COUNTING FLAGS IN TRIANGLE-FREE DIGRAPHS

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ABSTRACT. Motivated by the Caccetta-Häggkvist Conjecture, we prove that every digraph on n vertices with minimum outdegree $0.3465n$ contains an oriented triangle. This improves the bound of $0.3532n$ of Hamburger, Haxell and Kostochka. The main new tool we use in our proof is the theory of flag algebras developed recently by Razborov.

1. Introduction

A *digraph* is a directed graph with no loops, no parallel edges, and no counter-parallel edges. We write $V(D)$ and $E(D)$ for the set of vertices and for the set of edges of a digraph D. The *outneighborhood* $\Gamma^+(u)$ of a vertex $u \in V(D)$ is defined as $\Gamma^+(u) = \{v \in V(D) : uv \in E(D)\}$. For a set $U \subseteq V(D)$, we define its *common neighborhood* $\Gamma^+(U) = \bigcap_{u \in U} \Gamma^+(u)$. The *outdegree* of a vertex u is defined $\deg^+(u) = |\Gamma^+(u)|$. A digraph D is *outregular* if $\deg^+(u) = \deg^+(v)$ for any $u, v \in V(D)$. For a digraph D we write $\delta^+(D)$ for its minimum outdegree, i.e., $\delta^+(D) = \min_{u \in V(D)} \deg^+(u)$. A *cycle* of length t is a digraph C_t whose vertices can be labelled as $v_0, \ldots, v_{t-1}$ so that $v_i v_j$ is a directed edge of C_t if and only if $i + 1 \equiv j \pmod{t}$. A *triangle* is a cycle of length three. Finally, a digraph is *acyclic* if it does not contain any cycle.

One of the most intriguing problems of extremal (di)graph theory is the following conjecture of Caccetta and Häggkvist [2] dating back to 1978.

Conjecture 1.1. *Every n-vertex digraph with minimum outdegree at least r has a cycle with length at most $\lceil n/r \rceil$.*

If correct, the above bound is tight. We refer to [14] for a thorough survey on the Conjecture 1.1.

The case when $r = n/3$ is of particular interest. It asserts that any n-vertex digraph with minimum outdegree at least $n/3$ contains a triangle. Our main result gives a new minimum outdegree bound for this case of the Caccetta-Häggkvist Conjecture.

Theorem 1.2. *Every n-vertex digraph with minimum outdegree at least $0.3465n$ contains a triangle.*

This improves previous minimum-degree bounds established by Caccetta and Häggkvist [2] ($0.3820n$), Bondy [1] ($0.3798n$), Shen [12] ($0.3543n$) and Hamburger, Haxell, and Kostochka [5] ($0.3532n$).

The proof of Theorem 1.2 uses the theory of flag algebras which was recently developed by Razborov [9]. Flag algebras provide general formalism which allows one to deal with problems in extremal combinatorics. Razborov used this approach to solve a long-standing open problem on density of triangles in graphs [11], and a special case of the Turán's problem for 3-uniform hypergraphs [10]. The main ingredient of our proof is, similarly to [10], an approach called by Razborov the "semidefinite method". The other

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two ingredients are (using the language of Razborov) "induction" and a recent result of Chudnovsky, Seymour and Sullivan [3] on eliminating cycles in triangle-free digraphs. Brute force computer search was used to combine these techniques to give the bound. However, the resulting proof is close to being computer-free, only with Maple used to verify several hundred addition and multiplication operations involving five-to-nine digit numbers.

The paper is organized as follows. In Section 2 we survey some of the theory of flag algebras needed for our purposes. Section 3 treats the structure of triangle-free digraphs. It contains a statement of the key Theorem 3.5 and gives a short proof of Theorem 1.2 based on it. Finally, in Section 4 we give a proof of Theorem 3.5.

2. Flag algebras

We refer the reader to [9] for a thorough treatise of the matter of flag algebras. Here, we present only what is needed for our proof of Theorem 1.2, following closely [9]. Furthermore, we restrict our presentation only to the theory $\mathcal{T}$ of triangle-free digraphs. The theory $\mathcal{T}$ is a vertex uniform theory[i] with amalgamation property[ii], which allows us to use full strength of the results from [9].

Given a digraph D and a set $U \subseteq V(D)$ we write $D \setminus U$ for the digraph obtained from D by deleting the vertices of U.

A *type* of order k is a triangle-free k-vertex digraph σ on the vertex set $V(\sigma) = [k]$. The symbol $|\sigma|$ denotes the order of σ, i.e., $|\sigma| = k$. Suppose that an injective map $\eta : [k'] \to [k]$ is given. Then a *restriction* $\sigma|_\eta$ of the type σ is a type on the vertex set $[k']$ such that η is an isomorphism between $\sigma|_\eta$ and $\sigma[\mathrm{Im}(\eta)]$.

Suppose that σ is a type of order k. Then a *σ-flag* is a pair $F = (D, \theta)$, where D is a triangle-free digraph and $\theta : [k] \to V(D)$ is an injective digraph homomorphism such that $\sigma \cong D[\mathrm{Im}(\theta)]$. We write $\mathcal{F}^\sigma$ for the set of all σ-flags; $\mathcal{F}^\sigma_\ell$ is its restriction to σ-flags of order ℓ. For two σ-flags $F_1, F_2 \in \mathcal{F}^\sigma$, $F_1 = (D_1, \theta_1)$, $F_2 = (D_2, \theta_2)$, we write $F_1 \cong_\sigma F_2$ if there exists a digraph isomorphism which is consistent with the labellings θ_1 and θ_2. A *restriction* of a σ-flag $F = (D, \theta)$ to a set V, $\mathrm{Im}(\theta) \subseteq V \subseteq V(D)$, is a σ-flag $F|_V = (D[V], \theta)$.

A given type σ of order k can be regarded as a σ-flag. In view of this, any injective map $\eta : [k'] \to [k]$ naturally defines a $\sigma|_\eta$-flag of order k denoted by (σ, η).

We shall now enhance $\mathcal{F}^\sigma$ with the structure of an algebra. Given two σ-flags $F = (D, \theta) \in \mathcal{F}^\sigma_\ell$ and $F' \in \mathcal{F}^\sigma_{\ell'}$, $\ell' \le \ell$ we define the number $p(F'; F)$ by

$$p(F'; F) = \mathbf{P}\left[F|_{\mathrm{Im}(\theta) \cup \mathbf{V}} \cong_\sigma F'\right] ,$$

where $\mathbf{V}$ is an $(\ell' - |\sigma|)$-element subset of $V(D) - \mathrm{Im}(\theta)$ taken uniformly at random. (Following [9] we use bold letters to denote random objects.) Likewise, for three flags $F_1 \in \mathcal{F}^\sigma_{\ell_1}, F_2 \in \mathcal{F}^\sigma_{\ell_2}$, $F \in \mathcal{F}^\sigma_\ell$, $\ell \ge \ell_1 + \ell_2 - |\sigma|$ we define the quantity $p(F_1, F_2; F)$ as

$$p(F_1, F_2; F) = \mathbf{P}\left[F|_{\mathrm{Im}(\theta) \cup \mathbf{V}_1} \cong_\sigma F_1 \text{ and } F|_{\mathrm{Im}(\theta) \cup \mathbf{V}_2} \cong_\sigma F_1\right] .$$

where $(\mathbf{V}_1, \mathbf{V}_2)$ is a pair of disjoint subsets of $V(D) - \mathrm{Im}(\theta)$ of cardinality $\ell_1 - |\sigma|$ and $\ell_2 - |\sigma|$ respectively, drawn uniformly at random from the space of all such possible pairs.

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[i] Razborov [9] calls a theory vertex uniform if it has a unique model of order one. Indeed, there is a single triangle-free digraph (up to isomorphism) of order one.

[ii] Amalgamation property, as defined by Razborov [9], reads in the model of triangle-free digraphs as that the disjoint union of two triangle-free digraphs is a triangle-free digraph. Some properties listed in this section require the underlying theory to be vertex uniform with amalgamation property.

For each σ-flag F we can group all the values $p(F;\tilde{F})$ $(\tilde{F} \in \mathcal{F}^\sigma)$ by defining $p^F \in [0,1]^{\mathcal{F}^\sigma}$ as $p^F(\tilde{F}) = p(F;\tilde{F})$.

The following chain rule follows directly from the definition (cf. [9, Lemma 2.2]).

