An Extremal Problem Motivated by Triangle-Free Strongly Regular Graphs

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Abstract

We introduce the following combinatorial problem. Let $G$ be a triangle-free regular graph with edge density $\rho$. What is the minimum value $a(\rho)$ for which there always exist two non-adjacent vertices such that the density of their common neighborhood is $\leq a(\rho)$? We prove a variety of upper bounds on the function $a(\rho)$ that are tight for the values $\rho = 2/5, 5/16, 3/10, 11/50$, with $C_5$, Clebsch, Petersen and Higman-Sims being respective extremal configurations. Our proofs are entirely combinatorial and are largely based on counting densities in the style of flag algebras. For small values of $\rho$, our bound attaches a combinatorial meaning to so-called Krein conditions that might be interesting in its own right. We also prove that for any $\epsilon > 0$ there are only finitely many values of $\rho$ with $a(\rho) \geq \epsilon$ but this finiteness result is somewhat purely existential (the bound is double exponential in $1/\epsilon$).

1. Introduction

Triangle-free strongly regular graphs (TFSR graphs), sometimes also called SRNT (for strongly regular no triangles) is a fascinating object in algebraic combinatorics. Except for the trivial bipartite series, there are only seven such graphs known (see e.g. [God95]). At the same time, the existing feasibility conditions still leave out many possibilities for the triple $^2 (n, k, c)$.

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1In this paper all densities are normalized by $n, \frac{n^2}{2}$ etc. rather than by $n - 1, \binom{n}{2},\ldots$.

2It is well-known and will be reminded later that $n$ is actually determined by $k, c$. 

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where \( n \) is the number of vertices, \( k \) is the vertex degree and \( c \) is the number of common neighbours of two non-adjacent vertices. For example, there are about 60 prospective values for \((n, k, c)\) with \( \lambda_1 \leq 10 \), where \( \lambda_1 \) is the second largest eigenvalue of \( G \) (also computable from \( k, c \)) [Big11, Tables 1,2]. The most prominent of them is probably the hypothetical Moore graph \((c = 1)\) of degree \( k = 57 \). This situation is in sharp contrast with general strongly regular graphs (or, for that matter, with finite simple groups) where non-trivial infinite series are abundant, see e.g. [GR01, Chapter 10].

Somewhat superficially, the methods employed for studying (triangle-free) strongly regular graphs can be categorized in “combinatorial” and “arithmetic/algebraic” methods. The latter are based upon spectral properties of \( G \) or modular counting. The former are to a large extent based on calculating various quantities (that we will highly prefer to normalize in such a way that they become densities in \([0, 1]\)), and these calculations look remarkably similar to those used in asymptotic extremal combinatorics, particularly in the proofs based on flag algebras. The unspoken purpose of this paper is to highlight and distill these connections between the two areas. To that end, we introduce and study a natural extremal problem corresponding to strong regularity.

Before going into some technical details, it might be helpful to digress on the apparent contradiction of studying highly regular and inherently finite objects with methods that are quite analytical and continuous in their nature. The key to resolving this is the simple observation that has been used in extremal combinatorics many times: any finite graph (or, for that matter, more complicated combinatorial object) can be alternately viewed as an analytical object called its stepfunction graphon [Lov12, §7.1] or, in other words, infinite blow-up. It is obtained by replacing every vertex with a measurable set of appropriate measure. To this object we can already apply all methods based on density calculations, and the conversion of the results back to the finite world is straightforward.

Let us now fix some notation. All graphs \( G \) in this paper are simple and, unless otherwise noted, triangle-free. By \( n = n(G) \) we always denote the number of vertices, and let
\[
\rho = \rho(G) \overset{\text{def}}{=} \frac{2|E(G)|}{n(G)^2}
\]
be the edge density of \( G \). Note that the normalizing factor here is \( \frac{n^2}{2} \), not
(n \choose 2)$: the previous paragraph provides a good clue as why this is much more natural choice. A $\rho$-regular graph is a regular graph $G$ with $\rho(G) = \rho$. We let
\[ a(G) \overset{\text{def}}{=} \min_{(u,v) \notin E(G)} \frac{|N_G(u) \cap N_G(v)|}{n(G)}, \]
where $N_G(v)$ is the vertex neighbourhood of $v$. For a rational number $\rho \in [0, 1/2]$, we let
\[ a(\rho) \overset{\text{def}}{=} \max \{ a(G) \mid G \text{ is a triangle-free } \rho\text{-regular graph} \} \quad (1) \]
Our goal is to give upper bounds on $a(\rho)$.

**Remark 1** We stress that we do have here maximum, not just supremum, this will be proven below (see Corollary 4.5). In particular, $a(\rho)$ is also rational. Another finiteness result (Corollary 4.6) says that for every $\epsilon > 0$ there exist only finitely many rationals $\rho$ with $a(\rho) \geq \epsilon$. While this result is of somewhat existential nature (the bound is double exponential in $1/\epsilon$), it demonstrates, somewhat surprisingly, that our relaxed version of strong regularity still implies at least some rigidity properties that might be expected from much more regular structures in algebraic combinatorics.

**Remark 2** The definition of $a(G)$ readily extends to graphons, and it is natural to ask whether this would allow us to extend the definition of $a(\rho)$ to irrational $\rho$ or at least come up with interesting constructions beyond finite graphs: such constructions are definitely not unheard of in the extremal combinatorics. Somewhat surprisingly (again), the answer to both questions is negative. Namely, we have the dichotomy: every triangle-free graphon $W$ (we do not even need regularity here) is either a finite stepfunction of a finite vertex-weighted graph or satisfies $a(W) = 0$ (Theorem 4.7).

**Remark 3** Every TFSR graph $G$ with parameters $(n, k, c)$, where $k$ is the degree and $c$ is the size of common neighbourhoods of non-adjacent vertices leads to the lower bound $a(k/n) \geq c/n$. Thus, optimistically, one could view upper bounding the function $a(\rho)$ as an approach to finding more feasibility conditions for TFSR graphs based on entirely combinatorial methods. This hope is somewhat supported by the fact that our bound is tight for the values corresponding to four (out of seven) known TSFR graphs, as well as an infinite sequence of values not ruled out by other conditions.
Remark 4  As we will see below, in the definition (1) we can replace ordinary 
$\rho$-regular triangle-free graphs with weighted twin-free $\rho$-regular triangle-free 
graphs that can be additionally assumed to be maximal. A complete description 
of such graphs with $\rho > 1/3$ was obtained in [BT05]. Along with very 
simple Lemma 4.4 below, this allows us to completely compute the value of 
$a(\rho)$ for $\rho > 1/3$ and, in particular, determine those values of $\rho$ for which 
a(\rho) > 0. Using relatively simple methods from Section 5.1, we can prove 
the bounds $a(\rho) \leq \frac{\rho}{3} \ (1/3 \leq \rho \leq 3/8)$, $a(\rho) \leq 3\rho - 1 \ (3/8 \leq \rho \leq 2/5)$ and 
a(\rho) = 0 (2/5 < \rho < 1/2). But since they are significantly inferior (that is, 
for $\rho < 2/5$) to those that follow from [BT05], we will save space and in the 
rest of the paper focus on the range $\rho \leq 1/3$.

Our main result is shown on Figure 1. The analytical expressions for 
our upper bound $a_0(\rho)$ will be given in Theorem 3.1; for now let us briefly 
comment on a few features of Figure 1.

Remark 5  The bound is tight for the values $\rho = \frac{11}{50}, \frac{3}{10}, \frac{5}{16}$ corresponding to 
Higman-Sims, Petersen and Clebsch, respectively. It is piecewise linear for 
$\rho \geq 9/32$ and involves three algebraic functions of degree $\leq 4$ when $\rho \leq 9/32$. 

Figure 1: The main result
Remark 6 Let us explain the reasons for using the term “Krein bound”. It may not be seen well on Figure 1 but this curve has a singular point at

\[ \rho_0 \overset{\text{def}}{=} \frac{3}{98} (10 - \sqrt{2}) \approx 0.263. \]

For \( \rho \geq \rho_0 \), \( a_0(\rho) \) is a solution to a polynomial equation \( g_K(\rho, a) = 0 \) that is most likely an artifact of the proof method (and it gets superseded at \( \rho \approx 0.271 \) by other methods anyway). The bound for \( \rho \leq \rho_0 \) is more interesting.

The Krein parameters is an important invariant of associative schemes in the algebraic combinatorics. They are always non-negative, and this provides very powerful Krein conditions necessary for the existence of schemes with given parameters. For strongly regular graphs there are just two of them, \( K_1 \) and \( K_2 \) (see e.g. [GR01]), and in the special case of triangle-free graphs we are interested in this paper they can be further simplified [Big11]. The formulas from [Big11] are reproduced in the accompanying Maple worksheet to be found at http://people.cs.uchicago.edu/~razborov/files/tfsr.mw, it also contains supporting computations for the next paragraph.

More precisely, \( K_1, K_2 \) are rational functions of \( k, c \) and non-trivial eigenvalues \( \lambda_1, \lambda_2 \) of the adjacency matrix. When written as functions of \( k, c \), they become (conjugate) algebraic quadratic functions and thus do not seem to possess any obvious combinatorial meaning. Their \textit{product}, however, is the rational function in \( k, c \):

\[ K_1 K_2 = (k - 1)(k - c)(k^2 - k(3c + 1) - c^3 + 4c^2 - c) \geq 0 \]

Re-writing the non-trivial term here in the variables \( \rho = k/n, c = a/n \) (and recalling that \( n = 1 + \frac{k(k-1+c)}{c} \)), we will get a constraint \( f_K(\rho, a) \geq 0 \) that holds for all TFSR graphs. What we prove with purely combinatorial methods is that for \( \rho \leq \rho_0 \) (and less us remark that all hypothetical TFSR graphs are confined to that region) this inequality holds in much less rigid setting.

As a by-side heuristical remark, this bound was discovered by flag-algebraic computer experiments with particular values of \( \rho \) corresponding to potential TFSR graphs from [Big11, Tables 1,2]. The result turned out to be tight precisely for those values for which \( c = \lambda_1(\lambda_1 - 1) \), which is equivalent to \( K_2 = 0 \). The connection to Krein parameters and, as a consequence, the hypothesis \( f_K(\rho, a) \geq 0 \) suggested itself immediately.
2. Preliminaries

We utilize all notation introduced in the previous section. In particular, all graphs \( G = (V(G), E(G)) \) are simple and, unless otherwise noted, triangle-free, and \( n = n(G) \) is the number of vertices.

