EXACT SOLUTIONS FOR THE NP-HARD WASSERSTEIN BARYCENTER PROBLEM USING A DOUBLY NONNEGATIVE RELAXATION AND A SPLITTING METHOD *

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Abstract.

The so-called *simplified* Wasserstein barycenter problem, also known as the cheapest hub problem, consists in selecting one point from each of k given sets, each set consisting of n points, with the aim of minimizing the sum of distances to the barycenter of the k chosen points. This problem is known to be NP-hard. We compute the Wasserstein barycenter by exploiting the Euclidean distance matrix structure to obtain a facially reduced doubly nonnegative, **DNN**, relaxation. The facial reduction provides a natural splitting for applying the symmetric alternating directions method of multipliers (**sADMM**) to the **DNN** relaxation. The **sADMM** method exploits structure in the subproblems to find strong upper and lower bounds. In addition, we extend the problem to allow varying n_j points for the j-th set.

The purpose of this paper is twofold. First we want to illustrate the strength of this **DNN** relaxation with the natural splitting approach mentioned above. Our numerical tests then illustrate the surprising success on random problems, as we generally, efficiently, find the provable exact solution of this NP-hard problem. Comparisons with current commercial software illustrate this surprising efficiency. However, we demonstrate and prove that there is a duality gap for problems with *enough* multiple optimal solutions, and that this arises from problems with highly symmetrized structure.

1. Introduction. We consider the so-called *simplified Wasserstein barycenter,* ***WBP*** problem of finding the optimal barycenter of k points, where exactly one point is chosen from k sets of points, each set consisting of n points. This is a simplification of more general problems of *optimal mass transportation* and the problems of summarizing and combining probability measures that occurs in e.g., statistics and machine learning. In [3, Def. 1.4] this problem is called the *cheapest-hub problem*, and further in [3], a reduction to **WBP** is derived from the *k-clique problem* thus proving NP-hardness.[1] Algorithms for **WBP** with exponential dependence in d are discussed in [3, Sect. 1.3.1].[2] There are many important applications in molecular conformation e.g., [6], clustering [18], supervised and unsupervised learning, etc. For additional details on the theory and applications of optimal transport theory see e.g., [2, 10, 14], lecture link, Introduction to Transportation Problems link, and the many references therein.

The purpose of this paper is twofold. First, we provide a successful framework for handling quadratic hard discrete optimization problems; and second, we illustrate the surprising success when applied to our specific **WBP**.

We model our problem as a quadratic objective, quadratic constrained $\{0, 1\}$ discrete optimization problem, i.e., we obtain a *binary quadratic* model. We then get a convex relaxation for this hard discrete optimization problem by lifting to the doubly nonnegative, **DNN**, cone, the cone of nonnegative elementwise, positive semidefinite symmetric matrices. Strict feasibility fails for the relaxation, so we apply *facial reduction,* ***FR***. This results in many constraints becoming redundant and also gives rise to a *natural splitting* that can be exploited by the symmetric alternating directions method of multipliers (**sADMM**). We exploit the structure, and include redundant constraints on the subproblems of the splitting and on the dual variables. The **sADMM** algorithm allows for efficient upper and provable lower bounding techniques for the original hard **WBP** problem. This helps the algorithm stop early.

Our Extensive tests on random problems are surprisingly efficient and successful, i.e., the relaxation with the upper and lower bounding techniques provide a provable optimal solution to the original hard **WBP** for *surprisingly many* instances; essentially for all our randomly generated instances. For example, to solve the original hard discrete optimization problem to optimality for our algorithm for a random problem with $k = n = 25$ in dimension $d = 25$ took of the order of 10 seconds. In contrast, using the well known solver GUROBI, on three problems, with sizes $n = k = 5, 7, 8$, respectively, it took approximately: $2, 570, 46692$

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[1] Recall that the *k-clique problem* is the problem of finding k vertices in a graph such that each pair is close in the sense of being *adjacent*.

[2] We discuss this further below as the complexity of our algorithm does *not* depend on d.

seconds, respectively (using the same laptop for both tests). (Detailed numerics for our algorithm are provided below Subsection 4.4.)

Though generically we are surprisingly successful in finding the exact solutions to the NP-hard problem, the **DNN** relaxation can fail to find the exact solution for problems with special structure, i.e., there can be a positive duality gap between the optimal value of the original hard problem and the lower bound found from the **DNN** relaxation. In Corollary 5.2 we include a constructive proof for a general hard $\{0,1\}$ problem that a sufficient number of linearly independent optimal solutions results in a duality gap between the original hard problem and its **DNN** relaxation. This is specialized to our NP-hard problem in Corollary 5.3. A specific instance is included. Note that we consider that we have an optimal solution to **WBP** if the upper and lower bounds are equal to machine precision as any other feasible solution cannot have a smaller objective value within machine precision.

1.1. Outline. We continue in Subsection 1.2 with preliminary notation. The main NP-hard Problem 2.1 and connections to Euclidean distance matrices, **EDM**, are given in Section 2. A regularized, facially reduced, doubly nonnegative, **DNN**, relaxation is derived in Section 3. The **FR** in the relaxation fits *naturally* with applying a splitting approach. This is presented in Section 4 along with special bounding techniques and heuristics on the dual multipliers for accelerating the splitting algorithm. The algorithm provides *provable* lower and upper bounds for the original NP-hard Problem 2.1 that are attained by dual and primal feasible solutions, respectively. Thus a *zero* gap (called a duality gap) proves optimality. Our empirics are given in Subsection 4.4.