Lemma 2.1. *Let $\ell' \le \tilde{\ell} \le \ell$, $F \in \mathcal{F}^\sigma_\ell$, $F' \in \mathcal{F}^\sigma_{\ell'}$ be given. Then*

$$p(F';F) = \sum_{\tilde{F} \in \mathcal{F}^\sigma_{\tilde{\ell}}} p(F';\tilde{F}) p(\tilde{F};F) .$$

In the space $\mathbb{R}\mathcal{F}^\sigma$ of finite formal linear combinations of σ-flags consider the subspace $\mathcal{K}^\sigma$ generated by all the elements of the form

$$F' - \sum_{\tilde{F} \in \mathcal{F}^\sigma_{\tilde{\ell}}} p(F';\tilde{F})\tilde{F} , \tag{2.1}$$

where the σ-flag $F' \in \mathcal{F}^\sigma_{\ell'}$ is arbitrary, and $\ell' \le \tilde{\ell}$.

We set $\mathcal{A}^\sigma = \mathbb{R}\mathcal{F}^\sigma / \mathcal{K}^\sigma$. $\mathcal{A}^\sigma$ shall be the desired algebra. The additive structure of $\mathcal{A}^\sigma$ is inherited from $\mathbb{R}\mathcal{F}^\sigma$. To define the multiplicative structure, consider the bilinear mapping $\cdot : \mathcal{F}^\sigma \otimes \mathcal{F}^\sigma \to \mathcal{A}^\sigma$ defined on the basis as follows: for arbitrary $F_1 \in \mathcal{F}^\sigma_{\ell_1}$, $F_2 \in \mathcal{F}^\sigma_{\ell_2}$ take $\ell \ge \ell_1 + \ell_2 - |\sigma|$ and define

$$F_1 \cdot F_2 = \sum_{F \in \mathcal{F}^\sigma_\ell} p(F_1, F_2; F) F .$$

It is shown in [9] that the expression on the right-hand side does not depend on the choice of ℓ (modulo $\mathcal{K}^\sigma$). Since $\mathcal{K}^\sigma$ is absorbing on both sides, this defines a multiplication $\cdot : \mathcal{A}^\sigma \otimes \mathcal{A}^\sigma \to \mathcal{A}^\sigma$. $\mathcal{A}^\sigma$ is a commutative algebra. The unit element, denoted 1_σ, is the only element of $\mathcal{F}^\sigma_{|\sigma|}$.

2.1. **Convergence.** We write $\mathrm{Hom}(\mathcal{A}^\sigma, \mathbb{R})$ for the set of all algebra homomorphisms from $\mathcal{A}^\sigma$ to $\mathbb{R}$. The set $\mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R}) \subseteq \mathrm{Hom}(\mathcal{A}^\sigma, \mathbb{R})$ contains those homomorphisms ρ which have the property that $\rho(F) \ge 0$ for every $F \in \mathcal{F}^\sigma$. Note that $\mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R}) \subseteq \mathrm{Hom}(\mathcal{A}^\sigma, \mathbb{R})$ can be viewed as a subset of $[0, +\infty)^{\mathcal{F}^\sigma}$. In fact, it is not difficult to show that $\mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R}) \subseteq [0,1]^{\mathcal{F}^\sigma}$.

A partial preorder $\le_\sigma$ on $\mathcal{A}^\sigma$ is defined by $a \le_\sigma b$, for $a, b \in \mathcal{A}^\sigma$, if $\rho(a) \le \rho(b)$ for every $\rho \in \mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$. Observe that if $f_1, f_2 \in \mathcal{A}^\sigma$ are such that $f_2 - f_1 = \sum_{F \in \mathcal{F}^\sigma} c_F F$, where each $c_F \in \mathbb{R}$ is nonnegative, then $f_1 \le_\sigma f_2$.

We say that a sequence of σ-flags $\{F_n\}_{n=1}^\infty$ *converges* to a point $x \in [0,1]^{\mathcal{F}^\sigma}$ if the sequence $\{p^{F_n}\}_{n=1}^\infty$ converges to x in the product topology on $[0,1]^{\mathcal{F}^\sigma}$. This is denoted by writing $\lim_n F_n = x$. It turns out that a sequence of σ-flags can converge only to a point in $\mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R}) \subseteq [0,1]^{\mathcal{F}^\sigma}$. On the other hand, every point of $\mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$ is a limit of some sequence of σ-flags (cf. [7, Theorem 2.5], [9, Theorem 3.3]).

Theorem 2.2. *Suppose that $\{D_n\}_{n=1}^\infty$ is a sequence of σ-flags. Then there exists a subsequence $\{D_{n_i}\}_{i=1}^\infty$ and a point $\rho \in \mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$ such that $\{D_{n_i}\}_{i=1}^\infty$ converges to ρ.*

Conversely, for any $\rho \in \mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$ there exists a sequence of growing σ-flags which converges to ρ.

2.2. **Frequently used symbols.** Let us now introduce notation for the most frequently used flags. The symbols ϱ, α and β stand for the unlabelled directed edge, the 1-labelled directed edge with the label on the tail of the edge and the 2-labelled directed edge with the label 1 on the tail of the edge, respectively. The symbol γ denotes the 1-labelled non-edge. A *fork* κ consists of three vertices a, b, c and two edges ab, ac. We say that the vertex a is the *center* of κ, and the 1-labelled fork with the center being its labelled vertex is denoted by a symbol χ.

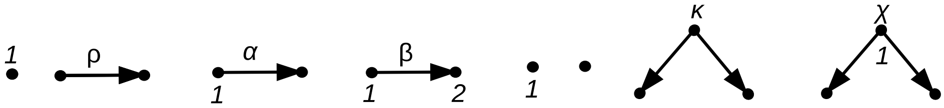

FIGURE 1. Frequently used types and flags.

The symbol 1 denotes (besides the usual meaning), the unique type of order one, i.e., the labelled vertex.

2.3. **Averaging.** Suppose that a type σ of order k and its restriction $\sigma_0 = \sigma|_\eta$ of order k' are given. We define the *unlabelling* of a flag $F = (D, \theta) \in \mathcal{F}^\sigma$ as a flag $F|_\eta = (D, \theta\eta) \in \mathcal{F}^{\sigma_0}$. Let $\boldsymbol{\theta}' : [k] \to V(D)$ be an injective extension of the map $\theta\eta : [k'] \to V(D)$ taken uniformly at random from the space of all such maps. The *normalizing factor* $q_{\sigma,\eta}(F)$ is the probability that $(D, \boldsymbol{\theta}')$ and F are isomorphic σ-flags. The *averaging operator* $[\![]\!]_{\sigma,\eta} : \mathcal{A}^\sigma \to \mathcal{A}^{\sigma_0}$ is linear, and defined on the basis by

$$[\![F]\!]_{\sigma,\eta} = q_{\sigma,\eta}(F)F|_\eta \,.$$

When $k' = 0$ we write $[\![]\!]_\sigma$ instead of $[\![]\!]_{\sigma,\eta}$ for brevity.

2.4. **Random homomorphisms.** The crucial notion in the theory of flag algebras is that of random extensions of homomorphisms (also called random rooted homomorphisms). Suppose that σ is a type of order k, let $\sigma_0 = \sigma|_\eta$ be its restriction. Fix a homomorphism $\rho \in \mathrm{Hom}^+(\mathcal{A}^{\sigma_0}, \mathbb{R})$ with $\rho((\sigma,\eta)) > 0$. Then we say that a probability measure $\mathbf{P}^{\sigma,\eta}$ defined on the Borel sets of $\mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$ *extends* ρ if

$$\int_{\mathrm{Hom}^+(\mathcal{A}^\sigma,\mathbb{R})} \rho(f)\mathbf{P}^{\sigma,\eta}(d\rho) = \frac{\rho([\![f]\!]_{\sigma,\eta})}{\rho([\![1_\sigma]\!]_{\sigma,\eta})} \,,$$

for any $f \in \mathcal{A}^\sigma$.

Theorem 2.3. *Let σ be a type of order k, and let $\sigma_0 = \sigma|_\eta$ be its restriction. Fix a homomorphism $\rho \in \mathrm{Hom}^+(\mathcal{A}^{\sigma_0}, \mathbb{R})$ with $\rho((\sigma,\eta)) > 0$. Then there exists a probability measure $\mathbf{P}^{\sigma,\eta}$ defined on the Borel sets of $\mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$ which extends ρ.*

The *random homomorphism rooted at ρ* is a random homomorphism given by the distribution $\mathbf{P}^{\sigma,\eta}$ and is denoted by $\boldsymbol{\rho}^{\sigma,\eta}$. For such a random homomorphism $\boldsymbol{\rho}^{\sigma,\eta}$ it holds that

$$\mathbf{E}[\boldsymbol{\rho}^{\sigma,\eta}(f)] = \frac{\rho([\![f]\!]_{\sigma,\eta})}{\rho([\![1_\sigma]\!]_{\sigma,\eta})} \,, \tag{2.2}$$

for any $f \in \mathcal{A}^\sigma$.