Let us now remind some rudimentary notions from the language of flag algebras (see [Raz07, §2.1]) restricted to graphs. A type \( \sigma \) is simply a totally labelled graph, that is a graph on the vertex set \([k] \defeq \{1, 2, \ldots, k\}\) for some \( k \) called the size of \( \sigma \). Figure 2 shows all types used in this paper, including the trivial type 0 of size 0.

![Figure 2: Types](image)

A flag is a graph partially labelled by labels from \([k]\) for some \( k \geq 0\). Every flag \( F \) belongs to the unique type obtained by removing all unlabelled vertices. Figure 3 lists all flags we need in this paper.

Mnemonic rules used in this notation are reasonably consistent: the subscript, when present, normally denotes the overall number of vertices in the flag. The first part of the superscript denotes the type of the flag. The remaining part, when present, helps to identify the flag in case of ambiguity. For example, there is only one flag \( P_3^N \) based on the path of length 2 and the type \( N \). There are, however, two flags based on its complement \( \bar{P}_3 \), and \( \bar{P}_3^{N,c} [\bar{P}_3^{N,b}] \) is the flag in which the first labelled vertex is the central [border, respectively] vertex in \( \bar{P}_3 \).
Figure 3: Flags
Also, for $S \subseteq [3]$ we denote by $F^T_S$ the flag with 3 labelled independent vertices and one unlabelled vertex connected to the vertices from $S$. Thus, $S^T_4 = F^T_{1,2,3}$ and $T^T_4 = F^T_{[3]}$.

Let $F$ be a flag of type $\sigma$ with $k$ labelled vertices and $\ell - k$ unlabelled ones, and $v_1, \ldots, v_k$ be (not necessarily distinct) vertices in the target graph $G$ that span the type $\sigma$, that is $(v_i, v_j) \in E(G)$ if and only if $(i, j) \in E(\sigma)$. Then we let $F(v_1, \ldots, v_k)$ be the probability that after picking $w_{k+1}, \ldots, w_{\ell} \in V(G)$ independently at random, the $\sigma$-flag induced in $G$ by $v_1, \ldots, v_k, w_{k+1}, \ldots, w_{\ell}$ is isomorphic (in the label-preserving way) to $F$. We stress that $w_{k+1}, \ldots, w_{\ell}$ are chosen completely independently at random; in particular some or all of them may be among $\{v_1, \ldots, v_k\}$. When this happens, we treat colliding vertices as non-adjacent twins.

We will also need some basic operations on flags (multiplication, evaluation and lifting operators, to be exact) but since they will not be needed until Section 5.2, we defer it until then.

In this notation $\rho = \frac{2|E(G)|}{n^2}$ is the edge density, $e(v) = \frac{|N_G(v)|}{n}$ is the relative degree of $v$ and $P^N_3(u, v) = \frac{|N_G(u) \cap N_G(v)|}{n^2}$ is the relative size of the common neighbourhood of $u$ and $v$. A graph $G$ is $\rho$-regular if $e(v) \equiv \rho$. Etc.

Warning. When evaluating [the density of] say $C_4$, we must take into account not only induced copies, but also contributions made by paths $P_3$ (one collapsing diagonal) and even by edges (both diagonals collapsing).

We let

$$a(G) \overset{\text{def}}{=} \min_{(u,v) \notin E(G)} P^N_3(u,v)$$

and, for a rational $\rho \in [0, 1/2]$, we also let

$$a(\rho) \overset{\text{def}}{=} \max \{a(G) \mid G \text{ a triangle-free } \rho\text{-regular graph} \}$$

(we will prove below that the maximum value here is actually attained).

3. The statement of the main result

Many of our statements and proofs, particularly for small values of $\rho$, involve rather cumbersome computations. As we already noted in the introduction, a Maple worksheet with supporting evidence can be found at http://people.cs.uchicago.edu/~razborov/files/tfsr.mw.
Let
\[ f_K(\rho, a) \overset{\text{def}}{=} a^3 + (3\rho - 4)a^2 + (5\rho - 1)a - 4\rho^3 + \rho^2. \]

Then
\[ f_K(\rho, \rho^2) = \rho^3(\rho^3 + 3\rho^2 - 4\rho + 1) > 0 \]
(since \( \rho \leq 1/3 \)) while
\[ f_K(\rho, \rho^2) = \rho^5(1 - 2\rho)/ (1 - \rho)^3 < 0. \]

Let \( \text{Krein}(\rho) \) be the largest (actually, the only) root of the cubic polynomial equation \( f_K(\rho, z) = 0 \) in the interval \( z \in [\rho^2, z_{\rho^2}] \).

Next, let
\[ g_K(\rho, a) \overset{\text{def}}{=} a^4 + a^3((4\sqrt{2} - 8)\rho + 7 - 4\sqrt{2}) + a^2\rho((6 - 4\sqrt{2})\rho + 8\sqrt{2} - 13) + a\rho^2 + (15 - 10\sqrt{2})\rho + 2\sqrt{2} - 3) + \rho^3((8\sqrt{2} - 12)\rho + 3 - 2\sqrt{2}) \]
(the meaning of this expression might become clearer in Section 5.2.1). We again have \( g_K(\rho, \rho^2) > 0 \),
\[ g_K(\rho, \frac{\rho^2}{1 - \rho}) = -\frac{\rho^7(1 - 2\rho)}{(1 - \rho)^4} < 0, \quad (4) \]
and we define \( \hat{\text{Krein}}(\rho) \) as the largest (unique) root of the equation \( g_K(\rho, z) = 0 \) in the interval \( z \in [\rho^2, \frac{\rho^2}{1 - \rho}] \).

We note that \( \hat{\text{Krein}}(\rho_0) = \hat{\text{Krein}}(\rho_0) = \frac{\rho_0}{3} \) (recall that \( \rho_0 \) is given by (2)), and that they have the same first derivative at \( \rho = \rho_0 \) as well. It should also be noted that \( \hat{\text{Krein}}(\rho) \geq \text{Krein}(\rho) \) and that they are very close to each other. For example, let
\[ \rho_1 \approx 0.271 \]
bethe appropriate root of the equation \( g_K(\rho, \frac{1 - 3\rho}{2}) = 0 \); this is the point at which Krein bounds yield to more combinatorial methods, see Figure 1. Then in the relevant interval \( \rho \in [\rho_0, \rho_1] \) we have \( \hat{\text{Krein}}(\rho) \leq \text{Krein}(\rho) + 3 \cdot 10^{-6} \).

\(^3\)This is the non-trivial factor in (3) re-written in terms of \( \rho, a \).

\(^4\)The left end of this interval is determined entirely by convenience, but the right end represents a trivial upper bound on \( a(\rho) \) resulting from double counting copies of \( C_4 \). See the calculation after (41) for more details.
We finally let

\[ \text{Improved}(\rho) \overset{\text{def}}{=} \frac{15 - 22\rho - 2\sqrt{242\rho - 27} - 508\rho^2}{74}, \]

and let

\[ \rho_2 \overset{\text{def}}{=} \frac{66 + 2\sqrt{13}}{269} \approx 0.272 \]

be the root of the equation \( \text{Improved}(\rho) = \frac{1 - 3\rho}{2} \).

We can now explain Figure 1 as follows:

**Theorem 3.1** For \( \rho \leq 1/3 \) we have \( a(\rho) \leq a_0(\rho) \), where

\[
a_0(\rho) \overset{\text{def}}{=} \begin{cases}
    \text{Krein}(\rho), & \rho \in [0, \rho_0] \\
    \text{Krein}(\rho), & \rho \in [\rho_0, \rho_1] \\
    \frac{1 - 3\rho}{2}, & \rho \in [\rho_1, \rho_2] \\
    \text{Improved}(\rho), & \rho \in [\rho_2, 9/32] \\
    \rho/3, & \rho \in [9/32, 3/10] \\
    2\rho - \frac{1}{2}, & \rho \in [3/10, 5/16] \\
    \frac{2}{5}\rho, & \rho \in [5/16, 1/3].
  \end{cases}
\]

4. **Finiteness results**

Before embarking on the proof of Theorem 3.1, let us fulfill the promise made in Remarks 1 and 2.

Throughout the paper we will be mostly working with (vertex)-weighted graphs, i.e. with graphs \( G \) equipped with a probability measure \( \mu \) on \( V(G) \), ordinary graphs corresponding to the uniform measure. The flag-algebraic notation \( F(v_1, \ldots, v_k) \) introduced in Section 2 readily extends to this case simply by changing the sampling distribution from uniform to \( \mu \).

The *twin relation* \( \approx \) on \( G \) is given by \( u \approx v \) iff \( N_G(u) = N_G(v) \), and a graph \( G \) is *twin-free* if its twin relation is trivial. Factoring a graph by its twin relation gives us a *twin-free weighted* graph \( G^{\text{red}} \) that preserves all properties of the original graph \( G \) (like the values \( \rho(G) \) and \( a(G) \), \( \rho \)-regularity or triangle-freeness) we are interested in this paper.

Our main technical argument in this section is the following
**Theorem 4.1** Let \((G, \mu)\) be a vertex-weighted triangle-free twin-free graph and \(a \overset{\text{def}}{=} a(G, \mu)\). Then

\[ n(G) \leq (2a^{-1})^{1+a^{-1}} + 2a^{-1}. \]

**Proof.** Let \(n \overset{\text{def}}{=} n(G)\) and \(V(G) \overset{\text{def}}{=} \{v_1, \ldots, v_n\}\), where \(\mu(v_1) \geq \ldots \geq \mu(v_n)\). Choose the maximal \(k\) with the property \(\mu(\{v_k, \ldots, v_n\}) \geq a/2\). Then, by averaging, we have \(1 - a/2 \leq \frac{a/2}{n-k+1}\) which is equivalent to

\[ n \leq 2a^{-1}(n - k + 1). \]

Hence, denoting

\[ W_0 \overset{\text{def}}{=} \{v_{k+1}, \ldots, v_n\} \]

(note for the record that \(\mu(W_0) < a/2\)), it suffices to prove that

\[ |W_0| \leq (2a^{-1})^{a^{-1}}. \] (5)

For \(W \subseteq V(G)\) let us define

\[ K(W) \overset{\text{def}}{=} \bigcap_{w \in W} N_G(w); \]

note that \(K(W) \cap W = \emptyset\). The bound (5) will almost immediately follow from the following two claims.

