = 0$ if $x \le \binom{s-1}{t}$. Further, the derivative is positive if $x > \binom{s-1}{t}$ and thus it's enough to show strict convexity on $(\binom{s-1}{t},\infty)$. For convenience we'll denote $f_t^{-1}(x)$ by u, and we may assume that $u > s-1$. Note that

$$(f_s \circ f_t^{-1})'(x) = f_s'(u)\cdot u', \qquad \text{and} \qquad u' = \frac{1}{f_t'(u)}.$$

Thus

$$\begin{aligned}(f_s\circ f_t^{-1})'' &= f_s''(u)\cdot(u')^2 + f_s'(u)\cdot u'' = f_s''(u)\cdot\frac{1}{(f_t'(u))^2} - \frac{f_s'(u)}{(f_t'(u))^2}\cdot f_t''(u)\cdot u' \\ &= \frac{f_s''(u)f_t'(u) - f_s'(u)f_t''(u)}{(f_t'(u))^3}.\end{aligned}$$

Since $u > t-1$, we have $f_t'(u) > 0$ so we need only that the numerator of the above is positive. To this end, since $s > t$, note that

$$\begin{aligned}&f_s''(u)f_t'(u) - f_s'(u)f_t''(u) \\ &\qquad = \frac{2}{s!t!}\Bigg[\sum_{\substack{0\le i<j\le s-1\\ 0\le k\le t-1}} u(u-1)\cdots\cancel{(u-i)}\cdots\cancel{(u-j)}\cdots(u-s+1)\cdot \\ &\qquad\qquad\qquad\qquad \cdot u(u-1)\cdots\cancel{(u-k)}\cdots(u-t+1) \\ &\qquad\quad - \sum_{\substack{0\le i\le s-1\\ 0\le j<k\le t-1}} u(u-1)\cdots\cancel{(u-i)}\cdots(u-s+1)\cdot \\ &\qquad\qquad\qquad\qquad \cdot u(u-1)\cdots\cancel{(u-j)}\cdots\cancel{(u-k)}\cdots(u-t+1)\Bigg].\end{aligned}$$

We'll show that this is non-negative by proving that all the negative terms are canceled by positive ones. If we write $T_{ij|k}$ for a typical term in the first sum and $T_{i|jk}$ for one in the second, then we see that all the terms with $i, j, k < t$ cancel since $T_{i|jk}$ cancels with $T_{jk|i}$. The remaining negative terms are of the form $T_{i|jk}$ with $i \geq t$. We have that each such term $T_{i|jk}$ cancels with $T_{ji|k}$. Strictness of convexity is guaranteed since some strictly positive terms remain, e.g., the $T_{ij|k}$ with $i = k$ and $j \geq t$. □

We are now ready for the proof of the main theorem of this section, which we recall here.

Theorem 1.7. *Given $2 \leq t \leq r$, for all $\varepsilon > 0$ there exists $\delta > 0$ such that if G is a graph on n vertices having*

$$k_t(G) \geq (1+\varepsilon)\frac{n}{r+1}\binom{r+1}{t}$$

then $s_{r+1}(G) \geq \delta n$.

Proof. As in Theorem 1.6,

$$n\binom{r}{t-1}(1+\varepsilon) \leq t k_t(G) = \sum_v k_t(v) \leq \sum_v \binom{d(v)}{t-1}.$$

Define $\ell(v) = f_{t-1}(d(v)) = \binom{d(v)}{t-1}$. We have

$$\sum_v \ell(v) \geq n\binom{r}{t-1}(1+\varepsilon) \qquad \text{and} \qquad s_{r+1} = \sum_v \binom{d(v)}{r+1} = \sum_v \binom{f_{t-1}^{-1}(\ell(v))}{r+1}.$$

The last equality is true term-by-term noting that if $d(v) < t-1$, and hence $d(v) \neq f_{t-1}^{-1}(f_{t-1}(d(v)))$, the v term in both these sums is zero.

