MINIMUM ENERGY CONFIGURATIONS ON A TORIC LATTICE AS A QUADRATIC ASSIGNMENT PROBLEM.
PART II: SYMMETRY REDUCTION OF SEMIDEFINITE PROGRAMMING RELAXATIONS

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ABSTRACT

The Jordan reduction, a symmetry reduction method for semidefinite programming, was recently introduced for symmetric cones by Parrilo and Permenter in [17]. We extend this method to the doubly nonnegative cone and investigate its application to a strong relaxation of the quadratic assignment problem. This reduction is then used to efficiently calculate better bounds for certain discrete energy minimization problems, which initially have the form of semidefinite programs too large to be solved directly.

Keywords quadratic assignment problem · semidefinite programming · discrete energy minimization · symmetry reduction

AMS subject classification 90C22; 20B40

1 Introduction

This paper studies symmetry reduction of semidefinite programs (SDPs) where the matrix variable is also entry-wise nonnegative, i.e. symmetry reduction of conic linear programming over the doubly nonnegative cone. Such problems appear naturally in the study of convex relaxations of combinatorial problems. In particular, we are interested in such relaxations of the quadratic assignment problem (QAP):

\[ QAP(A, B) = \min_{\varphi \in S_n} \sum_{i,j=1}^{n} a_{ij} b_{\varphi(i),\varphi(j)}, \]

where \( A = (a_{ij}) \) and \( B = (b_{ij}) \) are square \( n \times n \) matrices, and \( S_n \) denotes the symmetric group (i.e. all permutations) on \( n \) elements.

Specifically, we are interested in the SDP relaxation of the QAP by Zhao et al. [23], applied to a problem in discrete energy minimization. This problem may be described as follows, with reference to Figure 1: given a toric grid of fixed size, and a number of repulsive particles, how should one place the particles on grid points in such a way as to minimize the total energy of the system. Here, the energy between two particles is inversely proportional to the (Lee) distance between them, where the Lee distance is simply the shortest path between the two particles on the grid.

This problem is of interest in physics (see [4]), as well as in computer graphics (grey-scale printing) [21]. It may be seen as a discrete variant on the Thomson problem on the torus, better known as the poppy-seed bagel problem (a humorous reference to the question of how to spread poppy-seeds evenly on a bagel) [15].

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In terms of the QAP, the matrix $B = (b_{ij})$ is indexed by the grid points, and $b_{ij}$ ($i \neq j$) is the inverse of the Lee distance (shortest path on the grid) between grid points $i$ and $j$. The diagonal of $B$ is set to zero. The matrix $A$ is zero except for a square block of all-ones in the upper left corner, of size equal to the number of particles. It is easy to see that the QAP objective function value is twice the total energy of the system, if the energy between any two particles equals the inverse Lee distance between them.

In part I of this paper [5], we compared the SDP bound by Zhao et al. [23] for this specific QAP to bounds from the literature, including bounds from [4]. We showed that the SDP bounds improve on the best-known bounds for several grid sizes and numbers of particles. The actual computation of the SDP bounds was only possible through symmetry reduction, since the original sizes of the SDPs were mostly prohibitively large. Indeed, in the SDP relaxation, the matrix variables are of order the number of grid points on the torus squared. Thus, for the $12 \times 10$ grid in Figure 1, the SDP matrix variables will be of the order $120^2 = 14,400$, well beyond the range of SDP solvers.

In this, the second part of the paper, we describe the symmetry reduction process in detail.

Symmetry reduction for SDP was first introduced by Schrijver in 1979 in [20]; see for example the chapter [2] by Bachoc, Gijswijt, Schrijver and Vallentin for a review of later developments up to 2012. The specific case of SDP relaxations of quadratic assignment problems was investigated by De Klerk and Sotirov in [10, 11].

Parrilo and Permenter [17] recently introduced a new — and more general — form of symmetry reduction, called Jordan reduction. We will extend their approach to obtain the required symmetry reduction of our energy minimization QAP.

Outline and contributions of this paper

In the next section, we recap relevant definitions and results on the Jordan reduction of Parrilo and Permenter [17]. In Section 3, we subsequently extend this approach — which was formulated for symmetric cones — to the doubly nonnegative cone. This allows us to finally apply the method to the SDP relaxation of the general QAP due to Zhao et al. [23] in Section 4, and specifically to the energy minimization QAP on the toric grid in Section 5. We describe the final block-diagonalization in Section 5.3, that in fact reduces the SDP relaxation to a much more tractable second-order cone program.

Our main contribution is to give a reduction of the SDP relaxation of the energy minimization QAP that allows computation of moderate sized instances, as detailed in the first part of this paper [5]. More generally, our extension of the Jordan reduction method of Parrilo and Permenter [17] in Section 3 should lead to additional applications in SDP relaxations of other combinatorial problems.

2 Preliminaries on Jordan symmetry reduction

We will study conic optimization problems in the form

$$\inf \left\{ \langle C, X \rangle \mid \langle A_i, X \rangle = b_i \text{ for } i \in [m] \right\} \quad \text{=} \quad \inf \left\{ \langle C, X \rangle \mid X \in X_0 + \mathcal{L} \right\} ,$$

where $X \in K$.
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where \([m] = \{1, \ldots, m\}, \mathcal{K} \subseteq \mathcal{V}\) is a closed, convex cone in a real Hilbert space \(\mathcal{V}\), \(X_0 \in \mathcal{V}\) satisfies \(\langle A_i, X_0 \rangle = b_i\) for all \(i \in [m]\), and \(\mathcal{L} \subseteq \mathcal{V}\) is the nullspace of the linear operator \(A\), where \(A(X) = (\langle A_i, X \rangle)_{i=1}^m\). The objective function is given using the inner product \(\langle \cdot, \cdot \rangle\) of \(\mathcal{V}\), with which one defines the dual cone as:

\[\mathcal{K}^* := \{Y \in \mathcal{V} \mid \langle X, Y \rangle \geq 0 \ \forall X \in \mathcal{K}\}.
\]

In this paper, we will mostly deal with the case where \(\mathcal{V}\) is the space \(S^n\) of \(n \times n\) symmetric matrices equipped with the Euclidean inner product, and where \(\mathcal{K}\) is the cone of doubly nonnegative matrices.

### 2.1 Constraint Set Invariance

Parrilo and Permenter \[17\] introduced a set of three conditions a subspace has to fulfill, such that it is be possible to use it for symmetry reduction. Here we revisit some of their results.

**Definition 2.1.** A projection is a linear transformation \(P: \mathcal{V} \to \mathcal{V}\) which is idempotent, i.e. \(P^2 = P\).

**Definition 2.2** (Definition 2.1. in \[17\]). A projection \(P: \mathcal{V} \to \mathcal{V}\) fulfills the Constraint Set Invariance Conditions (CSICs) for \((\mathcal{K}, X_0 + \mathcal{L}, \mathcal{C})\) if

\[
\begin{align*}
(i) \ \text{The projection is positive:} & \ P(\mathcal{K}) \subseteq \mathcal{K}, \\
(ii) \ P(X_0 + \mathcal{L}) \subseteq X_0 + \mathcal{L}, \\
(iii) \ P^*(C + \mathcal{L}^\perp) \subseteq C + \mathcal{L}^\perp,
\end{align*}
\]

where \(P^*\) is the adjoint of \(P\), which satisfies \(\langle P(X), Y \rangle = \langle X, P^*(Y) \rangle\) for all \(X, Y \in \mathcal{V}\).