**Claim 4.2** For any \(W \subseteq V(G)\) and \(v^* \not\in W \cup K(W)\) we have

\[ \mu \left( \left( \bigcup_{v \in K(W)} N_G(v) \right) \cup N_G(v^*) \right) \geq \mu \left( \bigcup_{v \in K(W)} N_G(v) \right) + a. \]

**Proof of Claim 4.2.** Since \(v^* \not\in K(W)\), there exists \(w \in W\) such that \((v^*, w) \not\in E(G)\); moreover, \(w \neq v^*\) since \(v^* \not\in W\). Now, all vertices in \(N_G(v^*) \cap N_G(w)\) contribute to the difference \(N_G(v^*) \setminus \bigcup_{v \in K(W)} N_G(v)\) (since \(w \in W\) and \(G\) is triangle-free).\(\blacksquare\)

**Claim 4.3** For every \(W \subseteq V(G)\) with \(\mu(W) \leq a/2\) and \(|W| \geq 2\) there exists \(v^* \not\in W \cup K(W)\) such that\(^5\)

\[ |W \cap N_G(v^*)| \geq \frac{a}{2}|W|. \]

\(^5\)note that this bound is about absolute sizes, not about measures.
Proof of Claim 4.3. Let
\[ L(W) \overset{\text{def}}{=} \{ v \not\in W \mid N_G(v) \cap W \not\subseteq \{ \emptyset, W \} \}. \]

Note that \( L(W) \) is disjoint from both \( W \) and \( K(W) \) and that there are no edges between \( K(W) \) and \( L(W) \). The desired vertex \( v^* \) will belong to \( L(W) \), and we consider two (similar) cases.

**Case 1.** \( K(W) = \emptyset \).
In this case we have
\[ L(W) = \left( \bigcup_{w \in W} N_G(w) \right) \setminus W. \tag{6} \]

W.l.o.g. we can assume that \( n \geq 3 \) which implies (since \( G \) is twin-free) that \( G \) is not a star. That is, for every \( w \in V(G) \) there exists \( v \neq w \) non-adjacent to it and hence we have the bound \( e(w) \geq \Delta^N(v, w) \geq a \) on the minimum degree. Along with (6) and the assumption \( \mu(W) \leq a/2 \), we get \( \mu(N_G(w) \cap L(W)) \geq a/2 \) for any \( w \in W \). Now the existence of the required \( v^* \in L(W) \) follows by standard double counting of edges between \( W \) and \( L(W) \) (note that, unlike \( L(W) \), the set \( W \) is not weighted in this argument according to \( \mu \)).

**Case 2.** \( K(W) \neq \emptyset \).
Then \( W \) is independent and the condition \( v \not\in W \) in the definition of \( L(W) \) can be dropped. Fix arbitrarily \( w \neq w' \in W \) (this is how we use the assumption \(|W| \geq 2\)). Then \( w, w' \) are not twins and \( N_G(w) \Delta N_G(w') \subseteq L(W) \), hence \( L(W) \neq \emptyset \). Fix arbitrarily \( v \in L(W) \) and \( w \in W \) with \( (v, w) \notin E(G) \). Then
\[ N_G(v) \cap N_G(w) \subseteq L(W) \tag{7} \]
(since \( W \) is independent and there are no edges between \( L(W) \) and \( K(W) \)) hence \( \mu(L(W)) \geq a \). We claim that actually \( \mu(N_G(w) \cap L(W)) \geq a \) for every \( w \in W \). Indeed, if \( N_G(w) \supseteq L(W) \) this follows from the bound we have just proved, and if there exists \( v \in L(W) \) with \( (v, w) \notin E(G) \), this follows from (7). The analysis of Case 2 is now completed by the same averaging argument as in Case 1 (with the final bound improved by a factor of two). □

Claim 4.3

The rest of the proof of Theorem 4.1 is easy. We start with the set \( W_0 \) and then, using Claims 4.3 and 4.2, recursively construct sets \( W_0 \supset W_1 \supset \)
such that \(|W_r| \geq (a/2)^r|W_0|\) and

\[
\mu \left( \bigcup_{v \in K(W_r)} N_G(v) \right) \geq ar. \tag{8}
\]

More specifically, once \(W_r\) is constructed and \(|W_r| \geq 2\), we pick up a vertex \(v^*\) guaranteed by Claim 4.3 and set \(W_{r+1} := W \cap N_G(v^*)\). Then the bound (8) follows from Claim 4.2 by an obvious induction.

This process may terminate for only one reason: when the assumption \(|W_r| \geq 2\) no longer holds. On the other hand, due to (8), it must terminate within \(a^{-1}\) steps. The bound (5) follows, and this also completes the proof of Theorem 4.1.

Remark 7 The bound in Theorem 4.1 is essentially tight. Indeed, let us consider the graph \(G_h\) on \(n = 2h + 2^h\) vertices

\[\{u_{i\epsilon} \mid i \in [h], \epsilon \in \{0, 1\}\} \cup \{v_a \mid a \in \{0, 1\}^h\},\]

and let \(E(G_h)\) consist of the matching \(\{(u_{i0}, u_{i1}) \mid i \in [h]\}\) \(\cup\) \(\{(v_a, v_{a-\epsilon}) \mid a \in \{0, 1\}^h\}\) as well as the cross-edges \(\{(u_{i\epsilon}, v_a) \mid a(i) = \epsilon\}\). Then \(G\) is a triangle-free twin-free graph and for every \((w, w') \notin E(G), N_G(w) \cap N_G(w')\) either contains an \(u\)-vertex or contains at least \(2^{h-2}\) \(v\)-vertices. Hence if we set up the weights

\[\mu(u_{i\epsilon}) = \frac{1}{4^h}\]

and \(\mu(v_a) = 2^{-h-1}\), we will have \(a(G, \mu) \geq \frac{1}{4^h}\) and \(n(G)\) is inverse exponential in \(a(G, \mu)^{-1}\).

Before deriving consequences mentioned in the introduction, we need a simple exercise in linear algebra (and optimization).

Lemma 4.4 Let \(G\) be a finite graph. Then there exists at most one value \(\rho = \rho_G\) for which there exist vertex weights \(\mu\) such that \((G, \mu)\) is \(\rho\)-regular. Whenever \(\rho_G\) exists, it is a rational number. Moreover, in that case there are rational weights \(\eta\) such that \((G, \eta)\) is \(\rho_G\)-regular and

\[a(G, \eta) = \max \{a(G, \mu) \mid (G, \mu) \text{ is } \rho_G \text{-regular}\}.\]

\(^6\)We could have shaved off an extra factor \(2^{r-1}\) by observing that Case 1 in Claim 4.3 may occur at most once.
Proof. Fix an arbitrary system of weights \( \mu \) for which \((G, \mu)\) is \(\rho\)-regular for some \(\rho\). Let \(A\) be the adjacency matrix of \(G\), \(\mu\) be the (column) vector comprised of vertex weights and \(j\) be the identically one vector. Then the regularity condition reads as \(A\mu = \rho \cdot j\). Since \(j\) is in the space spanned by the columns of \(A\), there exists a \textbf{rational} vector \(\eta\) such that \(A\eta = j\). Now, on the one hand \(\eta^T A \mu = \rho \cdot (\eta^T j)\) and, on the other hand, \(\eta^T A \mu = j^T \mu = 1\) (the latter equality holds since \(\mu\) is a probability measure). Hence \(\rho = (\eta^T j)^{-1}\) is a rational number not depending on \(\mu\).

For the second part, we note that the linear program

\[
\begin{align*}
\eta(v) &\geq 0 & (v \in V(G)) \\
\sum_v \eta(v) &= 1 \\
e(v) &= \rho & (v \in V(G)) \\
P_3^N(v, w) &\geq a & ((v, w) \not\in E(G))
\end{align*}
\]

with rational coefficients in the variables \(\eta(v)\) is feasible since \(\mu\) is its solution. Hence it also has an optimal solution with rational coefficients.\(\blacksquare\)

Let us now derive consequences.

**Corollary 4.5** For every rational \(\rho\) there exists a finite triangle-free \(\rho\)-regular graph \(G\) such that \(a(G)\) attains the maximum value \(a(\rho)\) among all such graphs.

**Proof.** We can assume w.l.o.g. that \(a(\rho) > 0\). Let \(\{G_n\}\) be an increasing sequence of graphs such that \(\lim_{n \to \infty} a(G_n) = a(\rho)\). Then Theorem 4.1 implies that \(\{G_n^{\text{red}}\}\) may assume only finitely many values. Hence (by going to a subsequence) we can also assume that all \(G_n\) correspond to different vertex weights \(\mu_n\) of the same (twin-free) graph \(G\). But now Lemma 4.4 implies the existence of rational weights \(\eta(v)\), say \(\eta(v) = \frac{N_v}{N}\) for integers \(N_v, N\) such that \(a(G, \eta) = a(\rho)\). We convert \((G, \eta)\) to an ordinary graph replacing every vertex \(v\) with a cloud of \(N_v\) twin clones.\(\blacksquare\)

**Corollary 4.6** For every \(\epsilon > 0\) there are only finitely many \(\rho\) with \(a(\rho) \geq \epsilon\). In other words, \(0\) is the only accumulation point of \(\text{im}(a)\).
Proof. According to Lemma 4.4, the edge density $\rho$ is completely determined by the skeleton $G$ of a $\rho$-regular weighted graph $(G, \mu)$, and then Theorem 4.1 implies that there are only finitely many such $G$.\[\blacksquare\]

Now we prove that there are no “inherently infinite” triangle-free graphons $W$ with $a(W) > 0$. Since this result is somewhat tangential to the rest of the paper, we will be rather sketchy and in particular we refer the reader to [Lov12] for all missing definitions.

A graphon $W : [0,1] \times [0,1] \rightarrow [0,1]$ is triangle-free if
$$\int \int \int W(x, y)W(y, z)W(x, z)dx dy dz = 0.$$ Given a graphon $W$, let $P_3^N : [0,1] \times [0,1] \rightarrow [0,1]$ be defined by $P_3^N(x, y) = \int W(x, z)W(y, z)dz$; Fubini’s theorem implies that $P_3^N$ is defined a.e. and is measurable. We define $a(W)$ as the maximum value $a$ such that
$$\lambda \left( \left\{ (x, y) \in [0,1]^2 \big| W(x, y) < 1 \implies P_3^N(x, y) \geq a \right\} \right) = 1.$$ (9)

To every finite vertex-weighted graph $(G, \mu)$ we can associate the naturally defined step-function graphon $W_{G, \mu}$ (see [Lov12, §7.1] or Section 1 above), and two graphons are isomorphic if they have the same sampling statistics [Lov12, §7.3].