We define

$$\tilde{f}_{r+1,t-1}(\ell) = f_{r+1}(f_{t-1}^{-1}(\ell)).$$

We will determine the minimum of $\sum_{i=1}^n \tilde{f}_{r+1,t-1}(\ell_i)$ subject to $\sum_{i=1}^n \ell_i \geq n\binom{r}{t-1}(1+\varepsilon)$. To be precise, we solve the relaxation where $\ell_i \in \mathbb{R}_{\geq 0}$. Since $\tilde{f}_{r+1,t-1}$ is convex by Lemma 2.1, we have

$$\sum_{i=1}^n \tilde{f}_{r+1,t-1}(\ell_i) \geq n\tilde{f}_{r+1,t-1}\Big(\sum_{i=1}^n \ell_i\Big) \geq n\tilde{f}_{r+1,t-1}\Big(\binom{r}{t-1}(1+\varepsilon)\Big).$$

Thus we are done, setting $\delta = \tilde{f}_{r+1,t-1}\Big(\binom{r}{t-1}(1+\varepsilon)\Big)$. □

3 Many stars, no K_{r+1}

In this section, we work on the problem of determining $\mathrm{ex}_{S_t}(n, K_{r+1})$. We first prove that any extremal graph is complete r-partite. Our proof of this is a modification of a proof of Turán's Theorem that can be found, for example, in [1]. This simplifies the problem of finding the largest number of S_ts. We then address the graphon version of the problem, determining $\mathrm{ex}_{S_t}(W, K_{r+1})$.

3.1 Optimal graphs are complete multipartite

We begin by proving any graph achieving $\mathrm{ex}_{S_t}(n, K_{r+1})$ is complete multipartite.

Theorem 3.1. *If G is a K_{r+1}-graph on $n \geq t+1$ vertices with the maximum number of S_ts subject to these conditions, then non-adjacency is an equivalence relation, i.e., G is complete multipartite.*

Proof. We start by proving the base case when $n = t+1$. In that situation, $s_t(G)$ is the same as the number of dominating vertices in G, which is at most the minimum of r and n. If $t \geq r$, i.e., $n \geq r+1$, we cannot have more than r dominating vertices or G would contain a K_{r+1}. Thus, the unique optimal graph is the r-partite graph $K_{t+r-2,1,1,\ldots,1}$. If $t < r$, then K_n contains no K_{r+1} and has n dominating vertices.

Let G be a K_{r+1}-free graph on n vertices with $s_t(G) = \mathrm{ex}_{S_t}(n, K_{r+1})$. We will consider modifications of G obtained by deleting some vertices and cloning others. We start by determining the effect of these operations on $s_t(G)$. For $x \in V(G)$, let $G \oplus x$ be the graph G' consisting of G together with a new vertex x' such that $N_{G'}(x') = N_G(x)$. Note that, in particular, $x \not\sim_{G'} x'$. Also, if G is K_{r+1}-free then so are both $G \setminus x$ and $G \oplus x$.

The number of $K_{1,t}$s with center at vertex v is $\binom{d(v)}{t}$. If we increase the degree of a vertex v from d to $d+1$ then the number of S_ts centered at v will increase by $\binom{d+1}{t} - \binom{d}{t} = \binom{d}{t-1}$. Likewise, if we decrease the degree of a vertex from d to $d-1$, the number of S_ts centered at the vertex will decrease by $\binom{d}{t} - \binom{d-1}{t} = \binom{d-1}{t-1}$. The effect on $s_t(G)$ of deleting or cloning a vertex x is felt both at x and the neighbors of x. To be precise,

$$s_t(G \setminus x) = s_t(G) - B_G^-(x) \qquad \text{and} \qquad s_t(G \oplus x) = s_t(G) + B_G^+(x),$$

where

$$B_G^+(x) = \binom{d(x)}{t} + \sum_{v \in N_G(x)} \binom{d(v)}{t-1} \qquad \text{and} \qquad B_G^-(x) = \binom{d(x)}{t} + \sum_{v \in N_G(x)} \binom{d(v)-1}{t-1}.$$

Note that $B_G^+(x) \geq B_G^-(x)$.