2.5. **Minimum outdegree and outdegree distribution.** Random homomorphisms allow us to define *minimum outdegree* $\delta_\alpha(\rho)$ of a homomorphism $\rho \in \mathrm{Hom}^+(\mathcal{A}^0, \mathbb{R})$. This is defined by

$$\delta_\alpha(\rho) = \max\{a : \mathbf{P}[\boldsymbol{\rho}^1(\alpha) < a] = 0\} \,.$$

It is not true that if a sequence $\{D_n\}_{n=1}^\infty$ of digraphs converges to ϕ then $\lim_{n\to\infty} \delta^+(D_n)/|V(D_n)| = \delta_\alpha(\phi)$. Indeed, let us try to add to every digraph D_n an isolated vertex to get a modified digraph D_n'. Then $\delta^+(D_n') = 0$, but the object ϕ is a limit of the sequence $\{D_n'\}_{n=1}^\infty$ as well. However, the converse is true: if all digraphs D_n have large minimum outdegree, then $\delta_\alpha(\phi)$ is large as well ([9]).

Theorem 2.4. *Suppose that* $\{D_n\}_{n=1}^{\infty}$ *is a sequence which converges to* ϕ*. Then*

$$\delta_\alpha(\phi) \geq \liminf_{n\to\infty} \frac{\delta^+(D_n)}{|V(D_n)|} .$$

As discussed above, the dual statement to Theorem 2.4 does not hold in general. However, a weaker statement is true. For each $\phi \in \mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$ there exists a sequence $\{D_n\}_{n=1}^{\infty}$ of digraphs which converges to ϕ, such that $\lim_n \delta^+(D_n)/|V(D_n)| = \delta_\alpha(\phi)$.

Theorem 2.5. *Suppose that* $\phi \in \mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$ *is given. Then there exists a sequence* $\{D_n\}_{n=1}^{\infty}$ *of triangle-free digraphs which converges to* ϕ*, and such that*

$$\lim_{n\to\infty} \frac{\delta^+(D_n)}{|V(D_n)|} = \delta_\alpha(\phi) .$$

To prove Theorem 2.5 it is enough to consider digraphs D_n generated at random according to a distribution given by ϕ; the way how to generate the digraphs D_n is described in [7, Section 2.6]. It can be checked that $\lim_n D_n = \phi$ and $\lim_n \delta^+(D_n)/|V(D_n)| = \delta_\alpha(\phi)$ almost surely. The calculations needed to this end are very similar to those carried in [7] and we omit them.

Suppose that a sequence of triangle-free digraphs $\{D_n\}_{n=1}^{\infty}$ converges to ϕ. We shall need to relate the outdegree distributions in the graphs D_n to the distribution of $\boldsymbol{\phi}^{\mathbf{1}}(\alpha)$. For a triangle-free digraph F of order n and for a number $c \in [0,1]$ we write

$$S(F,c) := \frac{|\{v \in V(F) \,:\, \deg^+(v) \leq cn\}|}{n} .$$

As a consequence of [9, Theorem 3.12] we get the following.

Lemma 2.6. *Let* $\{D_n\}_{n=1}^{\infty}$ *be an arbitrary sequence of triangle-free graphs such that* $\lim D_n = \phi$*. Then*

$$\mathbf{P}[\boldsymbol{\phi}^{\mathbf{1}}(\alpha) \leq c] \geq \liminf_{n\to\infty} S(F,c) .$$

2.6. **Cauchy-Schwarz Inequality.** One of the most frequently used tools in extremal combinatorics is the Cauchy-Schwarz Inequality. Recently, Lovász and Szegedy [8] made some progress on formalizing its importance in the context of extremal graph theory. They have shown that every linear inequality between subgraph densities that holds asymptotically for all graphs can be approximated (with arbitrary precision) with an inequality which can be proven using only finitely many applications of the Cauchy-Schwarz Inequality. However, their result does not apply to problems which involve the minimum degree condition. In the language of flag algebras the Cauchy-Schwarz Inequality reads as follows (cf. [9, Theorem 3.14]).

Theorem 2.7. *Suppose that* σ *is a type and* $\sigma_0 = \sigma|_\eta$ *its restriction. Then for arbitrary* $f \in \mathcal{A}^\sigma$ *and for arbitrary* $\rho \in \mathrm{Hom}^+(\mathcal{A}^{\sigma_0}, \mathbb{R})$ *it holds*

$$\rho\left([\![f^2]\!]_{\sigma,\eta}\right) \geq 0 .$$

2.7. **Inductive arguments.** Another tool commonly used in the area of extremal combinatorics is mathematical induction. To formalize such arguments in flag algebras framework, Razborov [9] introduces the notion of *an upward operator*. We will only use two special instances of this operator defined below.

Let σ be a type of order k, and $\eta : [k'] \to [k]$ an injective mapping. For a σ-flag $F = (D,\theta)$ let $F\downarrow_\eta$ be a $\sigma|_\eta$-flag defined by

$$F\downarrow_\eta := F|_\eta \setminus \theta([k] \setminus \mathrm{Im}(\eta)) .$$

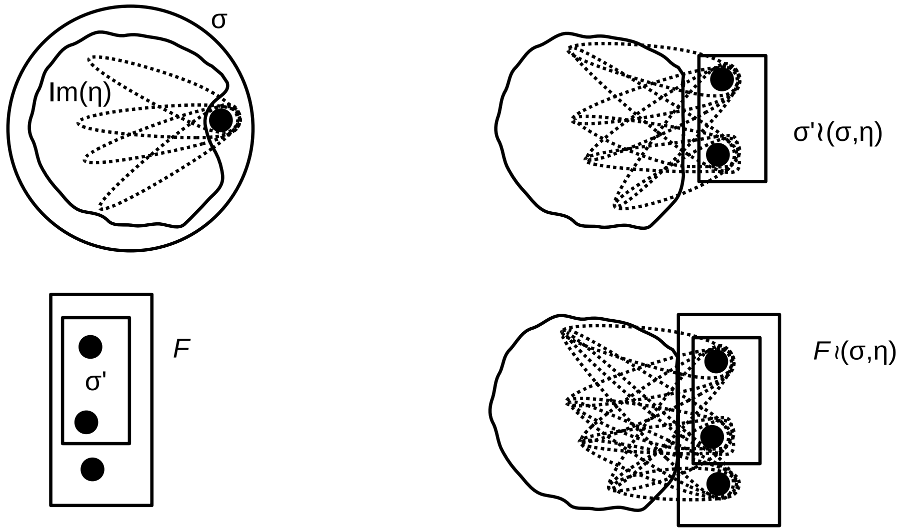

FIGURE 2. The operation $F \wr (\sigma, \eta)$.

Let $\pi^{\sigma,\eta} : \mathcal{A}^{\sigma|_\eta} \to \mathcal{A}^\sigma$ be defined by its action on $\mathcal{F}^{\sigma|_\eta}$ as follows

$$\pi^{\sigma,\eta}(F) = \sum_{\substack{\hat{F} \in F^\sigma \\ \hat{F}\downarrow_\eta = F}} \hat{F} ,$$

for $F \in \mathcal{F}^{\sigma|_\eta}$.

We will use the following properties of $\pi^{\sigma,\eta}$ established in [9, Theorem 3.18, Corollary 3.19].