Theorem 4.7 Let $W$ be a triangle-free graphon. Then we have the following dichotomy: either $a(W) = 0$ or $W$ is isomorphic to $W_{G, \mu}$ for some finite vertex-weighted triangle-free graph $(G, \mu)$.

Proof. (sketch) Assume that $a(W) > 0$, that is (9) holds for some $a > 0$. Let $G_n$ be the random sample from the graphon $W$; this is a probability measure on the set $G_n$ of triangle-free graphs on $n$ vertices up to isomorphism. A standard application of Chernoff’s bound along with (9) gives us that
$$\Pr[a(G_n) \leq a/2] \leq \exp(-\Omega(n)).$$ (10)

Now, if we equip $\prod_{n \in \mathbb{N}} G_n$ with the product measure $\prod_n G_n$, then the fundamental fact from the theory of graph limits is that the sequence of graphs $G_n$ sampled according to this measure converges to $W$ with probability 1, and the same holds for their twin-free reductions $G_n^{\text{red}}$. Since the series $\sum_n \exp(-\Omega(n))$ converges, Theorem 4.1 along with (10) implies that the number of vertices in $G_n^{\text{red}}$ is bounded, also with probability 1. Then a simple compactness argument shows that it contains a sub-sequence converging to $W_{G, \mu}$ for some finite weighted graph $(G, \mu)$.\[\blacksquare\]
5. The proof of Theorem 3.1

We fix a triangle-free $\rho$-regular graph $G$, and for the reasons explained in Remark 4, we assume that $\rho \leq \frac{1}{3}$. We have to prove that $a(G) \leq a_0(\rho)$, that is there exists a pair of non-adjacent vertices $u, v$ with $P^N_3(u, v) \leq a_0(\rho)$. We work in the set-up of Section 4, that is we replace $G$ with its weighted twin-free reduction $(G, \mu)$; the weights $\mu$ will be dropped from notation whenever it may not create confusion. We also let $a \overset{\text{def}}{=} a(G, \mu) > 0$ throughout.

5.1. $\rho \geq \rho_1$: exploiting combinatorial structure

The only way in which we will be using twin-freeness is the following claim (that was already implicitly used in the proof of Theorem 4.1).

Claim 5.1 For any two non-adjacent vertices $u \neq v$, $P^N_3(u, v) \leq \rho - a$.

Proof. First we have $P^N_3(u, v) + \bar{P}^{N,c}_3(u, v) = e(v) = \rho$. Thus it remains to prove that $\bar{P}^{N,c}_3(u, v) \geq a$. But since $u$ and $v$ are not twins and $e(u) = e(v)$, there exists a vertex $w \in N_G(u) \setminus N_G(v)$. Then $a \leq P^N_3(v, w) \leq \bar{P}^{N,c}_3(u, v)$, the last inequality holds since $G$ is triangle-free.\[\text{\[11\]}\]

5.2. $\rho \geq \rho_1$: exploiting combinatorial structure

The only way in which we will be using twin-freeness is the following claim (that was already implicitly used in the proof of Theorem 4.1).

Claim 5.2 For any $w \in P$ there exists $v_3 \in I$ such that $(w, v_3) \notin E$.

Proof. The assumptions $\rho \leq \frac{1}{3}$ and $a > 0$ imply, along with (11), that $I^N_3(v_1, v_2) > \rho$. As $e(w) = \rho$, Claim 5.2 follows.\[\text{\[12\]}\]

Before proceeding further, let us remark that $a_0(\rho) \geq \frac{\rho}{3}$ for $\rho \in [\rho_1, 1/3]$ (verifications of computationally unpleasant statements like this one can be found in the Maple worksheet at http://people.cs.uchicago.edu/~razborov/files/tfsr.mw). Hence we can and will assume w.l.o.g. that

$$a > \frac{\rho}{3} \quad \text{(12)}$$

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Claim 5.3 For any \( v_3 \in I \) we have \( S^I_4(v_1, v_2, v_3) > 0 \), that is there exists a vertex \( w \in P \) adjacent to \( v_3 \).

Proof. Since \( P \) is non-empty, we can assume w.l.o.g. that \( \exists w \in P ((v_3, w) \not\in E) \) (otherwise we are done). Now we have the computation (again, since \( G \) is triangle-free)

\[
\rho = c(v_3) \geq P_3^N(v_3, v_1) + P_3^N(v_3, v_2) + P_3^N(v_3, w) - S^I_4(v_1, v_2, v_3) \\
\geq 3a - S^I_4(v_1, v_2, v_3). \tag{13}
\]

The claim now follows from (12). \( \blacksquare \)

Let now \( c \overset{\text{def}}{=} |P| \) be the size of \( P \) (weights are ignored). Claims 5.2 and 5.3 together imply that \( c \geq 2 \). The rest of the analysis depends on whether \( c = 2 \), \( c = 3 \) or \( c \geq 4 \).

5.1.1. \( c = 2 \)

Let \( P = \{w, w'\} \), where \( \mu(w) \geq \mu(w') \), and note that \( \mu(w') \leq \frac{a}{2} \). By Claim 5.2, there exists \( v_3 \in I \) such that \((w, v_3) \not\in E\). We have \( S^I_4(v_1, v_2, v_3) \leq \mu(w') \leq \frac{a}{2} \). Along with (13), this gives us the bound

\[
a \leq \frac{2}{5} \rho. \tag{14}
\]

By Claim 5.3, for any \( v_3 \in I \) we have either \((w, v_3) \in E(G)\) or \((w', v_3) \in E(G)\). In other words, the neighbourhoods of \( v_1, v_2, w, w' \) cover the whole graph or, equivalently, \( I^N_3(v_1, v_2) + I^N_3(w, w') = 1 \). Now, \( I^N_3(v_1, v_2) = 1 - 2\rho + a \) by (11), and for \((w, w')\) this calculation still works in the “right” direction: \( I^N_3(w, w') = 1 - 2\rho + P_3^N(w, w') \geq 1 - 2\rho + a \). Thus we get \( a \leq 2\rho - \frac{1}{2} \).

Along with (14), we get that \( a \leq \min \left( \frac{2}{5} \rho, 2\rho - \frac{1}{2} \right) \leq a_0(\rho) \) (see the Maple worksheet) and this completes the analysis of the case \( c = 2 \).
5.1.2.  \( c = 3 \)

Let \( P = \{w_1, w_2, w_3\} \). We abbreviate \( F_{ij}^T(w_1, w_2, w_3) \) to \( F_i \), \( F_{ij}^{(1,2,3)}(w_1, w_2, w_3) \) to \( F_{ij} \) and \( F_{(1,2,3)}^T(w_1, w_2, w_3) (= S_4^T(w_1, w_2, w_3)) \) to \( f_3 \). In our claims below we will always assume that \( \{i, j, k\} = \{1, 2, 3\} \) is an arbitrary permutation on three elements.

We begin with noticing that Claim 5.1 applied to the pair \((w_i, w_k)\) gives us \( F_{ik} + f_3 \leq \rho - a \) that can be re-written (since \( F_i + F_{ij} + F_{ik} + f_3 = e(w_i) = \rho \)) as

\[
F_i + F_{ij} \geq a. \tag{15}
\]

On the other hand, the bound \( P_3^N(w_i, w_j) \geq a \) re-writes as

\[
F_{ij} + f_3 \geq a. \tag{16}
\]

We also note that (15) (along with its analogue obtained by changing \( F_i \) to \( F_j \)) implies

\[
F_{ij} = 0 \implies (F_i \geq a \land F_j \geq a). \tag{17}
\]

**Claim 5.4** \( F_{ij} > 0 \implies F_k \geq a. \)

**Proof.** Let \( v \) be any vertex contributing to \( F_{ij} \), that is \( (w_i, v), (w_j, v) \in E(G) \) while \( (w_k, v) \notin E(G) \). Then \( a \leq P_3^N(w_k, v) \leq F_k. \)

Now, (17) along with Claim 5.4 imply that there exist at least two indices \( i \in [3] \) with \( F_i \geq a \). Assume w.l.o.g. that \( F_1, F_2 \geq a \). Our goal (that, somewhat surprisingly, is the most complicated part of the analysis) is to show that in fact \( F_3 \geq a \) as well.

**Claim 5.5** \( F_i > 0. \)

**Proof.** When \( i = 1 \) or \( i = 2 \), we already have the stronger fact \( F_i \geq a \) so we are only left to show that \( F_3 > 0 \). Assume the contrary. Then \( F_{12} = 0 \) by Claim 5.4, hence \( f_3 \geq a \) by (16). Also, \( F_{13} \geq a \) and \( F_{23} \geq a \) by (15) (with \( i = 3 \)). Summing all this up, \( \rho = e(w_3) = F_{13} + F_{23} + f_3 \geq 3a \), contrary to the assumption (12).\]

The next claim, as well as Claim 5.13 below, could have been also written very concisely at the expense of introducing a few more flags; we did not do this since those flags are not used anywhere else in the paper.
Claim 5.6 There is an edge between [the sets of vertices corresponding to] $F_i$ and $F_j$.

Proof. Since $\{i,j\} \cap \{1,2\} \neq \emptyset$, we can assume w.l.o.g. that $i = 1$. We have

$$\rho = e(w_1) = F_1 + F_{1j} + F_{1k} + f_3$$

and $F_1 \geq a$, $F_{1j} + f_3 \geq a$ (by (16)). Hence $F_{1k} < a$ due to (12). Let now $v$ be an arbitrary vertex contributing to $F_j$ that exists by Claim 5.5. We have

$P^N(v, w_1) \geq a$, and all contributions to it come from either $F_{1k}$ or $F_1$. Since $F_{1k} < a$, $v$ must have at least one neighbor in $F_1$.

Claim 5.7 $F_i + F_{ij} + F_{ik} \geq 2a$.

Proof. Let $v, v'$ be as in Claim 5.6 with $i := k$, i.e. $(v, v') \in E(G)$, $v$ contributes to $F_k$ and $v'$ contributes to $F_j$. Then $2a \leq P^N(v, i, v) + P^N(v, i, v') \leq F_i + F_{ij} + F_{ik}$ simply because $(v, v')$ is an edge, and this implies that the sets corresponding to $P^N(v, i, v)$, $P^N(v, i, v')$ are disjoint.

Claim 5.8 $F_{ij} > 0$.

Proof. Assuming the contrary, we get $f_3 \geq a$ from (16) and $F_i + F_{ik} \geq 2a$ from Claim 5.7. This (again) contradicts $e(w_i) = \rho < 3a$.