Suppose that, in G, there exists vertices x, y, and z such that $x \not\sim y$ and $y \not\sim z$, but $x \sim z$. Consider first the case that either $B_G^+(x) > B_G^-(y)$ or $B_G^+(z) > B_G^-(y)$. Without loss of generality, we assume $B_G^+(x) > B_G^-(y)$ and let $G' = (G \setminus y) \oplus x$. The graph G' has n vertices and is K_{r+1}-free, yet

$$\begin{aligned} s_t(G') - s_t(G) &= B_G^+(x) - B_{G\oplus x}^-(y) \\ &= B_G^+(x) - B_G^-(y) \\ &> 0, \end{aligned}$$

a contradiction to assumption on G. The second equality follows since $x \not\sim_G y$.

Otherwise, we have $B^-_G(y) \geq B^+_G(x), B^+_G(z)$. In this case, we let $G'' = (G \setminus \{x, z\}) \oplus y \oplus y$. We have

$$\begin{aligned} s_t(G'') - s_t(G) &= 2B^+_G(y) - B^-_G(x) - B^-_{G\setminus x}(z) \\ &\geq 2B^+_G(y) - B^+_G(x) - B^+_{G\setminus x}(z) \\ &\geq 2B^+_G(y) - B^+_G(x) - B^+_G(z) \\ &\geq 0, \end{aligned}$$

where the equality holds since $x \not\sim_G y$ and $z \not\sim_G y$. If any of the above inequalities are strict, we have a contradiction, and thus we are done unless $B^+_G(y) = B^-_G(y)$, $B^+_G(x) = B^-_G(x)$, and $B^+_G(z) = B^-_{G\setminus x}(z)$. Since $B^+_G(x) = B^-_G(x)$, we know that if $v \sim_G x$, then $\binom{d(v)}{t-1} = \binom{d(v)-1}{t-1}$, i.e., $d(v) < t-1$. Since $z \sim_G x$, we have $d(z) < t-1$. By the same argument, we also have that $d(v) < t-1$ for all neighbors in G of z. Putting this together, we have $B^+(z) = 0$. Roughly speaking, this says that z is useless. In particular, $s_t(G \setminus z) = s_t(G)$.

We construct a graph on n vertices by picking an optimal graph H on $n-1$ vertices which will have at least as many S_ts as $G \setminus z$. We will then clone a vertex in H so as to construct a graph on n vertices with more S_ts than G. By induction on n, the optimal graph H' on $n-1$ vertices is complete multipartite and contains at least one vertex x of degree at least t. Cloning x gives

$$s_t(H \oplus x) > s_t(H) \geq s_t(G \setminus z) = s_t(G),$$

a contradiction. $\square$

3.2 The graphon problem

Knowing that the optimal graph is complete multipartite leaves only the question of what part sizes are optimal. We solve the problem asymptotically, i.e., we show that there are optimal proportions $\alpha_1, \alpha_2, \ldots, \alpha_r$ for the part sizes. Somewhat more surprisingly, we will show that there are cases where it is *not* the case that the optimal proportions are all $\alpha_i = 1/r$.

