NEW LOWER BOUNDS AND ASYMPTOTICS FOR THE CP-RANK

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ABSTRACT. Let p_n denote the largest possible cp-rank of an $n \times n$ completely positive matrix. This matrix parameter has its significance both in theory and applications, as it sheds light on the geometry and structure of the solution set of hard optimization problems in their completely positive formulation. Known bounds for p_n are $s_n = \binom{n+1}{2} - 4$, the current best upper bound, and the Drew-Johnson-Loewy (DJL) lower bound $d_n = \lfloor \frac{n^2}{4} \rfloor$. The famous DJL conjecture (1994) states that $p_n = d_n$. Here we show $p_n = \frac{n^2}{2} + \mathcal{O}(n^{3/2}) = 2d_n + \mathcal{O}(n^{3/2})$, and construct counterexamples to the DJL conjecture for all $n \geq 12$ (for orders seven through eleven counterexamples were already given in [3]).

1. Introduction: motivation, notations

1.1. Motivation: The cp-cone and copositive optimization. In this article we consider completely positive matrices M and their cp-rank. An $n \times n$ matrix M is said to be *completely positive* if there exists a nonnegative (not necessarily square) matrix V such that $\mathsf{M} = \mathsf{V}\mathsf{V}^\top$ ($^\top$ denotes transposition). This form of factorization is more restrictive than the general question of nonnegative matrix factorization where M could be rectangular; in fact, complete positivity of M implies positive-semidefiniteness and nonnegativity of all entries of M. Typically, a completely positive matrix $\mathsf{M} = \mathsf{V}\mathsf{V}^\top$ may have many such factorizations, and the *cp-rank* of

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M, cpr M, is the minimum number of columns in such a nonnegative factor V (for completeness, we define cpr $\mathsf{M} = 0$ if M is a square zero matrix and cpr $\mathsf{M} = \infty$ if M is not completely positive). The set $\mathcal{CP}_n$ of all completely positive $n \times n$ matrices forms a proper cone (i.e., it is pointed, convex, and solid in the sense that it has nonempty interior). With respect to the *Frobenius* inner product $\langle \mathsf{A}, \mathsf{B} \rangle := \mathrm{trace}(\mathsf{AB})$, this cone is dual to the cone $\mathcal{COP}_n$ of symmetric *copositive matrices* of order n. An $n \times n$ matrix S is said to be copositive if $\mathbf{x}^\top \mathsf{S} \mathbf{x} \geq 0$ for every nonnegative vector $\mathbf{x} \in \mathbb{R}^n$.

Copositive and completely positive matrices are central in the rapidly evolving field of *copositive optimization* which links discrete and continuous optimization, and has numerous real-world applications. For recent surveys and structured bibliographies, we refer to [4, 5, 6, 9], and for a fundamental text book to [2].

A conic optimization problem of the form

$$\inf\{\langle \mathsf{C}, \mathsf{X} \rangle : \langle \mathsf{A}_i, \mathsf{X} \rangle = b_i,\ i \in \{1, \dots, m\},\ \mathsf{X} \in \mathcal{CP}_n\} \tag{1}$$

is called *completely positive optimization problem*, but sometimes also *copositive optimization problem*, because the corresponding dual problem is given as

$$\sup\left\{ \sum_{i=1}^m b_i y_i : \mathbf{y} \in \mathbb{R}^m,\ \mathsf{S} = \mathsf{C} - \sum_{i=1}^m y_i \mathsf{A}_i \in \mathcal{COP}_n \right\}. \tag{2}$$

Both problems consist in optimizing a linear form over a feasible set which can be described as the intersection of an affine subspace with one of the cones $\mathcal{COP}_n$ or $\mathcal{CP}_n$. Hence at least one optimal solution (if this exists at all) must be contained in the boundary of these cones. Moreover, if strong duality for (1) and (2) holds, then there exists a primal-dual optimal pair $(\mathsf{X}^*, \mathsf{S}^*) \in \mathcal{CP}_n \times \mathcal{COP}_n$ with $\langle \mathsf{S}^*, \mathsf{X}^* \rangle = 0$ or $\mathsf{S}^* \perp \mathsf{X}^*$, which relation can be exploited to obtain information about X^* if we have some knowledge on S^*.

As remarked above, the conic primal-dual pair (1) and (2) serves to reformulate NP-hard optimization problems. Since everything else is linear, it is quite obvious that this approach shifts the whole complexity of the hard optimization problem into the (boundaries of the) cones $\mathcal{CP}_n$ and $\mathcal{COP}_n$. These boundaries are much more complex than the boundaries of the symmetric, self-dual cones used in polynomial-time conic optimization (such as Linear or Semidefinite Optimization, or optimization over the Minkowski cone). For instance, while the boundary of the semidefinite cone consists of matrices which are rank-deficient, the boundary of the completely positive cone $\mathcal{CP}_n$ also contains nonsingular matrices like the identity matrix, or matrices with all entries strictly positive like the all-ones matrix. So, neither linear constraints on the entries nor rank restrictions are sufficient to characterize or elucidate geometric properties of completely positive matrices. Therefore, the cp-rank was early recognized as a useful matrix parameter to shed more light upon the structure and the properties of completely positive matrices, and consequently has received considerable attention by researchers over the past decades.

Determining the maximum possible cp-rank of $n \times n$ completely positive matrices,

$$p_n := \max \{\text{cpr } \mathsf{M} : \mathsf{M} \in \mathcal{CP}_n\},$$

is still an open problem for general n. It is known [2, Theorem 3.3] that $p_n = n$ if $n \leq 4$, whereas this equality does no longer hold for $n \geq 5$. Let $d_n := \left\lfloor \frac{n^2}{4} \right\rfloor$ and $s_n := \binom{n+1}{2} - 4$. For $n \geq 5$, it is known that

$$d_n \leq p_n \leq s_n , \tag{3}$$

and that $d_n = p_n$ in case $n = 5$ [15]. It is still unknown whether $d_6 = p_6$ although the bracket (3) was reduced in the recent paper [14] where also the upper bound $p_n \leq s_n$ was established for the first time.

The famous Drew-Johnson-Loewy (DJL) conjecture [8] is by now twenty years old. It states that $d_n = p_n$ is true for all $n \geq 5$, and some evidence in support of the DJL conjecture is found in [1, 7, 8, 13], see also [2, Section 3.3]. In a recent paper [3] it was shown that the DJL conjecture does not hold for orders n ranging between seven and eleven by constructing examples which establish $p_n > d_n$.

1.2. **Notations, terminology and paper structure.** Some notation and terminology: we abbreviate $[r:s] = \{r, r+1, \dots, s\}$ for integers $r \leq s$. Let $\mathbf{e}_i \in \mathbb{R}^n$ be the ith column vector of the $n \times n$ identity matrix I_n and $\boldsymbol{\eta}_n = \sum_{i=1}^n \mathbf{e}_i$. By $\mathsf{E}_n = \boldsymbol{\eta}_n \boldsymbol{\eta}_n^\top$ we denote the $n \times n$ matrix of all ones. The nonnegative orthant is denoted by $\mathbb{R}^n_+$ which contains the standard simplex

$$\Delta_n := \left\{ \mathbf{x} \in \mathbb{R}^n_+ : \boldsymbol{\eta}_n^\top \mathbf{x} = 1 \right\} .$$

The matrix $\mathrm{Diag}(\mathbf{y})$ is a diagonal matrix containing the entries of $\mathbf{y}$ on the diagonal. The Kronecker product is denoted by $\otimes$, and

$$\mathsf{A} \oplus \mathsf{B} = \begin{bmatrix} \mathsf{A} & \mathsf{O} \\ \mathsf{O}^\top & \mathsf{B} \end{bmatrix}$$

means the direct sum of two square matrices. For a given $\mathbf{x} \in \mathbb{R}^k_+$, we define the *zero-norm* $\|\mathbf{x}\|_0$ as the number of positive entries $x_i > 0$. Given a square matrix $\mathsf{S} \in \mathcal{COP}_n$, we will use the phrase "zero(es) of S" as an abbreviation of "zero(es) $\mathbf{x} \in \Delta_n$ of the quadratic form $\mathbf{x}^\top \mathsf{S} \mathbf{x}$"; this terminology differs slightly from that in [11] but is more convenient for our purposes.

The paper is organized as follows: In Section 2 we look at copositive matrices S with finitely many (but many) zeroes. Such matrices S lie on the boundary of the copositive cone, and elementary conic duality therefore tells us that there are nontrivial completely positive matrices M such that $\mathsf{M} \perp \mathsf{S}$. There is a strong connection between the zeroes of S and the cp-rank of M, which is established through Lemma 2.2. Lemma 2.3 deals with cp-ranks of Khatri-Rao-like products (defined in Subsection 2.2) of matrices, which are necessary to make assertions about cp-ranks of high-order matrices. Combination of these auxiliary results culminates in Theorem 2.2 and in Corollary 2.1, which refutes the DJL conjecture for $n \geq 7$ and shows that the largest possible cp-rank p_n lies asymptotically much closer to the upper bound s_n than to the lower bound d_n.

Section 3 improves the lower bound for p_n in the following way: in Section 2 only identity matrices are used as building blocks to construct matrices of higher order. This is sufficient to prove the assertions of Section 2, but better results can be obtained by using, as building blocks, matrices with cp-ranks that exceed their orders. Some of these building-block-matrices are new in the literature, some of them were already used in [3]. To further illustrate the advantage of the approach in this article, an explicit construction of a matrix of order twelve with high cp-rank is presented in an appendix. Note that in contrast to [3], for general order n, we need not construct the matrices explicitly but rather can invoke the existence result in Lemma 2.2.

2. Main results

2.1. **Rank, two-rank and cp-rank.** Our method of finding matrices of high cp-rank builds upon two observations: (1) For certain matrices $\mathsf{M} \in \mathcal{CP}_n$, only multiples of vectors from a finite set $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$ may appear as columns of a factor V in any factorization $\mathsf{M} = \mathsf{V}\mathsf{V}^\top = \sum_{i=1}^k y_i \mathbf{u}_i \mathbf{u}_i^\top$, where $\mathbf{y} = [y_1, \ldots, y_k]^\top \in \mathbb{R}^k_+$. This property is shared by all matrices in a certain convex subcone of $\mathcal{CP}_n$ determined by the set $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$. (2) This subcone contains matrices with cp-rank bounded below by a number computable from the set $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$; so the cp-rank will be high if this number is large.

This argument is made precise in the following results, starting from the observation in a more general context, that a convex cone spanned by some finite set of vectors of rank r always contains a vector which is *not* a positive linear combination of *less than* r vectors from this finite set; a converse of Caratheodory's theorem in some sense.