Now we finally have

Claim 5.9 $F_i \geq a$.

Proof. Immediate from Claims 5.4 and 5.8.

Claim 5.10 $\mu(w_i) + F_{jk} \geq 4a - \rho$.

Proof. Let (by Claim 5.9) $v$ be any vertex contributing to $F_i$. Then we have the computation (cf. (13)):

$$\rho = e(v) = T^4(v_1, v_2, v) + P^N_3(v_1, v) + P^N_3(v_2, v) - S^4(v_1, v_2, v) \geq T^4(v_1, v_2, v) + 2a - \mu(w_i).$$

(18)
On the other hand,
\[ 2a \leq P^N_3(v, w_j) + P^N_3(v, w_k) \leq T^L_4(v_1, v_2, v) + F_{jk} \]  \hspace{1cm} (19)
(note that \( v \) may not be connected to vertices in \( F_{ij}, F_{ik}, f_3 \) as it would have created a triangle with \( w_i \)). The claim follows from comparing these two inequalities.

Let us now extend the notation \( f_3 = F_{(1,2,3)} \) to \( f_\nu \overset{\text{def}}{=} \sum_{S \in \binom{[\nu]}{\rho}} F_S \).

Then Claim 5.3 implies \( f_0 = 0 \) and hence
\[ f_1 + f_2 + f_3 = \mu(I) = 1 - 2\rho + a \]  \hspace{1cm} (20)

and also
\[ f_1 + 2f_2 + 3f_3 = \sum_i e(w_i) = 3\rho. \]  \hspace{1cm} (21)

Next, Claim 5.9 implies
\[ f_1 \geq 3a \]  \hspace{1cm} (22)

and Claim 5.10, after summing it over \( i \in [3] \) gives us
\[ f_2 \geq 11a - 3\rho. \]  \hspace{1cm} (23)

Resolving (20) and (21) in \( f_3 \), we get
\[ 2f_1 + f_2 = 3 - 9\rho + 3a. \]  \hspace{1cm} (24)

Comparing this with (22) and (23) gives us the bound
\[ a \leq \frac{3}{14}(1 - 2\rho) \]  \hspace{1cm} (25)

which is \( \leq a_0(\rho) \) as long as \( \rho \in [9/32, 1/3] \).

To complete the analysis of case \( c = 3 \) we still have to prove that \( a(\rho) \leq \text{Improved}(\rho) \) for \( \rho_1 \leq \rho \leq \frac{9}{32} \). As it uses some material from the proof of the Krein bound, we defer this to Section 5.2.2.
5.1.3. \( c \geq 4 \)

Fix arbitrarily distinct \( w_1, w_2, w_3, w_4 \in P \) and let us employ the same notation \( F_i, F_{ij}, F_{ijk}, F_{ijkl} \) as in the previous section, with the exception that now these flags belong to the type that consists of four independent vertices. Likewise, we always assume that \( \{i, j, k, \ell\} = \{1, 2, 3, 4\} \) and let

\[
f_{\nu} = \sum_{S \in \binom{\nu}{4}} F_S.
\]

Note that since we allow \( c > 4 \), this time \( f_0 \) need not necessarily be zero. We further let

\[
\hat{F}_S \overset{\text{def}}{=} \sum_{T \subseteq \{i, j, k, \ell\} \setminus S \neq \emptyset} F_T
\]

be the measure of \( \bigcup_{i \in S} N_G(w_i) \), and we also use abbreviations \( \hat{F}_i, \hat{F}_{ij}, \hat{F}_{ijk}, \hat{F}_{1234} \) in this case.

To start with, \( \hat{F}_i = \rho \) and Claim 5.1 implies \( \hat{F}_{ij} \geq \rho + a \).

Claim 5.11 \( \hat{F}_{ijk} \geq \rho + 2a \).

**Proof.** For \( S \subseteq \{i, j, k\} \), let \( F^*_S \overset{\text{def}}{=} F_S + F_{S \cup \{\ell\}} \) be the result of ignoring \( w_{\ell} \) and we (naturally) let

\[
f^*_\nu = \sum_{S \in \binom{\nu}{i, j, k}} F^*_S.
\]

Then (cf. (21))

\[
f_1^* + 2f_2^* + 3f_3^* = 3\rho,
\]

and also

\[
f_2^* + 3f_3^* = P_3^N(w_i, w_j) + P_3^N(w_i, w_k) + P_3^N(w_j, w_k) \leq 3(\rho - a)
\]

by Claim 5.1. Besides, \( \hat{F}_{ijk} = f_1^* + f_2^* + f_3^* \).

If \( f_2^* = 0 \), we are done: \( \hat{F}_{ijk} = 3\rho - 2f_3^* \geq 3\rho - 2(\rho - a) = \rho + 2a \).

Hence we can assume that \( f_2^* > 0 \), say, \( F_{ij}^* > 0 \). Pick an arbitrary vertex \( v \) corresponding to \( F_{ij}^* \) then, as before, \( \hat{F}_{ijk} = \hat{F}_{ij} + F_k^* \geq \rho + a + P_3^N(v, w_k) \geq \rho + 2a \).

**Lemma 5.12** \( \hat{F}_{1234} \geq \rho + 3a \).
Proof. First, \( \hat{F}_{1234} = \hat{F}_{jk\ell} + F_i \geq \rho + 2a + F_i \) by Claim 5.11. Hence we can assume that \( F_i < a \) (for all \( i \in [4] \), as usual). This implies that \( f_3 = 0 \) since if, say \( v \) were a vertex corresponding to the flag \( F_{jk\ell} \), we would have had \( P_3^N(v, w_3) \leq F_i \), in contradiction to the assumption \( F_i < a \).

Now, let \( \Gamma \) be the graph on \([4]\) with the set of edges

\[
E(\Gamma) = \{ (i, j) \mid F_{ij} > 0 \}.
\]

Analogously to (15), we have

\[
F_i + F_{ij} + F_{i\ell} \geq a
\]

(recall that \( F_{ij\ell} = 0 \)) and, analogously to Claim 5.4,

\[
F_{ij} > 0 \implies F_k + F_{k\ell} \geq a.
\]

Next, (26), along with \( F_i < a \), implies that the minimum degree of \( \Gamma \) is \( \geq 2 \), that is \( \Gamma \) is the complement of a matching. Hence there are only three possibilities: \( \Gamma = K_4 \), \( \Gamma = C_4 \) or \( \Gamma = K_4 - e \), and the last one is ruled out by (27) along with \( F_k < a \).

If \( \Gamma = K_4 \) then summing up (27) over all choices of \( k, \ell \), we get \( 3f_1 + 2f_2 \geq 12a \). Adding this with \( f_1 + 2f_2 + 4f_4 = 4\rho \), we get \( \hat{F}_{1234} = f_1 + f_2 + f_4 \geq \rho + 3a \). Thus it remains to deal with the case \( \Gamma = C_4 \), say \( E(\Gamma) = \{ (1, 2), (2, 3), (3, 4), (4, 1) \} \) (or, in other words, \( F_{13} = F_{24} = 0 \)).

First we observe (recall that \( f_3 = 0 \)) that

\[
f_4 = P_3^N(w_1, w_3)(= P_3^N(w_2, w_4)) \geq a.
\]

Next, since \( F_{i,i+2} = 0 \), (26) amounts to

\[
F_i + F_{i,i+1} \geq a
\]

(all summations in indices are mod 4) and hence \( 2F_i + F_{i,i+1} + F_{i,i-1} + f_4 \geq 3a \). Comparing with

\[
F_i + F_{i,i+1} + F_{i,i-1} + f_4 = e(w_i) = \rho,
\]

we see that \( F_i \geq 3a - \rho \) which is strictly positive by the assumption (12). Likewise, \( F_{i,i+1} = \rho - f_4 - (F_i + F_{i,i-1}) \leq \rho - 2a < a \).

Claim 5.13 There is an edge between \( F_i \) and \( F_{i+1} \).
**Proof of Claim 5.13.** This is similar to the proof of Claim 5.6. Pick up a vertex \( v \) contributing to \( F_i \) \((F_i > 0 \text{ as we just observed})\). Then \( P_3^N(w_{i+1}, v) \leq F_{i+1} + F_{i+1,i+2} \) and since we already know that \( F_{i+1,i+2} < a \), there exists a vertex corresponding to \( F_{i+1} \) and adjacent to \( v \).

**Claim 5.14** \( F_i + F_{i+1} + F_{i,i+1} \geq 2a \).

**Proof of Claim 5.14.** This is similar to the proof of Claim 5.7. Pick vertices \( v, v' \) witnessing Claim 5.13 with \( i := i + 2 \), so that in particular \((v, w_{i+2}), (v', w_{i-1}), (v, v')\) are all in \( E(G) \) while \((v, w_{i+1}), (v', w_i)\) are not (since \( v, v' \) correspond to the flags \( F_{i+2}, F_{i-1} \), respectively). Then

\[
2a \leq P_3^N(v, w_{i+1}) + P_3^N(v', w_i) \leq F_i + F_{i+1} + F_{i,i+1}
\]

since \( P_3^N(v, w_{i+1}) \leq F_{i+1} + F_{i,i+1} \), \( P_3^N(v', w_i) \leq F_i + F_{i,i+1} \) and the corresponding sets are disjoint since \((v, v')\) is an edge.

Now we can complete the proof of Lemma 5.12:

\[
\tilde{F}_{1234} = (F_1 + F_{12} + F_{14} + F_{1234}) + (F_2 + F_{23}) + (F_3 + F_4 + F_{34}) \geq \rho + 3a
\]

by (28) and Claim 5.14.

This also completes the proof of Theorem 3.1 for \( \rho \geq \rho_1 \) (that is, modulo the bound \( \text{Improved}(\rho) \) deferred to Section 5.2.2). Indeed, since \( \tilde{F}_{1234} \leq \mu(I) = 1 - 2\rho + a \), Lemma 5.12 implies \( a \leq \frac{1-3\rho}{2} \) which is \( \leq a_0(\rho) \) as long as \( \rho \in [\rho_1, 1/3] \).

### 5.2. Analytical lower bounds

In this section we prove the bounds \( a(\rho) \leq \text{Krein}(\rho) \) \((\rho \leq \rho_0)\), \( a(\rho) \leq \text{Krein}(\rho) \) \((\rho \in [\rho_0, \rho_1])\) and \( a(\rho) \leq \text{Improved}(\rho) \) \((\rho \in [\rho_2, 9/32])\). We keep all the notation and conventions from the previous section.