The optimization problem we are trying to solve then is (asymptotically, and ignoring a factor of $1/t!$)

$$\begin{array}{lrcl} \text{Maximize} & F(\rho_1, \rho_2, \ldots, \rho_r) & = & \displaystyle\sum_{i=1}^{r} \rho_i (1-\rho_i)^t \\ \text{subject to} & \rho_i & \geq & 0 \\ & \displaystyle\sum_{i=1}^{r} \rho_i & = & 1. \end{array} \tag{1}$$

We will naturally start by finding the interior critical points, which must satisfy

$$\nabla F(\rho) = \lambda(1, 1, \ldots, 1)$$

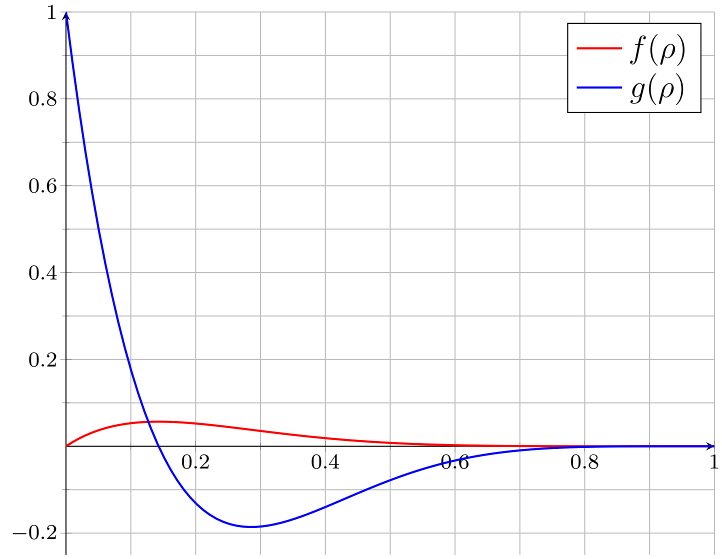

Figure 1: Graphs of $f(\rho)$ and $g(\rho)$ with $t = 6$

for some λ. Writing $f(\rho) = (1-\rho)^t\rho$ we require that the vector $(f'(\rho_1), f'(\rho_2), \ldots, f'(\rho_r))$ is constant.

We start with a basic lemma concerning the derivatives of f.

Lemma 3.2. *With $f(\rho) = (1-\rho)^t\rho$ and $k \geq 1$ we have*

$$f^{(k)}(\rho) = (-1)^k t_{(k-1)}(1-\rho)^{t-k}((t+1)\rho - k).$$

In particular the first and second derivatives of f are

$$g(\rho) = f'(\rho) = (1-\rho)^{t-1}(1-(t+1)\rho))$$
$$h(\rho) = f''(\rho) = t(1-\rho)^{t-2}((t+1)\rho - 2).$$

Proof. Straightforward. $\square$

We denote values of $g(\rho)$ by ϕ. If ϕ is a value of g with $\phi > 0$ there is exactly one solution of $g(\rho) = \phi$, whereas if $\phi \in (\phi_{\min}, 0]$ (where $\phi_{\min} = g(2/(t+1))$ is the minimum value of $g(\rho)$ on $[0,1]$) then there are exactly two solutions. One of these solutions satisfies $1/(t+1) \leq \rho < 2/(t+1)$, and the other satisfies $2/(t+1) < \rho \leq 1$.

Corollary 3.3. *Interior critical points for* (1) *are either of the form $(1/r, 1/r, \ldots, 1/r)$, the Turán solution, or $(\alpha, \alpha, \ldots, \alpha, \beta, \beta, \ldots, \beta)$, where $\alpha < 2/(t+1) < \beta$ and for some $\phi \in (\phi_{min}, 0]$ we have $g(\alpha) = \phi = g(\beta)$, which we will refer to as a skew solution. In the skew solution case we also require that $a\alpha + b\beta = 1$, where a is the number of αs and b is the number of βs.*

In this section we will prove the following theorem describing the optimal solution to (1). We establish our result for all r and t sufficiently large. The following definition gives the r and t for which our theorem holds.

Definition. We call a pair (r, t) *legal* if $r \geq 6$ and also

$$t \geq \begin{cases} 3 & \text{if } r \geq 9, \\ 4 & \text{if } r = 8, \\ 5 & \text{if } r = 7, \text{ and} \\ 37 & \text{if } r = 6. \end{cases}$$

It is in Lemma 3.9 below that legal pairs come up.