Lemma 2.1. *Let V be a real vector space, let $\{\mathbf{v}_i : i \in [1:k]\} \subseteq V$ be a set of vectors of rank r, and define for $\mathbf{y} \in \mathbb{R}^k_+$*

$$P_{\mathbf{y}} := \left\{ \mathbf{x} \in \mathbb{R}^k_+ : \sum_{i=1}^k x_i \mathbf{v}_i = \sum_{i=1}^k y_i \mathbf{v}_i \right\}.$$

Then there exists $\mathbf{y} \in \mathbb{R}^k_+$ such that

$$\min_{\mathbf{x} \in P_{\mathbf{y}}} \|\mathbf{x}\|_0 = r\,.$$

Proof. First we show that $\min_{\mathbf{x} \in P_{\mathbf{y}}} \|\mathbf{x}\|_0 \le r$ for all $\mathbf{y} \in \mathbb{R}^n_+$ (this is basically Caratheodory's theorem, we include the short argument for the readers' convenience). To this end, choose an $\mathbf{x} \in P_{\mathbf{y}}$ with $m = \|\mathbf{x}\|_0$ minimal over $P_{\mathbf{y}}$. We assume without loss of generality $x_i > 0$ for all $i \le m$. If $m > r$ would hold, then there were $\mu_i \in \mathbb{R}$ with $\sum\limits_{i=1}^m \mu_i \mathbf{v}_i = \mathbf{o}$ with some $\mu_i > 0$. Further without loss of generality we assume (for some $s \in [1:m]$) that $\mu_i \le 0$ for $i < s$ while $\mu_i > 0$ and $\frac{x_i}{\mu_i} \ge \frac{x_m}{\mu_m} > 0$ for all $i \in [s:m]$. Define $z_i := x_i - \frac{x_m}{\mu_m}\mu_i \ge 0$ for all $i \in [1:m]$ and $z_i := 0$ for $i > m$, so that $\|\mathbf{z}\|_0 \le m-1$ (as also $z_m = 0$). But straightforward calculations show $\sum_i z_i \mathbf{v}_i = \sum_i x_i \mathbf{v}_i$, so $\mathbf{z} \in P_{\mathbf{y}}$, in contradiction to the assumptions. Next we use the fact that a vector space over an infinite scalar field is never the union of a finite number of proper subspaces, see [10, p.211]. Define the cone

$C := \left\{\sum_{i=1}^m y_i \mathbf{v}_i : \mathbf{y} \in \mathbb{R}^m_+\right\} \subseteq V$ and observe that the linear subspace $L = C - C$ is r-dimensional. If we had $\min\limits_{\mathbf{x}\in P_{\mathbf{y}}} \|\mathbf{x}\|_0 < r$ for all $\mathbf{y} \in \mathbb{R}^m_+$, then C (and thus also L) would have to be a subset of

$$U := \bigcup_{\substack{I \subseteq [1:m]\\ |I| \le r-1}} \left\{ \sum_{i=1}^m x_i \mathbf{v}_i : \mathbf{x} \in \mathbb{R}^m,\, x_i = 0 \text{ for all } i \in [1:m] \setminus I \right\},$$

which is impossible, since U is a union of finitely many proper subspaces of L (of dimension at most $r-1$). □

For a matrix $\mathsf{A} = [\mathbf{a}_1, \ldots, \mathbf{a}_k]^\top$ we let $\mathsf{A}^{\langle 2\rangle} := [\mathbf{a}_1 \otimes \mathbf{a}_1, \ldots, \mathbf{a}_k \otimes \mathbf{a}_k]^\top$, and define the *two-rank* of A as

$$\operatorname{rank}^{(2)} \mathsf{A} := \operatorname{rank} \mathsf{A}^{\langle 2\rangle}\,.$$

For illustration, denote by $\mathsf{B}_i = \mathbf{e}_i\mathbf{e}_i^\top \in \mathbb{R}^{n\times n}$. Then $\mathsf{I}_n^{\langle 2\rangle} = [\mathsf{B}_1|\cdots|\mathsf{B}_n]$. Note that always $\operatorname{rank}^{(2)} \mathsf{A} \ge \operatorname{rank} \mathsf{A}$ with equality if $\operatorname{rank} \mathsf{A} = k$, i.e., if A itself has full row rank, then also $\mathsf{A}^{\langle 2\rangle}$ has (the same) full row rank. Furthermore we note for later use the trivial relations $\operatorname{rank}^{(2)}(\alpha\mathsf{A}) = \operatorname{rank}^{(2)} \mathsf{A}$ if $\alpha > 0$,

$$\operatorname{rank}^{(2)} \begin{bmatrix} \mathsf{A} \\ \mathsf{B} \end{bmatrix} \ge \operatorname{rank}^{(2)} \mathsf{B}\,,$$

and a slightly less trivial one: $\operatorname{rank}^{(2)} [\mathsf{A}|\mathsf{B}] \ge \operatorname{rank}^{(2)} \mathsf{B}$.

Lemma 2.2. *Let $\mathsf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_k]^\top \in \mathbb{R}^{k\times n}_+$, where $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$ are all the zeroes of some copositive matrix $\mathsf{S} \in \mathcal{COP}_n$.*
Then there exists a diagonal matrix $\mathsf{D} = \operatorname{Diag}(\mathbf{y})$ with $\mathbf{y} \in \mathbb{R}^k_+$ such that the completely positive matrix $\mathsf{M} = \mathsf{U}^\top\mathsf{D}\mathsf{U}$ satisfies cpr M = rank$^{(2)}$ U.

Proof. Consider any $\mathsf{M} = \mathsf{U}^\top\operatorname{Diag}(\mathbf{y})\mathsf{U}$. We observe that $\langle \mathsf{M}, \mathsf{S}\rangle = 0$, i.e., that $\mathsf{M} \perp \mathsf{S}$ holds. Therefore by [3, Lemma 2.1] we conclude that any cp-factorization of M is of the form

$$\mathsf{M} = \mathsf{U}^\top\operatorname{Diag}(\mathbf{x})\mathsf{U} = \sum_{i=1}^k x_i \mathbf{u}_i\mathbf{u}_i^\top$$

with some $\mathbf{x} \in \mathbb{R}^k_+$. For any $\mathbf{x}$ corresponding to a minimal cp-factorization of M we then have $\operatorname{cpr} \mathsf{M} = \|\mathbf{x}\|_0$. Since the rank of the set $\{\mathbf{u}_i\mathbf{u}_i^\top : i \in [1:k]\}$ equals $\operatorname{rank}^{(2)} \mathsf{U}$, as is seen by identifying $\mathbf{u}_i\mathbf{u}_i^\top$ with $\mathbf{u}_i \otimes \mathbf{u}_i = \operatorname{vec}(\mathbf{u}_i\mathbf{u}_i^\top)$, we can invoke Lemma 2.1 to obtain the desired conclusion. □

2.2. **Direct sums and Khatri-Rao-like products.** For matrices $\mathsf{U} \in \mathbb{R}^{k\times n}$ and $\mathsf{V} \in \mathbb{R}^{\ell\times m}$ we construct the following $k\ell \times (n+m)$-matrix, denoted as $\mathsf{U} \circledast \mathsf{V} = [\mathsf{U}\otimes \boldsymbol{\eta}_\ell | \boldsymbol{\eta}_k \otimes \mathsf{V}]$; recall that $\boldsymbol{\eta}_d$ denotes the all ones vector in $\mathbb{R}^d$. Note that both $\mathsf{U}\otimes\mathsf{V}$ and $\mathsf{U}^{\langle 2\rangle} \circledast \mathsf{V}^{\langle 2\rangle}$ are, up to permutations of columns, submatrices of $(\mathsf{U}\circledast\mathsf{V})^{\langle 2\rangle}$, and all these matrices have the same number $k\ell$ of rows. Further note that using the Khatri-Rao product $\star$, see. e.g. [12], we can write

$$\mathsf{U}\circledast\mathsf{V} = [\mathsf{U}|\boldsymbol{\eta}_k] \star [\boldsymbol{\eta}_\ell|\mathsf{V}] \quad \text{and} \quad (\mathsf{U}^{\langle 2\rangle})^\top = [\mathbf{u}_1|\mathbf{u}_2|\cdots|\mathbf{u}_k] \star [\mathbf{u}_1|\mathbf{u}_2|\cdots|\mathbf{u}_k]\,.$$

Recall that a matrix $\mathsf{A} \in \mathbb{R}^{k\times n}_+$ is *row-stochastic* if $\mathsf{A}\boldsymbol{\eta}_n = \boldsymbol{\eta}_k$ holds.

Lemma 2.3. *Let $\alpha > 0$ and $\beta > 0$ and consider two row-stochastic matrices $\mathsf{U} \in \mathbb{R}^{k\times n}$ and $\mathsf{V} \in \mathbb{R}^{\ell\times m}$. Then for the $k\ell \times (n+m)$-matrix $\mathsf{W} = (\alpha\mathsf{U})\circledast(\beta\mathsf{V})$ and the $(k+\ell)\times(n+m)$-matrix $\widetilde{\mathsf{W}} = \mathsf{U}\oplus\mathsf{V}$ we have*

(a) *$\operatorname{rank}\mathsf{W} = \operatorname{rank}\mathsf{U} + \operatorname{rank}\mathsf{V} - 1$ and $\frac{1}{\alpha+\beta}\mathsf{W}$ is row-stochastic,*
(b) *$\operatorname{rank}^{(2)}\mathsf{W} \geq \operatorname{rank}\mathsf{U}\operatorname{rank}\mathsf{V} + \operatorname{rank}^{(2)}\mathsf{U} - \operatorname{rank}\mathsf{U} + \operatorname{rank}^{(2)}\mathsf{V} - \operatorname{rank}\mathsf{V}$,*
(c) *$\operatorname{rank}\widetilde{\mathsf{W}} = \operatorname{rank}\mathsf{U} + \operatorname{rank}\mathsf{V}$, $\operatorname{rank}^{(2)}\widetilde{\mathsf{W}} = \operatorname{rank}^{(2)}\mathsf{U} + \operatorname{rank}^{(2)}\mathsf{V}$ and $\widetilde{\mathsf{W}}$ is row-stochastic.*
(d) *If the rows of U (resp. V) are all the zeroes of some $\mathsf{S}_\mathsf{U} \in \mathcal{COP}_n$ (resp. $\mathsf{S}_\mathsf{V} \in \mathcal{COP}_m$), then there are copositive matrices $\{\mathsf{S},\widetilde{\mathsf{S}}\} \subset \mathcal{COP}_{n+m}$ such that the rows of $\frac{1}{\alpha+\beta}\mathsf{W}$ are all the zeroes of S and the rows of $\widetilde{\mathsf{W}}$ are all the zeroes of $\widetilde{\mathsf{S}}$.*

Proof. It is clear that $\frac{1}{\alpha+\beta}\mathsf{W}$ is row-stochastic. Let $r_\mathsf{U} := \operatorname{rank}\mathsf{U}$ and $r_\mathsf{V} := \operatorname{rank}\mathsf{V}$. Since the rank of the first n (resp. last m) columns of W is r_U (resp. r_V), $\operatorname{rank}\mathsf{W}$ can be smaller than $r_\mathsf{U}+r_\mathsf{V}$ only if some nonzero linear combination of the first n columns of W equals some linear combination of the last m columns of W.

So assume that there are $\mathbf{x}\in\mathbb{R}^n$ and $\mathbf{y}\in\mathbb{R}^m$, such that $(\mathsf{U}\otimes\boldsymbol{\eta}_\ell)\mathbf{x} = (\mathsf{U}\otimes\boldsymbol{\eta}_\ell)(\mathbf{x}\otimes 1) = \mathsf{U}\mathbf{x}\otimes\boldsymbol{\eta}_\ell$ and $(\boldsymbol{\eta}_k\otimes\mathsf{V})\mathbf{y} = (\boldsymbol{\eta}_k\otimes\mathsf{V})(1\otimes\mathbf{y}) = \boldsymbol{\eta}_k\otimes\mathsf{V}\mathbf{y}$ are both equal to $\mathbf{w}\in\mathbb{R}^{k\ell}\setminus\{\mathbf{o}\}$. From $\mathbf{w} = \mathsf{U}\mathbf{x}\otimes\boldsymbol{\eta}_\ell$ we deduce that $w_i = w_j$ if $\lceil\frac{i}{\ell}\rceil = \lceil\frac{j}{\ell}\rceil$, and from $\mathbf{w} = \boldsymbol{\eta}_k\otimes\mathsf{V}\mathbf{y}$ we deduce $w_i = w_j$ if $i\equiv j \bmod \ell$, and the only nonzero vectors satisfying both conditions are of the form $\mathbf{w} = c\boldsymbol{\eta}_{k\ell}$ with $c\neq 0$. Therefore $\operatorname{rank}\mathsf{W} = r_\mathsf{U}+r_\mathsf{V}-1$, which concludes the proof of (a).