Theorem 2.8. *Let σ_0 be a type, $\phi \in \mathrm{Hom}(\mathcal{A}^{\sigma_0}, \mathbb{R})$, and $k_1 \le k_2$ be two nonnegative integers. Let (σ_1, η_1) and (σ_2, η_2) be two extensions of σ_0 of orders k_1 and k_2, respectively, such that $\phi((\sigma_i, \eta_i)) > 0$ $(i = 1, 2)$, and $\eta : [k_1] \to [k_2]$ an injective mapping such that $\sigma_2|_\eta = \sigma_1$ and $\eta_2 = \eta \circ \eta_1$.*

a) *For every $f \in \mathcal{A}^{\sigma_0}$ we have*

$$\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\sigma_1},\boldsymbol{\eta_1}}(\pi^{\sigma_1,\eta_1}(f)) = \phi(f)] = 1 .$$

b) *For any $f \in \mathcal{A}^{\sigma_1}$ we have*

$$\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\sigma_1},\boldsymbol{\eta_1}}(f) = 0] = 1 \quad \Rightarrow \quad \mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\sigma_2},\boldsymbol{\eta_2}}(\pi^{\sigma_2,\eta}(f)) = 0] = 1 .$$

2.8. **A product operation.** Let σ be a type of order k and let $\eta : [k-1] \to [k]$ be an injective mapping. For a σ'-flag F with $|\sigma'| = k'$, we now define type $\sigma' \wr (\sigma, \eta)$ and a $(\sigma' \wr (\sigma, \eta))$-flag $F \wr (\sigma, \eta)$. In fact, we define only $F \wr (\sigma, \eta)$ as this gives a complete description of $\sigma' \wr (\sigma, \eta)$. The function $\mathrm{add}_{k-1} : \mathbb{Z} \to \mathbb{Z}$ maps x to $x + k - 1$. $F \wr (\sigma, \eta)$ denotes the unique flag $\hat{F} = (D, \theta)$ such that $\theta : [k-1+k'] \to V(D)$ is injective, $(D|_{\theta([k-1]) \cup \{v\}}, \theta([k-1])) \cong (\sigma, \eta)$ for every $v \in V(D) \setminus \theta([k-1])$, and $(D \setminus \theta([k-1]), \theta \circ \mathrm{add}_{k-1}) \cong F$. For $F \in \mathcal{F}^{\sigma'}$ we have $F \wr (\sigma, \eta) \in \mathcal{F}^{\sigma' \wr (\sigma, \eta)}$. The construction is illustrated on Figure 2. Let $\pi^{\wr(\sigma,\eta)}_{\sigma'} : \mathbb{R}\mathcal{F}^{\sigma'} \to \mathbb{R}\mathcal{F}^{\sigma' \wr (\sigma,\eta)}$ be the linear extension of the map $F \mapsto F \wr (\sigma, \eta)$. Note that $\mathcal{K}^{\sigma'}$ does not necessarily lie in the kernel of $\pi^{\wr(\sigma,\eta)}_{\sigma'}$.

Let $\phi \in \mathrm{Hom}(\mathcal{A}^{\sigma|_\eta}, \mathbb{R})$. If $\phi((\sigma, \eta)) \neq 0$ we define

$$\phi^{\wr(\sigma,\eta)}(F) := \phi(\pi^{\wr(\sigma,\eta)}(F)) / (\phi((\sigma, \eta)))^{l-k+1}$$

for a flag $F \in \mathcal{F}^0$ of order l. If $\phi((\sigma, \eta)) = 0$ we define $\phi^{\wr(\sigma,\eta)}(f) := 0$ for every $f \in \mathcal{F}^0$ instead. By [9, Theorems 2.6 and 4.1], we have the following.

Theorem 2.9. *Let σ be a type of order k and let $\eta : [k-1] \to [k]$ be an injective map.*

a) *For every $\phi \in \mathrm{Hom}(\mathcal{A}^{\sigma|_\eta}, \mathbb{R})$ we have*

$$\phi^{\wr(\sigma,\eta)} \in \mathrm{Hom}(\mathcal{A}^0, \mathbb{R}) .$$

b) *For every $\phi \in \mathrm{Hom}(\mathcal{A}^{\sigma|_\eta}, \mathbb{R})$ and type σ' and $f \in \mathcal{A}^{\sigma'}$ we have*

$$\mathbf{P}\left[\boldsymbol{\phi}^{\boldsymbol{\sigma'}\wr(\boldsymbol{\sigma},\boldsymbol{\eta}),\,\boldsymbol{\eta}}\left(\pi_{\sigma'}^{\wr(\sigma,\eta)}(f)\right) \geq 0\right] = 1 \quad \Rightarrow \quad \mathbf{P}\left[\left(\boldsymbol{\phi}^{\wr(\boldsymbol{\sigma},\boldsymbol{\eta})}\right)^{\boldsymbol{\sigma'}}(f) \geq 0\right] = 1 .$$

3. The structure of triangle-free digraphs

We first make several observations which will later allow us to restrict our attention only to special classes of digraphs.

Observation 3.1. *Let D be a triangle-free digraph with $\delta^+(D) \geq k$. Then there exists a triangle-free digraph D' on the same vertex set with outdegree of every vertex equal to k.*

Indeed, to obtain the digraph D' it suffices to remove for every vertex v arbitrary $\deg^+(v) - k$ edges leaving v.

Suppose that D is an n-vertex digraph. We replace every vertex $v \in V(D)$ by a copy D_v of the digraph D and every directed edge by uv of the original digraph D by a complete directed bipartite graph from D_u to D_v. This construction yields a digraph $D^{(2)}$ on n^2 vertices. It is easy to check that $\delta^+(D^{(2)}) = \delta^+(D)n$. Moreover if D is triangle-free, then so is $D^{(2)}$.

Using this procedure repeatedly we get the following.

Observation 3.2. *Suppose that there exists a triangle-free n-vertex digraph D with minimum outdegree at least cn. Then for any m_0 there exists a triangle-free digraph D' of order $m > m_0$ with minimum outdegree at least cm.*

Moreover, if D was outregular, then so is D'.

3.1. Triangle-free and acyclic digraphs.

A recent result of Chudnovsky, Seymour and Sullivan [3] asserts that one can delete k edges from a triangle-free digraph D with at most k non-edges to make it acyclic. Hamburger, Haxell and Kostochka [5] used this result to refine a proof of Shen [12], and consequently to obtain the previously best-known bound on the Caccetta-Häggkvist conjecture. They used the following corollary of the Chudnovsky-Seymour-Sullivan Theorem.

Lemma 3.3. *Suppose D is a triangle-free digraph with k non-edges. Then there is a vertex $v \in V(D)$ with $\deg^+(v) < \sqrt{2k}$.*

We refer the reader to [5] for a proof. The above lemma can be stated in the language of flag algebras and homomorphisms as follows.

Lemma 3.4. *For every $\phi \in \mathrm{Hom}^+(\mathcal{A}^0, \mathbb{R})$ we have for every $\epsilon_0 > 0$ that*

$$\mathbf{P}\left[\boldsymbol{\phi}^{\mathbf{1}}(\alpha) < \sqrt{1 - \phi(\varrho)} + \epsilon_0\right] > 0 .$$

Proof. By Theorem 2.2 there exists a sequence $\{D_n\}_{n=1}^{\infty}$ of triangle-free graphs such that $\lim D_n = \phi$. By the definition of convergence, for every $\epsilon > 0$, there exists a number n_0 such that for every digraph D_n $(n > n_0)$ contains at most $(1 - \phi(\varrho) + \epsilon)|V(D_n)|^2/2$ non-edges. A repeated application of Lemma 3.3 gives that there exists a set $S_n \subseteq V(D_n)$, $|S_n| \geq \epsilon|V(D_n)|$ such that $\deg^+(v) \leq \left(\sqrt{1 - \phi(\varrho) + \epsilon} + \epsilon\right)|V(D_n)|$ for every $v \in S_n$. By Lemma 2.6, we conclude that

$$\mathbf{P}\left[\boldsymbol{\phi}^{\mathbf{1}}(\alpha) \leq \left(\sqrt{1 - \phi(\varrho) + \epsilon} + \epsilon\right)\right] \geq \epsilon .$$

□

3.2. **Caccetta-Häggkvist Conjecture in the language of flag algebras.** Theorem 3.5 below is the main technical result of the paper. It translates Theorem 1.2 into the limit setting.

Theorem 3.5. *It holds in $\mathcal{T}$ that*

$$\max_{\rho \in \mathrm{Hom}^+(\mathcal{A}^0,\mathbb{R})} \delta_\alpha(\rho) < 0.3465 .$$

Theorem 3.5 is proven in Section 4. We now demonstrate that it implies Theorem 1.2.