Note that this definition is symmetric going from primal to dual, since

\[P(\mathcal{K}) \subseteq \mathcal{K} \iff P^*(\mathcal{K}^*) \subseteq \mathcal{K}^*.
\]

These projections send feasible solutions to feasible solutions with the same objective value, as the next result shows.

**Proposition 2.3** (Proposition 1.4.1 in \[18\]). If a projection \(P: \mathcal{V} \to \mathcal{V}\) fulfills the CSICs, then

- \(P((X_0 + \mathcal{L}) \cap \mathcal{K}) \subseteq (X_0 + \mathcal{L}) \cap \mathcal{K},\)
- \(P^*((C + \mathcal{L}^\perp) \cap \mathcal{K}^*) \subseteq (C + \mathcal{L}^\perp) \cap \mathcal{K}^*,\)
- For \(X \in X_0 + \mathcal{L}\): \(\langle C, X \rangle = \langle C, P(X) \rangle,\)
- For \(Y \in C + \mathcal{L}^\perp\): \(\langle X_0, Y \rangle = \langle X_0, P^*(Y) \rangle.\)

To make things easier, we restrict ourselves to orthogonal projections \(P_S\) to a subspace \(S \subseteq \mathcal{V}\), which are exactly the projections of which the range and kernel are orthogonal, or equivalently the projections which are self-adjoint, i.e. \(P_S = P_S^*\). If the projection \(P_S\) fulfills the CSICs we call the subspace \(S\) admissible, following \[17\]. In this case, the CSICs may be rewritten as follows.

**Theorem 2.4** (Theorem 5.2.4 in \[18\]). Consider the conic optimization problem (2.1) and let \(S \subseteq \mathcal{V}\) be the range of an orthogonal projection \(P_S: \mathcal{V} \to \mathcal{V}\). Let \(P_L\) denote the orthogonal projection onto \(\mathcal{L}\), etc., and define \(C_L = P_L(C)\) and \(X_0, L^\perp = P_L(X_0)\). Then \(S\) is an admissible subspace if, and only if,

\[
\begin{align*}
(a) \ C_L, X_0, L^\perp & \subseteq S, \\
(b) \ P_L(S) & \subseteq S, \\
(c) \ P_S(\mathcal{K}) & \subseteq \mathcal{K}.
\end{align*}
\]

Restricting the conic program to an admissible subspace \(S\) thus results in another, potentially significantly smaller program, with the same optimal value.

\[
\inf \langle P_S(C), X \rangle \\
\text{s.t. } X \in P_S(X_0) + \mathcal{L} \cap \mathcal{S}, \\
X \in \mathcal{K} \cap \mathcal{S}.
\]
2.2 The reduction for Jordan-Algebras

Next we review some results from [18] for the situation where the space $V$ is an Euclidian Jordan algebra $J$, that is a commutative algebra (with product denoted by ‘$\circ$’) over $\mathbb{R}$ satisfying the Jordan identity
\[(x \circ y) \circ x^2 = x \circ (y \circ x^2),\]
and an inner product with $(x \circ y, z) = (y, x \circ z)$. For every such algebra we can define $K$ as the cone of squares of $J$ given by $K = \{ x \circ x \mid x \in J \}$, which always is a symmetric cone, i.e. a self-dual and homogenous convex cone (see for example [12]).

The only example relevant for us is the case $J = S^n$, the symmetric $n \times n$-matrices with real entries, with product defined by
\[X \circ Y := \frac{1}{2} (XY + YX),\]
and the inner product the Euclidean (trace) inner product $\langle X, Y \rangle = \text{trace}(XY)$. It is easy to see (e.g. from the spectral decomposition) that its cone of squares is exactly the positive semidefinite cone $S^n_+$.

Since the product of a Jordan algebra is commutative, we have
\[2x \circ y = x \circ y + y \circ x = (x + y)^2 - x^2 - y^2,\]
which means that subspaces are closed under multiplication, if and only if they include all squares. Similarly isomorphisms between (euclidian) Jordan algebras are exactly the bijective linear maps satisfying $\phi(x^2) = (\phi(x))^2$.

**Definition 2.5.** A Jordan algebra $J$ is called special, if it is isomorphic to the algebra one gets from a real associative algebra by equipping the latter with the product $x \circ y = \frac{1}{2} (xy + yx)$.

There is only a single (up to isomorphisms) simple Jordan algebra which is not special, the algebra of Hermitian $3 \times 3$-matrices of Octonions $H_3(\mathbb{O})$. The for us relevant case $J = S^n$ is special.

**Definition 2.6.** A subspace (not necessarily a subalgebra) $S$ of a Jordan algebra is called unital, if there is an an element $e \in S$ such that $e \circ a = a \circ e = a$ for all $a \in S$.

An important fact for us is that every Euclidean Jordan algebra is unital.

One main result of [18] is an alternative description of the CSICs when the ambient space is a special Euclidean Jordan algebra. In this case the condition $P_S(K) \subseteq K$ in Theorem 2.4 — with $K$ the cone of squares in $J$ — is equivalent to $S$ being closed under taking squares, i.e. to $S$ being a Jordan sub-algebra of $J$.

This gives an algorithm for finding the minimal admissible subspace, which is defined as follows.

**Definition 2.7.** The unique minimal admissible subspace is
\[S_{\min} := \bigcap_{S \text{ is admissible}} S.\]

As mentioned before, we may now formulate an algorithm for $S_{\min}$.

**Theorem 2.8 (Theorem 3.2 in [17]).** If $V = J$ is an Euclidian, special Jordan algebra, then $S_{\min}$ is the output of Algorithm 1.

**Algorithm 1: Finding $S_{\min}$**

1. $S \leftarrow \text{span}\{C_L, X_{0,L} \}$
2. repeat
3. $S \leftarrow S + P_L(S)$
4. $S \leftarrow S + \text{span}\{X^2 \mid X \in S\}$
5. until converged;

2.3 A combinatorial reduction algorithm

The fourth step of Algorithm 1 is not linear, and hard to implement. But, conveniently, Permenter does introduce three combinatorial algorithms in his PhD thesis ([18], Chapter 7) for the cone $S^n_+$, which all find orthogonal 0/1-bases for an optimal unital admissible subspace with certain additional properties. Here we will only mention one of the algorithms, since the other ones cannot give us better reductions for our special case.
Partition subspaces

The second combinatorial algorithm by Permenter [18] finds an optimal unital partition subspace, which is a subspace with 0/1-basis, the elements of which sum to the all-one matrix. We can describe the basis uniquely with a partition of the coordinates of \( S^n \), i.e. of \([n] \times [n]\), simply by having one part for every basis element with ones in the corresponding coordinates. For example the following spaces are partition subspaces:

\[
P_1 = \begin{pmatrix} a & a & b \\ a & a & b \\ b & b & c \end{pmatrix}, \quad P_2 = \begin{pmatrix} a & b & b \\ b & a & b \\ b & b & c \end{pmatrix}, \quad P_3 = P_1 \land P_2 = \begin{pmatrix} a & b & c \\ b & a & c \\ c & c & d \end{pmatrix},
\]

where \( P_1 \land P_2 \) is the coarsest partition space refining both \( P_1 \) and \( P_2 \).