Let us continue a bit our crash course on flag algebras we began in Section 2. For the readers familiar with the general theory, let us remark that what follows below is its “light” and slightly informal version obtained by evaluating general formulas on the step-function graphon \( W_{G,}\mu\).

The product \( F_1(v_1, v_2, \ldots, v_k)F_2(v_1, v_2, \ldots, v_k) \), where \( F_1 \) and \( F_2 \) are flags of the same type and \( v_1, \ldots, v_k \in V(G) \) induce this type in \( G \), can be always
expressed as a fixed (that is, not depending on $G, v_1, \ldots, v_k$) linear combination of expressions of the form $F(v_1, \ldots, v_k)$ (cf. [Raz07, eq. (5)]). The idea is simple: by definition, $F_1(v_1, v_2, \ldots, v_k)F_2(v_1, v_2, \ldots, v_k)$ is equal to the probability of the event $E$ stating that the $\sigma$-flag induced by $w_1^{(1)}, \ldots, w_{\ell_1-k}^{(1)}$ is isomorphic, in the label-preserving way, to $F_1$ and the $\sigma$-flag induced by $w_1^{(2)}, \ldots, w_{\ell_2-k}^{(2)}$ is isomorphic to $F_2$. Here $\ell_i$ is the number of vertices in $F_i$, and $w_1^{(1)}, \ldots, w_{\ell_1-k}^{(1)}, w_1^{(2)}, \ldots, w_{\ell_2-k}^{(2)}$ is an i.i.d. sample from $V(G)$ according to the distribution $\mu$.

Now we can realize the same distribution differently. Namely, at the first step we sample $\ell_1 + \ell_2 - 2k$ unsorted vertices $w_1, \ldots, w_{\ell_1+\ell_2-2k}$ i.i.d. under $\mu$. Then, at the second step we distribute among them $\ell_1 - k$ superscripts (1) and $\ell_2 - k$ superscripts (2), uniformly at random. By symmetry, this gives us an identical distribution and, also by symmetry, the conditional probability of the event $E$ after the first step depends only on the isomorphism type of the flag $F$ with $\ell \equiv \ell_1 + \ell_2 - k$ vertices induced by $v_1, \ldots, v_k, w_1, \ldots, w_{\ell_1+\ell_2-2k}$. This allows us to write

$$F_1(v_1, \ldots, v_k)F_2(v_1, \ldots, v_k) = \sum_{F \in \mathcal{F}_\ell^\sigma} p(F_1, F_2; F) F(v_1, \ldots, v_k),$$

where $\mathcal{F}_\ell^\sigma$ is the set of all $\sigma$-flags (up to isomorphism) on $\ell$ vertices, and $p(F_1, F_2; F)$ are the coefficients uniquely determined by the second stage of the above experiment: the probability that after randomly splitting unlabelled vertices of the flag $F$ into two groups of sizes $\ell_1 - k$ and $\ell_2 - k$, we get an isomorphic copy of $F_1$ and an isomorphic copy of $F_2$. For example, $e^2 = P_3^{1,c}$ in the sense that for every triangle-free graph $G$ (otherwise we would get an extra term $K_4^3$) and every $v \in V(G)$ we have $e(v)^2 = P_3^{1,c}(v)$.

We also need the averaging or unlabeling operator, cf. [Raz07, §2.2] $^7 f \mapsto [f]_{\sigma, \eta}$. Let $\sigma$ be a type of size $k$, and $\eta: [k'] \rightarrow [k]$ be an injective mapping, usually written as $[\eta_1, \ldots, \eta_{k'}]$ or even $\eta_1$ when $k = 1$ (here $\eta_1, \ldots, \eta_{k'}$ are pairwise different elements of $[k]$). Then we have the naturally defined type $\sigma|_\eta$ of size $k'$ given by $(i, j) \in E(\sigma|_\eta)$ if and only if $(\eta_i, \eta_j) \in E(\sigma)$. Assume now that $F$ is a $\sigma$-flag with $\ell$ vertices and $w_1, \ldots, w_{k'} \in V(G)$ span the type $\sigma|_\eta$. We are interested in the expectation $\mathbf{E}[F(\bar{v}_1, \ldots, \bar{v}_k)]$, where $\bar{v}_j$ is fixed to $w_j$ if $j = \eta_i$ and is picked i.i.d. according to the measure $\mu$ when $j \not\in \text{im}(\eta)$.

\footnote{For the reader familiar with graph limits, let us remark that their operator is different but connected to ours via a simple Möbius transformation, followed by summation over several types.}
It may be the case that for certain choices of \( \bar{v}_j \) the tuple \( \bar{v}_1, \ldots, \bar{v}_k \) does not even span the type \( \sigma \). In that case we let \( F(\bar{v}_1, \ldots, \bar{v}_k) \) def = 0.

Similarly to the case of multiplication, the expectation is the result of the following two-step experiment: first we pick up i.i.d. the missing \( k - k' \) entries \( \bar{v}_j \) (\( j \not\in \text{im}(\eta) \)) and then we pick, also i.i.d. w.r.t. \( \mu \), the \( \ell - k \) vertices \( w_{k+1}, \ldots, w_\ell \) stipulated in the definition of \( F(v_1, \ldots, v_k) \). Reversing the steps as before, we arrive at the following formula.

Let \( F|_\eta \) be the \( \sigma|_\eta \)-flag with the same underlying graph as \( F \) and the labelling \( \theta \circ \eta : [k'] \rightarrow V(F) \), where \( \theta : [k] \rightarrow V(F) \) is the labelling of \( F \). Let the coefficient \( q_{\sigma, \eta}(F) \in [0, 1] \) be determined by the following experiment: we pick up a labelling \( \Theta : [k] \rightarrow V(F) \) at random, but under the condition that it is consistent with \( \theta \) on \( \text{im}(\eta) \). Then \( q_{\sigma, \eta}(F) \) is the probability that \( \Theta \) spans a copy of \( \sigma \) and the resulting \( \sigma|_\eta \)-flag is isomorphic to \( F \). We have

\[
E[F(\bar{v}_1, \ldots, \bar{v}_k)] = q_{\sigma, \eta}(F) \cdot F|_\eta(v_{\eta_1}, \ldots, v_{\eta_{\ell}});
\]

accordingly, we let

\[
[F]_{\sigma, \eta} \text{ def } = q_{\sigma, \eta} 
\cdot F|_\eta,
\]

extended by linearity to linear combinations of \( \sigma \)-flags. When \( \eta \) is empty, the notation is simplified to \([F]_\sigma \). Besides, it is often handy to introduce a special notation for flags in which unlabelled vertices are supposed to be ordered:

\[
\langle \sigma, \eta \rangle \text{ def } = [1_{\sigma}]_{\sigma, \eta} = q_{\sigma, \nu}(1_{\sigma}) \cdot (\sigma, \eta),
\]

where the pair \((\sigma, \eta)\) is viewed as a \( \sigma|_\eta \)-flag and \( 1_{\sigma} \) is trivial (that is, completely labelled) \( \sigma \)-flag.

Examples: \([c]_1 = \rho, \ [P_3^{1,b}]_1 = \frac{2}{3} P_3 \) and \([S_4^T]_{I,[3,1]} = \frac{1}{2} S_4^N \).

Finally, we also need the lifting operator \( \pi^{\sigma, \eta} \), where \( \sigma, \eta \) are as above. Namely, for a \( \sigma|_\eta \)-flag \( F \), let

\[
\pi^{\sigma, \eta}(F)(v_1, \ldots, v_k) \text{ def } = F(v_{\eta_1}, \ldots, v_{\eta_{\ell}})
\]

be the result of forgetting certain vertices among \( v_1, \ldots, v_k \) and possibly re-enumerating the remaining ones according to \( \eta \). This time the formula is slightly different. Let \( F \downarrow_\eta \) be another \( \sigma|_\eta \)-flag, defined similarly to \( F|_\eta \) but with the difference that we not only unlabel vertices outside of \( \text{im}(\eta) \) but actually remove them from the flag. Then

\[
\pi^{\sigma, \eta}(F) \text{ def } = \sum \{ \hat{F} \in \mathcal{F}_{\ell+k-k'} \mid \hat{F} \downarrow_\eta = F \},
\]
where $\ell$ is the number of vertices in $F$.

Remarkably, unlike $\llbracket J \rrbracket_{\sigma,\eta}$, $\pi_{\sigma,\eta}$ does respect the multiplicative structure. When $\eta$ is empty, we again abbreviate $\pi_{\sigma,\eta}$ to $\pi_{\sigma}$.

The main tool in flag algebras is the light version of the Cauchy-Schwartz inequality formalized as

$$\llbracket J^2 \rrbracket_{\sigma,\eta} \geq 0,$$

and the power of the method relies on the fact that positive linear combinations of these inequalities can be arranged as a semi-definite programming problem. But the resulting proofs are often very non-instructive, so in this paper we have decided to use more human-oriented language of optimization. Let us stress that, if desired, the argument can be also re-cast as a purely symbolic sum-of-squares computation based on statements of the form (30).

After this preliminary work, let us return to the problem at hand. As in the previous section, we fix arbitrarily two non-adjoint vertices $v_1, v_2$ with $P^N_3(v_1, v_2) = a$ and let $P \overset{\text{def}}{=} \mathcal{N}_G(v_1) \cap \mathcal{N}_G(v_2)$, $I \overset{\text{def}}{=} \mathcal{V}(G) \setminus (\mathcal{N}_G(v_1) \cup \mathcal{N}_G(v_2))$. Recall that $\mu(P) = a$ and $\mu(I) = 1 - 2\rho + a$.

### 5.2.1. Krein bounds

We are going to estimate the quantity $\llbracket S^T_4 (T^T_4 + S^T_4) \rrbracket_{I, [1,2]}(v_1, v_2)$ from both sides and compare results.

The upper bound does not depend on whether $\rho \leq \rho_0$ or not and it consists of several typical flag-algebraic computations.

**Convention.** When the parameters $(v_1, v_2, \ldots, v_k)$ in flags are omitted, this means that the inequality in question holds for their arbitrary choice. We specify them explicitly when the fact depends on the specific property $P^N_3(v_1, v_2) = a$ of $v_1$ and $v_2$.