In Section 5 we prove that multiple optimal solutions can lead to duality gaps. We include specific instances. Our concluding remarks are in Section 6.

1.2. Notation. We let $S \in \mathbb{S}^n$ denote a matrix in the space of $n \times n$ symmetric matrices equipped with the *trace inner product* $\langle S, T\rangle = \operatorname{tr} ST$; we use $\operatorname{diag}(S) \in \mathbb{R}^n$ to denote the linear mapping to the diagonal of S; the adjoint mapping is $\operatorname{diag}^*(v) = \operatorname{Diag}(v) \in \mathbb{S}^n$. We let $[k] = \{1, 2, \ldots, k\}$.

The convex cone of positive semidefinite matrices is denoted $\mathbb{S}^n_+ \subset \mathbb{S}^n$, and we use $X \succeq 0$ for $X \in \mathbb{S}^n_+$. Similarly, for positive definite matrices we use $\mathbb{S}^n_{++}, X \succ 0$. We let $\mathcal{N}^n$ denote $n \times n$ nonnegative symmetric matrices. The cone of doubly nonnegative matrices is $\mathbf{DNN} = \mathbb{S}^n_+ \cap \mathcal{N}^n$.

For a set of points $p_i \in \mathbb{R}^d$, we let $P = \begin{bmatrix} p_1 & p_2 & \ldots & p_t \end{bmatrix}^T \in \mathbb{R}^{t\times d}$ denote the *configuration matrix*. Here d is the *embedding dimension*. Without loss of generality, we can assume the points span $\mathbb{R}^d$, and we can translate the points and assume they are centered, i.e.,

$$P^T e_t = 0.^3$$

Here we let e_t, *vector of ones* of dimension t and we use e if the dimension is clear. And we use e_0, 0*-th unit vector* of appropriate size. We denote the corresponding *Gram matrix*, $G = PP^T$. Then the classical result of Schoenberg [17, Sect. 3], see e.g. [1], relates a *Euclidean distance matrix*, ***EDM***, with a Gram matrix by applying

$$D = \mathcal{K}(G) = \operatorname{diag}(G)e^T + e\operatorname{diag}(G)^T - 2G.$$

Moreover, this mapping is one-one and onto between the $t(n-1)$ dimensinal *centered subspace*, $\mathcal{S}^n_C$ and *hollow subspace*, $\mathcal{S}^n_H$

$$\mathcal{S}^n_C = \{X \in \mathbb{S}^n \,:\, Xe = 0\}, \quad \mathcal{S}^n_H = \{X \in \mathbb{S}^n \,:\, \operatorname{diag} X = 0\}; \quad \mathcal{K}(\mathcal{S}^n_C) = \mathcal{S}^n_H.$$

Here we denote the *triangular number*, $t(k) = k(k+1)/2$. Note that the centered assumption $P^T e = 0 \iff G = PP^T \in \mathcal{S}^n_C$. Further notation is introduced as needed.

2. Simplified Wasserstein barycenters, WBP. We now present the main problem and the connections to Euclidean distance matrices, **EDM**. We follow the notation in [3, Sect. 1.2] and refer to our main problem as the simplified Wasserstein barycenter problem, or Wasserstein barycenter for short.

[3] The translation is given by

$$P^T \mapsto P^T - ve^T,$$

where $v := \frac{1}{n}P^T e$ is the barycenter of the points.

2.1. Main problem and EDM connection. Our main optimization problem is to find a point in each of k sets to obtain an optimal barycenter. We can think of this as finding a *hub of hubs*. That is, suppose that there are k areas with n airports in each area.[4] We want to choose exactly one airport to act as a minor hub in each of the k areas so that the barycenter for these k minor hubs would serve as a major (best) hub for the k minor hubs. .

Problem 2.1 (*simplified Wasserstein barycenter,* ***WBP***). Suppose that we are given a finite number of sets $S_1, ..., S_k$, each consisting of n points in $\mathbb{R}^d$. Find the optimal barycenter point y after choosing exactly one point from each set:

$$p_W^* := \min_{\substack{p_i \in S_i \\ i \in [k]}} \min_{y \in \mathbb{R}^d} \sum_{i \in [k]} \|p_i - y\|^2 =: \min_{\substack{p_{j_i} \in S_i \\ i \in [k]}} F(p_{j_1}, p_{j_2}, \ldots, p_{j_k}), \tag{2.1}$$

thus defining F. Here

$$P^T = \begin{bmatrix} p_1 & \ldots & p_N \end{bmatrix} \in \mathbb{R}^{d \times N}, D, G, \tag{2.2}$$

denote the corresponding (configuration) matrix of points, **EDM**, and Gram matrix, respectively. We allow the set sizes, $n_j, j \in [k]$, to vary and let $N = \sum_{j \in [k]} n_j$.