Next we denote $\rho_\mathsf{U} = \operatorname{rank}^{(2)}\mathsf{U}$ and $\rho_\mathsf{V} = \operatorname{rank}^{(2)}\mathsf{V}$, and assume that the rows of U and V are arranged in a way such that the matrices $\widetilde{\mathsf{U}} = \mathsf{U}_{[1:r_\mathsf{U}]\times[1:n]}$, $\widetilde{\mathsf{V}} =$

$\mathsf{V}_{[1:r_\mathsf{V}]\times[1:m]}$, $\widehat{\mathsf{U}} = \mathsf{U}_{[r_\mathsf{U}+1:\rho_\mathsf{U}]\times[1:n]}$ and $\widehat{\mathsf{V}} = \mathsf{V}_{[r_\mathsf{V}+1:\rho_\mathsf{V}]\times[1:m]}$ satisfy

$$\operatorname{rank}\widetilde{\mathsf{U}} = r_\mathsf{U},\ \operatorname{rank}\widetilde{\mathsf{V}} = r_\mathsf{V},\ \operatorname{rank}^{(2)}\begin{bmatrix}\widetilde{\mathsf{U}}\\ \widehat{\mathsf{U}}\end{bmatrix} = \rho_\mathsf{U},\ \operatorname{rank}^{(2)}\begin{bmatrix}\widetilde{\mathsf{V}}\\ \widehat{\mathsf{V}}\end{bmatrix} = \rho_\mathsf{V}.$$

Moreover let $\mathbf{u}_1 = \mathbf{e}_1^\top\mathsf{U}$ and $\mathbf{v}_1 = \mathbf{e}_1^\top\mathsf{V}$ be the first rows of U and V. Now consider the following $(r_\mathsf{U}r_\mathsf{V} + \rho_\mathsf{U} - r_\mathsf{U} + \rho_\mathsf{V} - r_\mathsf{V}) \times (n+m)$-submatrix of W:

$$\overline{\mathsf{W}} = \begin{bmatrix} \widetilde{\mathsf{U}}\otimes\boldsymbol{\eta}_{r_\mathsf{V}} & \boldsymbol{\eta}_{r_\mathsf{U}}\otimes\widetilde{\mathsf{V}} \\ \mathbf{u}_1\otimes\boldsymbol{\eta}_{\rho_\mathsf{V}-r_\mathsf{V}} & \widehat{\mathsf{V}} \\ \widehat{\mathsf{U}} & \boldsymbol{\eta}_{\rho_\mathsf{U}-r_\mathsf{U}}\otimes\mathbf{v}_1 \end{bmatrix} = \begin{bmatrix} \widetilde{\mathsf{U}}\circledast\widetilde{\mathsf{V}} \\ \mathbf{u}_1\circledast\widehat{\mathsf{V}} \\ \widehat{\mathsf{U}}\circledast\mathbf{v}_1 \end{bmatrix}.$$

Noting that $\widetilde{\mathsf{U}}\otimes\widetilde{\mathsf{V}}$ is a submatrix of $(\widetilde{\mathsf{U}}\circledast\widetilde{\mathsf{V}})^{\langle 2\rangle}$, where the latter has $r_\mathsf{U}r_\mathsf{V}$ rows, we deduce $\operatorname{rank}(\widetilde{\mathsf{U}}\circledast\widetilde{\mathsf{V}})^{\langle 2\rangle} = r_\mathsf{U}r_\mathsf{V}$ from

$$r_\mathsf{U}r_\mathsf{V} = \operatorname{rank}\widetilde{\mathsf{U}}\operatorname{rank}\widetilde{\mathsf{V}} = \operatorname{rank}(\widetilde{\mathsf{U}}\otimes\widetilde{\mathsf{V}}) \le \operatorname{rank}(\widetilde{\mathsf{U}}\circledast\widetilde{\mathsf{V}})^{\langle 2\rangle} \le r_\mathsf{U}r_\mathsf{V}.$$

Next consider the submatrix $\begin{bmatrix} \widetilde{\mathsf{U}}^{\langle 2\rangle}\circledast\widetilde{\mathsf{V}}^{\langle 2\rangle} \\ \mathbf{u}_1^{\langle 2\rangle}\circledast\widehat{\mathsf{V}}^{\langle 2\rangle} \\ \widehat{\mathsf{U}}^{\langle 2\rangle}\circledast\mathbf{v}_1^{\langle 2\rangle} \end{bmatrix}$ of $\overline{\mathsf{W}}^{\langle 2\rangle} = \begin{bmatrix} (\widetilde{\mathsf{U}}\circledast\widetilde{\mathsf{V}})^{\langle 2\rangle} \\ (\mathbf{u}_1\circledast\widehat{\mathsf{V}})^{\langle 2\rangle} \\ (\widehat{\mathsf{U}}\circledast\mathbf{v}_1)^{\langle 2\rangle} \end{bmatrix}$. If for $\mathbf{x} \in \mathbb{R}^{r_\mathsf{U}r_\mathsf{V}}$, $\mathbf{y} \in \mathbb{R}^{\rho_\mathsf{V}-r_\mathsf{V}}$, $\mathbf{z} \in \mathbb{R}^{\rho_\mathsf{U}-r_\mathsf{U}}$ we have $\mathbf{o} = [\mathbf{x}^\top, \mathbf{y}^\top, \mathbf{z}^\top]\overline{\mathsf{W}}^{\langle 2\rangle}$, then also

$$\begin{aligned}\mathbf{o} &= \mathbf{x}^\top(\widetilde{\mathsf{U}}^{\langle 2\rangle}\circledast\widetilde{\mathsf{V}}^{\langle 2\rangle}) + \mathbf{y}^\top(\mathbf{u}_1^{\langle 2\rangle}\circledast\widehat{\mathsf{V}}^{\langle 2\rangle}) + \mathbf{z}^\top(\widehat{\mathsf{U}}^{\langle 2\rangle}\circledast\mathbf{v}_1^{\langle 2\rangle}) \\ &= \mathbf{x}^\top(\widetilde{\mathsf{U}}^{\langle 2\rangle}\circledast\widetilde{\mathsf{V}}^{\langle 2\rangle}) + (\mathbf{y}^\top\boldsymbol{\eta}_{\rho_\mathsf{V}-r_\mathsf{V}}\mathbf{u}_1^{\langle 2\rangle})\circledast(\mathbf{y}^\top\widehat{\mathsf{V}}^{\langle 2\rangle}) + (\mathbf{z}^\top\widehat{\mathsf{U}}^{\langle 2\rangle})\circledast(\mathbf{z}^\top\boldsymbol{\eta}_{\rho_\mathsf{U}-r_\mathsf{U}}\mathbf{v}_1^{\langle 2\rangle})\end{aligned}$$

must hold. Therefore $\mathbf{y}^\top\widehat{\mathsf{V}}^{\langle 2\rangle}$ belongs to the row space of $\widetilde{\mathsf{V}}^{\langle 2\rangle}$, and $\mathbf{z}^\top\widehat{\mathsf{U}}^{\langle 2\rangle}$ belongs to the row space of $\widetilde{\mathsf{U}}^{\langle 2\rangle}$, implying $\mathbf{y} = \mathbf{o}$ and $\mathbf{z} = \mathbf{o}$, because, by assumption, the rows of both $\begin{bmatrix}\widetilde{\mathsf{U}}^{\langle 2\rangle}\\ \widehat{\mathsf{U}}^{\langle 2\rangle}\end{bmatrix}$ and $\begin{bmatrix}\widetilde{\mathsf{V}}^{\langle 2\rangle}\\ \widehat{\mathsf{V}}^{\langle 2\rangle}\end{bmatrix}$ are linearly independent. Then by linear independence of the first $r_\mathsf{U}r_\mathsf{V}$ rows of $\overline{\mathsf{W}}^{\langle 2\rangle}$ also $\mathbf{x} = \mathbf{o}$ must hold. Thus $\operatorname{rank}^{(2)}\mathsf{W} \ge \operatorname{rank}^{(2)}\overline{\mathsf{W}} = r_\mathsf{U}r_\mathsf{V} + \rho_\mathsf{U} - r_\mathsf{U} + \rho_\mathsf{V} - r_\mathsf{V}$, which completes the proof of (b).

For the proof of (c) we use that for any matrices A,B we have $\operatorname{rank}(\mathsf{A}\oplus\mathsf{B}) = \operatorname{rank}\mathsf{A} + \operatorname{rank}\mathsf{B}$, and that the matrix $(\mathsf{A}\oplus\mathsf{B})^{\langle 2\rangle}$ and its submatrix $\mathsf{A}^{\langle 2\rangle}\oplus\mathsf{B}^{\langle 2\rangle}$ have the same rank. Furthermore $\widetilde{\mathsf{W}}\boldsymbol{\eta}_{n+m} = \boldsymbol{\eta}_{k+\ell}$ is easily checked.

Finally, for the proof of (d) we define matrices

$$\mathsf{S} := \begin{bmatrix} \mathsf{S}_\mathsf{U} + \frac{\beta}{\alpha}\mathsf{E}_n & -\boldsymbol{\eta}_n\boldsymbol{\eta}_m^\top \\ -\boldsymbol{\eta}_m\boldsymbol{\eta}_n^\top & \mathsf{S}_\mathsf{V} + \frac{\alpha}{\beta}\mathsf{E}_m \end{bmatrix}, \quad \text{and} \quad \widetilde{\mathsf{S}} := \begin{bmatrix} \mathsf{S}_\mathsf{U} & \boldsymbol{\eta}_n\boldsymbol{\eta}_m^\top \\ \boldsymbol{\eta}_m\boldsymbol{\eta}_n^\top & \mathsf{S}_\mathsf{V} \end{bmatrix}.$$

Take any $\mathbf{z} = [\lambda\mathbf{x}^\top, (1-\lambda)\mathbf{y}^\top]^\top$ with $(\mathbf{x},\mathbf{y}) \in \Delta_n \times \Delta_m$ and $0 \le \lambda \le 1$. Then

$$\mathbf{z}^\top\mathsf{S}\mathbf{z} = \lambda^2\mathbf{x}^\top\mathsf{S}_\mathsf{U}\,\mathbf{x} + (1-\lambda)^2\mathbf{y}^\top\mathsf{S}_\mathsf{V}\,\mathbf{y} + \frac{(\alpha+\beta)^2}{\alpha\beta}\left(\lambda - \frac{\alpha}{\alpha+\beta}\right)^2 \ge 0\,,$$

with equality if and only if $\lambda = \frac{\alpha}{\alpha+\beta}$, and $\mathbf{x}^\top$ (resp. $\mathbf{y}^\top$) is one of the rows of U (resp. V), i.e. if and only if $\mathbf{z}^\top$ is one of the rows of $\frac{1}{\alpha+\beta}\mathsf{W}$.
Furthermore, with $\mathbf{z}$ as above, we have

$$\mathbf{z}^\top \widetilde{\mathsf{S}}\mathbf{z} = \lambda^2 \mathbf{x}^\top \mathsf{S}_{\mathsf{U}}\,\mathbf{x} + (1-\lambda)^2 \mathbf{y}^\top \mathsf{S}_{\mathsf{V}}\,\mathbf{y} + 2\lambda(1-\lambda) \geq 0\,,$$

with equality if and only if $\lambda \in \{0,1\}$, and, depending on the value of λ, either $\mathbf{x}^\top$ is one of the rows of U or $\mathbf{y}^\top$ is one of the rows of V, i.e. if and only if $\mathbf{z}^\top$ is one of the rows of $\widetilde{\mathsf{W}}$. □

2.3. **Zeroes and characteristic triples.** We now define the set $\mathcal{Z}$ as follows: denote by $\mathcal{R}$ all row-stochastic matrices and let

$$\mathcal{R}_0 := \{\mathsf{U} \in \mathcal{R} : \text{the rows of } \mathsf{U} \text{ are all the zeroes of some copositive matrix}\}$$

as well as $\mathcal{Z} := \{\alpha\mathsf{U} : \alpha > 0\,,\ \mathsf{U} \in \mathcal{R}_0\}$.
The matrices in $\mathcal{Z}$ are exactly those that are needed for applications of Lemma 2.2. Moreover, with Lemma 2.3 we have a means of constructing new elements[1] of $\mathcal{Z}$ from known ones: $\{\mathsf{U},\mathsf{V}\} \subset \mathcal{Z} \Rightarrow \mathsf{U} \circledast \mathsf{V} \in \mathcal{Z}$. For our purpose of showing the existence of matrices of large cp-rank, only certain characteristics of a matrix $\mathsf{U} \in \mathcal{Z}$ are important: (a) the number of columns of U (say n); (b) the $\operatorname{rank}\mathsf{U}$ (say r); and (c) an integer lower bound ρ for $\operatorname{rank}^{(2)}\mathsf{U}$ (where we require $\rho \geq \operatorname{rank}\mathsf{U}$); these three integers we collect in a *characteristic triple*

$$c = (\pi_1(c), \pi_2(c), \pi_3(c)) := (n, r, \rho)\,.$$

Some $\mathsf{U} \in \mathcal{Z}$ may have more than one characteristic triple, namely if and only if $\operatorname{rank}\mathsf{U} < \operatorname{rank}^{(2)}\mathsf{U}$. By abuse of notation, we define a binary operation on any two characteristic triples,

$$(n_1, r_1, \rho_1) \circledast (n_2, r_2, \rho_2) := (n_1 + n_2, r_1 + r_2 - 1, r_1 r_2 + \rho_1 - r_1 + \rho_2 - r_2)\,; \qquad (4)$$

note that $1 \leq r_1 + r_2 - 1 \leq r_1 r_2 + \rho_1 - r_1 + \rho_2 - r_2$ if both $1 \leq r_1 \leq \rho_1$ and $1 \leq r_2 \leq \rho_2$ holds. The operation $\circledast$ obviously obeys the commutative and (only a little

[1] There is also another closure property which we won't use: If P and D are a permutation matrix and a positive diagonal matrix of suitable orders, then $\mathsf{U} \in \mathcal{Z} \Rightarrow \mathsf{PUD} \in \mathcal{Z}$.

less obvious) the associative law.[2] Clearly also the binary operation $(n_1, r_1, \rho_1) \oplus (n_2, r_2, \rho_2) := (n_1 + n_2, r_1 + r_2, \rho_1 + \rho_2)$ is associative and commutative. It follows from Lemma 2.3 that if c, c' are characteristic triples of $\mathsf{U}, \mathsf{V} \in \mathcal{Z}$, then $c \circledast c'$ is a characteristic triple of $\mathsf{U} \circledast \mathsf{V}$ and $c \oplus c'$ is a characteristic triple of $\mathsf{U} \oplus \mathsf{V}$.