For our purposes an important special case is a so-called Jordan configuration, defined as follows.

**Definition 2.9.** A partition \( P \) of \( A \times A \), where \( A \) is a finite set, is called a Jordan configuration, if its characteristic matrices \( B_P \) satisfy

- \( X = X^T \) for all \( X \in B_P \),
- \( XY + YX \in \text{span } B_P \) for all \( X, Y \in B_P \),
- \( I \in \text{span } B_P \).

In words, a Jordan configuration is a basis of a unital partition subspace that is also a Jordan subalgebra of \( S^n \).

A more general example of a partition space, also of interest to us, is a so-called coherent algebra.

**Definition 2.10.** A partition \( P \) of \( A \times A \), where \( A \) is a finite set, is called a coherent configuration, if its characteristic matrices \( B_P \) satisfy

- If \( X \in B_P \) then also \( X^T \in B_P \),
- \( XY \in \text{span } B_P \) for all \( X, Y \in B_P \),
- \( I \in \text{span } B_P \).

Thus, a coherent configuration gives a 0/1 basis of a partition subspace that is also a matrix \(*\)-algebra, namely the associated coherent algebra. Note that the symmetric part of a coherent configuration is a Jordan configuration. It is an open question if the converse is also true [7], [18, p. 218].

To restrict the algorithm to partition subspaces, we need more notation: \( \text{part}(A) \) is the smallest partition space containing the matrix (or subspace) \( A \), which is simply the partition space given by the unique entries of \( A \).

**Algorithm 2: Partition algorithm**

1. \( P \leftarrow \text{part}(C_L) \land \text{part}(X_0, C_L) \)
2. repeat
3. \( P \leftarrow P \land \text{part}(P_L(P)) \)
4. \( P \leftarrow P \land \text{part}(\text{span}\{X^2 \mid X \in P\}) \)
5. until converged;

There are two basic ways to implement this algorithm: One can use polynomial matrices, or randomization. For the first variant one introduces (commuting) variables \( t_i \) for each element of a basis \( B_1, \ldots, B_k \) of \( P \), and then refines the partition with \( \text{part}(P_L(\sum_{i=1}^k t_i B_i)) = \text{part}(\sum_{i=1}^k t_i P_L(B_i)) \) and \( \text{part}((\sum_{i=1}^k t_i B_i)^2) \). If we for example take \( P_2 \) from the example above, one has

\[
\begin{pmatrix} t_a & t_b & t_b \\ t_b & t_a & t_b \\ t_b & t_b & t_c \end{pmatrix}^2 = \begin{pmatrix} t_a^2 + 2t_b^2 & 2t_a t_b + t_b^2 & t_a t_b + t_b^2 + t_b t_c \\ 2t_a t_b + t_b^2 & 2t_a^2 + t_b^2 & t_a t_b + t_b^2 + t_b t_c \\ 2t_a t_b + t_b^2 + t_b t_c & t_a t_b + t_b^2 + t_b t_c & 2t_b^2 + t_c^2 \end{pmatrix},
\]

of which the unique polynomials induce the partition \( P_3 \).

The second variant refines the partition with a random element in the partition space after projecting it to \( L \) and after squaring it. While one has to be more careful about rounding errors here, it is both easier to implement and much faster.
Algorithm 3: Partition algorithm, randomized

1 \( P \leftarrow \text{part}(C_L) \wedge \text{part}(X_{0,L^+}) \)
2 repeat
3 \( X \leftarrow \text{random element of } P \)
4 \( P \leftarrow P \wedge \text{part}(P_L(X)) \)
5 \( P \leftarrow P \wedge \text{part}(X^2) \)
6 until converged;

Remark 2.11. We note that the first variant of the partition algorithm presented here is very similar to the Weisfeiler-Leman (WL) algorithm [22], that finds the coarsest coherent configuration refining a given partition of \([n] \times [n]\). The only difference is that the WL algorithm uses non-commuting variables \(t_i\), as opposed to commuting ones; see [1] on details of the implementation of the WL algorithm.

3 EXTENSION TO THE DOUBLY NONNEGATIVE CONE

We will now fix the cone \(K\) in (2.1) to be the doubly nonnegative cone \(D^n := S^n_+ \cap \mathbb{R}^{n \times n}_+\). Since we will refer to nonnegative, symmetric matrices frequently, we also introduce the notation \(N^n = S^n \cap \mathbb{R}^{n \times n}_+\). Even though \(D^n\) is not a cone of squares in a Euclidean Jordan algebra, one may readily adapt some of the results of the last section to this setting.

We start with an elementary, but important observation.

Proposition 3.1. Assume that a subspace \(S \subseteq S^n\) has a basis of nonnegative matrices with pairwise disjoint supports. Then the orthogonal projection \(P_S\) onto \(S\) satisfies \(P_S(D^n) \subseteq D^n\) if it satisfies \(P_S(S^n_+) \subseteq S^n_+\).

Proof. If \(S\) has a basis of nonnegative matrices with disjoint supports, then it has an orthonormal basis with this property, say \(A_i (i \in [d])\), and the orthogonal projection is of the form

\[ P_S(X) = \sum_{i=1}^{d} \langle A_i, X \rangle A_i. \]

Since the Euclidean inner product of two nonnegative matrices is nonnegative, we have

\[ P_S(N^n) \subseteq N^n, \]

and, since \(D_n \subseteq S^n_+\), and \(P_S(S^n_+) \subseteq S^n_+\) by assumption,

\[ P_S(D^n) \subseteq S^n_+ \cap N^n = D^n. \]

If we consider partition subspaces, we may therefore use results on admissible partition subspaces for the case \(K = S^n_+\), as follows.

Corollary 3.2. Consider a conic optimization problem of the form (2.1), with \(V = S^n\), and \(K = S^n_+\), and let \(S\) be an admissible partition subspace for this problem. Then, \(S\) is also a admissible partition subspace for the related problem where we replace \(K = S^n_+\) by \(K = D^n\).

The important practical implication is that we may use Algorithm 3 to find the minimal admissible Jordan configuration for conic optimization problems on the cone \(D^n\). In the next section we will do precisely this for an SDP relaxation of the quadratic assignment problem.

It it instructive though, to ask how restrictive it is to only consider admissible partition subspaces. In what follows, we show that, the partition subspace structure is actually imposed by some relatively weak assumptions.

To this end, we recall a result on nonnegative projection matrices, taken from [13, Theorem 2.38], but originally due to Belitskii and Lyubich (cf. [3, p. 108]).

Proposition 3.3 (Theorem 2.1.11 in [3]). The general form of a nonnegative projection matrix is

\[ P = (A + B)C^T \]

where \(r = \text{rank}(P)\), \(A, B, C \in \mathbb{R}^{n \times r}_+\), \(A^T A = I\), \(C^T A = I\), \(B^T A = 0\) and \(B^T C = 0\).
As a consequence, a nonnegative projection matrix has the following structure.

**Corollary 3.4.** Any \( n \times n \) symmetric nonnegative projection matrix \( P \) with \( r \)-dimensional range takes the form \( P = C C^T \) for some \( C \in \mathbb{R}^{n \times r}_+ \) such that \( C^T C = I \). In particular, the columns of \( C \) form a nonnegative, orthonormal basis of the range of \( P \), and these basis vectors therefore have disjoint supports.