By Lemma 2.2 below, the optimal Wasserstein barycenter is the standard barycenter of the k optimal points. It is known [3, Sect. 1.2] that the problem can be phrased using inter-point squared distances. We include a proof to emphasize the connection between Gram and Euclidean distance matrices.[5] We start by recording the following minimal property of the standard barycenter with respect to sum of squared distances.

LEMMA 2.2. *Suppose that we are given k points $q_i \in \mathbb{R}^d, i = 1, \ldots k$. Let $\bar{y} = \frac{1}{k}\sum_{i=1}^k q_i$ denote the barycenter. Then*

$$\bar{y} = \operatorname*{argmin}_y \sum_{i=1}^k \frac{1}{2}\|q_i - y\|^2.$$

Proof. The result follows from the stationary point equation $\sum_{i=1}^k (q_i - \bar{y}) = 0$. ∎

We now have the following useful lemma.

Lemma 2.3. Let $Q^T = [q_1 \ldots q_k] \in \mathbb{R}^{d \times k}$ and let G_Q and D_Q be, respectively, the Gram and the EDM matrices corresponding to the columns in Q^T. Further, let $y = \frac{1}{k}Q^T e$ be the barycenter. Then

$$2k \sum_{i=1}^k ||q_i - y||^2 = e^T D_Q e = 2k \operatorname{tr}(G_Q) - 2e^T G_Q e. \tag{2.3}$$

Proof. Let $J = I - ee^T/k$ be the orthogonal projection onto $e^\perp$. Hence, $J^2 = J^T = J$. Moreover, the i-th row $(JQ)_i = (Q - \frac{1}{k}ee^T Q)_i = (q_i - y)^T$. Now

$$\sum_{i=1}^k ||q_i - y||^2 = \operatorname{tr}(JQQ^T J) = \operatorname{tr}(JG_Q) = \operatorname{tr}(G_Q) - \frac{1}{k}e^T G_Q e.$$

But $D_Q = \mathcal{K}(G_Q) = e \operatorname{diag}(G_Q)^T + \operatorname{diag}(G_Q)e^T - 2G_Q$. Therefore, $e^T D_Q e = 2k \operatorname{tr}(G_Q) - 2e^T G_Q e$. ∎

The following Corollary 2.4 illustrates the connection between the simple Wasserstein barycenter problem[6] of finding the optimal barycenter and the k-clique problem of finding k pairwise adjacent vertices.

COROLLARY 2.4. *Let $N = \sum_{j \in [k]} n_j$, and let $S_j = \{p_{j_i}\}_{i=1}^{n_j}, j \in [k]$ be given. Consider the main problem (2.1) and let y denote the optimal Wasserstein barycenter. The problem of finding y is equivalent to finding exactly one point in each set that minimizes the sum of squared distances in the following:*

$$(WIQP) \qquad 2Np_W^* = p^* := \min_{\substack{p_t \in S_t \\ t \in [k]}} \sum_{i,j \in [k]} \|p_i - p_j\|^2. \tag{2.4}$$

[4] We extend the prolem to allow for different sizes for the sets.
[5] As noted earlier, This is called the *cheapest-hub* problem in [3, Sect. 1.2].
[6] We refer to this as the Wasserstein barycenter problem.

Proof. Suppose that $P^T = \begin{bmatrix} p_1 & \dots & p_k \end{bmatrix} \in \mathbb{R}^{d\times k}$ is a fixed matrix of optimal solution vectors to (2.1), and let y be the barycenter. Without loss of generality, since distances do not change after a translation, we translate all the points $p_t, t \in [k]$, by y and obtain $y = 0$. This implies that the corresponding Gram matrix $Ge = PP^Te = 0$. This combined with (2.1) and (2.3) and the corresponding distance matrix D yield

$$\begin{array}{rcl} \sum_{i,j\in[k]} \|p_i - p_j\|^2 & = & e^T De \\ & = & e^T(\operatorname{diag}(G)e^T + e\operatorname{diag}(G)^T - 2G)e \\ & = & 2N\operatorname{diag}(G)^T e \\ & = & 2N\operatorname{tr} G \\ & = & 2N\sum_{i\in[k]} \|p_i\|^2 \\ & = & 2Np_W^*, \end{array} \tag{2.5}$$

where the last equality follows from Lemma 2.2. ∎

2.2. A reformulation using a Euclidean distance matrix. In this paper we work with the optimal value p^* and now provide a reformulation of (2.4) using an **EDM**. Define

$$x := \begin{pmatrix} v_1 \\ \vdots \\ v_k \end{pmatrix} \in \mathbb{R}^N,\ v_i \in \mathbb{R}^{n_i}, \quad A := \operatorname{blkdiag}(e_{n_1}^T, ..., e_{n_k}^T) \in \mathbb{R}^{k\times N}. \tag{2.6}$$

And we note that $A = I \otimes e^T \in \mathbb{R}^{k\times kn}$, if $n_i = n, \forall i$, where we denote *Kronecker product*, $\otimes$. Note that we get $A^Te = e$. Then, the constraints of picking exactly one point from each set can be recast as:

$$Ax = e,\ x \in \{0,1\}^N. \tag{2.7}$$

Recalling Corollary 2.4 and (2.5) in the proof, we see that (2.1) can be formulated as a binary-constrained quadratic program (***BCQP***) using the Euclidean distance matrix D formed from all N points $P^T = \begin{bmatrix} p_1 & \dots & p_{n_1} & p_{n_1+1} & \dots & p_{n_1+n_2} & \dots & \dots & p_N \end{bmatrix}$:

$$\begin{array}{rcll} p^* = & \min & x^TDx = \langle D, xx^T\rangle \\ & \text{s.t.} & Ax = e \\ & & x \in \{0,1\}^N. \end{array} \qquad (\textbf{BCQP}) \tag{2.8}$$

For simplicity in the sequel we often assume that the cardinality of all sets are equal.