Proof of Theorem 1.2. Suppose for contradiction that there exist a triangle-free n-vertex digraph D with $\delta^+(D) = cn$, $c \geq 0.3465$. By Observation 3.1 there exists an infinite sequence $D_1, D_2, \dots$ of triangle-free digraphs with increasing orders such that the digraph D_i of order n_i has minimum outdegree at least cn_i. By Theorem 2.2, this sequence contains a subsequence $D_{k_1}, D_{k_2}, \dots$ with $\lim_{i\to\infty} D_{k_i} = \rho \in \mathrm{Hom}^+(\mathcal{A}^0,\mathbb{R})$. Since the minimum outdegree ratio translates to the limit object ρ by Theorem 2.4, we have $\delta_\alpha(\rho) \geq 0.3465$ which violates Theorem 3.5. □

4. Proof of theorem 3.5

Let $\rho \in \mathrm{Hom}^+(\mathcal{A}^0,\mathbb{R})$ be such that the maximum value of $\delta_\alpha(\rho)$ is attained. Such ρ exists by [9, Theorem 3.15]. We set $c := \delta_\alpha(\rho)$. By considering a sequence of graphs converging to ρ and using Theorems 2.2 and 2.5, and Observation 3.1, we assume without loss of generality that

$$\mathbf{P}[\boldsymbol{\rho}^{\mathbf{1}}(\alpha) = c] = 1 . \tag{4.1}$$

We proceed by deriving a series of inequalities on the values of ρ in Sections 4.2–4.5. We will concentrate our attention on inequalities which can be expressed in terms of values of ρ on the elements of $\mathcal{F}_4^0$. To be able to write down these inequalities we will need to enumerate elements of $\mathcal{F}_4^0$, and also the elements of $\mathcal{F}_3^\beta$ and $\mathcal{F}_3^1$, which is done in the following subsection.

4.1. **Notation.** The elements of $\mathcal{F}_3^\beta$ are denoted by $K_0, \dots, K_7$. The vertex set of each of these graphs is $\{1, 2, a\}$, where 1 and 2 are labelled vertices, inducing β. and the edge set of each of these graphs is listed in the table below.

K_0	$\{12\}$	K_3	$\{12, 1a\}$	K_6	$\{12, a1\}$
K_1	$\{12, 2a\}$	K_4	$\{12, 1a, 2a\}$	K_7	$\{12, a1, a2\}$
K_2	$\{12, a2\}$	K_5	$\{12, 1a, a2\}$		

The symbols $L_0, \dots L_{13}$ denote the elements of $\mathcal{F}_3^1$, considered as graphs on the vertex set $\{1, a, b\}$, where 1 is the labelled vertex. The edge sets are given below.

L_0	$\{\}$	L_5	$\{b1\}$	L_{10}	$\{1a, b1\}$
L_1	$\{ab\}$	L_6	$\{b1, ab\}$	L_{11}	$\{1a, b1, ba\}$
L_2	$\{1b\}$	L_7	$\{b1, ba\}$	L_{12}	$\{a1, b1\}$
L_3	$\{1b, ab\}$	L_8	$\{1a, 1b\}$	L_{13}	$\{a1, b1, ab\}$
L_4	$\{1b, ba\}$	L_9	$\{1a, 1b, ab\}$		

Finally, we enumerate the elements of $\mathcal{F}_4^0$, i.e., all isomorphism types of triangle-free digraphs on the vertex set $\{a, b, c, d\}$. The table below gives edge sets of each of these thirty-two digraphs $H_0, \dots, H_{31}$.

H_0	$\{\}$	H_{11}	$\{ad, bc, cd\}$	H_{22}	$\{ac, ad, bc, bd, cd\}$
H_1	$\{cd\}$	H_{12}	$\{ad, bc, bd\}$	H_{23}	$\{ac, ad, bc, db\}$
H_2	$\{bd, cd\}$	H_{13}	$\{ad, bc, bd, cd\}$	H_{24}	$\{ac, ad, bc, db, dc\}$
H_3	$\{bd, dc\}$	H_{14}	$\{ad, bc, bd, dc\}$	H_{25}	$\{ac, da, bc, db\}$
H_4	$\{db, dc\}$	H_{15}	$\{ad, bc, db\}$	H_{26}	$\{ac, da, bc, db, dc\}$
H_5	$\{ad, bd, cd\}$	H_{16}	$\{ad, bc, db, dc\}$	H_{27}	$\{ac, ad, cb, db, cd\}$
H_6	$\{ad, bd, dc\}$	H_{17}	$\{da, bc, bd\}$	H_{28}	$\{ac, da, cb, bd\}$
H_7	$\{ad, db, dc\}$	H_{18}	$\{da, bc, bd, cd\}$	H_{29}	$\{ac, da, cb, db, dc\}$
H_8	$\{da, db, dc\}$	H_{19}	$\{da, bc, bd, dc\}$	H_{30}	$\{ca, da, cb, db, cd\}$
H_9	$\{bc, bd, cd\}$	H_{20}	$\{da, bc, db, dc\}$	H_{31}	$\{ab, ac, ad, bc, bd, cd\}$
H_{10}	$\{ad, bc\}$	H_{21}	$\{ac, ad, bc, bd\}$		

For brevity, $\rho(H_i)$ denotes ρ_i for $i = 0, 1, \dots, 31$, and $\bar{\rho} = (\rho_0, \rho_1, \dots, \rho_{31})$.

4.2. **Cauchy-Schwarz inequalities.** Let $\bar{a} \in \mathbb{R}^8$ be a (row) vector and let $\bar{K} = (K_0, \dots, K_7)$. Direct computation shows that $24\rho(\llbracket(\bar{a}\bar{K}^\intercal)^2\rrbracket_\beta) = \bar{a}(CS(\bar{\rho}))\bar{a}^\intercal$, where $CS(\bar{\rho})$ is the matrix given in Table 1; the entry $CS(\bar{\rho})_{ij}$ is $\rho(24\llbracket K_i \cdot K_j\rrbracket_\beta)$ computed by expanding $\llbracket K_i \cdot K_j\rrbracket_\beta \in \mathbb{R}\mathcal{F}_4^0$ as a sum of elements of $\mathcal{F}_4^0$.

From Theorem 2.7 we deduce the following corollary.

Corollary 4.1. *For every $\bar{a} \in \mathbb{R}^8$ we have*

$$\bar{a}(CS(\bar{\rho}))\bar{a}^\intercal \geq 0. \tag{4.2}$$

4.3. **Out-Regularity.**

Lemma 4.2. *For every $f \in \mathcal{A}^1$ we have $\rho(\llbracket f \cdot (\alpha - c)\rrbracket_1) = 0$.*

Proof. As $\boldsymbol{\rho}^1(f \cdot (\alpha - c)) = \boldsymbol{\rho}^1(f)\boldsymbol{\rho}^1(\alpha - c)$ and $\boldsymbol{\rho}^1(\alpha - c) = 0$ with probability one, by (4.1) we have

$$\mathbf{E}[\boldsymbol{\rho}^1(f \cdot (\alpha - c))] = 0, \tag{4.3}$$

The lemma follows from (2.2) and (4.3). □

Let $\bar{b} \in \mathbb{R}^{14}$ be a vector, let $\bar{L} = (L_0, \dots, L_{13})$. We have $24\rho(\llbracket\bar{b}\bar{L}^\intercal \cdot (\alpha - c)\rrbracket_1) = \bar{b}(B_{Reg} - cA_{Reg})\bar{\rho}^\intercal$, where the matrices A_{Reg} and B_{Reg} are given in Table 2. Thus Lemma 4.2 implies the following.

Corollary 4.3. *For every $\bar{b} \in \mathbb{R}^{14}$ we have*

$$\bar{b}(B_{Reg} - cA_{Reg})\bar{\rho}^\intercal \geq 0\ . \tag{4.4}$$

4.4. **Induction.** In this section we formalize the inductive argument of Shen [12] in the language of flag algebras and generalize it. Let $F = (D, \theta)$ be a σ-flag. We say that F is a *σ-source* if no edge of D has a tail in $V(D) \setminus \mathrm{Im}(\theta)$ and a head in $\mathrm{Im}(\theta)$. The set of all σ-sources of order k is denoted by $\mathcal{F}_k^{\sigma,\to}$. Recall that $c = \delta_\alpha(\rho)$.