As we have already implicitly computed in the previous section,

$$\llbracket (S^T_4)^2 \rrbracket_{I, [1,2]} = \frac{1}{3} K^N_{32} = \frac{1}{2} \llbracket K^P_{32} \rrbracket_{P, [1,2]}.$$

Similarly,

$$\llbracket S^T_4 T^T_4 \rrbracket_{I, [1,2]} = \frac{1}{2} \llbracket U^P_5 \rrbracket_{P, [1,2]}.$$

Altogether we have

$$\llbracket S^T_4 (S^T_4 + T^T_4) \rrbracket_{I, [1,2]} = \frac{1}{2} \llbracket K^P_{32} + U^P_5 \rrbracket_{P, [1,2]}.$$  (31)
On the other hand, we note that \( P_{3}^{E,b} = \pi_{E,3}^{2}(e) = \rho \) and since \( \frac{1}{2} P_{3}^{1,b} = [P_{3}^{E,b}]_{E,1} = [\pi_{E,1}^{1}(e)]_{E,1} \), we also have (due to regularity) \( P_{3}^{1,b} = 2\rho^2 \). Hence

\[
2\rho^2 = \pi^{p,3}(P_{3}^{1,b}) = K_{32}^{P} + U_{5}^{P} + V_{5}^{P,1} + V_{5}^{P,2}.
\]

(32)

Let us compute the right-hand side here. We have

\[
V_{5}^{P,1} = 2[\{D_{5}^{P,1}\}]_{D,1,2,3}
\]

(\( D_{5}^{P,1} \)) (\( v_{1}, v_{2} \)) = \pi_{5,1,2}(P_{3}^{N,b})(v_{1}, v_{2}) = \rho - a \quad (33)

(see the definition (29)) and

\[
V_{5}^{D,1} = \pi_{5,3,4}(P_{3}^{N}) \geq a.
\]

Putting these together, we have

\[
V_{5}^{P,1}(v_{1}, v_{2}, w) \geq 2a(\rho - a) \quad (w \in P)
\]

and, by symmetry, the same holds for \( V_{5}^{P,2} \). Comparing with (32), we find that

\[
(K_{32}^{P} + U_{5}^{P})(v_{1}, v_{2}, w) \leq 2\rho^2 - 4a(\rho - a) = 2((\rho - a)^2 + a^2).
\]

(34)

Averaging this over all \( w \in P \) and taking into account (31), we arrive at our first main estimate

\[
[S_{4}^{T}(S_{4}^{T} + T_{4}^{T})]_{D,1,2}(v_{1}, v_{2}) \leq a((\rho - a)^2 + a^2).
\]

(35)

For the lower bound we first claim that

\[
T_{4}^{T} \leq S_{4}^{T} + \rho - 2a.
\]

(36)

This was already established in (18), but let us re-cup the argument using the full notation:

\[
\rho = \pi^{I,3}(e) = T_{4}^{T} + \pi_{I}^{I,1,3}(P_{3}^{N}) + \pi_{I}^{I,2,3}(P_{3}^{N}) - S_{4}^{T} \geq T_{4}^{T} + 2a - S_{4}^{T}.
\]

Next, we need a lower bound on \( T_{4}^{N}(v_{1}, v_{2}) = [T_{4}^{T}]_{D,1,2}(v_{1}, v_{2}) \), that is on the density of those edges that have both ends in \( I \). For that we first classify all edges of \( G \) according to the number of vertices they have in \( I \):

\[
\pi^{N}(\rho) = T_{4}^{N} + \left( S_{4}^{N} + \sum_{i=1}^{2} V_{4}^{N,i} \right) + P_{4}^{N}.
\]

(37)
Now, \[ S_4^N(v_1, v_2) = 2 \sum_{e \in \Pi_3^N} \mathbb{P}_{\mathcal{P}_1, \mathcal{P}_3}(v_1, v_2) = 2a\rho. \]

Further we note that
\[
\rho(\rho - a) = \sum_{i=1}^2 \mathbb{P}_{\mathcal{P}_3^N}(v_1, v_2) = \frac{1}{2} \left( V_4^N + P_4^N \right)(v_1, v_2) \quad (i = 1, 2). \tag{38}
\]

Summing this over \(i = 1, 2\) and plugging our findings into (37), we get
\[
\rho = T_4^N(v_1, v_2) + 2a\rho + 4\rho(\rho - a) - P_4^N(v_1, v_2). \tag{39}
\]

So, the only thing that still remains is to estimate \(P_4^N(v_1, v_2)\) but this time from below. For that it is sufficient to compute its contribution to the right-hand side of (38) (letting, say, \(i := 1\)):
\[
a(\rho - a) \leq \sum_{i=1}^2 \mathbb{P}_{\mathcal{P}_3^N}(v_1, v_2) = \frac{1}{2} P_4^N(v_1, v_2).
\]

Substituting this into (39), we arrive at our estimate on the number of edges entirely within \(I\):
\[
\begin{align*}
\left[ T_4^T \right]_{I, [1, 2]}(v_1, v_2) &= T_4^N(v_1, v_2) \\
&\geq \rho - 2a\rho - 4\rho(\rho - a) + 2a(\rho - a) = \rho - 2(\rho^2 + (\rho - a)^2).
\end{align*}
\tag{40}
\]

We are now prepared to bound \( [S_4^T(S_4^T + T_4^T)]_{I, [1, 2]}(v_1, v_2) \) from below. As a piece of intuition, let us re-normalize \(S_4^T\) and \(T_4^T\) by the known values \(\langle I, [1, 2] \rangle = 1 + a - 2\rho\) so that they become random variables in the triangle
\[
\mathbb{T} = \{(x, y) \mid y \geq 0, \ y \leq x + \rho - 2a, \ x \leq a\}.
\]

Then we know the expectation of \(S_4^T\), have the lower bound (40) on the expectation of \(T_4^T\), and we need to bound the expectation of \(S_4^T(S_4^T + T_4^T)\), also from below. This leads to an optimization problem that we are going to solve; it is important that the constraints on the random variable \((S_4^T, T_4^T) \in \mathbb{T}\) listed in the previous sentence are the only constraints we are going to use, no combinatorial specifics will be used in this analysis.

For that purpose we are going to employ duality, i.e. we are looking for coefficients \(\alpha, \beta, \gamma\) depending on \(a, \rho\) only such that
\[
L(x, y) \overset{\text{def}}{=} x(x + y) - (\alpha x + \beta y + \gamma)
\]

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is non-negative on $T$, and applying $[\cdot]_{\|.\|_2}$ to this relation produces “the best possible result”. As we mentioned above, an alternative would be to write down an explicit “sum-of-squares” expression: the resulting proof would be shorter but it would be less intuitive.

Let us first observe the obvious upper bound

$$a \leq \frac{\rho^2}{1 - \rho},$$

it follows from the computation $3\rho^2 = 3[\mathbb{P}_3^1]_1 = P_3 = 3[\mathbb{P}_3^N]_N \geq 3a(1 - \rho)$.

Next, the right-hand side of (40) is a concave quadratic function in $a$, with two roots $a_1(\rho) \equiv \rho - \sqrt{2\rho - 4\rho^2}$, $a_2(\rho) \equiv \rho + \sqrt{2\rho - 4\rho^2}$. Further, $a_1(\rho) \leq a_0(\rho) \leq \frac{\rho^2}{1 - \rho} \leq a_2(\rho)$. Hence we can assume w.l.o.g. that the right-hand side in (40) is non-negative. Therefore, by decreasing $T_4^T$ if necessary (recall that we now treat $S_4^T, T_4^T$ as formal random variables), we can assume that the bound (40) on its expectation is actually tight.

Next, we note that since the quadratic form $x(x + y)$ is indefinite, the function $L(x, y)$ attains its minimum somewhere on the border of the compact region $T$. Since $L$ is linear on the line $x = a$ we can further assume that the minimum is attained at one of the lines $y = 0$ or $y = x + \rho - 2a$. Note further that along both these lines $L$ is convex.

We begin more specific calculations with the bound $g_K(\rho, a) \geq 0$ that is less interesting but also less computationally heavy. As a motivation for the forthcoming computations, we are looking for two points $(x_0, 0), (x_1, x_1 + \rho - 2a)$ on the lines $T_4^T = 0, T_4^T = S_4^T + \rho - 2a$ that are collinear (cf. (40)) with the point $(c_x, c_y)$, where

$$c_x \equiv \frac{\rho}{1 - 2\rho + a}, \quad c_y \equiv \frac{\rho - 2(\rho^2 + (\rho - a))^2}{1 - 2\rho + a}.$$

and such that the function $L(x, 0)$ has a double root at $x_0$ while $L(x, x + \rho - 2a)$ has a double root at $x_1$. Solving all this in $\alpha, \beta, \gamma, x_0, x_1$ gives us (see the
The remarks above imply that indeed $L(x, y)|_T \geq 0$ hence we have

$$\|S^T_4(S^T_1 + T^T_1)\|_{1,2} \geq \alpha a \rho + \beta (\rho - 2(\rho^2 + (\rho - a)^2)) + \gamma (1 - 2\rho + a). \quad (43)$$

Subtracting this from (35) and multiplying the result by $\frac{1^{-2\rho + a}}{2} > 0$, we get $g_K(\rho, a) \geq 0$. Given the way the function $\text{Krein}$ was defined, $g_K(\rho, a) < 0$ whenever $a \in \left(\text{Krein}(\rho), \frac{\rho^2}{1-\rho}\right)$. The required bound $a \leq \text{Krein}(\rho)$ now follows from (41).

The improvement $f_K(\rho, a) \geq 0$ takes place when the right-hand side in (42) is $> a$ since then we can hope to utilize the condition $S^T_4 \leq a$. As above, we first explicitly write down a solution of the system obtained by replacing the equation $L'(x, 0)|_{x=x_0} = 0$ with $x_0 = a$ and only then justify the result.