Remark 2.5 (difficulty of the Wasserstein barycenter problem). We first note that A in (2.6) is *totally unimodular*, i.e., every square submatrix has $\det(A_I) \in \{0, \pm 1\}$. Therefore, the basic feasible solutions, *vertices of the feasible set*, of the LP relaxation $Ax = e$, $x \geqslant 0$, are $\{0,1\}$ variables. Therefore, these discrete optimization problems with a linear objective yield vertices as optimal solutions and can be solved with simplex type methods while yielding $\{0,1\}$ solutions.

For our problem we have a quadratic objective function. And, by the properties of distance matrices, it is concave on the span of the feasible set of the LP relaxation. Therefore, minima are attained at extreme points, i.e., at vertices, at $\{0,1\}$ points. But solving the concave minimization problem is a hard problem. Note that the *width* of P is hidden in the rank when forming the Gram matrix $G = PP^T$ and so hidden in the rank of the rank-two update **EDM**

$$D = \operatorname{diag}(G)e^T + e\operatorname{diag}(G)^T - 2G, \quad \operatorname{rank}(D) \in [\operatorname{rank}(G), \operatorname{rank}(G) + 2].$$

In summary, the problem appears to be NP-hard due to the minimization of a quadratic function, [15], and the binary $0,1$ constraints. This is in contrast to the linear programming approaches for the generalized transportation problems solved in e.g., [10] and the references therein. However, the properties of total unimodularity and concavity both promote binary valued optimal points.

3. Facially reduced DNN relaxation. We now introduce a regularized convex relaxation to the hard binary quadratic constrained problem introduced in (2.8). We start with the SDP relaxation using a standard lifting approach. We regularize using *facial reduction,* ***FR***, and include the so-called *gangster constraint*. We then strengthen this by including nonnegativity constraints, i.e., we get the *doubly nonnegative,* ***DNN*** relaxation.

As stated above, for simplicity of notation we consider all sets to have the same cardinality, $n_1 = \ldots = n_k, N = \sum_j n_j$.

3.1. Semidefinite programming (SDP) relaxation. We begin with deriving an SDP relaxation of our formulation in (2.8). We start with a feasible vector $x \in \mathbb{R}^{kn}$ and set $\begin{pmatrix} x_0 \\ x \end{pmatrix} = \begin{pmatrix} 1 \\ x \end{pmatrix}$. We then lift the vector to a rank-1 matrix $Y_x := \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T$. The convex hull of the lifted vertices of the feasible set of (2.8) yields an equivalent polyhedral set in $\mathbb{S}^{N+1}$. It is difficult and expensive to find this polyhedral set. To obtain a tractable convex relaxation, we relax the implicit nonconvex rank-1 constraint on Y_x and linearize the objective function. Let

$$\hat{D} := \begin{bmatrix} 0 & 0 \\ 0 & D \end{bmatrix} \in \mathbb{S}^{kn+1}. \tag{3.1}$$

The objective function of (2.8) now becomes $\langle D, xx^T \rangle = \langle \hat{D}, Y_x \rangle$. After the lifting, we impose the constraints that we have from x onto Y, e.g., these include the $\{0,1\}$-constraints $x_i^2 - x_i = 0$, and the linear constraints $Ax = e$.

3.1.1. SDP reformulation. Define the linear transformation

$$\text{arrow} : \mathbb{S}^{n+1} \to \mathbb{R}^{n+1} : \begin{bmatrix} s_0 & s^T \\ s & \bar{S} \end{bmatrix} \mapsto \begin{pmatrix} s_0 \\ \text{diag}(\bar{S}) - s \end{pmatrix}.$$

For convenience, we define

$$\text{arrow}_0 : \mathbb{S}^{n+1} \to \mathbb{R}^{n+1} : \begin{bmatrix} s_0 & s^T \\ s & \bar{S} \end{bmatrix} \mapsto \begin{pmatrix} 0 \\ \text{diag}(\bar{S}) - s \end{pmatrix}.$$

We now show that, as long as the rank-one condition holds, the binary constraint on vector x is equivalent to the arrow constraint on the lifted matrix, $\text{arrow}\,(Y_x) = e_0$.