Lemma 4.4. *Let σ be a type of order k such that 1 has indegree $k-1$ in σ. Let $F_0 = (D, \theta)$ be a σ-flag with $|V(D)| = k+1$ such that every vertex of $\mathrm{Im}(\theta)$ is connected to the unique vertex in $V(D) \setminus \mathrm{Im}(\theta)$ by an outgoing edge. Let*

$$f(\sigma) := -c + \sum\{F :\ F \in \mathcal{F}_{k+1}^{\sigma,\to},\ F \ncong F_0\} + cF_0\ . \tag{4.5}$$

Then $\rho(\llbracket f(\sigma)\rrbracket_\sigma) \geq 0$.

$$
\begin{bmatrix}
2\rho_1+4\rho_{10} & \rho_3+\rho_{11}+\rho_{15} & 2\rho_2+\rho_{11}+\rho_{12} & 2\rho_4+\rho_{12}+\rho_{17} & \rho_9+\rho_{13}+\rho_{18} & \rho_9+\rho_{14}+\rho_{19} & \rho_3+\rho_{15}+\rho_{17} & \rho_9+\rho_{16}+\rho_{20} \\
\rho_3+\rho_{11}+\rho_{15} & 2\rho_7+2\rho_{16} & 2\rho_6+\rho_{14} & \rho_{17}+\rho_{23}+2\rho_{25} & \rho_{19}+\rho_{24}+\rho_{27} & \rho_{18}+\rho_{27} & \rho_{15}+\rho_{23}+4\rho_{28} & \rho_{18}+\rho_{29} \\
2\rho_2+\rho_{11}+\rho_{12} & 2\rho_6+\rho_{14} & 6\rho_5+2\rho_{13} & \rho_{12}+4\rho_{21}+\rho_{23} & \rho_{14}+2\rho_{22} & \rho_{13}+2\rho_{22}+\rho_{24} & \rho_{11}+\rho_{23}+2\rho_{25} & \rho_{13}+\rho_{24}+2\rho_{26} \\
2\rho_4+\rho_{12}+\rho_{17} & \rho_{17}+\rho_{23}+2\rho_{25} & \rho_{12}+4\rho_{21}+\rho_{23} & 6\rho_8+2\rho_{20} & \rho_{20}+2\rho_{26}+\rho_{29} & \rho_{20}+\rho_{29}+2\rho_{30} & 2\rho_7+\rho_{19} & \rho_{19}+2\rho_{30} \\
\rho_9+\rho_{13}+\rho_{18} & \rho_{19}+\rho_{24}+\rho_{27} & \rho_{14}+2\rho_{22} & \rho_{20}+2\rho_{26}+\rho_{29} & 2\rho_{30}+2\rho_{31} & \rho_{29}+\rho_{31} & \rho_{16}+\rho_{24} & \rho_{27}+\rho_{31} \\
\rho_9+\rho_{14}+\rho_{19} & \rho_{18}+\rho_{27} & \rho_{13}+2\rho_{22}+\rho_{24} & \rho_{20}+\rho_{29}+2\rho_{30} & \rho_{29}+\rho_{31} & 2\rho_{26}+2\rho_{31} & \rho_{16}+\rho_{27} & \rho_{24}+\rho_{31} \\
\rho_3+\rho_{15}+\rho_{17} & \rho_{15}+\rho_{23}+4\rho_{28} & \rho_{11}+\rho_{23}+2\rho_{25} & 2\rho_7+\rho_{19} & \rho_{16}+\rho_{24} & \rho_{16}+\rho_{27} & 2\rho_6+2\rho_{18} & \rho_{14}+\rho_{27}+\rho_{29} \\
\rho_9+\rho_{16}+\rho_{20} & \rho_{18}+\rho_{29} & \rho_{13}+\rho_{24}+2\rho_{26} & \rho_{19}+2\rho_{30} & \rho_{27}+\rho_{31} & \rho_{24}+\rho_{31} & \rho_{14}+\rho_{27}+\rho_{29} & 2\rho_{22}+2\rho_{31}
\end{bmatrix}
$$

TABLE 1. The matrix $CS(\bar\rho)$.

Proof. We consider two cases. The case when $\rho((\sigma,0)) = 0$ is trivial, as then $\rho(\llbracket f(\sigma)\rrbracket_\sigma) = 0$. Therefore, it suffices to consider the case $\rho((\sigma,0)) > 0$.

Let us first prove that

$$\mathbf{P}[\boldsymbol{\rho}^{\boldsymbol{\sigma}}(f(\sigma)) \ge 0] = 1\ . \tag{4.6}$$

For $i \in [k+1]$ we write $\xi_i : \{1\} \to [k+1]$ for the map $1 \mapsto i$. If $\phi \in \mathrm{Hom}^+(\mathcal{A}^\sigma,\mathbb{R})$ is such that $\phi(F_0) = 0$, then

$$\phi(\pi^{\sigma,\xi_1}(\alpha)) \le \phi\left(\sum\{F:\ F \in \mathcal{F}^{\sigma,\to}_{k+1},\ F \not\cong F_0\}\right)\ , \tag{4.7}$$

using triangle-freeness. It follows from (4.1), (4.5), and (4.7) that $\mathbf{P}[\boldsymbol{\rho}^{\boldsymbol{\sigma}}(f(\sigma)) < 0 \& \boldsymbol{\rho}^{\boldsymbol{\sigma}}(F_0) = 0] = 0$. It therefore suffices to show that

$$\mathbf{P}[\boldsymbol{\rho}^{\boldsymbol{\sigma}}(f(\sigma)) < 0 \,\&\, \boldsymbol{\rho}^{\boldsymbol{\sigma}}(F_0) > 0] = 0\ . \tag{4.8}$$

We restrict our attention to the case $\mathbf{P}[\boldsymbol{\rho}^{\boldsymbol{\sigma}}(F_0) > 0] > 0$, as otherwise is (4.8) trivial. Let σ' be a type of order $k+1$ such that $(\sigma',\eta') \cong F_0$ and $\mathrm{Im}(\eta') = [k]$. By Theorem 2.8 b) and (4.1) we have

$$\mathbf{P}[\boldsymbol{\rho}^{\boldsymbol{\sigma'}}(\pi^{\sigma',\xi_{k+1}}(\alpha - c)) = 0] = 1\ .$$

It follows that,

$$\mathbf{P}^\sigma[\mathbf{P}^{\sigma',\eta'}[(\boldsymbol{\rho}^{\boldsymbol{\sigma}})^{\boldsymbol{\sigma'},\boldsymbol{\eta'}}(\pi^{\sigma',\xi_{k+1}}(\alpha - c)) = 0]] = 1\ .$$

Thus (4.8) is established by the following claim.

Claim 4.4.1. *For every $\phi \in \mathrm{Hom}^+(\mathcal{A}^\sigma,\mathbb{R})$ such that $\phi(F_0) > 0$ and*

$$\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\sigma'},\boldsymbol{\eta'}}(\pi^{\sigma',\xi_{k+1}}(\alpha - c)) = 0] = 1 \tag{4.9}$$

$$
A_{Reg} = \begin{bmatrix}
12 & 6 & 3 & 3 & 3 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 3 & 4 & 2 & 2 & 1 & 1 & 2 & 1 & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 3 & 4 & 2 & 2 & 1 & 1 & 2 & 1 & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 0 & 6 & 2 & 0 & 0 & 0 & 0 & 2 & 2 & 4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 4 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 2 & 2 & 1 & 2 & 1 & 0 & 0 & 0 & 2 & 1 & 2 & 0 & 2 & 4 & 1 & 0 & 0 \\
0 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 3 & 4 & 2 & 2 & 1 & 1 & 2 & 1 & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 2 & 2 & 1 & 2 & 1 & 0 & 0 & 0 & 2 & 1 & 2 & 0 & 2 & 4 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 6 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 4 & 4 & 0 & 2 & 0 & 2 & 2 & 0 & 0 & 2 & 4 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 3 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 2 & 2 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 2 & 0 & 2 & 0 & 2 & 2 & 0 & 2 & 2 & 4 \\
0 & 0 & 0 & 1 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 2 & 2 & 1 & 2 & 1 & 0 & 0 & 0 & 2 & 1 & 2 & 0 & 2 & 4 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 2 & 0 & 2 & 0 & 2 & 2 & 0 & 2 & 2 & 4 \\
0 & 0 & 1 & 0 & 0 & 3 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 2 & 0 & 2 & 0 & 2 & 2 & 0 & 2 & 2 & 4
\end{bmatrix}
$$

$$
B_{Reg} = \begin{bmatrix}
0 & 1 & 2 & 1 & 0 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 4 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 2 & 0 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 2 & 2 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 2 & 3 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 2 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1
\end{bmatrix}
$$

TABLE 2. The matrices A_{Reg} and B_{Reg}.

we have

$$\phi(f(\sigma)) \geq 0 \, .$$

Proof of Claim 4.4.1. Note that $\pi^{\sigma',\eta'}(cF_0) = \pi_1^{\wr(\sigma',\eta')}(c)$. Then

$$
\begin{aligned}
\pi^{\sigma',\eta'}(f(\sigma)) &= \pi^{\sigma',\eta'}\left(\sum\{F : \ F \in \mathcal{F}_{k+1}^{\sigma,\to}, \ F \not\cong F_0\} + cF_0 - c\right) \\
&\geq_{\sigma'} \pi^{\sigma',\xi_{k+1}}(\alpha - c) - \pi_1^{\wr(\sigma',\eta')}(\alpha - c) \, , \qquad (4.10)
\end{aligned}
$$

using triangle-freeness. It follows that for every $\phi \in \mathrm{Hom}^+(\mathcal{A}^\sigma, \mathbb{R})$ it holds

$$\mathbf{P}\left[\boldsymbol{\phi}^{\boldsymbol{\sigma'},\boldsymbol{\eta'}}\left(\pi^{\sigma',\eta'}(f(\sigma))\right) \geq \boldsymbol{\phi}^{\boldsymbol{\sigma'},\boldsymbol{\eta'}}\left(\pi^{\sigma',\xi_{k+1}}(\alpha - c) - \pi_1^{\wr(\sigma',\eta')}(\alpha - c)\right)\right] = 1 \, . \qquad (4.11)$$