**Proof.** With reference to (3.1), one has

\[
P = P^T \implies PA = P^TA \iff (A + B)C^T A = C(A^T + B^T)A \iff A + B = C.
\]

Thus by (3.1) one has \( P = C C^T \), and \( C^T C = I \). Since nonnegative vectors can only be orthogonal if they have disjoint supports, the columns of \( C \) have this property.

Finally, recall that a projection matrix is symmetric if and only if it corresponds to an orthogonal projection.

One may easily extend this to orthogonal projection operators, as follows.

**Proposition 3.5.** Assume that a given orthogonal projection \( P_S \) with range \( S \subseteq \mathbb{S}^n \) satisfies \( P_S(N^n) \subseteq N^n \). Then:

1. \( S \) has a basis of nonnegative matrices with disjoint supports.
2. If, in addition, \( S \) contains the all ones matrix \( J \), then it is a partition subspace.
3. If, in addition to the condition in item 2), \( P_S(S_+^n) \subseteq S_+^n \) and \( S \) contains the identity matrix, then \( S \) is a Jordan configuration.

**Proof.** Since \( P_S \) is self-adjoint, we may write it as a symmetric matrix, say \( M_{P_S} \), with respect to the standard orthonormal basis of \( \mathbb{S}^n \). For a \( X \in \mathbb{S}^n \), we define the vector \( \text{svec}(X) \in \mathbb{R}^{\frac{1}{2}n(n+1)} \) as

\[
\text{svec}(X) = \left( X_{11}, \sqrt{2}X_{21}, \ldots, \sqrt{2}X_{n1}, X_{22}, \sqrt{2}X_{32}, \ldots, \sqrt{2}X_{n2}, \ldots, X_{nn} \right)^T.
\]

Thus \( \text{svec}(X) \) gives the coordinates of \( X \) in the standard orthonormal basis of \( \mathbb{S}^n \). One therefore has

\[
\text{svec}(P_S(X)) = M_{P_S} \cdot \text{svec}(X) \quad \forall X \in \mathbb{S}^n.
\]

Choosing \( \text{svec}(X) \) as the standard unit vectors in \( \mathbb{R}^{\frac{1}{2}n(n+1)} \) makes it clear that \( M_{P_S} \in N^{\frac{1}{2}n(n+1)} \). Thus the first claim now follows from Corollary 3.4, namely that \( S \) has a basis of nonnegative matrices with pairwise disjoint supports. If \( S \) contains the all-ones matrix \( J \), then it must hold that these basis matrices are 0/1, proving the second claim.

Finally, to prove the third claim, we recall that \( S \) unital and \( P_S(S_+^n) \subseteq S_+^n \) implies that \( S \) is a Euclidean Jordan algebra. Since it has a 0/1 basis, it is in fact a Jordan configuration if we also assume \( I \in S \).

The last proposition shows that partition subspaces are closely related to nonnegative projections. The question remains if there exists an orthogonal projection \( P_S : \mathbb{S}^n \to \mathbb{S}^n \) with range \( S \subseteq \mathbb{S}^n \) that satisfies \( P_S(D^n) \subseteq D^n \), but not \( P_S(N^n) \subseteq N^n \). If the answer is no, then all admissible subspaces that contain \( J \) and \( I \) are automatically Jordan configurations for conic problems over the doubly nonnegative cone, by the proposition.

4 Reducing the semidefinite relaxation of the quadratic assignment problem

A semidefinite programming relaxation for QAP(\( A, B \)) (see (1.1)), due to Zhao, Karisch, Rendl and Wolkowicz [23], is

\[
\min \langle B \otimes A, Y \rangle \quad \text{s.t.} \quad \langle I_n \otimes E_{jj}, Y \rangle = 1 \text{ for } j \in [n], \\
\langle E_{jj} \otimes I_n, Y \rangle = 1 \text{ for } j \in [n], \\
\langle I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n, Y \rangle = 0, \\
\langle J_n^2, Y \rangle = n^2, \\
Y \in D^{n^2},
\]

where \( A, B \in \mathbb{S}^n \). We refer to Part I of this paper [5] and to [19] for more details of this relaxation.
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First, we have to transform this program into conic form. We get a feasible solution \( X_0 \) by forming the outer product of a vectorized permutation-matrix, for example we can set

\[
X_0 = \text{vec}(I_n)\text{vec}(I_n)^T.
\]

We get the space \( \mathcal{L} \), as seen earlier, by

\[
\mathcal{L} = \{ X \in \mathbb{S}^n \mid \langle A_i, X \rangle = 0 \quad \forall i \in [m]\},
\]

where

\[
\{A_i\}_{i \in [m]} = \{ J_{n^2}, I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n, I_n \otimes E_{jj} \text{ and } E_{jj} \otimes I_n \mid j \in [n]\}
\]

are the data-matrices of the constraints of the SDP relaxation (4.1). Accordingly the orthogonal complement is exactly

\[
\mathcal{L}^\perp = \text{span}\{A_1, \ldots, A_m\}.
\]

**Theorem 4.1.** Any admissible subspace, say \( S \subset \mathbb{S}^n \), for the QAP relaxation (4.1) with \( n > 2 \), has a basis of nonnegative matrices with disjoint supports, provided that \( P_S(\mathbb{S}^n) \subseteq \mathbb{S}^n \) where \( P_S : \mathbb{S}^n \to \mathbb{S}^n \) is the orthogonal projection onto \( S \). If, in addition, \( P_S(\mathbb{S}^n) \subseteq \mathbb{S}^n \) and \( S \) is unital, then \( S \) is a Jordan configuration.

**Proof.** Let \( S \) be an admissible subspace for the QAP relaxation (4.1) with \( n > 2 \), and assume \( P_S(\mathbb{S}^n) \subseteq \mathbb{S}^n \). The first claim of the theorem is an immediate consequence of Proposition 3.5.

If we further assume \( P_S(\mathbb{S}^n) \subseteq 2 \mathbb{S}^n \) and \( S \) unital, then \( S \) is closed under taking squares, i.e. it is a Jordan subalgebra of \( \mathbb{S}^n \) [18, Lemma 5.2.2]. Thus \( S \) contains \( X_{0,\mathcal{L}^\perp} \) and its square, which we will now calculate. To project \( X_0 = \text{vec}(I_n)\text{vec}(I_n)^T \) onto \( \mathcal{L}^\perp \), the span of the constraint matrices, we first notice only two of them have nonzero entries outside of the diagonal, the all one matrix \( I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n \), and the matrix \( I_n \otimes J_n + J_n \otimes I_n \), which we will call \( T \) from now on. The matrices \( I_n \otimes E_{jj} \text{ for } j = 1, \ldots, n \text{ sum to the identity matrix } I_{n^2} \), meaning we can easily find an orthogonal basis of the off diagonal part of \( \mathcal{L}^\perp \):

\[
B_1 = T,
\]

\[
B_2 = J_{n^2} - I_{n^2} - T.
\]

Since \( \langle T, X_0 \rangle = 0 \) and \( \langle J_{n^2}, X_0 \rangle = n^2 \) we get

\[
\langle B_2, X_0 \rangle = \langle J_{n^2}, X_0 \rangle - \langle I_{n^2}, X_0 \rangle = n^2 - n.
\]