Our strategy is to fix a subset $\mathcal{U} \subseteq \mathcal{Z}$ together with a set C of characteristic triples, containing one characteristic triple for each $\mathsf{U} \in \mathcal{U}$, and construct the $\circledast$-semigroups generated by $\mathcal{U}$ and C. From the latter, we fix the first component $\pi_1(c) = n$, the column number of some $\mathsf{U} \in \mathcal{U}$ accordingly picked, and search a triple $c \in C$ with a large third component $\pi_3(c) \leq \operatorname{rank}^{(2)} \mathsf{U}$. There are no limitations on the second component $\pi_2(c) = \operatorname{rank} \mathsf{U}$, and typically the chosen U will not have full column rank.

We start considering semigroups generated by a single $\mathsf{U} \in \mathcal{Z}$, and therefore define $\mathsf{U}^{\circledast 1} = \mathsf{U}$ and inductively $\mathsf{U}^{\circledast (n+1)} = \mathsf{U} \circledast \mathsf{U}^{\circledast n}$ for $n \geq 1$. Similarly we define $c^{\circledast n}$, where c is a characteristic triple.

Theorem 2.1. *Let $\mathsf{U} \in \mathcal{Z}$, and (n, r, ρ) be (one of) its characteristic triple(s). Then for any $i \in \mathbb{N}$ there is a matrix $\mathsf{M} \in \mathcal{CP}_{ni}$ satisfying*

$$cpr\, \mathsf{M} \geq \tfrac{1}{2}(r-1)^2 i(i-1) + (\rho - 1)i + 1\,.$$

Proof. The result follows from

$$(n, r, \rho)^{\circledast i} = (ni, (r-1)i + 1, \tfrac{1}{2}(r-1)^2 i(i-1) + (\rho-1)i + 1)\,,$$

which is easily proved by induction, using (4). □

For any $n \geq 1$ we have $\mathsf{I}_n \in \mathcal{Z}$, since the rows of I_n are the only zeroes of the copositive matrix $\mathsf{E}_n - \mathsf{I}_n$. The (unique) characteristic triple of I_n is (n, n, n). Putting $\mathsf{U} = \mathsf{I}_n$ in Theorem 2.1, we see $\operatorname{rank}^{(2)} \mathsf{I}_n^{\circledast i} \geq \rho_{i,n}$ where

$$\rho_{i,n} := \tfrac{1}{2}(n-1)^2 i(i-1) + (n-1)i + 1 = \tfrac{(ni)^2}{2} - ni(i + \tfrac{n}{2}) + 2ni + \tfrac{i(i-3)}{2} + 1\,. \quad (5)$$

Next, counterexamples to the DJL-conjecture for infinitely many n, and in particular for $n = 12$, are presented.

[2]The binary operation $\circledast$ on the set $\mathcal{Z}$ is associative but not commutative, but there are always permutation matrices $\mathsf{P}_1, \mathsf{P}_2$ such that $\mathsf{B} \circledast \mathsf{A} = \mathsf{P}_1(\mathsf{A} \circledast \mathsf{B})\mathsf{P}_2$. Clearly, row and column permutations of U do neither affect $\operatorname{rank} \mathsf{U}$ nor $\operatorname{rank}^{(2)} \mathsf{U}$.

Example 2.1. ($p_{12} \geq 37 > 36 = d_{12}$) *We have* $\mathrm{rank}^{(2)}\, \mathsf{I}_4^{\circledast 3} \geq 37$ *by (5); more precisely, we have* $(4,4,4)^{\circledast 3} = (12,10,37)$ *and thus there is a completely positive matrix of order 12, rank 10 and cp-rank at least* 37*, which may be written as* $(\mathsf{I}_4^{\circledast 3})^\top \mathrm{Diag}(\mathbf{x})(\mathsf{I}_4^{\circledast 3})$ *for some* $\mathbf{x} \in \mathbb{R}^{64}_+$. *An explicit construction will be given in Appendix A.*

Similarly we obtain $p_{4i} \geq \rho_{i,4} = \frac{9}{32}(4i)^2 - \frac{3}{8}(4i) + 1 > \lfloor \frac{1}{4}(4i)^2 \rfloor = d_{4i}$ *for* $i \geq 3$ *and* $p_{3n} \geq \rho_{3,n} = \frac{1}{3}(3n)^2 - 3n + 1 > \lfloor \frac{1}{4}(3n)^2 \rfloor = d_{3n}$ *for* $n \geq 4$.

We continue this argument and maximize, for fixed $N := ni$, the second term in formula (5) for $\rho_{i,n}$, namely $-ni(i + \frac{n}{2})$, with the result $n^* = \sqrt{2N}, i^* = \sqrt{\frac{N}{2}}$, and

$$\rho_{i^*,n^*} = \frac{N^2}{2} - N\sqrt{2N} + \frac{9}{4}N - \frac{3}{4}\sqrt{2N} + 1 \tag{6}$$

which yields good lower bounds for the cp-rank if both i^* and n^* are integers, i.e., if $n = 2m$ (and $N = 2m^2$) for $m \in \mathbb{N}$. We will re-encounter the three leading terms of (6) in the estimate (10) of Corollary 2.1 below; for an improvement see (12) in Section 3.

Still better lower bounds could probably be obtained by considering products of possibly different characteristic triples (just before we only considered powers of a single characteristic triple). Let S be the semigroup generated by the set of characteristic triples $\{(i,i,i) : i \in \mathbb{N}\}$. So any $c \in S$ is a finite $\circledast$-product of these (i,i,i), allowing repetition of factors, and $\pi_1(c) - \pi_2(c) + 1$ is the number of factors, counted with multiplicity. The factorization need however not be unique, as is seen from the example $(12,10,30) = (1,1,1) \circledast (5,5,5) \circledast (6,6,6) = (2,2,2) \circledast (3,3,3) \circledast (7,7,7)$. The best lower bound for p_n that we can get from S is then

$$b_n := \max\{\pi_3(c) : \pi_1(c) = n,\ c \in S\}. \tag{7}$$

Lemma 2.4. *The maximum* b_n *is for some* $j \geq 1$ *attained at a characteristic triple* c *of the form* $c = (i_1,i_1,i_1) \circledast \cdots \circledast (i_j,i_j,i_j)$*, where* $i_1 \leq \cdots \leq i_j$ *and* $i_j - i_1 \leq 1$.

Proof. There is nothing to show if $j = 1$. So assume $j = 2$. If we had $i_2 - i_1 > 1$, then $\tilde{c} := (i_1{+}1, i_1{+}1, i_1{+}1) \circledast (i_2{-}1, i_2{-}1, i_2{-}1)$ fulfils $\pi_1(c) = \pi_1(\tilde{c})$, $\pi_2(c) = \pi_2(\tilde{c})$, and $\pi_3(c) = i_1 i_2 < (i_1{+}1)(i_2{-}1) = \pi_3(\tilde{c})$ in contrast to the maximality of $\pi_3(c)$. If $j > 2$ then for some characteristic triple c' we have $c = (i_1,i_1,i_1) \circledast (i_j,i_j,i_j) \circledast c'$, which, in case of $i_j - i_1 > 1$ we compare with $\tilde{c} := (i_1{+}1, i_1{+}1, i_1{+}1) \circledast (i_2{-}1, i_2{-}1, i_2{-}1) \circledast c'$, obtaining as above $\pi_1(c) = \pi_1(\tilde{c})$, $\pi_2(c) = \pi_2(\tilde{c})$, and $\pi_3(c) < \pi_3(\tilde{c})$ in contrast to the maximality of $\pi_3(c)$. Here we used the following property: if c', $\gamma = (n, r, \rho)$ and $\tilde{\gamma} = (n, r, \tilde{\rho})$ are characteristic triples with $\tilde{\rho} > \rho$, then $\pi_3(\tilde{\gamma} \circledast c') > \pi_3(\gamma \circledast c')$. □

We remark that the characteristic triples that maximize (7) are in general not uniquely determined by Lemma 2.4. For example, $b_{37} = 442$ is attained twice, at $(7,7,7)^{\circledast 3} \circledast (8,8,8)^{\circledast 2} = (37,33,442)$ and at $(9,9,9)^{\circledast 3} \circledast (10,10,10) = (37,34,442)$.

2.4. **New bounds for the cp-rank.** In the following theorem we provide precise asymptotic estimates for b_n as defined in (7).

Theorem 2.2. *For $n \geq 5$, we have*

$$-\sqrt{2n} + \frac{1}{16} \leq b_n - \frac{n^2}{2} + n\sqrt{2n} - \frac{9}{4}n \leq -\frac{5}{8}\sqrt{2n} + \frac{3}{2}\,. \tag{8}$$

Moreover $b_n \leq$ cpr M for some $\mathsf{M} \in \mathcal{CP}_n$ of the form $\mathsf{M} = \mathsf{U}^\top \mathsf{D} \mathsf{U}$, where D is a nonnegative diagonal matrix and $\mathsf{U} \in \mathcal{Z}$ is a binary matrix, i.e., has all entries in $\{0,1\}$.

Proof. From Lemma 2.4 we know that $b_n = \pi_3(c)$ for some characteristic triple $c \in S$ of the form

$$c = (n, n-k+1, \rho_{m,k,i}) = (m,m,m)^{\circledast i} \circledast (m+1, m+1, m+1)^{\circledast k-i},$$

where $m \geq 1$, $k \geq 1$, $1 \leq i \leq k$ and $n = mi + (m+1)(k-i) = mk + k - i$. Then the binary matrix $\mathsf{U} := \mathsf{I}_m^{\circledast i} \circledast \mathsf{I}_{m+1}^{\circledast k-i} \in \mathcal{Z}$ satisfies $\operatorname{rank}^{(2)} \mathsf{U} \geq b_n$, and by Lemma 2.2 there is a nonnegative diagonal matrix D such that we have $b_n \leq \operatorname{cpr} \mathsf{U}^\top \mathsf{D} \mathsf{U}$, which settles the second assertion of the theorem. We now turn to the asserted inequalities. Putting $r_1 = (m-1)i + 1$, $r_2 = m(k-i) + 1$, $\rho_1 = \rho_{i,m}$ and $\rho_2 = \rho_{k-i,m+1}$ from (5) yields

$$\begin{aligned}
\rho_{m,k,i} &= r_1 r_2 + \rho_1 - r_1 + \rho_2 - r_2 \\
&= (i(m-1)+1)((k-i)m+1) + \tfrac{1}{2}(m-1)^2 i(i-1) + \tfrac{1}{2}m^2(k-i)(k-i-1) \\
&= \frac{1}{2}(n-k)^2 + \frac{3}{2}(n-k) - mn + \frac{1}{2}m(m+1)k + 1 =: f_n(m,k).
\end{aligned}$$

Denoting $\widehat{X}_n := \{(m,k,i) \in [1,\infty[^3 \colon i \leq k, mk + k - i = n\}$ and $X_n := \widehat{X}_n \cap \mathbb{N}^3$ we note that

$$b_n = \max_{(m,k,i) \in X_n} f_n(m,k) \leq \max_{(m,k,i) \in \widehat{X}_n} f_n(m,k) \leq \max_{k \in [1,n]} \left(\max_{m \in [\frac{n}{k}-1, \frac{n}{k}]} f_n(m,k) \right).$$