Using (4.9), the identity (4.11) can be rewritten as

$$\mathbf{P}\left[\boldsymbol{\phi}^{\boldsymbol{\sigma'},\boldsymbol{\eta'}}\left(\pi^{\sigma',\eta'}(f(\sigma))\right) \geq \boldsymbol{\phi}^{\boldsymbol{\sigma'},\boldsymbol{\eta'}}\left(\pi_1^{\wr(\sigma',\eta')}(c - \alpha)\right)\right] = 1 \, . \qquad (4.12)$$

Note that $1 \wr (\sigma', \eta') = \sigma'$. Further, it is easy to check that

$$\pi_1^{\wr(\sigma',\eta')}(\alpha) \leq_{\sigma'} \pi^{\sigma',\xi_{k+1}}(\alpha) \, , \text{ and} \qquad (4.13)$$

$$\pi_1^{\wr(\sigma',\eta')}(c) = \pi^{\sigma',\xi_{k+1}}(c) \, . \qquad (4.14)$$

Plugging (4.13) and (4.14) into (4.9), we get $\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\sigma'},\boldsymbol{\eta'}}(\pi_1^{\wr(\sigma',\eta')}(c-\alpha)) \geq 0] = 1$. This allows us to conclude from (4.12) that $\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\sigma'},\boldsymbol{\eta'}}\left(\pi^{\sigma',\eta'}(f(\sigma))\right) \geq 0] = 1$. Now, Theorem 2.8 a) asserts that $\phi(f(\sigma)) \geq 0$. $\square$

The inequality $\rho([\![f(\sigma)]\!]_\sigma) \geq 0$ follows from (4.6) by (2.2). $\square$

Let T and V denote the types of order 3 such that $E(T) = \{23, 21, 31\}$ and $E(V) = \{21, 31\}$. Note that T and V are the only types of order 3 satisfying the conditions of Lemma 4.4. We have

$$\begin{aligned}\rho([\![f(T)]\!]_T) =&(1-c)\rho_9 - c\rho_{13} - c\rho_{14} - c\rho_{16} + (1-c)\rho_{18} + (1-c)\rho_{19} + (1-c)\rho_{20}\\ &- 2c\rho_{22} - 2c\rho_{24} - 2c\rho_{26} + (1-2c)\rho_{27} + (1-2c)\rho_{29} + (2-2c)\rho_{30} - 3c\rho_{31},\end{aligned} \tag{4.15}$$

and

$$\begin{aligned}\rho([\![f(V)]\!]_V) =&(1-c)\rho_2 - 3c\rho_5 + (1-c)\rho_6 - c\rho_{11} + (1-c)\rho_{12} - 2c\rho_{13} + (1-c)\rho_{14}\\ &+ (2-2c)\rho_{21} - c\rho_{22} - c\rho_{23} - c\rho_{24} - c\rho_{25} - c\rho_{26}\ .\end{aligned} \tag{4.16}$$

Denote the right sides of the identities (4.15) and (4.16), considered as functions of $\bar{\rho}$, by $Ind_T(\bar{\rho})$ and $Ind_V(\bar{\rho})$, respectively. By Lemma 4.4 we have the following.

Corollary 4.5. *$Ind_T(\bar{\rho}) \geq 0$ and $Ind_V(\bar{\rho}) \geq 0$.*

4.5. **Density of Forks.** We use Lemma 3.4 to obtain a lower bound on $\rho(\kappa)$.

Lemma 4.6. *If $c \geq 1/3$ then $\rho(\kappa) \geq 3(3c-1)^2$.*

Proof. We begin with an auxiliary claim.

Claim 4.6.1. *Let $\phi \in \mathrm{Hom}^+(\mathcal{A}^1, \mathbb{R})$ be such that $\phi((\beta,1)) > 0$, and*

$$\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\beta},\mathbf{1}}(\pi^{\beta,2}(\alpha)) = c] = 1\ . \tag{4.17}$$

Then

$$\phi(\gamma) \geq c - \sqrt{\phi(\chi)}\ .$$

Proof of Claim 4.6.1. By Lemma 3.4 applied to $\phi^{\wr(\beta,1)}$ we have for every $\epsilon > 0$ that

$$\mathbf{P}[(\boldsymbol{\phi}^{\wr(\boldsymbol{\beta},\mathbf{1})})^{\mathbf{1}}(\alpha) < \sqrt{1 - \phi^{\wr(\beta,1)}(\varrho)} + \epsilon] > 0\ .$$

By the counterpositive of Theorem 2.9 b) and the definition of $\phi^{\wr(\beta,1)}$ it follows that for every $\epsilon > 0$ we have

$$\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\beta},\mathbf{1}}(\pi_1^{\wr(\beta,1)}(\alpha)) < \sqrt{\phi(\pi^{\wr(\beta,1)}(1-\varrho))} + \epsilon] > 0\ . \tag{4.18}$$

Note that $\pi^{\wr(\beta,1)}(1-\varrho) = \chi$. It follows from (4.17) and (4.18) that

$$\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\beta},\mathbf{1}}(\pi^{\beta,2}(\alpha) - \pi^{\wr(\beta,1)}(\alpha)) > c - \sqrt{\phi(\chi)} - \epsilon] > 0\ , \tag{4.19}$$

for any $\epsilon > 0$. We have $\pi^{\beta,2}(\alpha) - \pi^{\wr(\beta,1)}(\alpha) \leq_\beta \pi^{\beta,1}(\gamma)$. Thus,

$$\mathbf{P}[\boldsymbol{\phi}^{\boldsymbol{\beta},\mathbf{1}}(\pi^{\beta,1}(\gamma)) > c - \sqrt{\phi(\chi)} - \epsilon] > 0\ , \tag{4.20}$$

for any $\epsilon > 0$.

We claim that $\phi(\gamma) \geq c - \sqrt{\phi(\chi)}$. Indeed, suppose for contradiction that $\phi(\gamma) = c - \sqrt{\phi(\chi)} - \epsilon'$ for some $\epsilon' > 0$. By Theorem 2.8 a) we conclude that

$$\mathbf{P}\left[\boldsymbol{\phi}^{\boldsymbol{\beta},\mathbf{1}}\left(\pi^{\beta,1}(\gamma) - c + \sqrt{\phi(\chi)} + \epsilon'\right) = 0\right] = 1\ ,$$

a contradiction to (4.20). □

Note that homomorphisms in $\{\boldsymbol{\rho}^{\mathbf{1}}\}$ satisfy $\rho^1((\beta,1)) > 0$ and (4.17) almost surely. Therefore, by Claim 4.6.1, $\mathbf{P}[\boldsymbol{\rho}^{\mathbf{1}}(\gamma) + \sqrt{\boldsymbol{\rho}^{\mathbf{1}}(\chi)} \geq c] = 1$. It follows that $\mathbf{E}[\sqrt{\boldsymbol{\rho}^{\mathbf{1}}(\chi)}] \geq 3c-1$, and the lemma is implied by Jensen's inequality, as $\rho(\kappa) = 3\mathbf{E}[\boldsymbol{\rho}^{\mathbf{1}}(\chi)]$. □

Expanding $J-3(3c-1)^2$ in the basis $\mathcal{F}_4^0$ we get

$$\begin{aligned}4\rho(J-3(3c-1)^2) =& \rho_4+\rho_7+3\rho_8+\rho_{12}+\rho_{17}+\rho_{19}+2\rho_{20}+2\rho_{21}\\ &+\rho_{23}+\rho_{25}+\rho_{26}+\rho_{29}+2\rho_{30}-12(3c-1)^2\sum_{i=0}^{31}\rho_i\,.\end{aligned}$$

Denote the right side of the above identity by $Fork(\bar{\rho})$. The next statement follows directly from Lemma 4.6.

Corollary 4.7. *If* $c\geq 1/3$ *then* $Fork(\bar{\rho})\geq 0$.