Hence the off-diagonal part of \( X_{0,\mathcal{L}^\perp} \) is the matrix

\[
\frac{\langle B_2, X_0 \rangle}{\langle B_2, B_2 \rangle} B_2 = \frac{\frac{n^2 - n}{n^2 - 2n(n^2 - n)}}{B_2} = \frac{1}{n^2 - n} B_2.
\]

The diagonal part of \( X_{0,\mathcal{L}^\perp} \) is the matrix \( \frac{1}{n} I_{n^2} \), since

\[
\langle E_{jj} \otimes I_n, \frac{1}{n} I_{n^2} - X_0 \rangle = \langle E_{jj} \otimes I_n, \frac{1}{n} I_{n^2} \rangle - \langle E_{jj} \otimes I_n, X_0 \rangle = 1 - 1 = 0,
\]

and analogously \( \langle I_n \otimes E_{jj}, \frac{1}{n} I_{n^2} - X_0 \rangle = 0 \). Combining the two parts we see

\[
X_{0,\mathcal{L}^\perp} = \frac{1}{n^2 - n} B_2 + \frac{1}{n} I_{n^2}.
\]

Straightforward calculation now yields

\[
X_{0,\mathcal{L}^\perp}^2 = \frac{n^2 - 2n + 1}{n^2(n - 1)^2} J_{n^2} - \frac{n - 1}{n(n - 1)^2} (I_n \otimes J_n + J_n \otimes I_n) + \frac{1}{(n - 1)^2} I,
\]

\[
X_{0,\mathcal{L}^\perp}^4 = \frac{1}{(n - 1)^2} X_{0,\mathcal{L}^\perp}^2 + \frac{n - 2}{(n - 1)^2} J_{n^2}.
\]

Thus \( S \) contains the all-ones matrix if \( n > 2 \), since

\[
\frac{n - 2}{n(n - 1)^2} J_{n^2} = X_{0,\mathcal{L}^\perp}^4 - \frac{1}{(n - 1)^2} X_{0,\mathcal{L}^\perp}^2,
\]

and the right-hand-side terms both belong to \( S \). By Corollary ??, \( S \) must therefore have a 0/1 basis, i.e. it must be a partition subspace. To show that it is in fact a Jordan configuration, we only need to show still that it contains the identity matrix. To this end, it suffices to note that all the diagonal entries of \( X_{0,\mathcal{L}^\perp}^2 \) are the same, and different from the off-diagonal entries. Since \( S \) has a 0/1 basis, it must therefore contain the identity.
The important practical implication of this theorem is that the optimal admissible Jordan configuration $S$ of the QAP relaxation (4.1) may be computed using Algorithm 3. The resulting reduction is at least as good as the known ones from the literature, as we now show.

**Corollary 4.2.** This symmetry reduction of the QAP relaxation (4.1) via Algorithm 3 is at least as good as both the group symmetry reduction (see [10, 11]) and the reduction to the coherent algebra containing the data matrices of the program (via the Weisfeiler-Leman algorithm [22]).

**Proof.** The symmetric part of a coherent configuration is a Jordan configuration, and the partition given by the orbitals of a group leaving the program invariant is a coherent configuration. 

4.1 Results of reductions of QAPLib problems

In practice the (partition) Jordan reduction is not much stronger than group symmetry reduction, and reduction to the smallest coherent algebra containing the data matrices. When comparing reductions for data from QAPLib [6], only one single reduction (esc16f), of the ones that were symmetry reduced before, was stronger, the others were exactly the same as reported in [10], where the reduction was done using group symmetry. But we managed to reduce some larger instances for the first time. We also do gain a large speed up in determining the reduction, since we avoid having to determine the automorphism groups of matrices. In Table 1 we give the dimension of the smallest admissible partition subspace for each problem (for which we determined a reduction), the original number of variables of the problem, and the time needed for the reduction.

One of the QAPLib instances, that was not symmetry reduced before, is tai64c. The reduction for this problem worked particularly well, as can be seen in Table 1. It is an an example of the energy minimization problem discussed in detail in Part I of the paper [5], for grid size $8 \times 8$. This gave us the motivation to explore this special case further. This is done in the next section.

5 Reducing the relaxation of the energy minimization problem

In this section we take a look at the specific case of the energy minimization problem introduced in part I of this paper [5], and described in the introduction. Recall from the introduction, and with reference to Figure 1, that this is an instance of the QAP (4.1) where $B = (b_{ij})$ is indexed by toric grid points, and $b_{ij}$ ($i \neq j$) equals the inverse of the Lee distance (shortest path on the grid) between grid points $i$ and $j$. (The diagonal of $B$ is zero.) The matrix $A$ is zero except for a square block of all-ones in the upper left corner, of size equal to the number of particles on the toric grid.

5.1 Symmetric circulant matrices

First, we need some well-known properties of (symmetric) circulant matrices, which will appear later in the construction of the admissible subspaces of the relaxation of the energy minimization problem.

**Definition 5.1.** An $n \times n$ matrix $C$ is called circulant, if each row is rotated one element to the right relative to the row above, i.e. $C_{ij} = c_{j-i\mod n}$ for all $i, j$ and fitting $c_k, k = 0, \ldots, n - 1$.

**Proposition 5.2.** A symmetric circulant $n \times n$ matrix $C$ has at most $\left\lfloor \frac{n}{2} \right\rfloor + 1 = \left\lfloor \frac{n+1}{2} \right\rfloor$ unique entries, and $c_k = c_{n-k}$.

**Proof.** Let $j \geq i$ and $k = j - i$. By definition we have $c_k = C_{ij} = C_{ji} = c_{n-(j-i)} = c_{n-k}$. Hence $C$ is given by $c_0, \ldots, c_{\left\lfloor \frac{n}{2} \right\rfloor}$.

This allows us to construct symmetric circulant matrices from a given $c \in \mathbb{R}^{\left\lfloor \frac{n}{2} \right\rfloor}$. We call this function $C = \text{circ}_{n}(c_0, \ldots, c_{\left\lfloor \frac{n}{2} \right\rfloor})$.

**Proposition 5.3** (E.g. Theorem 7 in [14]). The product of two circulant matrices is a circulant matrix, and the product commutes. The product of symmetric circulant matrices is symmetric.