Proposition 3.1. The following holds:

$$\left\{ Y \in \mathbb{S}_+^{kn+1} : \text{rank}(Y) = 1, \text{arrow}\,(Y) = e_0 \right\} = \left\{ Y = \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T : x \in \{0,1\}^{kn} \right\}.$$

Proof. ($\supseteq$): This is clear from the definitions.
($\subseteq$): Since Y is symmetric, positive semidefinite and has rank 1, there exist $x_0 \in \mathbb{R}$ and $x \in \mathbb{R}^{kn}$ such that $Y = \begin{pmatrix} x_0 \\ x \end{pmatrix} \begin{pmatrix} x_0 \\ x \end{pmatrix}^T$. Since $\text{arrow}\,(Y) = e_0$, $x_0^2 = 1$ and $x \circ x = x_0 x$. If $x_0 = 1, x \in \{0,1\}^{kn}$; otherwise $x_0 = -1$ and $x \in \{0,-1\}^n$ and it is easy to verify that

$$\left\{ \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T : x \in \{0,1\}^{kn} \right\} = \left\{ \begin{pmatrix} -1 \\ x \end{pmatrix} \begin{pmatrix} -1 \\ x \end{pmatrix}^T : x \in \{0,-1\}^n \right\}.$$

□

For the "only-one-element-from-each-set" linear equality constraint $Ax = e$ (see (2.7)), we use the following positive semidefinite matrix

$$K := \begin{bmatrix} -e^T \\ A^T \end{bmatrix} \begin{bmatrix} -e^T \\ A^T \end{bmatrix}^T \in \mathbb{S}_+^{kn+1}. \tag{3.2}$$

We observe that

$$
\begin{aligned}
Ax = e \quad &\iff \quad \begin{pmatrix}1\\ x\end{pmatrix}^T \begin{bmatrix}-e^T\\ A^T\end{bmatrix} = 0 \\
&\iff \quad Y_x K = \begin{pmatrix}1\\ x\end{pmatrix}\begin{pmatrix}1\\ x\end{pmatrix}^T \begin{bmatrix}-e^T\\ A^T\end{bmatrix}\begin{bmatrix}-e^T\\ A^T\end{bmatrix}^T = 0 \\
&\iff \quad KY_x = 0,
\end{aligned} \tag{3.3}
$$

i.e., $\mathrm{range}(Y_x) \subseteq \mathrm{null}(K) = \mathrm{null}\left(\begin{bmatrix}-e & A\end{bmatrix}\right)$. Moreover, this emphasizes that strict feasibility fails for feasible Y even if we ignore the rank-1 constraint. If we choose V full column rank so that $\mathrm{range}(V) = \mathrm{null}(K)$, then we can *facially reduce* the problem using the substitution

$$
Y \leftarrow VRV^T \in V\mathbb{S}_+^{nk+1-k}V^T \trianglelefteq \mathbb{S}_+^{kn+1}, \tag{3.4}
$$

where $\trianglelefteq$ denotes *face of*. This makes the constraint $KY = 0$ redundant. More detailed discussion for constructing the facial vector V is provided later in Subsection 3.2.1.

Then the rank restricted SDP reformulation of (2.8) becomes

$$
\begin{array}{rlll}
p^* = & \min & \langle \hat{D}, Y\rangle & \\
& & \mathrm{arrow}\,(Y) = e_0 & \\
\text{(SDP)} & & \mathrm{rank}(Y) = 1 & \\
& & KY = 0 & \\
& & Y \in \mathbb{S}_+^{kn+1}. &
\end{array}
$$

3.1.2. Relaxing the rank-1 constraint. Since the **NP**-hardness of the SDP formulation comes from the rank-1 constraint, we now relax the problem by deleting this constraint. The SDP relaxation of the above model is

$$
\begin{array}{rlll}
p^* = & \min_{Y\in\mathbb{S}^{kn+1}} & \langle \hat{D}, Y\rangle & \\
& & \mathrm{arrow}\,(Y) = e_0 & \\
\text{(SDP relax)} & & KY = 0 & \\
& & Y \succeq 0. &
\end{array} \tag{3.5}
$$

However, the improved processing efficiency of this convex relaxation trades off with the accuracy of solving the original NP-hard problem. The rank of an optimal Y can now be greater than one. The idea now is to impose a "correct" amount of redundant constraints in the SDP model that reduces the rank of an optimal solution as much as possible, but does not hurt the processing efficiency of the model too much. Note that if we have ignored the rank one constraint and replaced the $KY = 0$ constraint using facial reduction and substituting $Y = VRV^T$, then strict feasibility holds, i.e., the barycenter of the the lifted vertices of the feasible set of (2.8) yields an $\hat{R}, Y = V\hat{R}V^T$, that satisfies strict feasibility, e.g., [9].

3.1.3. The gangster constraint. The *gangster constraint* is essentially a trivial projection that fixes at 0 (shoots holes at) certain entries of the matrix. The entries are given in the *gangster index*, $\mathcal{J}$. By abuse of notation, we allow one entry to be fixed at 1. The gangster constraint in our case comes from the linear constraint $Ax = e$ combined with the binary constraint on x. We let $S \circ T$ denote the Hadamard (elementwise) product.

Proposition 3.2. Let x be feasible for **BCQP**. Then

$$
[A^TA - I] \circ xx^T = 0,
$$

and $A^TA - I \succcurlyeq 0, xx^T \succcurlyeq 0$.

Proof. Recall that $x \in \mathbb{R}_+^{kn}$. We now use basic properties of the Kronecker product, e.g., [16], and see that

$$
A = I_k \otimes e^T,\ A^T = I_k \otimes e, \quad A^TA = I_k \otimes ee^T,
$$

i.e., $A^TA = \text{BlkDiag}(ee^T, \ldots, ee^T)$, a block diagonal structure, and the columns of A are unit vectors. Therefore $A^Te_k = e_{nk}$ and $\text{Diag}(\text{diag}(A^TA)) = I_{kn}$. The nonnegativity results follow from the definition, as does $Y_{00} = 1$.