4.6. **Combining the ingredients.** Let $R(c)$ denote the set of vectors $\bar{r}\in\mathbb{R}^{32}$ such that

(P1) $\bar{r}\geq\bar{0}$,
(P2) $\|\bar{r}\|_1=1$,
(P3) $\bar{a}(CS(\bar{r}))\bar{a}^{\intercal}\geq 0$ for every $\bar{a}\in\mathbb{R}^8$,
(P4) $\bar{b}(B_{Reg}-cA_{Reg})\bar{r}^{\intercal}\geq 0$ for every $\bar{b}\in\mathbb{R}^{14}$,
(P5) $Ind_T(\bar{r})\geq 0$ and $Ind_V(\bar{r})\geq 0$, and
(P6) $Fork(\bar{r})\geq 0$.

Corollaries 4.1, 4.3, 4.5 and 4.7 imply that $\bar{\rho}\in R(c)$ for $c\geq 1/3$. Therefore the following proposition implies Theorem 3.5.

Proposition 4.8. $R(c)=\varnothing$ *for* $c\geq 0.3465$.

Proof. Let

$$\begin{aligned}
\bar{a}_1&=(\ -69.83,\ -27.04,\ 3.45,\ -53.59,\ 1.74,\ 28.78,\ -9.28,\ 59.66\ )\,,\\
\bar{a}_2&=(\ -44.57,\ -25.93,\ -24.40,\ -30.16,\ 2.40,\ 5.40,\ 15.67,\ 37.27\ )\,,\\
\bar{a}_3&=(\ 86.95,\ 58.70,\ 35.15,\ 52.46,\ -18.52,\ 3.32,\ -52.56,\ -57.83\ )\,,\\
\bar{a}_4&=(\ -1.29,\ 0.17,\ 57.48,\ -26.29,\ 10.28,\ 26.90,\ -27.33,\ -9.15\ )\,,
\end{aligned}$$

$\bar{b}=(0,0,-17448,-16496,26501,-24163,-8929,-54193,-30136,7267,-24582,-42769,22644,0)$,

$$c_T=39648\,,\qquad c_V=19877\,,\ \text{and}\qquad d=2078\,.$$

Further, let

$$F(c,\bar{r}):=\left(\sum_{i=1}^{4}\bar{a}_i(CS(\bar{r}))\bar{a}_i^{\intercal}\right)+\bar{b}(B_{Reg}-cA_{Reg})\bar{r}^{\intercal}+c_TInd_T(\bar{r})+c_VInd_V(\bar{r})+d\cdot Fork(\bar{r})\,.$$

By definition of $R(c)$, we have $F(c,\bar{r})\geq 0$ for every $\bar{r}\in R(c)$. Moreover, it is not hard to directly verify that for fixed $\bar{r}\geq\bar{0}$ and $c\geq 1/3$ the function $F(c,\bar{r})$ is a non-increasing function of c. (See Maple worksheet [6].) On the other hand computing $F(0.3465,\bar{r})$ we get

$$\begin{array}{rrrrrrrr}
- & 38.906394\,\bar{r}_0 & - & 25.96859\,\bar{r}_1 & - & 4156.34069\,\bar{r}_2 & - & 16.447994\,\bar{r}_3\\
- & 1172.27439\,\bar{r}_4 & - & 577.3814\,\bar{r}_5 & - & 4.57689\,\bar{r}_6 & - & 10.55419\,\bar{r}_7\\
- & 4042.1489\,\bar{r}_8 & - & 10.328894\,\bar{r}_9 & - & 13.03079\,\bar{r}_{10} & - & 1327.03609\,\bar{r}_{11}\\
- & 2658.54869\,\bar{r}_{12} & - & 9.71489\,\bar{r}_{13} & - & 14574.68439\,\bar{r}_{14} & - & 7.032994\,\bar{r}_{15}\\
- & 6.85949\,\bar{r}_{16} & - & 11279.04479\,\bar{r}_{17} & - & 7.458494\,\bar{r}_{18} & - & 15538.64129\,\bar{r}_{19}\\
- & 19.61149\,\bar{r}_{20} & - & 15.87099\,\bar{r}_{21} & - & 12.39949\,\bar{r}_{22} & - & 9949.057894\,\bar{r}_{23}\\
- & 9.5492\,\bar{r}_{24} & - & 12.55709400\,\bar{r}_{25} & - & 17.24429\,\bar{r}_{26} & - & 9.535194\,\bar{r}_{27}\\
- & 1.24639\,\bar{r}_{28} & - & 3070.47399\,\bar{r}_{29} & - & 17.36519\,\bar{r}_{30} & - & 13.03819\,\bar{r}_{31}\,.
\end{array} \tag{4.21}$$

Note that the coefficients in (4.21) are exact (see [6] for calculations). The expression (4.21) is bounded from above by $F(0.3465, \bar{r}) \leq -1.24639\|\bar{r}\|_1 < 0$. Proposition 4.8 follows. □

5. Concluding remarks

5.1. **The algorithm.** We now sketch how we used a computer to aid us with our search for the right system of arguments. For a fixed value of c, the conditions (P1), (P2) and (P4)–(P6) in the definition of $R(c)$ give a polytope in $\mathbb{R}^{32}$, which is denoted by $R'(c)$. It is defined by 68 linear identities and inequalities. Therefore, it is not hard to check whether $R'(c)$ is empty, while it is much harder to verify if $R'(c)$ contains a point, satisfying condition (P3) for every $\bar{a} \in \mathbb{R}^8$. On the other hand checking, whether a *particular* point $\bar{r} \in \mathbb{R}^{32}$ satisfies (P3) for all choices $\bar{a}$ amounts to checking whether $CS(\bar{r})$ is positive semi-definite. If $CS(\bar{r})$ is not positive semi-definite then any eigenvector of $CS(\bar{r})$ corresponding to a negative eigenvalue serves as a certificate that $\bar{r} \notin R(c)$.

The algorithm which we use to find vectors $\bar{a}_1, \dots, \bar{a}_4$, given in the proof of Proposition 4.8, exploits the above observation, and proceeds as follows. Suppose that vectors $\bar{a}_1, \bar{a}_2, \dots, \bar{a}_k$ have been defined. Let $R_k(c)$ be the polytope in $\mathbb{R}^{32}$ defined by conditions (P1), (P2) and (P4)–(P6), and condition (P3), restricted to vectors $\bar{a}_1, \bar{a}_2, \dots, \bar{a}_k$. Using binary search we find c_k, an approximation of $\max\{c \mid R_k(c) \neq \varnothing\}$. We proceed to find an arbitrary point $\bar{r}_k \in R_k(c_k)$ and define $\bar{a}_{k+1}$ to be an eigenvector corresponding to some negative eigenvalue of $CS(\bar{r}_k)$. We repeat the process until $c_k - c_{k+1}$ falls below a prespecified threshold.

5.2. **Improving the bound.** It is possible to improve the bound we establish in Theorem 1.2 slightly at the expense of a more involved proof. As the improvements we were able to produce were not significant and relied on technical and computational tweaks, rather than new ideas, we have chosen to avoid overcomplicating the argument. Let us, however, point out a few ways in which one can attempt to improve Theorem 1.2.

1. Instead of concentrating on the values ρ takes on elements of $\mathcal{F}_4^0$, one can examine $\mathcal{F}_5^0$, instead. This leads to significant increase of matrices CS, A_{Reg} and B_{Reg} in size, and makes it harder to guarantee the absence of rounding errors.

2. One can attempt to generalize Lemma 4.4. We initially considered a much more general class of induction hypotheses and performed search over the corresponding parameters in a similar manner to the search over parameters in Cauchy-Schwarz inequalities described in Section 5.1. This did not, however, lead to any improvements of the bound.

3. Chudnovsky, Seymour and Sullivan [3] conjecture that one can delete $k/2$ edges from a triangle-free digraph D with at most k non-edges to make it acyclic. This conjecture implies improvements of Lemmas 3.3 and 3.4. Dunkum, Hamburger and Pór [4] have recently shown that deleting $0.88k$ edges suffices, and Shen [13] further improved this bound to $0.865k$. These results allow us to improve Lemma 3.4, but such an improvement in turn only produces a tiny decrease in the bound Theorem 1.2. However, the proofs in [3, 4] can both be recast in the language of flag algebras. It might be interesting see if one can obtain a generalization of Lemma 3.3 in this manner and use it to improve Theorem 1.2.

5.3. **Acknowledgement.** The computer search for the coefficients of the vector $F(c, \bar{r})$ was done using QSopt linear programming solver. We would like to thank its author William Cook for making the tool available and answering our questions concerning its usage.

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