For fixed k, $f_n(m,k)$ is a convex function of m, and

$$f_n\left(\frac{n}{k},k\right) = f_n\left(\frac{n}{k}-1,k\right) = \frac{n^2}{2} - nk + \frac{k^2}{2} + 2n - \frac{3k}{2} - \frac{n^2}{2k} + 1 := g_n(k)\,,$$

therefore $b_n \le \max_{k\in[1,n]} g_n(k)$. We collect some facts about g_n, assuming $n \ge 5$. From $g_n'(k) = k - n - \frac{3}{2} + \frac{n^2}{2k^2}$, $g_n''(k) = 1 - \frac{n^2}{k^3}$ and $g_n'''(k) = \frac{3n^2}{k^4}$ we deduce that g_n is strictly concave on $[1, n^{\frac{2}{3}}]$ and strictly convex on $[n^{\frac{2}{3}}, n]$, and that g_n' is strictly convex on $[1,n]$ with $g_n'(1) = \frac{n^2-1}{2} - n > 0$ and $g_n'(n) = -1 < 0$ so that there is only one zero of g_n' in $[1,n]$ which is the only maximizer of g_n on $[1,n]$, and this maximizer must lie in the interval $A_n := [z_n + \frac{1}{4} - \frac{1}{z_n}, z_n + \frac{1}{4}]$, where $z_n = \sqrt{\frac{n}{2}}$. Indeed,

$$g_n'\left(z_n + \frac{1}{4}\right) = \frac{1}{2}\frac{n^2}{z_n^2}\left(1 + \frac{1}{4z_n}\right)^{-2} - n + z_n - \frac{5}{4} \in \left[-\frac{9}{8}, -\frac{7}{8}\right]\,,$$

where for the latter inclusion we used $(1-y)^2 \le (1+y)^{-2} \le 1 - 2y + 3y^2$ for $y \in [0,1]$; we need $y = \frac{1}{4z_n}$. So we have shown $g_n'(\sup A_n) < 0$. Furthermore, for $k \in A_n$ we have

$$g_n''(k) \le 1 - n^2\left(z_n + \frac{1}{4}\right)^{-3} = 1 - 4z_n\left(1 + \frac{1}{4z_n}\right)^{-3} \le 1 - 4z_n\left(1 - \frac{3}{4z_n}\right) = 4 - 4z_n\,,$$

and by the mean value theorem for some $k \in A_n$

$$g_n'\left(z_n + \frac{1}{4} - \frac{1}{z_n}\right) = g_n'\left(z_n + \frac{1}{4}\right) - \frac{1}{z_n}g_n''(k) \ge -\frac{9}{8} + 4 - \frac{4}{z_n} \ge \frac{1}{3}\,.$$

We conclude $g_n'(\sup A_n) < 0 < g_n'(\inf A_n)$ so that A_n must contain the minimizer of g_n. Now $z_n + \frac{1}{4} < n^{\frac{2}{3}}$ for $n \ge 5$, and by concavity of g_n on $[1, n^{\frac{2}{3}}]$ we get

$$\begin{aligned}
\max_{k\in[1,n]} g_n(k) &= \max_{k\in A_n} g_n(k) \le g_n\left(z_n + \frac{1}{4}\right) + \frac{9}{8z_n} \\
&= \frac{n^2}{2} - n\left(z_n + \frac{1}{4}\right) + \frac{(z_n+\frac{1}{4})^2}{2} + 2n - \frac{3(z_n+\frac{1}{4})}{2} - \frac{n^2}{2(z_n+\frac{1}{4})} + 1 + \frac{9}{8z_n} \\
&\le \frac{n^2}{2} - 2nz_n + \frac{9}{4}n - \frac{5}{4}z_n + \frac{3}{2}\,,
\end{aligned}$$

where we used $\frac{n^2}{2}\left(z_n + \frac{1}{4}\right)^{-1} = nz_n\left(1 + \frac{1}{4z_n}\right)^{-1} \ge nz_n\left(1 - \frac{1}{4z_n}\right) = nz_n - \frac{n}{4}$, and $\frac{21}{32} + \frac{9}{8z_n} \le \frac{3}{2}$ for $n \ge 5$. This proves the rightmost inequality in (8).

Turning now to the left inequality in (8), we note that for any $(m,k,i) \in X_n$ we have $b_n \ge f_n(m,k)$. The preceding calculations suggest to choose

$$k_n := z_n + \alpha_n \in \left[z_n - \frac{1}{4}, z_n + \frac{3}{4}\right] \cap \mathbb{N}\,, \quad m_n := \frac{n}{z_n} + \beta_n \in \left]\frac{n}{k_n} - 1, \frac{n}{k_n}\right] \cap \mathbb{N}$$

and $i_n := m_n k_n + k_n - n \in [1:k_n]$. Clearly $\alpha_n \in \left[-\frac{1}{4}, \frac{3}{4}\right]$, and because we have $\left|\frac{n}{k_n} - \frac{n}{z_n}\right| = 2|\alpha_n|\frac{z_n}{z_n+\alpha_n} \leq \frac{3}{2}$ for $(\alpha_n, z_n) \in \left[-\frac{1}{4}, \frac{3}{4}\right] \times [1, \infty[$, we get $\beta_n \in \left[-\frac{5}{2}, \frac{3}{2}\right]$. We obtain

$$\begin{aligned} f_n(m_n, k_n) &= \frac{n^2}{2} - nk_n - nm_n + \frac{1}{2}m_n^2 k_n + \frac{1}{2}k_n^2 + \frac{3n}{2} + \frac{1}{2}m_n k_n - \frac{3}{2}k_n + 1 \\ &= \frac{n^2}{2} - 2nz_n + \frac{9}{4}n + \gamma_n z_n + \delta_n \\ &\geq \frac{n^2}{2} - 2nz_n + \frac{9}{4}n - 2z_n + \frac{1}{16}, \end{aligned}$$

where we used

$$\gamma_n = \frac{1}{2}(\beta_n + 2\alpha_n)(\beta_n + 2\alpha_n + 1) + \alpha_n(1 - 2\alpha_n) - \frac{3}{2} \geq -\frac{1}{8} - \frac{3}{8} - \frac{3}{2} = -2$$

and, discussing behaviour for $(\alpha_n, \beta_n) \in \left[-\frac{1}{4}, \frac{3}{4}\right] \times \left[-\frac{5}{2}, \frac{3}{2}\right]$,

$$\delta_n = \frac{1}{2}\alpha_n\beta_n(\beta_n + 1) + \frac{1}{2}\alpha_n^2 - \frac{3}{2}\alpha_n + 1 \geq \frac{1}{16}\,.$$

The proof is now complete. □

Remark 2.1. *For later reference we add that* $\max_{(m,k,i)\in X_n} f_n(m, k)$ *is attained only in points* (m^*, k^*, i^*) *satisfying*

$$k^* \leq z_n + \frac{3}{2}\,.$$

To see this, let $k > z_n + \frac{3}{2}$*. Then, by straightforward but tedious calculations, we get* $f_n(m, k) \leq g_n(k) < g_n(z_n + \frac{3}{2}) \leq \frac{n^2}{2} - 2nz_n + \frac{9}{4}n - 2z_n + \frac{1}{16} \leq b_n$*, therefore* $f_n(m, k)$ *can not be maximal.*

Corollary 2.1. *The DJL-conjecture is false for* $n \geq 7$*. Asymptotically,* p_n *is much closer to the upper bound* $s_n = \binom{n+1}{2} - 4$ *than to the DJL lower bound* $d_n = \left\lfloor\frac{n^2}{4}\right\rfloor$*:*

$$p_n = \frac{n^2}{2} + \mathcal{O}\big(n^{3/2}\big) \quad \textit{and thus} \quad \lim_{n\to\infty} \frac{s_n - p_n}{p_n - d_n} = 0\,. \tag{9}$$

Proof. For $n \in [7:11]$ counterexamples were given in [3], and for $n = 12$ we gave a counterexample in Example 2.1. Furthermore, we derive from (8)

$$\frac{n^2}{2} + \mathcal{O}\big(n^{3/2}\big) = s_n \geq p_n \geq b_n \geq \frac{n^2}{2} - (n+1)\sqrt{2n} + \frac{9}{4}n + \frac{1}{16} > d_n\,, \tag{10}$$

where the latter inequality holds for $n \geq 13$ (again checked straightforwardly), showing the existence of counterexamples also for $n \geq 13$. Now (9) follows immediately. □

3. Improvement of lower bounds

3.1. **Semigroups of characteristic triples.** Up to now, we have used in our construction a very simple matrix sequence $\mathcal{I} := (\mathsf{I}_n)_{n\in\mathbb{N}}$. This was sufficient to disprove the DJL conjecture for large n and establishing the asymptotics in (9). Note that b_n is a lower bound for the cp-rank of matrices from a subset of $\mathcal{CP}_n$, namely for completely positive $n\times n$-matrices that have a representation as $\mathsf{U}^\top\mathsf{D}\mathsf{U}$, where D is a nonnegative diagonal matrix and $\mathsf{U}\in\mathcal{Z}$ is a binary matrix. No longer insisting on matrices in that subset, we will be able to further increase our lower bounds for p_n. So our strategy is to replace $\mathcal{I}$ by another sequence $\mathcal{J} = (\mathsf{J}_n)_{n\in\mathbb{N}}$ of not necessarily binary matrices, where we assume that J_n is of order n, all J_n have full column rank, and that we know the exact values of $\rho_n^{\mathcal{J}} := \operatorname{rank}^{(2)}\mathsf{J}_n$, not just lower bounds, with $\rho_n^{\mathcal{J}} > n$ for at least one n. Then we let $S^{\mathcal{J}}$ be the semigroup generated by the set of characteristic triples $\{(n,n,\rho_n^{\mathcal{J}}) : n\in\mathbb{N}\}$, and define

$$b_n^{\mathcal{J}} := \max\left\{\pi_3(c) : \pi_1(c) = n,\ c\in S^{\mathcal{J}}\right\}. \tag{11}$$

We recall that $S^{\mathcal{I}} = S$ and $b_n^{\mathcal{I}} = b_n$ from (7) in this notation, and of course $\rho_n^{\mathcal{I}} = n$. Further, for all such $\mathcal{J}$, from considering $\pi_2(c\circledast c')$, we deduce that any $c\in S^{\mathcal{J}}$ is $\circledast$-irreducible if and only if $\pi_1(c) = \pi_2(c)$. In other words, $(n,n,\rho)\in S^{\mathcal{J}}$ if and only if $\rho = \rho_n^{\mathcal{J}}$. Clearly we may again infer that there is $\mathsf{M} = \mathsf{U}^\top\mathsf{D}\mathsf{U}\in\mathcal{CP}_n$ satisfying $\operatorname{cpr}\mathsf{M}\geq b_n^{\mathcal{J}}$, where D is a nonnegative diagonal matrix and U is an element of the subsemigroup of $(\mathcal{Z},\circledast)$ generated by $\mathcal{J}$. Such U can be found as follows: take some maximizing characteristic triple $c\in S^{\mathcal{J}}$ satisfying $\pi_1(c) = n$ and $\pi_3(c) = b_n^{\mathcal{J}}$ (there may be more than one maximizing characteristic triple); use some factorization of c as a product of generators (again there may be more than one such factorization), say $c = c_1\circledast\cdots\circledast c_k$, for some $k\in\mathbb{N}$; and define $\mathsf{U} := \mathsf{J}_{\pi_1(c_1)}\circledast\cdots\circledast\mathsf{J}_{\pi_1(c_k)}$.
The next result is about the increase $b_n^{\mathcal{J}} - b_n$ of the lower bound that we may expect in the case that we have certain bounds for $\rho_n^{\mathcal{J}}$.

Lemma 3.1. *Assume that for some $\alpha,\beta>0$ we have $(\alpha+1)n-\beta\leq\rho_n^{\mathcal{J}}\leq(\alpha+1)n$ for $n\in\mathbb{N}$. Then $b_n^{\mathcal{J}}$ satisfies*

$$\alpha n - \beta\left(\sqrt{\frac{n}{2}}+\frac{3}{2}\right)\leq b_n^{\mathcal{J}} - b_n\leq\alpha n,$$

with b_n as defined in (7).