We call the Jordan algebra (with product $X \circ Y = \frac{1}{2}(XY + YX) = XY$) of symmetric circulant $n \times n$ matrices $\mathcal{C}^n$. We define a $0/1$-basis for $\mathcal{C}^n$ by

$$\left\{ C_i^n = \text{circ}_n(d_i) : i = 0, \ldots, \left\lfloor \frac{n}{2} \right\rfloor \right\},$$

where for $i \notin \{0, \frac{n}{2}\}$ we set $d_i = e_i \in \mathbb{R}^{\left\lfloor \frac{n}{2} \right\rfloor + 1}$, the vector with a one in position $i$, and zero otherwise. For $i = 0$ and $i = \frac{n}{2}$, if $n$ is even, we set $d_i = 2e_i$.
Table 1: Results for numerical symmetry reduction of QAPLib problems using Algorithm 3.

| QAP instance | Reduced Dimension dim $\left(2^{n^2} = (n^2 + 1)^2\right)$ | Original dimension dim $2n^2 = (n^2 + 1)$ | Runtime (s) |
|--------------|-----------------------------------------------------------|------------------------------------------|-------------|
| chr18b       | 14742                                                     | 52650                                    | 0.33        |
| esc16a       | 150                                                       | 32896                                    | 0.25        |
| esc16b       | 155                                                       | 32896                                    | 0.28        |
| esc16c       | 405                                                       | 32896                                    | 0.33        |
| esc16d       | 405                                                       | 32896                                    | 0.26        |
| esc16e       | 135                                                       | 32896                                    | 0.26        |
| esc16f       | 3                                                         | 32896                                    | 0.19        |
| esc16g       | 230                                                       | 32896                                    | 0.25        |
| esc16h       | 90                                                        | 32896                                    | 0.19        |
| esc16i       | 80                                                        | 32896                                    | 0.24        |
| esc16j       | 150                                                       | 32896                                    | 0.29        |
| esc32a       | 2112                                                      | 524800                                   | 3.94        |
| esc32b       | 96                                                        | 524800                                   | 3.95        |
| esc32c       | 366                                                       | 524800                                   | 4.09        |
| esc32d       | 342                                                       | 524800                                   | 3.95        |
| esc32e       | 120                                                       | 524800                                   | 3.93        |
| esc32f       | 180                                                       | 524800                                   | 4.00        |
| esc32g       | 666                                                       | 524800                                   | 4.11        |
| esc32h       | 679                                                       | 8390656                                  | 69.14       |
| krai30a      | 91950                                                     | 405450                                   | 2.82        |
| krai30b      | 48030                                                     | 405450                                   | 2.99        |
| kra32        | 28752                                                     | 524800                                   | 3.50        |
| krai30c      | 379350                                                    | 405450                                   | 4.30        |
| nug12        | 2952                                                      | 10440                                    | 0.15        |
| nug15        | 7425                                                      | 25425                                    | 0.22        |
| nug16b       | 4704                                                      | 32896                                    | 0.18        |
| nug20        | 21000                                                     | 80200                                    | 0.48        |
| nug21        | 27783                                                     | 97461                                    | 0.66        |
| nug22        | 29766                                                     | 117370                                   | 0.70        |
| nug24        | 41760                                                     | 166176                                   | 1.17        |
| nug25        | 28675                                                     | 195625                                   | 1.20        |
| nug27        | 75087                                                     | 266085                                   | 1.78        |
| nug28        | 78792                                                     | 307720                                   | 2.01        |
| nug29        | 105750                                                    | 405450                                   | 3.18        |
| scr12        | 2952                                                      | 10440                                    | 0.07        |
| scr15        | 13275                                                     | 25425                                    | 0.18        |
| scr20        | 21000                                                     | 80200                                    | 0.65        |
| sko42        | 397782                                                    | 1558730                                   | 14.17       |
| sko49        | 391069                                                    | 2883601                                   | 26.58       |
| sko56        | 1255968                                                   | 4918816                                   | 45.37       |
| sko64        | 1082880                                                   | 8390656                                   | 69.77       |
| ste36a       | 201712                                                    | 840456                                   | 6.61        |
| ste36b       | 201712                                                    | 840456                                   | 6.72        |
| ste36c       | 201712                                                    | 840456                                   | 6.28        |
| tai64c       | 75                                                        | 8390656                                   | 20.15       |
| tho30        | 112950                                                    | 405450                                   | 2.64        |
| tho40        | 333600                                                    | 1280800                                   | 9.55        |
| wil50        | 813750                                                    | 3126250                                   | 26.74       |
5.2 Admissible subspaces

To symmetry reduce all problems of this type, one can now try to find an admissible (unital) partition subspace \( S \) for every such problem. As a reminder, such a subspace needs to fulfill the three properties:

1. \( C_L := P_L(B \otimes A), X_{0,L} := X_0 - P_L(X_0) \in S \),
2. \( P_L(S) \subseteq S \),
3. \( \{ X^2 \mid X \in S \} \subseteq S \),

where \( L \) is the subspace given by the \( Y \in \mathbb{S}^{n^2} \) with

\[
\langle I_n \otimes E_{jj}, Y \rangle = 0 \text{ for } j \in [n], \\
\langle E_{jj} \otimes I_n, Y \rangle = 0 \text{ for } j \in [n], \\
\langle T, Y \rangle = 0, \\
\langle J_n, Y \rangle = 0,
\]

where \( T = I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n \), and \( X_0 \) is any symmetric matrix satisfying the linear constraints of the SDP \( \mathcal{L} \), e.g. \( X_0 = \text{vec}(I_n)\text{vec}(I_n)^T \). Recall that, for \( n = n_1n_2 \), the matrix \( B \in \mathbb{R}^{n \times n} \) is defined by

\[
B(x_1,y_1),(x_2,y_2) = \frac{1}{d_{\text{Lee}}}((x_1,y_1),(x_2,y_2)),
\]

where \( d_{\text{Lee}} \) is the Lee-distance (length of shortest path on the toric grid). The ordering of the indices \([n_1] \times [n_2] = [n]\) we left implicit in Part I of this paper, but now we fix it to \((x,y) \mapsto n_2(x-1) + y\). \( A \in \mathbb{R}^{n \times n} \) is the matrix with an \( m \times m \) all-one block in the top left corner, and otherwise zero.

In this section we will make use of Tensor products of algebras. As a reminder, if \( A_1, \ldots, A_{d_1} \in \mathbb{R}^{n_1 \times n_2} \) is a basis of a matrix algebra \( A \), and \( B_1, \ldots, B_{d_2} \in \mathbb{R}^{n_2 \times n_2} \) a basis of a matrix algebra \( B \), then \( A \otimes B \) is the \( n_1n_2 \times n_1n_2 \) matrix algebra with basis \( A_i \otimes B_j \), for \( i \in [d_1], j \in [d_2] \).

We restrict ourselves to a partition subspace, which means that the exact values of the entries of the matrix do not matter to us, only the pattern of unique elements. For the first of the three properties, we take a look at the structure of \( C := B \otimes A \).

**Lemma 5.4.** \( B \in \mathcal{C}^{n_1} \otimes \mathcal{C}^{n_2} \), i.e. \( B \) is a block matrix, with \( n_1 \) rows and \( n_2 \) columns of blocks, which are arranged in a symmetric circulant pattern, and each of these blocks is an \( n_2 \times n_2 \) symmetric circulant matrix.

**Proof.** The Lee-distance between \((x_1, y_1)\) and \((x_2, y_2)\) depends only on \( x_2 - x_1 \mod n_1 \) and \( y_2 - y_1 \mod n_2 \), and the order of the arguments do not matter. This means that both the submatrices for fixed \( x \) and for fixed \( y \) coordinates are symmetric circulant matrices:

\[
\left( B(i_1,y_1), (j_2,y_2) \right)_{1 \leq i_1,j_2 \leq n_1} \in \mathcal{C}^{n_1}, \\
\left( B(x_1,i_1), (x_2,j_2) \right)_{1 \leq i_1,j_2 \leq n_2} \in \mathcal{C}^{n_2}.
\]

The chosen ordering of the indices \((x,y) \mapsto n_2(x-1) + y\) thus results in \( B \in \mathcal{C}^{n_1} \otimes \mathcal{C}^{n_2} \).