Theorem 3.4. *Suppose (r, t) is a legal pair. The objective function F is maximized at an interior critical point. There are at most two possibilities for this critical point. One is the Turán solution. The only other possibility is the skew solution $(\alpha, \alpha, \ldots, \alpha, \beta)$ associated to $a = r - 1$ and $b = 1$ having $g(\alpha) = g(\beta)$ largest. If any skew solution exists, then this skew solution exists.*

Our approach will be to fix t, a, and b, and consider α, β as functions of ϕ. We are then looking for solutions to

$$L_{a,b}(\phi) = a\alpha + b\beta = 1,$$

which maximize

$$F_{a,b} = af(\alpha) + bf(\beta).$$

If the context makes it clear, we will omit the subscripts. We will then consider a critical point $(\alpha, \alpha, \ldots, \alpha, \beta, \beta, \ldots, \beta)$ with a copies of α and b copies of β and ϕ value $\phi = g(\alpha) = g(\beta)$. If $a < r-1$, we will show that there is a critical point associated to some $\phi' = g(\alpha') = g(\beta') > \phi$ with $a+1$ copies of α', $b-1$ copies of β', and a larger value for the objective function. Thus, we need only consider which critical point associated with the case $a = r - 1$ and $b = 1$ is best. We show it is the one with ϕ largest.

We begin with some preliminary lemmas.

Lemma 3.5. *For any a, b summing to r, we have*

$$\frac{dL_{a,b}}{d\phi} = \frac{a}{h(\alpha)} + \frac{b}{h(\beta)},$$

$$\frac{dF_{a,b}}{d\phi} = \phi \frac{dL_{a,b}}{d\phi}, \text{ and}$$

$$\frac{d^2 L_{a,b}}{d\phi^2} = \frac{ah'(\alpha)(h(\beta))^3 + bh'(\beta)(h(\alpha))^3}{-(h(\alpha)h(\beta))^3}.$$

Proof. Since $\phi = g(\alpha)$, we have that $d\alpha/d\phi = 1/h(\alpha)$. Similarly, $d\beta/d\phi = 1/h(\beta)$ from which the first equation follows. For the second,

$$\frac{dF}{d\phi} = ag(\alpha)\frac{d\alpha}{d\phi} + bg(\beta)\frac{d\beta}{d\phi} = \frac{a\phi}{h(\alpha)} + \frac{b\phi}{h(\beta)} = \phi\Big(\frac{a}{h(\alpha)} + \frac{b}{h(\beta)}\Big) = \phi\frac{dL}{d\phi}.$$

The third is a straightforward calculation. □

As a consequence, for $\phi_2 < \phi_1$, we have

$$F(\phi_1) - F(\phi_2) = \int_{\phi_2}^{\phi_1} \frac{dF}{d\phi}\,d\phi = \int_{\phi_2}^{\phi_1} \phi\frac{dL}{d\phi}\,d\phi = \phi L\Big|_{\phi_2}^{\phi_1} - \int_{\phi_2}^{\phi_1} L\,d\phi. \tag{2}$$

Note that, in the expression for $d^2L/d\phi^2$ in Lemma 3.5, the denominator and the first term on the numerator are always positive and the second term on the numerator is positive provided $\beta > 3/(t+1)$. Hence, for $\phi > \phi_{\text{key}} := g(3/(t+1))$, we see that L is a convex function of ϕ. Our proof will depend on the fact that if L is concave at ϕ, this requires $\phi \le \phi_{\text{key}}$.

Now we are ready to begin the proof in earnest. The following sequence of technical lemmas builds our understanding of the relationship between the values of the objective function at the possible internal critical points.