Proof. We are going to show by induction on k that

a) for each $c = (n, n+1-k, \rho) \in S^{\mathcal{J}}$ there is $c' = (n, n+1-k, \rho') \in S$ satisfying

$$\rho \leq \rho' + \alpha n,$$

b) for each $c' = (n, n+1-k, \rho') \in S$ there is $c = (n, n+1-k, \rho) \in S^{\mathcal{J}}$ satisfying

$$\rho' + \alpha n - \beta k \leq \rho.$$

Both assertions are true for $k = 1$, with $\rho = \rho_n^{\mathcal{J}}$ and $\rho' = n$. Next we assume a) proved up to k, and we use that $c = (n, n-k, \rho) \in S^{\mathcal{J}}$ has for some $i \in [1 : n-1]$ a representation $c = (i, i, \rho_i^{\mathcal{J}}) \circledast \bar{c}$, where $\bar{c} = (n-i, n-i-k+1, \bar{\rho}) \in S^{\mathcal{J}}$. By assumption, there is $\bar{c}' = (n-i, n-i-k+1, \bar{\rho}') \in S$ such that

$$\bar{\rho} \leq \bar{\rho}' + \alpha(n-i),$$

and then $c' := (i, i, i) \circledast \bar{c}' = (n, n-k, \rho') \in S$ satisfies

$$\rho - \rho' = \rho_i^{\mathcal{J}} - i + \bar{\rho} - \bar{\rho}' \leq \alpha i + \alpha(n-i) = \alpha n.$$

Next, assuming b) proved up to k, we use that $c' = (n, n-k, \rho') \in S$ has for some $i \in [1 : n-1]$ a representation $c' = (i, i, i) \circledast \bar{c}'$, where $\bar{c}' = (n-i, n-i-k+1, \bar{\rho}') \in S$. By assumption, there is $\bar{c} = (n-i, n-i-k+1, \bar{\rho}) \in S^{\mathcal{J}}$ such that

$$\bar{\rho}' + \alpha(n-i) - \beta k \leq \bar{\rho},$$

and then $c' := (i, i, \rho_i^{\mathcal{J}}) \circledast \bar{c} = (n, n-k, \rho) \in S^{\mathcal{J}}$ satisfies

$$\rho - \rho' = \rho_i^{\mathcal{J}} - i + \bar{\rho} - \bar{\rho}' \geq \alpha i - \beta + \alpha(n-i) - \beta k = \alpha n - \beta(k+1).$$

Now we use a) to obtain

$$b_n^{\mathcal{J}} = \max_{r,\rho} \left\{ \rho : (n, r, \rho) \in S^{\mathcal{J}} \right\} \leq \max_{r,\rho'} \{ \rho' + \alpha n : (n, r, \rho') \in S \} = b_n + \alpha n$$

and, using b) and Remark 2.1,

$$\begin{aligned} b_n + \alpha n - \beta \left(\sqrt{\frac{n}{2}} + \frac{3}{2} \right) &\leq \max_{k,\rho'} \{ \rho' + \alpha n - \beta k : (n, n+1-k, \rho') \in S \} \\ &\leq \max_{k,\rho} \left\{ \rho : (n, n+1-k, \rho) \in S^{\mathcal{J}} \right\} = b_n^{\mathcal{J}} . \end{aligned}$$

Hence the results. □

So by this method we always obtain an improvement which increases linearly in n, but we cannot hope for much more. The next theorem makes this more precise, and also provides a construction principle for such an improving sequence $\mathcal{J}$:

Theorem 3.1. *Suppose we choose $\mathcal{J} = (\mathsf{J}_n)_{n\in\mathbb{N}}$ as follows:*

- *Fix $n_0 \in \mathbb{N}$ and select $\mathsf{J}_n \in \mathcal{Z}$ with full column rank (and $\rho_n^{\mathcal{J}} = \mathrm{rank}^{(2)}\,\mathsf{J}_n$) for all $n \in [1\!:\!n_0]$, with $\rho_k^{\mathcal{J}} > k$ for at least one $k \in [1\!:\!n_0]$.*
- *Let $k_0 := \min\left\{n \in [1\!:\!n_0] : \frac{\rho_n^{\mathcal{J}}}{n} \geq \frac{\rho_\ell^{\mathcal{J}}}{\ell} \text{ for all } \ell \in [1\!:\!n_0]\right\}$.*
- *Write any $n > n_0$ as $n = ak_0 + b$, where $n_0 - k_0 < b \leq n_0$. Abbreviating*

$$q \odot \mathsf{A} := \mathsf{A} \oplus \mathsf{A} \oplus \cdots \oplus \mathsf{A}$$

for q such $\oplus$-operands A, define $\mathsf{J}_n = (a \odot \mathsf{J}_{k_0}) \oplus \mathsf{J}_b \in \mathcal{Z}$, which is a matrix of full column rank by Lemma 2.3, and let $\rho_n^{\mathcal{J}} = \mathrm{rank}^{(2)}\,\mathsf{J}_n = a\rho_{k_0}^{\mathcal{J}} + \rho_b^{\mathcal{J}}$.

Then $b_n^{\mathcal{J}} - b_n = \alpha n + \mathcal{O}(\sqrt{n})$ for some $\alpha > 0$ and thus

$$\frac{n^2}{2} + \frac{n}{2} - 4 \geq p_n \geq \frac{n^2}{2} - \sqrt{2}n^{3/2} + \gamma n + \mathcal{O}(\sqrt{n}) \tag{12}$$

for some $\gamma > \frac{9}{4}$ depending on the first n_0 matrices J_n, $n \in [1\!:\!n_0]$.

Proof. With $\alpha' := \frac{\rho_{k_0}^{\mathcal{J}}}{k_0} > 1$ we have $\rho_n^{\mathcal{J}} \leq \alpha' n$ for $n \in [1:n_0]$ by the definition of α', and $\rho_n^{\mathcal{J}} = a\rho_{k_0}^{\mathcal{J}} + \rho_b^{\mathcal{J}} \leq a\alpha' k_0 + \alpha' b = \alpha'(ak_0 + b) = \alpha' n$ also for $n > n_0$. With $\beta := \max\left\{\alpha' n - \rho_n^{\mathcal{J}} : n \in [1:n_0]\right\} \geq \alpha' - 1 > 0$ we have $\rho_n^{\mathcal{J}} \geq \alpha' n - \beta$ for $n \in [1\!:\!n_0]$, and $\rho_n^{\mathcal{J}} = a\rho_{k_0}^{\mathcal{J}} + \rho_b^{\mathcal{J}} \geq a\alpha' k_0 + \alpha' b - \beta = \alpha' n - \beta$ also for $n > n_0$. So the hypothesis of Lemma 3.1 is fulfilled with $\alpha := \alpha' - 1$ and β, and the results follow. □

3.2. **New building blocks and better bounds.** The following example shows the construction of a particular sequence $\mathcal{J} = (\mathsf{J}_n)_{n\in\mathbb{N}}$, and reports on the lower bounds $b_n^{\mathcal{J}}$ obtained from this sequence.

Example 3.1. *We let $n_0 = 26$. The construction of J_n for $n \in [1:n_0]$ will be divided into 3 steps, and J_n for $n > n_0$ will be constructed in a fourth step.*
Step 1: *We start with elementary* building blocks *$\mathsf{J}_n := \mathsf{I}_n$ for $n \in [1\!:\!5]$, and we add four more building blocks $\mathsf{J}_n \in \mathcal{Z}$ satisfying $\mathrm{rank}^{(2)}\,\mathsf{J}_n > n$. These we get by looking for copositive matrices having many zeroes, in particular we employ, using*

TABLE 1. Matrices J_n from Example 3.1. See text.

n	J_n	$\rho_n^{\mathcal{J}}$	n	J_n	$\rho_n^{\mathcal{J}}$	n	J_n	$\rho_n^{\mathcal{J}}$
$k \in [1:5]$	I_k	k	9	J_9	26	14	J_{14}	80
			10	$\mathsf{J}_9 \oplus \mathsf{J}_1$	27	15	J_{15}	95
6	J_6	8	11	J_{11}	32	26	$\mathsf{J}_{14} \oplus \mathsf{J}_{12}$	130
7	J_7	14	12	J_{12}	50	$k+15$, $k \in \mathbb{N} \backslash \{11\}$	$\mathsf{J}_k \oplus \mathsf{J}_{15}$	$\rho_k^{\mathcal{J}} + 95$
8	J_8	18	13	J_{13}	65			

the notation $\mathsf{C}(\mathbf{a})$ *with* $\mathbf{a} \in \mathbb{R}^n$ *from* [3],

$$\mathsf{S}_7 = \mathsf{C}([-153, 127, -27, -27, 127, -153, 162]^\top)\,,$$

$$\mathsf{S}_9 = \mathsf{C}([-1056, 959, -484, 231, 231, -484, 959, -1056, 1089]^\top)\,,$$

$$\mathsf{S}_{11} = \mathsf{C}([32, 18, 4, -24, -31, -31, -24, 4, 18, 32, 32]^\top)\,, \quad \textit{and}$$

$$\mathsf{S}_{15} = \mathsf{C}([a, a, b, a, c, b, a, a, b, c, a, b, a, a, d]^\top)\,, \text{ where } [a, b, c, d] = [-2609, 1803, 4009, 7318]\,.$$

Let the rows of $\mathsf{J}_7 \in \mathbb{R}^{14\times 7}$ *(resp.* $\mathsf{J}_9 \in \mathbb{R}^{27\times 9}$, $\mathsf{J}_{11} \in \mathbb{R}^{33\times 11}$, $\mathsf{J}_{15} \in \mathbb{R}^{360\times 15}$*) be the zeroes of* S_7, *(resp.* S_9, S_{11}, S_{15}*). Those matrices all have full column rank and satisfy* $\mathit{rank}^{(2)}\, \mathsf{J}_7 = 14$, $\mathit{rank}^{(2)}\, \mathsf{J}_9 = 26$, $\mathit{rank}^{(2)}\, \mathsf{J}_{11} = 32$ *and* $\mathit{rank}^{(2)}\, \mathsf{J}_{15} = 95$.

Step 2: *Now we delete some rows to close the gaps in column numbers, i.e., consider* $n \in \{6, 8, 12, 13, 14\}$. *Generally speaking, if* $\mathsf{U} \in \mathbb{R}^{k\times n}$ *collects in its rows all the zeroes of* $\mathsf{S} \in \mathbb{R}^{n\times n}$, *we define for a subset* $N \subseteq [1:n]$ *the complement* $N' = [1:n] \setminus N$ *and put* $K := \{\ell \in [1:k] : u_{\ell,i} = 0 \text{ for all } i \in N\}$. *Finally, we abbreviate by* $\Phi_N(\mathsf{U}) := \mathsf{U}_{K\times N'}$, *so that the rows of* $\Phi_N(\mathsf{U})$ *are the zeroes of the matrix* $\mathsf{S}_{N'\times N'}$. *The motivation is that if* U *has full rank and large two-rank, then in lucky cases the same will be true for* $\Phi_N(\mathsf{U})$ *for small sets* N. *Indeed,* $\mathsf{J}_6 := \Phi_{\{1\}}(\mathsf{J}_7) \in \mathbb{R}^{8\times 6}$, $\mathsf{J}_8 := \Phi_{\{1\}}(\mathsf{J}_9) \in \mathbb{R}^{18\times 8}$, $\mathsf{J}_{12} := \Phi_{\{1,2,3\}}(\mathsf{J}_{15}) \in \mathbb{R}^{60\times 12}$, $\mathsf{J}_{13} := \Phi_{\{1,2\}}(\mathsf{J}_{15}) \in \mathbb{R}^{108\times 13}$ *and* $\mathsf{J}_{14} := \Phi_{\{1\}}(\mathsf{J}_{15}) \in \mathbb{R}^{192\times 14}$ *have all full column rank and satisfy* $\mathit{rank}^{(2)}\, \mathsf{J}_6 = 8$, $\mathit{rank}^{(2)}\, \mathsf{J}_8 = 18$, $\mathit{rank}^{(2)}\, \mathsf{J}_{12} = 50$, $\mathit{rank}^{(2)}\, \mathsf{J}_{13} = 65$ *and* $\mathit{rank}^{(2)}\, \mathsf{J}_{14} = 80$.