Then

$$\begin{array}{rcl} Ax = e & \Longrightarrow & A^TAx = A^Te \\ & \Longrightarrow & A^TAx - Ix = A^Te - Ix \\ & \Longrightarrow & (A^TA - I)x = e_{nk} - x \\ & \Longrightarrow & (A^TA - I)xx^T = (e - x)x^T = ex^T - xx^T \\ & \Longrightarrow & \text{tr}[(A^TA - I)xx^T] = \text{tr}[ex^T - xx^T] = \sum_{i=1}^{kn} x_i - x_i^2 = 0 \\ & \Longrightarrow & (A^TA - I) \circ xx^T = 0. \end{array}$$

The final conclusion now follows from the nonnegativities in the Hadamard product. ∎

Define the gangster indices

$$\mathcal{J} := \left\{ (i,j) : \left(A^TA - I\right)_{ij} > 0 \right\}.$$

The gangster constraint on Y in (3.5) is $Y_{00} = 1$ and

$$\mathcal{J}(Y) = Y_{\mathcal{J}} = 0 \in \mathbb{R}^{|\mathcal{J}|}.$$

From Proposition 3.2, we see that the *gangster indices,* $\mathcal{J}$, are the nonzeros of the matrix $A^TA - I$, i.e., the set of off-diagonal indices of the n-by-n diagonal blocks of, all but the 0-th row and column, of Y_x. Our complete gangster index is $\hat{\mathcal{J}} := \{(0,0)\} \cup \mathcal{J}$. We define the *gangster constraint mapping,* $\mathcal{G}_{\mathcal{J}}$:

$$\mathcal{G}_{\mathcal{J}}(Y) = Y(\mathcal{J}) \in \mathbb{R}^{|\mathcal{J}|},$$

i.e., the elements of Y indexed by the index set $\mathcal{J}$.

Now the SDP relaxation model becomes

$$\begin{array}{rll} p^* = & \min_{Y \in \mathbb{S}^{kn+1}} & \langle \hat{D}, Y \rangle \\ & & Y_{00} = 1 \\ & & \text{arrow}_0(Y) = 0 \\ & & \mathcal{G}_{\mathcal{J}}(Y) = 0 \\ & & KY = 0 \\ & & Y \succeq 0. \end{array} \tag{3.6}$$

Proposition 3.3. Consider the SDP relaxation (3.6) but without the arrow_0 constraint. Then every optimal solution satisfies the constraint

$$\text{arrow}_0(Y) = 0,$$

i.e., it was a redundant constraint.

Proof. It follows from [6, Thm 2.1]. ∎

Our empirical tests on random problems without the arrow_0 constraint confirmed this result. However, the extra redundant constraint is useful for the subproblems in the splitting approach below.

3.2. Doubly nonnegative (DNN) relaxation. We now split the problem by using two variables $\{Y, R\}$ and apply a doubly nonnegative relaxation to (3.6). This *natural splitting* uses the facial reduction obtained in (3.4) but with orthonormal columns chosen for the facial vector V.

3.2.1. Formulating facial vector V for sparsity. In this subsection, we suggest strategies for constructing sparse versions of the *facial vector,* V. Recall that the columns of the facial vector V form an orthonormal basis for the nullspace of K.

For a typical matrix V see Figure 3.1 that is constructed using Lemma 3.4, below. Alternatively, we can use the MATLAB QR algorithm (with A specified as sparse) $[q, \sim] = qr(-e \quad A)$ and use the last part of q for the nullspace. This results in a relatively sparse orthonormal basis for the nullspace.

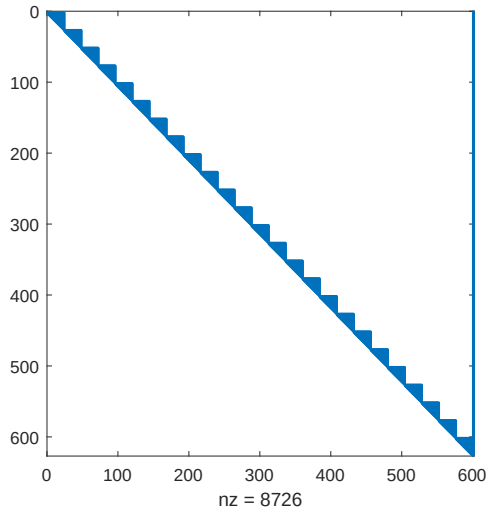

FIG. 3.1. *V matrix for k=25, n=25*

LEMMA 3.4. *Let k, n be given positive integers and from above let*

$$A = \left[I_k \otimes e_n^T \right], \; B = \begin{bmatrix} -e_k & A \end{bmatrix}.$$

Let $\mathcal{O} \in \mathbb{R}^{n-1 \times n-1}$ be the strictly upper triangular matrix of ones of order $n-1$. Set

$$v = \left(\frac{1}{\sqrt{j+j^2}} \right)_j \in \mathbb{R}^{n-1}, \; \bar{v} = \left(\frac{j}{\sqrt{j+j^2}} \right)_j \in \mathbb{R}^{n-1}, \; \beta = -1/\sqrt{n^2+nk}, \text{ and } \alpha = n\beta.$$