Performing the first step in this program gives us somewhat cumbersome rational functions that we attempt to simplify by introducing the abbreviations

$$u_0(\rho, a) \overset{\text{def}}{=} \frac{1}{4} (\rho + 2a - 2a \rho - 4\rho^2)$$

$$u_1(\rho, a) \overset{\text{def}}{=} \frac{1}{4} (3\rho - a - 7a^2 + 15a \rho - 12\rho^2)$$

$$u(\rho, a) \overset{\text{def}}{=} 4u_0(\rho, a) + u_1(\rho, a).$$
Then we get
\[
\begin{align*}
x_0 &= a \\
x_1 &= \frac{a(2a - \rho^2 - 3\rho a)}{u(\rho, a)} \\
\alpha &= 2a + \frac{7(\rho - a)(u_1(\rho, a)^2 - 2u_0(\rho, a)^2)}{u(\rho, a)^2} \\
\beta &= \frac{a(34u_0(\rho, a)^2 + 3u_1(\rho, a)^2 - 4u_0(\rho, a)u_1(\rho, a) - 2\rho(1 - 3\rho + a)^2)}{u(\rho, a)^2} \\
\gamma &= a^2 - \alpha a.
\end{align*}
\]

In order to analyze this solution, we first note that due to the bound just established we can assume w.l.o.g. that
\[
a \in [\text{Krein}(\rho), \overline{\text{Krein}}(\rho)].
\]

The function \(u_0(\rho, a)\) is linear and increasing in \(a\) and \(u_0(\rho,\text{Krein}(\rho)) > 0\) \((\rho \neq 0)\) hence \(u_0(\rho, a) \geq 0\). The function \(u_1(\rho, a)\) is quadratic concave in \(a\) and \(u_1(\rho,\text{Krein}(\rho)), u_1(\rho,\overline{\text{Krein}}(\rho)) \geq 0\). These two facts imply that \(u(\rho, a) > 0\) \((\rho > 0)\) hence our functions are at least well-defined.

Next, \(u_0, u_1 \geq 0\) imply that \(L'(x, 0)|_{x=a} = 2a - \alpha = \frac{7(\rho - a)}{u(\rho, a)^2}(\sqrt{2}u_0(\rho, a) + u_1(\rho, a))(\sqrt{2}u_0(\rho, a) - u_1(\rho, a))\) has the sign opposite to \(u_1(\rho, a) - \sqrt{2}u_0(\rho, a)\). This expression (that up to a constant positive factor is equal to \(c_x + (\sqrt{2} - 1)c_y - a\)) is also concave in \(a\). Moreover, it is non-negative for \(\rho \in [0, \rho_0], a \in [\text{Krein}(\rho), \overline{\text{Krein}}(\rho)]\) (at \(\rho = \rho_0\) the two bounds meet together: \(\text{Krein}(\rho_0) = \overline{\text{Krein}}(\rho_0) = \rho_0/3\) and also \(u_1(\rho, \rho/3) - \sqrt{2}u_0(\rho, \rho/3) = 0\)). This completes the proof of \(L'(x, 0)|_{x=a} \leq 0\) hence (given that \(L(a, 0) = 0\)) we have \(L(x, 0) \geq 0\) for \(x \leq a\). As we argued above, this gives us \(L|_T \geq 0\) which implies (43), with new values of \(\alpha, \beta, \gamma\). Comparing it with (40), we get \(f_K(\rho, a) \geq 0\), up to the positive multiplicative factor \(\frac{2a(\rho - a)}{u(\rho, a)}\). This concludes the proof of \(f_K(\rho, a) \geq 0\) whenever \(\rho \leq \rho_0\) and hence of the bound \(a \leq \text{Krein}(\rho)\) in that interval.

As a final remark, let us note that since the final bound \(f_K(\rho, a) \geq 0\) has a very clear meaning in algebraic combinatorics, it looks likely that the disappointingly complicated expressions we have encountered in proving it might also have a meaningful interpretation. But we have not pursued this systematically.
5.2.2. The improved bound for $c = 3$

Let us now finish the proof of the bound $a \leq \text{Improved}(\rho)$, $\rho \in [\rho_2, 9/32]$ left over from Section 5.1.2. We utilize all the notation introduced there and assume that $c = 3$. We also introduce the additional notation

$$a_i \overset{\text{def}}{=} \mu(w_i) \ (i = 1\ldots3)$$

for the weights of the vertices comprising the set $P$; thus, $\sum_{i=1}^{3} a_i = a$.

We want to obtain an upper bound on $T_4^N(v_1, v_2)$ and then compare it with (40). Let us split $I = J \cup K$, where $J$ corresponds to $f_1$ and $K$ corresponds to $f_2 + f_3$. Recalling that

$$T_4^N = [T_4^T]_{I, [1,2]},$$

let us split the right-hand side according to this partition as (with slight abuse of notation)

$$[T_4^T]_{I, [1,2]} = [T_4^T]_{J, [1,2]} + [T_4^T]_{K, [1,2]}.$$

When $v \in J$ corresponds to $F_i$, we have $S_4^T(v_1, v_2, v) = a_i$ and hence, by (36), $T_4^T(v_1, v_2, v) \leq \rho - 2a + a_i$. Thus

$$[T_4^T]_{J, [1,2]} \leq \sum_i F_i(\rho - 2a + a_i).$$

In order to bound $[T_4^T]_{K, [1,2]}$, we need to analyze edges between $K$ and $I$. First note that $K$ is independent (every two vertices in $K$ have a common neighbor in $P$). Furthermore, the only edges between $K$ and $J$ are between parts corresponding to $F_i$ and $F_{jk}$. Hence $[T_4^T]_{K, [1,2]} \leq \sum_i F_iF_{jk}$ and we arrive at the bound

$$T_4^N(v_1, v_2) \leq \sum_i F_i(\rho - 2a + F_{jk} + a_i). \quad (44)$$

Next, let us denote by $\epsilon_i$ the (non-negative!) deficits in Claim 5.10:

$$\epsilon_i \overset{\text{def}}{=} a_i + F_{jk} - 4a + \rho; \ \epsilon_i \geq 0.$$

Then (44) re-writes as follows:

$$T_4^N(v_1, v_2) \leq 2af_1 + \sum_{i=1}^{3} F_i\epsilon_i.$$
Let us now assume w.l.o.g. that $F_1 \geq F_2 \geq F_3$. Then, since all $\epsilon_i$ are non-negative,

$$\sum_{i=1}^{3} F_i \epsilon_i \leq F_1 \cdot \sum_{i=1}^{3} \epsilon_i = F_1 (f_2 - 11a + 3\rho) = F_1 (3 - 6\rho - 8a - 2f_1),$$

where the last equality follows from (24). Summarizing,

$$T_4^N(v_1, v_2) \leq 2af_1 + F_1 (3 - 6\rho - 8a - 2f_1) = F_1 (3 - 6\rho - 8a) - 2f_1 (F_1 - a) \leq F_1 (3 - 6\rho - 8a) - 2(F_1 + 2a)(F_1 - a),$$

where the last inequality holds since $F_1 \geq a$ and $f_1 = F_1 + F_2 + F_3 \geq F_1 + 2a$ by Claim 5.9. The right-hand side here is a concave quadratic function in $F_1$; maximizing, we find

$$T_4^N(v_1, v_2) \leq \frac{33}{2} a^2 + 15a\rho - \frac{15}{2} a + \frac{9}{8} \rho^2 - \frac{9}{2} \rho + \frac{9}{8}.$$

Comparing with (40), we get a constraint $Q(\rho, a) \geq 0$ that is quadratic concave in $a$, and $\text{Improved}(\rho)$ is its smallest root. Moreover, $Q \left( \rho, \frac{3}{14} (1 - 2\rho) \right) = -\frac{(11\rho - 2)(9 - 32\rho)}{49} \leq 0$ since $\rho_2 > \frac{2}{11}$. Hence the preliminary bound (25) can be improved to $a \leq \text{Improved}(\rho)$.

### 6. Conclusion

In this paper we have taken a prominent open problem in the algebraic graph theory and considered its natural semi-algebraic relaxation in the vein of extremal combinatorics. The resulting extremal problem displays a remarkably rich structure, and we proved upper bounds for it employing methods greatly varying depending on the range of edge density $\rho$. Many of these methods are based on counting techniques typical for extremal combinatorics, and one bound has a clean interpretation in terms of algebraic Krein constraints for the triangle-free case.

The main generic question left open by this work is perhaps how far can this connection between the two areas go. Can algebraic combinatorics be a source of other interesting extremal problems? In the other direction, perhaps flag algebras and other advanced techniques from extremal combinatorics can turn out to be useful for ruling out the existence of highly
regular combinatorial objects with given parameters? These questions are admittedly open-ended so we would like to stop it here and conclude with several concrete open problems regarding TFSR graphs and their relaxations introduced in this paper.

Can the Krein bound $a(\rho) \leq \text{Krein}(\rho)$ be improved for small values of $\rho$? Of particular interest are the values $\rho = \frac{16}{77}$, $\rho = \frac{5}{28}$ or $\rho = \frac{7}{50}$, ideally showing that $a\left(\frac{16}{77}\right) = \frac{4}{77}$, $a\left(\frac{5}{28}\right) = \frac{1}{28}$ or $a\left(\frac{7}{50}\right) = \frac{1}{50}$. In other words, can we show that like the four denser TFSR graphs, the M22 graph, the Gewirtz graph and the Hoffman graph are also extremal configurations for their respective edge densities?

Another obvious case of interest is $\rho = \frac{57}{3250}$ corresponding to the only hypothetical unknown Moore graph. More generally, can we rule out the existence of a TSFR graph for at least one additional pair $(\rho, a)$ by showing that actually $a(\rho) \leq a$?

For some “non-critical” (that is, not corresponding to TFSR graphs) $\rho$ it is sometimes also possible to come up with constructions providing non-trivial lower bounds on $a(\rho)$. A good example\(^8\) is provided by the Kneser graphs $KG_{3k-1,k}$ having $\rho = \frac{2k-1}{3k-1}$ and $a = \frac{1}{(3k-1)}$ but there does not seem to be any reasons to believe that they are optimal. Are there any other values of $\rho$ for which we can compute $a(\rho)$ exactly? Of particular interest here is the value $\rho = 1/3$ critical for the Erdős-Simonovits problem (see again [BT05, Problem 1] and the literature cited therein). Can we compute $a(1/3)$ or at least determine whether $a(1/3) = 0$ or not?

Speaking of which, is there any rational $\rho \in (0, 1/3]$ for which $a(\rho) = 0$? Equivalently, does there exist $\rho \in [0, 1/3]$ for which there are no triangle-free $\rho$-regular graphs (or, which is the same, weighted twin-free graphs) of diameter 2? Note for comparison that there are many such values for $\rho > 1/3$; in fact, all examples leading to non-zero $a(\rho)$ fall into one of a few infinite series.

We conclude by remarking in connection with this question that regular weighted triangle-free twin-free graphs of diameter 2 seem to be extremely rare: a simple computer search has shown that Petersen is the only such graph on $\leq 11$ vertices with $\rho \leq 1/3$.

\(^8\)Let us remind that we confine ourselves to the region $\rho \leq 1/3$. A complete description of all non-zero values $a(\rho)$ for $\rho > 1/3$ follows from [BT05].
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