Lemma 3.6. *If there is a critical point with parameters ϕ, a, and b, and $a < r-1$, then there is a critical point associated to ϕ', $a+1$, and $b-1$, with $\phi' > \phi$ and $F_{a,b}(\phi) < F_{a+1,b-1}(\phi')$.*

Proof. We have $L_{a,b}(\phi) = 1$ and $\alpha(\phi) < \beta(\phi)$, hence $L_{a+1,b-1} < 1$. Also, note that $F_{a+1,b-1}(\phi) = F_{a,b}(\phi) + f(\alpha) - f(\beta)$. By the Intermediate Value Theorem, there is a root of $L_{a+1,b-1} = 1$ between ϕ and 0. (Note that $L_{a+1,b-1}(0) \ge 2(a+1)/(t+1) + b - 1 > 1$.) Let ϕ' be the smallest such root. By (2), we have

$$\begin{aligned}
F_{a+1,b-1}(\phi') - F_{a+1,b-1}(\phi) &= \phi' L_{a+1,b-1}(\phi') - \phi L_{a+1,b-1}(\phi) - \int_{\phi}^{\phi'} L_{a+1,b-1}(\rho)\,d\rho \\
&= \phi' - \phi(1+\alpha-\beta) - \int_{\phi}^{\phi'} L_{a+1,b-1}(\rho)\,d\rho \\
&= \phi(\beta-\alpha) + (\phi'-\phi) - \int_{\phi}^{\phi'} L_{a+1,b-1}(\rho)\,d\rho \\
&> \phi(\beta-\alpha),
\end{aligned}$$

where the inequality is a consequence of the fact that $L_{a+1,b-1}(\rho) < 1$ for $\rho \in (\phi, \phi')$. Thus,

$$\begin{aligned}
F_{a+1,b-1}(\phi') - F_{a,b}(\phi) &= (F_{a+1,b-1}(\phi') - F_{a+1,b-1}(\phi)) + (F_{a+1,b-1}(\phi) - F_{a,b}(\phi)) \\
&> \phi(\beta-\alpha) + f(\alpha) - f(\beta).
\end{aligned}$$

So, it suffices to show

$$\frac{f(\beta) - f(\alpha)}{\beta - \alpha} \le \phi.$$

But by the Mean Value Theorem for some $\rho \in (\alpha, \beta)$, we have

$$\frac{f(\beta) - f(\alpha)}{\beta - \alpha} = g(\rho).$$

For all $\rho \in (\alpha, \beta)$, we have $g(\rho) < g(\alpha) = g(\beta) = \phi$ and so we are done. $\square$

Lemma 3.7. *If $\alpha < \beta \le 3/(t+1)$ satisfy $g(\alpha) = \phi = g(\beta)$, then*

$$\frac{2 - (t+1)\alpha}{(t+1)\beta - 2} \le 1.$$

Proof. First note that if $2/(t+1) \le \rho \le 3/(t+1)$ then we have

$$-h\Big(\frac{4}{t+1} - \rho\Big) = t\Big(1 + \rho - \frac{4}{t+1}\Big)^{t-2}((t+1)\rho - 2) \ge t(1-\rho)^{t-2}((t+1)\rho - 2) = h(\rho),$$

since by hypothesis $2\rho \ge \frac{4}{t+1}$. As a consequence if $2/(t+1) \le \rho \le 3/(t+1)$ then

$$g\Big(\frac{4}{t+1} - \beta\Big) \ge g(\beta), \text{ since } g(\beta) - g\Big(\frac{4}{t+1} - \beta\Big) = \int_{\frac{2}{t+1}}^{\beta} h(\rho) + h\Big(\frac{4}{t+1} - \rho\Big)\, d\rho \le 0.$$

Now to prove the result we note that since $g\big(\frac{4}{t+1} - \beta\big) \ge \phi = h(\beta)$ while $g(\alpha) = \phi$, and g is decreasing on the interval $\big(\frac{1}{t+1}, \frac{2}{t+1}\big)$ we must have $\alpha \ge \frac{4}{t+1} - \beta$, which implies the claim. $\square$