Let $\tilde{\mathcal{O}} = -\mathcal{O}\,\mathrm{Diag}(v) + \mathrm{Diag}(\bar{v})$ and set

$$\bar{\mathcal{O}} = \begin{bmatrix} -v^T \\ \tilde{\mathcal{O}} \end{bmatrix} = \begin{bmatrix} -v_1 & -v_2 & -v_3 & \cdots & -v_{n-1} \\ \bar{v}_1 & -v_2 & -v_3 & \cdots & -v_{n-1} \\ 0 & \bar{v}_2 & -v_3 & \cdots & -v_{n-1} \\ 0 & 0 & \bar{v}_3 & \cdots & -v_{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \bar{v}_{n-1} \end{bmatrix}.$$

Then we have

$$V = \begin{bmatrix} 0 & \alpha \\ I_k \otimes \bar{\mathcal{O}} & \beta e \end{bmatrix} \in \mathbb{R}^{nk+1 \times (n-1)k+1}, \quad V^T V = I, \; BV = 0.$$

Proof. Denote the j-th column of V by V_j and define $J_s := \{j_1^s, j_2^s, \ldots, j_{n-1}^s\}$, where $j_r^s = (n-1)(s-1)+r$. Notice that J_s is the index set of columns of V in s-th block. $j \in J_{k+1}$ means V_j is the last column of V.

We first prove that $V^T V = I$, i.e., column vectors of V is orthonormal. Let $i, j \in \{1, \ldots, (n-1)k+1\}$. We consider the following cases:

If $j \leqslant (n-1)k$, then

$$V_j^T V_j = j v_j^2 + \bar{v}_j^2 = \frac{j}{j+j^2} + \frac{j^2}{j+j^2} = 1.$$

If $j = (n-1)k+1$, then

$$V_j^T V_j = \alpha^2 + nk\beta^2 = (n^2+nk)\beta^2 = 1.$$

Now let $i < j$. If $i, j \in J_s$ for some $s \leqslant k$. Then,

$$\begin{aligned} V_i^T V_j &= i v_i v_j - \bar{v}_i v_j \\ &= i \cdot \frac{1}{\sqrt{i+i^2}} \frac{1}{\sqrt{j+j^2}} - \frac{i}{\sqrt{i+i^2}} \frac{1}{\sqrt{j+j^2}} = 0. \end{aligned}$$

If $j = (n-1)k + 1$. Then,

$$V_i^T V_j = -i v_i \beta + \bar{v}_i \beta = (-i v_i + i v_i)\beta = 0.$$

If $i \in J_s$, $j \in J_t$ with $s < t \leqslant k$. For each row, at least one of the vectors has 0 entry, so trivially $V_i^T V_j = 0$. This proves the orthonormality.

Secondly, we observe $BV = 0$, i.e., range $V \subseteq \text{null}(B)$. To this end, we will see that $BV_j = 0$ for each $j = 1, \ldots, (n-1)k + 1$. Fix $s \in \{1, \ldots, k\}$. If $j = (n-1)k + 1$,

$$\left(BV_j\right)_s = -\alpha + n\beta = -n\beta + n\beta = 0,$$

Now assume that $j \leqslant (n-1)k$. If $j \in J_s$, then

$$\left(BV_j\right)_s = -j v_j + \bar{v}_j = -j v_j + j v_j = 0, \text{ for each } i = 1, \ldots, k.$$

Otherwise, trivially $\left(BV_j\right)_s = 0$. This justifies $BV = 0$. ∎

We leave open the question on how to exploit the structure of V to obtain efficient matrix-matrix multiplications of the form VRV^T needed in our algorithm.

3.2.2. DNN reformulation via facial reduction. Recall that the lifting for Y_x has the form

$$Y_x = \begin{pmatrix} 1 \\ x \end{pmatrix} \begin{pmatrix} 1 \\ x \end{pmatrix}^T, \quad x \in \{0,1\}^{kn}.$$

Hence, we can impose the redundant elementwise **LP** relaxation bound constraint $0 \leqslant Y \leqslant 1$. Moreover, the constraint $KY = 0$ is equivalent to applying **FR**, i.e., we get

$$Y \succeq 0, KY = 0 \iff Y = VRV^T, R \in \mathbb{S}_+^{nk+1-k}.$$

We now observe a useful redundant trace constraint on Y and transform it onto R.