Step 3: *We further define* $\mathsf{J}_{10} := \mathsf{J}_9 \oplus \mathsf{J}_1 \in \mathbb{R}^{28\times 10}$, *satisfying* $\mathit{rank}\, \mathsf{J}_{10} = 10$ *and* $\mathit{rank}^{(2)}\, \mathsf{J}_{10} = 27$. *For* $n \in [16:25]$ *we define* $\mathsf{J}_n := \mathsf{J}_{n-15} \oplus \mathsf{J}_{15}$, *and, deviating from the latter pattern, we finally let* $\mathsf{J}_{26} := \mathsf{J}_{12} \oplus \mathsf{J}_{14}$, *because* $\mathit{rank}^{(2)}\, \mathsf{J}_{12} + \mathit{rank}^{(2)}\, \mathsf{J}_{14} = 130 > 127 = \mathit{rank}^{(2)}\, \mathsf{J}_{11} + \mathit{rank}^{(2)}\, \mathsf{J}_{15}$, *and this completes the construction of* J_n

TABLE 2. Several bounds for p_n, where $b_n^{\mathcal{J}}$ is a lower bound for $\mathrm{rank}^{(2)}\,\mathsf{U}_n$; see text.

n	d_n	b_n	$b_n^{\mathcal{J}}$	U_n	s_n	n	d_n	b_n	$b_n^{\mathcal{J}}$	U_n	s_n
6	9	9	9	$\mathsf{J}_3 \circledast \mathsf{J}_3$	17	40	400	526	664	$\mathsf{J}_{13}^{\circledast 2} \circledast \mathsf{J}_{14}$	816
7	12	12	**14**	J_7	24	45	506	681	871	$\mathsf{J}_{15}^{\circledast 3}$	1031
8	16	16	18	J_8	32	50	625	856	1043	$\mathsf{J}_5 \circledast \mathsf{J}_{15}^{\circledast 3}$	1271
9	20	20	26	J_9	41	55	756	1051	1277	$\mathsf{J}_{13} \circledast \mathsf{J}_{14}^{\circledast 3}$	1536
10	25	25	28	$\mathsf{J}_3 \circledast \mathsf{J}_7$	51	60	900	1270	1553	$\mathsf{J}_{15}^{\circledast 4}$	1826
11	30	30	35	$\mathsf{J}_2 \circledast \mathsf{J}_9$	62	65	1056	1510	1781	$\mathsf{J}_5 \circledast \mathsf{J}_{15}^{\circledast 4}$	2141
12	36	**37**	50	J_{12}	74	70	1225	1771	2086	$\mathsf{J}_{14}^{\circledast 5}$	2481
13	42	44	65	J_{13}	87	80	1600	2357	2726	$\mathsf{J}_{16}^{\circledast 5}$	3236
14	49	52	80	J_{14}	101	90	2025	3036	3505	$\mathsf{J}_{15}^{\circledast 6}$	4091
15	56	61	95	J_{15}	116	100	2500	3800	4290	$\mathsf{J}_{14}^{\circledast 5} \circledast \mathsf{J}_{15}^{\circledast 2}$	5046
16	64	70	96	J_{16}	132	120	3600	5601	6241	$\mathsf{J}_{15}^{\circledast 8}$	7256
17	72	80	110	$\mathsf{J}_2 \circledast \mathsf{J}_{15}$	149	140	4900	7758	8478	$\mathsf{J}_{15}^{\circledast 4} \circledast \mathsf{J}_{16}^{\circledast 5}$	9866
18	81	91	125	$\mathsf{J}_3 \circledast \mathsf{J}_{15}$	167	160	6400	10285	11076	$\mathsf{J}_{16}^{\circledast 10}$	12876
19	90	102	140	$\mathsf{J}_4 \circledast \mathsf{J}_{15}$	186	180	8100	13176	14065	$\mathsf{J}_{15}^{\circledast 12}$	16286
20	100	114	155	$\mathsf{J}_5 \circledast \mathsf{J}_{15}$	206	200	10000	16436	17366	$\mathsf{J}_{15}^{\circledast 8} \circledast \mathsf{J}_{16}^{\circledast 5}$	20096
21	110	127	172	$\mathsf{J}_6 \circledast \mathsf{J}_{15}$	227	250	15625	26203	27261	$\mathsf{J}_{18} \circledast \mathsf{J}_{22} \circledast \mathsf{J}_{30}^{\circledast 7}$	31371
22	121	140	192	$\mathsf{J}_7 \circledast \mathsf{J}_{15}$	249	300	22500	38305	39736	$\mathsf{J}_{30}^{\circledast 10}$	45146
23	132	155	210	$\mathsf{J}_8 \circledast \mathsf{J}_{15}$	272	350	30625	52754	54495	$\mathsf{J}_{20} \circledast \mathsf{J}_{30}^{\circledast 11}$	61421
24	144	171	232	$\mathsf{J}_9 \circledast \mathsf{J}_{15}$	296	400	40000	69562	71591	$\mathsf{J}_{30}^{\circledast 3} \circledast \mathsf{J}_{31}^{\circledast 10}$	80196
25	156	187	247	$\mathsf{J}_{10} \circledast \mathsf{J}_{15}$	321	450	50625	88741	91141	$\mathsf{J}_{30}^{\circledast 15}$	101471
26	169	204	273	$\mathsf{J}_{13} \circledast \mathsf{J}_{13}$	347	500	62500	110291	112860	$\mathsf{J}_{20} \circledast \mathsf{J}_{30}^{\circledast 16}$	125246
27	182	222	300	$\mathsf{J}_{13} \circledast \mathsf{J}_{14}$	374	550	75625	134221	137061	$\mathsf{J}_{30}^{\circledast 8} \circledast \mathsf{J}_{31}^{\circledast 10}$	151521
28	196	241	328	$\mathsf{J}_{14} \circledast \mathsf{J}_{14}$	402	600	90000	160534	163571	$\mathsf{J}_{30}^{\circledast 20}$	180296
29	210	260	356	$\mathsf{J}_{14} \circledast \mathsf{J}_{15}$	431	650	105625	189249	192390	$\mathsf{J}_{30} \circledast \mathsf{J}_{31}^{\circledast 20}$	211571
30	225	280	385	$\mathsf{J}_{15} \circledast \mathsf{J}_{15}$	461	700	122500	220357	223592	$\mathsf{J}_{32}^{\circledast 17} \circledast \mathsf{J}_{33}^{\circledast 2} \circledast \mathsf{J}_{45}^{\circledast 2}$	245346
31	240	301	400	$\mathsf{J}_{15} \circledast \mathsf{J}_{16}$	492	734	134689	242873	246353	$\mathsf{J}_{32} \circledast \mathsf{J}_{33} \circledast \mathsf{J}_{39} \circledast \mathsf{J}_{45}^{\circledast 14}$	269741
32	256	323	416	$\mathsf{J}_{16}^{\circledast 2}$	524	800	160000	289771	293751	$\mathsf{J}_{35} \circledast \mathsf{J}_{45}^{\circledast 17}$	320396
33	272	345	443	$\mathsf{J}_3 \circledast \mathsf{J}_{15}^{\circledast 2}$	557	850	180625	328085	332428	$\mathsf{J}_{44}^{\circledast 5} \circledast \mathsf{J}_{45}^{\circledast 14}$	361671
34	289	368	472	$\mathsf{J}_4 \circledast \mathsf{J}_{15}^{\circledast 2}$	591	900	202500	368803	373521	$\mathsf{J}_{45}^{\circledast 20}$	405446
35	306	392	501	$\mathsf{J}_5 \circledast \mathsf{J}_{15}^{\circledast 2}$	626	1000	250000	457489	462760	$\mathsf{J}_{45}^{\circledast 12} \circledast \mathsf{J}_{46}^{\circledast 10}$	500496

and $\rho_n^{\mathcal{J}} := \mathit{rank}^{(2)}\,\mathsf{J}_n$ *for* $n \in [1:26]$. *We remark that the matrices* $\mathsf{J}_i, i \in [7:11]$ *have also been used in the paper* [3] *to provide the first counterexamples to the DJL conjecture.*

Step 4: *We compute* $k_0 := \min\left\{n \in [1\!:\!26] : \frac{\rho^{\mathcal{J}}_n}{n} \geq \frac{\rho^{\mathcal{J}}_\ell}{\ell} \text{ for all } \ell \in [1\!:\!26]\right\} = 15$. *Any* $n > 26$ *is now written as* $n = 15a + b$, *where* $11 < b \leq 26$, *and accordingly we define* $\mathsf{J}_n = a \odot \mathsf{J}_{15} \oplus \mathsf{J}_b \in \mathcal{Z}$, *and let* $\rho^{\mathcal{J}}_n = \mathit{rank}^{(2)}\,\mathsf{J}_n = 95a + \rho^{\mathcal{J}}_b$. *This completes the construction of the full sequence* $\mathcal{J}$, *a summary of which can be found in Table 1. We note without proof that the sequence* $(\rho^{\mathcal{J}}_n)_{n\in\mathbb{N}}$ *satisfies* $\rho^{\mathcal{J}}_n \geq \rho^{\mathcal{J}}_i + \rho^{\mathcal{J}}_{n-i}$ *for any* $i, n \in \mathbb{N}$ *such that* $i < n$, *and so our construction can be seen as picking from the semigroup with binary operation* $\oplus$ *generated by* $\{\mathsf{J}_n : n \in [1\!:\!26]\}$ *for each column dimension one of the matrices of highest two-rank.*

The values of $b^{\mathcal{J}}_n$ *for some* $n \in [1\!:\!1000]$, *together with other bounds and matrices* U_n *achieving* $\mathit{rank}^{(2)}\,\mathsf{U}_n \geq b^{\mathcal{J}}_n$ *are given in Table 2. The data for all other* $n \in [36\!:\!999]$ *are available from the authors upon request. See also Figure 1. The matrices* U_n *listed in Table 2 have been obtained as outlined in the beginning of this section, and are therefore in general not unique. For instance, we could also have chosen* $\mathsf{U}_{11} = \mathsf{J}_4 \circledast \mathsf{J}_7$, *because* $(2,2,2) \circledast (9,9,26) = (4,4,4) \circledast (7,7,14) = (11,10,35)$. *Note that* $b^{\mathcal{J}}_{10} = 28$ *and* $b^{\mathcal{J}}_{11} = 35$ *provide better lower bounds for* p_{10} *and* p_{11} *than* 27 *and* 32, *the ones given in* [3]. *As may be seen from the right half of Table 2, the structure of maximizers of* (11) *is more complicated than the structure of maximizers of* (7). *Indeed, there is no simple analogue of Lemma 2.4, since a maximizing characteristic triple from* $S^{\mathcal{J}}$ *may need more than 2 different generators in any of its factorizations. In the range* $[1:1000]$ *we found that at most 4 different generators always suffice, and that 4 are necessary in 4 cases, the smallest of them being* $n = 734$.

In order to get a grip on the asymptotic behavior of $(b^{\mathcal{J}}_n)_{n\in\mathbb{N}}$ *we compute* $\alpha := \frac{\rho^{\mathcal{J}}_{15}}{15} - 1 = \frac{16}{3}$ *and* $\beta := \max\left\{(\alpha+1)n - \rho^{\mathcal{J}}_n : n \in [1\!:\!26]\right\} = 11(\alpha+1) - \rho^{\mathcal{J}}_{11} = \frac{113}{3}$. *Then* $(\alpha+1)n - \beta \leq \rho^{\mathcal{J}}_n \leq (\alpha+1)n$ *holds for* $n \in \mathbb{N}$, *and combining Theorem 2.2, Lemma 3.1 and Theorem 3.1, we get*

$$-\frac{119}{6}\sqrt{2n} - \frac{903}{16} \leq b^{\mathcal{J}}_n - \frac{n^2}{2} + n\sqrt{2n} - \frac{91}{12}n \leq -\frac{5}{8}\sqrt{2n} + \frac{3}{2}\,.$$

4. Conclusions

Summarizing our findings regarding the DJL conjecture: it is true for $n = 5$ [15]; it is false for $n \geq 7$ (see [3] for $n \leq 11$); and it is still unresolved for $n = 6$, despite recent efforts to reduce the gap between the bounds for p_6 [14]; see also [11].