In the case \( n_1 = n_2 \) we can restrict the algebra further.

**Lemma 5.5.** If \( n_1 = n_2 \), then

\[
B \in \mathcal{C}^{n_1 \times n_1} := \left\{ X \in \mathcal{C}^{n_1} \otimes \mathcal{C}^{n_1} : X_{(x_1,y_1),(x_2,y_2)} = X_{(y_1,x_1),(y_2,x_2)} \right\}, \tag{5.2}
\]

and \( \mathcal{C}^{n_1 \times n_1} \) is a Jordan sub-algebra of \( \mathcal{C}^{n_1} \otimes \mathcal{C}^{n_1} \).

**Proof.** \( B \) is has this symmetry by definition of the Lee-distance. \( \mathcal{C}^{n_1 \times n_1} \) is a sub-algebra, because it is the restriction of an algebra to the commutant of \( \{ P, I \} \), where \( P \) is the \( n \times n \) permutation matrix switching the indices corresponding to each \((x,y)\) with the one corresponding to \((y,x)\).

The other relevant Jordan algebra for our problem is described in the following proposition.

**Proposition 5.6.** The subspace of \( n \times n \) matrices with pattern
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form a Jordan algebra, say \( \mathcal{J}^{n,m} \). We call the 0/1-basis corresponding to this pattern \( J_A, J_B, J_C, J_D, J_E \).

**Proof.** A straightforward calculation shows that squaring such a matrix results in another matrix of the same pattern with parameters

\[
\begin{align*}
a' &= a^2 + (m-1)b^2 + (n-m)c^2, \\
b' &= 2ab + (m-2)b^2 + (n-m)c^2, \\
c' &= (a + (m-1)b)c + (d + (n-m-1)e)c, \\
d' &= d^2 + (n-m-1)e^2 + mc^2, \\
e' &= 2de + (n-m-2)e^2 + mc^2.
\end{align*}
\]

We now want to show that the space \( S := \mathcal{C}^{n_1} \otimes \mathcal{C}^{n_2} \otimes \mathcal{J}^{n,m} \), respectively \( S = \mathcal{C}^{n_1,n_1} \otimes \mathcal{J}^{n,m} \) if \( n_1 = n_2 \), is admissible. We do this by verifying the three conditions listed at the beginning of this section.

**Theorem 5.7.** The subspace \( S := \mathcal{C}^{n_1} \otimes \mathcal{C}^{n_2} \otimes \mathcal{J}^{n,m} \), respectively \( S = \mathcal{C}^{n_1,n_1} \otimes \mathcal{J}^{n,m} \) if \( n_1 = n_2 \) is admissible for \((4.1)\), where \( B \) and \( A \) are the matrices corresponding to the problem of minimizing the energy of \( m \) particles on an \( n_1 \times n_2 \) grid.

For \( 2 < m < n - 2 \) the dimension of \( S \) is \( 5\left[ \frac{n_1+1}{2} \right] \left[ \frac{n_2+1}{2} \right] \) in the case \( n_1 \neq n_2 \), and \( \frac{5}{2} \left[ \frac{n_1+1}{2} \right] \left( \left[ \frac{n_2+1}{2} \right] + 1 \right) \) in the case \( n_1 = n_2 \).

**Proof.** We first show that \( P_C(S) \subseteq S \). To this end, note that both \( T = I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n \) and \( J_n \) are elements of \( S \), since \( J_n = J_{n_1} \otimes I_{n_2} \) and \( I_n = I_{n_1} \otimes I_{n_2} \) are both in \( \mathcal{C}^{n_1} \otimes \mathcal{C}^{n_2} \) (and in \( \mathcal{C}^{n_1,n_1} \) if \( n_1 = n_2 \)), as well as in \( \mathcal{J}^{n,m} \) because \( I_n = J_A + J_D \) and \( J_n = I_n + J_B + J_C + J_E \). Thus \( T \) and \( J_n \) can be written as linear combination of Kronecker products of elements of \( \mathcal{C}^{n_1}, \mathcal{C}^{n_2} \) and \( \mathcal{J}^{n,m} \), and are as such elements of \( S \).

The other two constraints are given by matrices \( I_n \otimes E_{jj} \) and \( E_{jj} \otimes I_n \), which only overlap with the two basis elements \( C_0^{n_1} \otimes C_0^{n_2} \otimes J_A \) and \( C_0^{n_1} \otimes C_0^{n_2} \otimes J_D \). Since \( C_0^{n_1} \otimes C_0^{n_2} \otimes J_A = \sum_{j=1}^m I_n \otimes E_{jj} \) and \( C_0^{n_1} \otimes C_0^{n_2} \otimes J_D = \sum_{j=m+1}^n I_n \otimes E_{jj} \), both of these matrices are projected to zero.

Thus all basis elements of \( S \) are sent to elements of \( S \), and \( P_C(S) \subseteq S \).

Next, we show \( C_L \subseteq S \). By Lemma 5.4, Lemma 5.5 and the definition of \( A \), we know that \( C = B \otimes A \in S \). Since \( P_C(S) \subseteq S \), that \( C_L \subseteq S \) as well.

Next, we show that \( X_{0,L+} \subseteq S \). We calculated \( X_{0,L+} \) in Theorem 4.1 to be

\[
X_{0,L+} = \frac{1}{n^2 - m} (J_{n^2} - I_{n^2} - T) + \frac{1}{n} I_{n^2},
\]

and \( J_{n^2}, I_{n^2} \) and \( T \) are elements of \( S \). Thus we have \( X_{0,L+} \subseteq S \).

Finally, we note that \( S \) is a (Jordan) algebra. This completes the proof that \( S \) is admissible. The dimension of \( S \) follows from \( \mathcal{C}^n \) having dimension \( \left[ \frac{n+1}{2} \right] \) and \( \mathcal{J}^{n,m} \) having dimension 5. In the case \( n_1 = n_2 \) the dimension is lower, since we can combine the basis elements \( C_i^{n_1} \otimes C_j^{n_1} \) and \( C_j^{n_1} \otimes C_i^{n_1} \) for each pair \( i \neq j \). \qed
Thus we have found an admissible subspace \( S \) for \([4,1]\), where \( A \) and \( B \) are the matrices corresponding to the problem of minimizing the energy of \( m \) particles on an \( n_1 \times n_2 \) toric grid. Its dimension is of order \( \mathcal{O}(n_1 n_2) \), which is significantly less than the original number of variables \( \frac{n_1^2 n_2^2}{2} = \mathcal{O}(n_1^2 n_2^2) \). The number of variables can be reduced further by fixing the variables corresponding to nonzero entries of \( I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n \) to zero. Thus if \( \{B_1, \ldots, B_k\} \) is a 0/1-basis of an admissible subspace, then it is enough to optimize over variables in the subspace \( S_0 \) with basis

\[
\{ B_i : (B_i I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n) = 0 \}.
\]

This results in \( 3\lfloor \frac{n_1 + 1}{2} \rfloor \lfloor \frac{n_2 + 1}{2} \rfloor - 1 \) variables in the case \( n_1 \neq n_2 \), and \( 1.5 \lfloor \frac{n_1 + 1}{2} \rfloor (\lfloor \frac{n_2 + 1}{2} \rfloor + 1) - 1 \) variables in the case \( n_1 = n_2 \). A few examples can be seen in Table 2. Note that the resulting subspace is generally not a Jordan algebra anymore.