Lemma 3.8. *If $r - 1 \ge 2/((t+1)\alpha(\phi_{key}) - 1)$, i.e., $(t+1)\alpha(\phi_{key}) \ge (r+1)/(r-1)$, and $\phi \le \phi_{key}$ then $\frac{dL}{d\phi} \le 0$.*

Proof. We have, with $L = L_{r-1,1}$,

$$\begin{aligned} \frac{dL}{d\phi} &= \frac{r-1}{h(\alpha)} + \frac{1}{h(\beta)} \\ &= \frac{(r-1)t(1-\beta)^{t-2}((t+1)\beta - 2) + t(1-\alpha)^{t-2}((t+1)\alpha - 2)}{h(\alpha)h(\beta)}. \end{aligned}$$

The first term in the numerator is positive and the second is negative. The denominator is negative. Thus $\frac{dL}{d\phi} \le 0$ precisely if

$$(r-1)(1-\beta)^{t-2}((t+1)\beta - 2) \ge (1-\alpha)^{t-2}(2 - (t+1)\alpha),$$

i.e.,

$$\Big(\frac{1-\alpha}{1-\beta}\Big)^{t-2} \cdot \frac{2 - (t+1)\alpha}{(t+1)\beta - 2} = \frac{(t+1)\beta - 1}{(t+1)\alpha - 1} \cdot \frac{1-\beta}{1-\alpha} \cdot \frac{2 - (t+1)\alpha}{(t+1)\beta - 2} \le r - 1,$$

where we used the fact that

$$\Big(\frac{1-\alpha}{1-\beta}\Big)^{t-1} = \frac{(t+1)\beta-1}{(t+1)\alpha-1},$$

a simple consequence of the fact that $g(\alpha)=g(\beta)$. Both of the ratios $\frac{1-\beta}{1-\alpha}$ and $\frac{2-(t+1)\alpha}{(t+1)\beta-2}$ are at most one; the first because $\beta \ge \alpha$, the second because it is the content of Lemma 3.7, so it is sufficient to prove that $\frac{(t+1)\beta-1}{(t+1)\alpha-1} \le r-1$. But this fraction is clearly monotonically increasing in ϕ and we have, by hypothesis,

$$\frac{(t+1)\beta-1}{(t+1)\alpha-1} \le \frac{(t+1)\beta(\phi_{\text{key}})-1}{(t+1)\alpha(\phi_{\text{key}})-1} = \frac{2}{(t+1)\alpha(\phi_{\text{key}})-1} \le r-1.$$ □

Lemma 3.9. *The hypothesis of Lemma 3.8 holds, that is,*

$$(t+1)\alpha(\phi_{key}) \ge \frac{r+1}{r-1},$$

for all legal pairs (r,t).

Proof. It is sufficient to prove that, for legal pairs (r,t), we have

$$g\Big(\frac{r+1}{(r-1)(t-1)}\Big) \ge g\Big(\frac{3}{t+1}\Big).$$

Noting that both of these are negative, this is equivalent to

$$\frac{2}{r-1}\Big(1-\frac{r+1}{(r-1)(t+1)}\Big)^{t-1} \le 2\Big(1-\frac{3}{t+1}\Big)^{t-1},$$

i.e.,

$$\Big(\frac{t-\frac{2}{r-1}}{t-2}\Big)^{t-1} = \Big(1+\frac{1+\frac{r-3}{r-1}}{t-2}\Big)^{t-1} \le r-1.$$

The left-hand side converges, as t tends to infinity, to $\exp(1+(r-3)/(r-1))$. The smallest r for which $\exp(1+(r-3)/(r-1)) \le r-1$ is $r=6$. Checking of explicit values gives the conditions on r and t. □