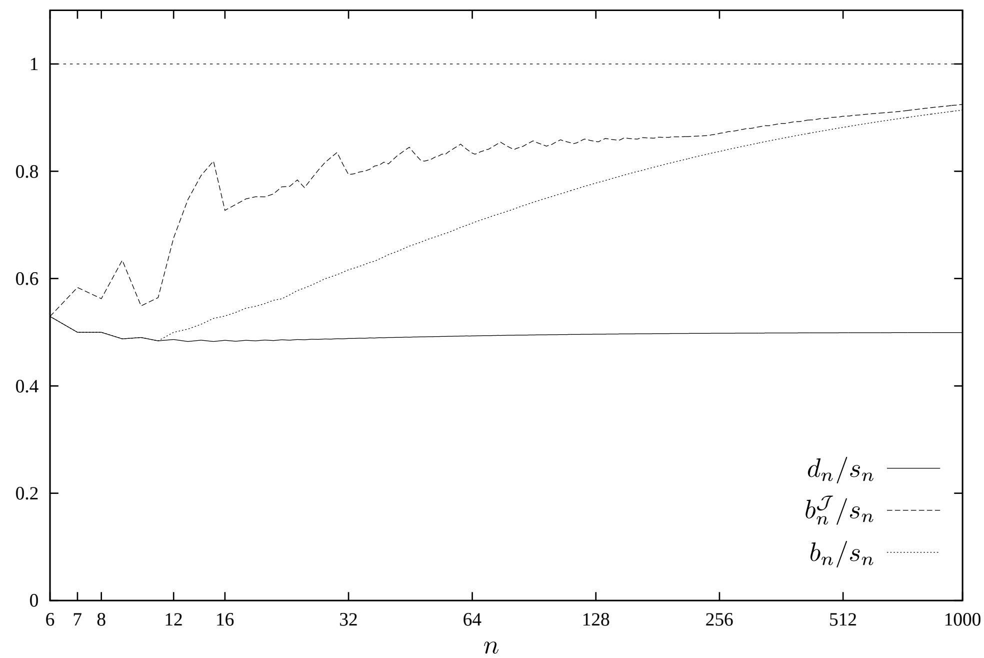

FIGURE 1. Three lower bounds on p_n compared to the best known upper bound s_n

APPENDIX A. CONSTRUCTING A 12×12-MATRIX OF CP-RANK 37.

Here we explicitly construct a matrix $\mathsf{M} \in \mathcal{CP}_{12}$ with cpr $\mathsf{M} = 37$, as announced in Example 2.1. Let the matrix $\mathsf{U} = \begin{bmatrix} \mathsf{U}_0 \\ \mathsf{U}_1 \\ \mathsf{U}_2 \\ \mathsf{U}_3 \end{bmatrix} \in \mathbb{R}^{64\times 12}$ be a rearrangement of the rows of $\mathsf{I}_4^{\circledast 3}$ (which are binary vectors with exactly one unit entry in each of the three four-entry blocks), satisfying $\mathsf{U}_i \in \mathbb{R}^{k_i \times 12}$, where $(k_0, \ldots, k_3) = (27, 27, 9, 1)$, and $\mathsf{U}_i(\mathbf{e}_1 + \mathbf{e}_5 + \mathbf{e}_9) = i\boldsymbol{\eta}_{k_i}$ for $i \in [0:3]$. Define the completely positive matrix

$$\mathsf{M} := 6\mathsf{U}_1^\top \mathsf{U}_1 + 6\mathsf{U}_2^\top \mathsf{U}_2 + \mathsf{U}_3^\top \mathsf{U}_3 = \begin{bmatrix} 91 & 0 & 0 & 0 & 19 & 24 & 24 & 24 & 19 & 24 & 24 & 24 \\ 0 & 42 & 0 & 0 & 24 & 6 & 6 & 6 & 24 & 6 & 6 & 6 \\ 0 & 0 & 42 & 0 & 24 & 6 & 6 & 6 & 24 & 6 & 6 & 6 \\ 0 & 0 & 0 & 42 & 24 & 6 & 6 & 6 & 24 & 6 & 6 & 6 \\ 19 & 24 & 24 & 24 & 91 & 0 & 0 & 0 & 19 & 24 & 24 & 24 \\ 24 & 6 & 6 & 6 & 0 & 42 & 0 & 0 & 24 & 6 & 6 & 6 \\ 24 & 6 & 6 & 6 & 0 & 0 & 42 & 0 & 24 & 6 & 6 & 6 \\ 24 & 6 & 6 & 6 & 0 & 0 & 0 & 42 & 24 & 6 & 6 & 6 \\ 19 & 24 & 24 & 24 & 19 & 24 & 24 & 24 & 91 & 0 & 0 & 0 \\ 24 & 6 & 6 & 6 & 24 & 6 & 6 & 6 & 0 & 42 & 0 & 0 \\ 24 & 6 & 6 & 6 & 24 & 6 & 6 & 6 & 0 & 0 & 42 & 0 \\ 24 & 6 & 6 & 6 & 24 & 6 & 6 & 6 & 0 & 0 & 0 & 42 \end{bmatrix},$$

(observe $\mathsf{M} = \mathsf{I}_3 \otimes \mathsf{A} + (\mathsf{E}_3 - \mathsf{I}_3) \otimes \mathsf{B}$ where A and B are the upper-left and upper-right corner 4×4 blocks) and let $\mathcal{K}_m = \{(r,s) \in [1:12]^2 : r < s, M_{rs} = m\}$ for $m \in \{6, 19, 24\}$. Clearly we have $|\mathcal{K}_6| = 27$ and $|\mathcal{K}_{24}| = 18$. Furthermore consider, by analogy of the construction in Lemma 2.3, the copositive matrix

$$\mathsf{S} = \begin{bmatrix} 3\mathsf{E}_4 - \mathsf{I}_4 & -\mathsf{E}_4 & -\mathsf{E}_4 \\ -\mathsf{E}_4 & 3\mathsf{E}_4 - \mathsf{I}_4 & -\mathsf{E}_4 \\ -\mathsf{E}_4 & -\mathsf{E}_4 & 3\mathsf{E}_4 - \mathsf{I}_4 \end{bmatrix} = \mathsf{I}_3 \otimes (3\mathsf{E}_4 - \mathsf{I}_4) - (\mathsf{E}_3 - \mathsf{I}_3) \otimes \mathsf{E}_4 = 4\mathsf{I}_3 \otimes \mathsf{E}_4 - \mathsf{I}_{12} - \mathsf{E}_{12}$$

which has exactly the rows of $\frac{1}{3}\mathsf{U}$ as zeroes (indeed, $\mathsf{S}\mathbf{u} = \boldsymbol{\eta}_{12} - \mathbf{u}$ for the rows $\mathbf{u}^\top$ of U). Therefore $\langle \mathsf{M}, \mathsf{S} \rangle = 0$. Further, form the (not copositive) 4×4 matrix $\mathsf{C} = \frac{1}{22} \begin{bmatrix} 5 & -6 & -6 & -6 \\ -6 & 5 & 5 & 5 \\ -6 & 5 & 5 & 5 \\ -6 & 5 & 5 & 5 \end{bmatrix}$ and $\bar{\mathsf{S}} = \mathsf{S} + \mathsf{E}_3 \otimes \mathsf{C}$. By computing all stationary points for the problem $\min\limits_{\mathbf{u} \in \Delta_{12}} \mathbf{u}^\top \bar{\mathsf{S}} \mathbf{u}$, it is straightforwardly checked that also $\bar{\mathsf{S}}$ is copositive. We further note $\langle \mathsf{M}, \bar{\mathsf{S}} \rangle = 0 + 3\langle \mathsf{A}, \mathsf{C} \rangle + 6\langle \mathsf{B}, \mathsf{C} \rangle = \frac{261}{22}$ and $\mathbf{u}^\top \bar{\mathsf{S}} \mathbf{u} = \frac{45}{22}$ for any row $\mathbf{u}^\top$ of U_0. Now consider any cp-factorization $\mathsf{M} = \mathsf{U}^\top \mathrm{Diag}(\mathbf{x}) \mathsf{U} = \sum_{i=1}^{64} x_i \mathbf{u}_i \mathbf{u}_i^\top$ with $\mathbf{x} \in \mathbb{R}^{64}_+$ and denote $\mathsf{M}_{123} := \mathsf{M} - \sum_{i=1}^{27} x_i \mathbf{u}_i \mathbf{u}_i^\top$. As also M_{123} is completely positive, we have $\langle \mathsf{M}_{123}, \bar{\mathsf{S}} \rangle \geq 0$ and thus $\sum_{i=1}^{27} x_i \leq \frac{261}{45} < 6$, so we have $(\mathsf{M}_{123})_{rs} > 0$ for all $(r,s) \in \mathcal{K}_6$. Now, for any $(r,s) \in \mathcal{K}_6$, there is exactly one row $\mathbf{u}^\top$ of $\begin{bmatrix} \mathsf{U}_1 \\ \mathsf{U}_2 \\ \mathsf{U}_3 \end{bmatrix}$ satisfying $u_r u_s > 0$ (which must be a row of U_1, e.g. $(\mathbf{e}_1 + \mathbf{e}_6 + \mathbf{e}_{10})^\top$ for $(6,10) \in \mathcal{K}_6$). This row $\mathbf{u}^\top$ moreover satisfies $u_\rho u_\sigma = 0$ for every $(\rho, \sigma) \in \mathcal{K}_6 \setminus \{(r,s)\}$. As $|\mathcal{K}_6| = 27$, the number of rows in U_1, we conclude that $0 < x_i \leq 6$ must hold for all $i \in [28:54]$, with $x_i < 6$ for some $i \in [28:54]$, if $x_i > 0$ for some $i \in [1:27]$. Further, consider any $(r,s) \in \mathcal{K}_{24}$. First we note $(\mathbf{u}_{64} \mathbf{u}_{64}^\top)_{rs} = 0$ because $\mathcal{K}_{24} \cap \{1,5,9\}^2 = \emptyset$. Moreover, by a similar reasoning also

$$\left(\sum_{i=1}^{27} x_i \mathbf{u}_i \mathbf{u}_i^\top \right)_{rs} = 0 \,.$$

Further, there are exactly three rows $\mathbf{u}^\top$ of U_1 such that $u_r u_s > 0$ (in case $(r,s) = (1,6)$, these are $(\mathbf{e}_1 + \mathbf{e}_6 + \mathbf{e}_{10})^\top$, $(\mathbf{e}_1 + \mathbf{e}_6 + \mathbf{e}_{11})^\top$ and $(\mathbf{e}_1 + \mathbf{e}_6 + \mathbf{e}_{12})^\top$) so that we arrive by above observations at

$$\left(\sum_{i=28}^{54} x_i \mathbf{u}_i \mathbf{u}_i^\top \right)_{rs} \leq 3 \cdot 6 = 18 \,.$$

Next denote $\mathsf{M}_{23} := \mathsf{M}_{123} - \sum_{i=28}^{54} x_i \mathbf{u}_i \mathbf{u}_i^\top$; then $(\mathsf{M}_{23})_{rs} \geq 24 - 18 = 6 > 0$ for any $(r,s) \in \mathcal{K}_{24}$. But for all $(r,s) \in \mathcal{K}_{24}$ there is exactly one row $\mathbf{u}^\top$ of $\begin{bmatrix} \mathsf{U}_2 \\ \mathsf{U}_3 \end{bmatrix}$

satisfying $u_r u_s > 0$ (which then must be a row of U_2). This row $\mathbf{u}^\top$ also satisfies $u_\rho u_\sigma > 0$ for exactly one other $(\rho, \sigma) \in \mathcal{K}_{24} \setminus \{(r,s)\}$, e.g., $\mathbf{u} = \mathbf{e}_1 + \mathbf{e}_5 + \mathbf{e}_{10}$ for $\{(1,10),(5,10)\} \subset \mathcal{K}_{24}$. We thus conclude that $x_i \geq 6$ must hold for all $i \in [55:63]$. However, if now $x_i = 0$ for all $i \in [1:27]$, we derive $x_i = 6$ for all $i \in [28:54]$ from the considerations on $\mathcal{K}_6$ and hence $(\mathsf{M}_{23})_{rs} = 24-18 = 6$ with equality in this case, which in turn implies $x_i = 6$ for all $i \in [55:63]$. But then $x_{64} = 19 - 3 \cdot 6 = 1 > 0$ must hold. Indeed, for any $(r,s) \in \mathcal{K}_{19}$, there are exactly three rows $\mathbf{u}$ of U_2 such that $u_r u_s > 0$ (in case $(r,s) = (1,5)$, these are $(\mathbf{e}_1 + \mathbf{e}_5 + \mathbf{e}_{10})^\top$, $(\mathbf{e}_1 + \mathbf{e}_5 + \mathbf{e}_{11})^\top$ and $(\mathbf{e}_1 + \mathbf{e}_5 + \mathbf{e}_{12})^\top$), and obviously, no row $\mathbf{u}^\top$ of $\begin{bmatrix} \mathsf{U}_0 \\ \mathsf{U}_1 \end{bmatrix}$ can satisfy $u_r u_s > 0$. Summarizing, we have $x_i > 0$ for all $i \in [28:63]$, and $x_i > 0$ for at least one $i \in [1:27] \cup \{64\}$, which means cpr $\mathsf{M} \geq 37$. From the definition of M we see that cpr $\mathsf{M} \leq 37$, so we finally conclude cpr $\mathsf{M} = 37$.

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