| \((n_1, n_2)\) | \(\text{dim}(S^2)\) | \(\text{dim}(S)\) | \(\text{dim}(S_0)\) |
|-----------------|-----------------|-----------------|-----------------|
| (4, 4)          | 32896           | 30              | 17             |
| (5, 5)          | 195625          | 30              | 17             |
| (6, 6)          | 840456          | 50              | 29             |
| (8, 8)          | 8390656         | 75              | 44             |
| (10, 10)        | 50005000        | 105             | 62             |
| (12, 12)        | 215001216       | 140             | 83             |
| (24, 24)        | 55037822976     | 455             | 272            |
| (100, 100)      | \(\approx 5 \cdot 10^{15}\) | 6630           | 3977           |
| (1000, 1000)    | \(\approx 5 \cdot 10^{23}\) | 628755         | 377252         |
| (6, 5)          | 405450          | 60              | 35             |
| (10, 5)         | 3126250         | 90              | 53             |
| (24, 12)        | 3439895040      | 455             | 272            |

5.3 Block diagonalization

We now want to block diagonalize the admissible subspace \( S := \mathbb{C}^{n_1} \otimes \mathbb{C}^{n_2} \otimes \mathcal{J}^{n,m} \), respectively \( S = \mathbb{C}^{n_1 n_2} \otimes \mathcal{J}^{n,m} \) if \( n_1 = n_2 \). We do this by making use of the fact that \( S \) is a tensor product of algebras, which allows us to block diagonalize each part on its own.

**Lemma 5.8** (See, for example, [14], [9]). The 0/1-basis \( \{C_i : i = 0, \ldots, \lfloor n/2 \rfloor \} \) of \( \mathbb{C}^n \) has a common set of eigenvectors, given by the columns of the discrete Fourier transform matrix:

\[
Q_{ij} := \frac{1}{\sqrt{n}} e^{-2\pi i j/n}, \quad i,j = 0, \ldots, n-1.
\]

The eigenvalues are

\[
\lambda_m(C_k^n) = 2 \cos(2\pi m k/n) \quad m = 0, \ldots, n-1, k = 0, \ldots, \lfloor n/2 \rfloor,
\]

and note that

\[
\lambda_m(C_k^n) = \lambda_{n-m}(C_k^n) \quad m = 1, \ldots, \lfloor n/2 \rfloor, k = 0, \ldots, \lfloor n/2 \rfloor.
\]

Thus we can block diagonalize \( \mathbb{C}^n \) by sending \( C_k^n \) to the vector

\[
\tilde{\lambda}(C_k^n) := (\lambda_0(C_k^n), \ldots, \lambda_{\lfloor n/2 \rfloor}(C_k^n)).
\]

To block diagonalize \( \mathcal{J}^{n,m} \), one may use the Jordan isomorphism \( \phi : \mathcal{J}^{n,m} \to \mathbb{R} \oplus \mathbb{R} \oplus S^2 \) given by

\[
\phi(J_A) = \begin{pmatrix} n-m & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \phi(J_B) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & m-1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \phi(J_C) = \sqrt{m(n-m)} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},
\]

\[
\phi(J_D) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \phi(J_E) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -m-1 \end{pmatrix}.
\]
This isomorphism was used implicitly in [8], but may also be verified directly by confirming that \( \phi(X^2) = [\phi(X)]^2 \) for all \( X \in J^{n,m} \).

We can now combine these block diagonalizations by noticing that it is enough to block diagonalize each of the algebras separately; see, for example, Section 7.2. in [10]. We obtain the final reduction shown in the next theorem. The proof is omitted since it is straightforward.

**Theorem 5.9.** The bound from (4.1), where the matrices \( A, B \) correspond to the energy minimization problem with parameters \( n_1, n_2, n = n_1 n_2 \) and \( m \), equals the optimal value of the following semidefinite program:

\[
\begin{align*}
\min_{y \in \mathbb{R}_{\geq 0}^m} & \quad 4nm(m-1) \sum_{i,j \in \Omega} \frac{y_{ij}B}{i+j} \\
\text{s.t.} & \quad y_{00} \mathbf{A} = y_{00} \mathbf{D} = \frac{1}{4n}, \\
& \quad 4n \sum_{j \in \Omega} c(x) y_{ij}x = n^2, \\
& \quad \text{for all } 0 \leq k \leq \left\lfloor \frac{n_1}{2} \right\rfloor, 0 \leq l \leq \left\lfloor \frac{n_2}{2} \right\rfloor:
\end{align*}
\]

\[
\sum_{0 \leq i \leq \left\lfloor \frac{n_1}{2} \right\rfloor} \sum_{0 \leq j \leq \left\lfloor \frac{n_2}{2} \right\rfloor} d_{ij} \left( M^{ij}(y) + (y_{ij} \mathbf{A} - y_{ij} \mathbf{B}) + (y_{ij} \mathbf{D} - y_{ij} \mathbf{E}) \right) \succeq 0,
\]

where

\[
c(x) := \begin{cases} 
    m, & \text{if } x = \mathbf{A} \\
    m(m-1), & \text{if } x = \mathbf{B} \\
    2m(n-m), & \text{if } x = \mathbf{C} \\
    (n-m), & \text{if } x = \mathbf{D} \\
    (n-m)(n-m-1), & \text{if } x = \mathbf{E}, 
\end{cases}
\]

and

\[
M^{ij}(y) := \begin{pmatrix} 
    y_{ij} \mathbf{A} + (m-1)y_{ij} \mathbf{B} & \sqrt{m(n-m)y_{ij}^2} \\
    \sqrt{m(n-m)y_{ij}^2} & y_{ij} \mathbf{D} + (n-m-1)y_{ij} \mathbf{E} 
\end{pmatrix},
\]

and the index set is

\[
\Omega = \left\{ ijx : x \in \{ A, B, C, D, E \}, 0 \leq i \leq \left\lfloor \frac{n_1}{2} \right\rfloor, 0 \leq j \leq \left\lfloor \frac{n_2}{2} \right\rfloor \right\} \\
\setminus \{(00B, 00C, 00E) \cup \{ y_{ijx} : x \in \{ A, D \}, i \neq 0 \wedge j \neq 0 \} \}.
\]

If in above constraints other indices appear, assume the corresponding variables are zero. If \( n_1 = n_2 \), then we can replace each pair \( y_{ijx}, y_{jix} \) by one variable \( y'_{ijx} = y_{ijx} + y_{jix} \), and the positive semidefinite constraints are unique only for \( k \leq l \).

### 6 Concluding remarks

The semidefinite program in Theorem 5.9 has block sizes of order at most \( 2 \times 2 \), and is therefore a second-order cone program, which can be solved very efficiently; see e.g. [16]. Thus, as reported in the first part of this paper [5], we were able to solve the SDP relaxation for toric grids of size \( 10 \times 10 \) (and beyond). Subsequently we were also able to prove optimality of certain configurations of particles on toric grids, e.g. for 4 particles on a \( 10 \times 10 \) grid. The interested reader is referred to [5] for more details on these results.

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