Corollary 3.10. *For any legal pair (r,t), there is no root of $L=L_{r-1,1}=1$ with $\phi \le \phi_{key}$ and $\frac{dL}{d\phi}>0$.*

Lemma 3.11. *For legal pairs (r,t), there are at most two roots of $L_{r-1,1}=1$.*

Proof. Suppose that there are at least three roots of $L_{r-1,1}=1$, and let $0>\phi_1>\phi_2>\phi_3$ be the three largest. We must have $\frac{dL}{d\phi}>0$ at ϕ_1, so by Corollary 3.10, $\phi_1>\phi_{\text{key}}$. As we observed after Lemma 3.5, for L to be concave requires $\phi \le \phi_{\text{key}}$. Between ϕ_1 and ϕ_3, L must be concave at some point, so $\phi_3<\phi_{\text{key}}$. Also, we must have $\frac{dL}{d\phi}>0$ at ϕ_3 and this combination is ruled out by Corollary 3.10. □

Corollary 3.12. *For legal pairs (r,t), if $L = L_{r-1,1} = 1$ has multiple solutions, then the one at which F is maximized is the one with ϕ largest.*

Proof. By the previous Lemma, there cannot be three roots of $L_{r-1,1} = 1$. If there are two, say $0 > \phi_1 > \phi_2$, then by (2), we have

$$F(\phi_1) - F(\phi_2) = \phi L\Big|_{\phi_2}^{\phi_1} - \int_{\phi_2}^{\phi_1} L\, d\phi = (\phi_1 - \phi_2) - \int_{\phi_2}^{\phi_1} L\, d\phi > 0,$$

since $L < 1$ for $\phi \in (\phi_2, \phi_1)$. □

Now we're ready to complete the proof of our main result.

Proof of Theorem 3.4. First we show that F is not maximized on the boundary of the domain. Suppose, without loss of generality, that $\rho_1 = 0$ and $\rho_r \neq 0$. Let $\rho_1' = \rho_r' = \frac{\rho_r}{2}$. Each term of the sum defining F, other than the first and last, remains unchanged. Originally, the first term was 0 and the last was $\rho_r(1-\rho_r)^t$. Now each term is $\frac{\rho_r}{2}(1-\frac{\rho_r}{2})^t$, giving a sum of $\rho_r(1-\frac{\rho_r}{2})^t > \rho_r(1-\rho_r)^t$. We conclude points on the boundary cannot be maximizers.

As the domain of F is closed and bounded and F is continuous, it must achieve its maximum and thus that maximum must occur at an interior point. By Corollary 3.3, such points only occur at points of the form $(\alpha, \alpha, \ldots, \alpha, \beta, \beta, \ldots, \beta)$ where $\alpha < 2/(t+1) < \beta$ and $g(\alpha) = \phi = g(\beta)$ or at points of the form $(1/r, 1/r, \ldots, 1/r)$.

If there are no critical points of the first type, then the only interior critical point is the Turán solution. In this case, F must attain its maximum here.

Otherwise, there exists at least one skew critical point $(\alpha, \alpha, \ldots, \alpha, \beta, \beta, \ldots, \beta)$, say with a many αs and b many βs. Repeatedly applying Lemma 3.6 and finally applying Corollary 3.12, we see that the critical point at which F attains its maximum is either the Turán solution or the one associated with $a = r-1$ and $b = 1$ having ϕ largest. □

Remark. There are examples where the Turán solution wins and examples where the skew solution is better. For example, among legal pairs, the Turán solution is best when $r = 7$ and $5 \leq t \leq 12$ and the skew solution is best when $r = 7$ and $t = 13$. Numerical evidence suggests that the Turán solution is better for small t and the skew solution takes over for large t.

There remain many, many open problems in this area, even for the stars without cliques problem discussed in this section. We are working on the details of what happens for non-legal pairs, and resolving the question of when the skew solution is best.

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