LEMMA 3.5. *Let* $Y \in \mathbb{S}^{kn+1}, Y = VRV^T, R \in \mathbb{S}^{nk+1-k}$. *Then*

$$KY = 0, \text{arrow}\,(Y) = e_0 \implies \text{tr}(Y) = \text{tr}(R) = k + 1.$$

Proof. Recall that $K := \begin{bmatrix} -e^T \\ A^T \end{bmatrix} \begin{bmatrix} -e^T \\ A^T \end{bmatrix}^T$. Since $\text{null}(K) = \text{null}\left(\begin{bmatrix} -e^T \\ A^T \end{bmatrix}^T \right)$, we have

$$0 = KY \iff 0 = \begin{bmatrix} -1 & e^T & \ldots & 0^T \\ \ldots & \ldots & \ldots & \ldots \\ -1 & 0^T & \ldots & e^T \end{bmatrix} \begin{bmatrix} Y_{0,0} & \ldots & Y_{0,nk} \\ \ldots & \ldots & \ldots \\ Y_{nk,0} & \ldots & Y_{nk,nk} \end{bmatrix}.$$

By expanding the first column of the product, we get $\sum_{i=1}^n Y_{jn+i,0} = 1, \forall j \in \{0, \ldots, k-1\}$. Since $\text{arrow}\,(Y) = e_0$, this implies that $\text{tr}(Y) = Y_{0,0} + \sum_{j=0}^{k-1} \sum_{i=1}^n Y_{jn+i,0} = 1 + k$. Since we choose the facial vector V to have orthonormal columns, the facial constraint yields

$$1 + k = \text{tr}(Y) = \text{tr}(VRV^T) = \text{tr}(RV^T V) = \text{tr}(R),$$ ∎

Next, we incorporate all these constraints into the SDP relaxation model to form the **DNN** relaxation model. Define the two set constraints

(3.7)
$$\mathcal{Y} := \{Y \in \mathbb{S}^{nk+1} : Y_{00} = 1, \mathcal{G}_{\mathcal{J}}(Y) = 0, \text{arrow}_0(Y) = 0, 0 \leqslant Y \leqslant 1\},\ \mathcal{R} := \{R \in \mathbb{S}_+^{nk+1-k} : \text{tr}(R) = k+1\}.$$

Our ***DNN*** *relaxation* model is:

(3.8) (**DNN**)
$$\begin{array}{lll} p^*_{\mathbf{DNN}} := \min_{R,Y} & \langle \hat{D}, Y\rangle \\ \text{s.t.} & Y = VRV^T \\ & Y \in \mathcal{Y} \\ & R \in \mathcal{R}. \end{array}$$

Observe that every feasible Y is both element-wise nonnegative and ***PSD***, i.e., this is a **DNN** relaxation. Moreover, by construction, **DNN** is trivially a feasible problem and the constraint $Y - VRV^T = 0$ is trivially surjective. Therefore, we have a regularized problem.

The splitting allows for the two cones to be handled separately. Combining them into one and applying e.g., an interior point approach is known to be very costly. And, one cannot get high dual feasibility accuracy and therefore the approximate optimal value we get is not a provable lower bound for Problem 2.1. In summary, the expense does not scale well with N, and we cannot apply weak duality and use the dual solution as both primal and dual feasibility are not highly accurate. We overcome this problem for the splitting method in Subsection 4.1.1 below.

3.2.3. Characterization of optimality for DNN relaxation. The generalized **KKT** optimality conditions hold for (3.8) with the normal cone $\mathcal{N}_{\mathcal{Y}\times\mathcal{R}}(Y,R)$. In addition, the interior of the closed convex feasible set $\text{int}\,(\mathcal{Y}\times\mathcal{R}) \neq \varnothing$ implies that

$$\mathcal{N}_{\mathcal{Y}\times\mathcal{R}}(Y,R) = \mathcal{N}_{\mathcal{Y}}(Y) \times \mathcal{N}_{\mathcal{R}}(R).$$

We can now use the corresponding Lagrangian with dual variable Z:

$$\mathcal{L}(Y,R,Z) = \langle \hat{D}, Y\rangle + \langle Z, Y - VRV^T\rangle + \iota_{\mathcal{Y}}(Y) + \iota_{\mathcal{R}}(R),$$

where $\iota_S(\cdot)$ is the *indicator function* for the set S. Therefore the first-order optimality conditions to the problem in (3.8) are: a primal-dual pair (Y,R,Z) is optimal if, and only if,

(3.9a) $Y = VRV^T, \quad R \in \mathcal{R},\ Y \in \mathcal{Y}$ (primal feasibility)

(3.9b) $0 \in -V^TZV + \mathcal{N}_{\mathcal{R}}(R)$ (dual R feasibility)

(3.9c) $0 \in \hat{D} + Z + \mathcal{N}_{\mathcal{Y}}(Y)$ (dual Y feasibility)

By the definition of the normal cone, we can easily obtain the following Proposition 3.6.

Proposition 3.6 (characterization of optimality for **DNN** in (3.8)). The primal-dual pair (R,Y,Z) is optimal for (3.8) if, and only if, (3.9) holds if, and only if,

(3.10a) $R = \mathcal{P}_{\mathcal{R}}(R + V^TZV)$

(3.10b) $Y = \mathcal{P}_{\mathcal{Y}}(Y - \hat{D} - Z)$

(3.10c) $Y = VRV^T.$

4. sADMM algorithm; bounding; empirics. The augmented Lagrangian corresponding to the **DNN** relaxation (3.8) with parameter $\beta > 0$ is

(4.1) $$\mathcal{L}_\beta(Y,R,Z) := \langle \hat{D}, Y\rangle + \langle Z, Y - VRV^T\rangle + \frac{\beta}{2}\|Y - VRV^T\|_F^2 + \iota_{\mathcal{Y}}(Y) + \iota_{\mathcal{R}}(R).$$

To solve our **DNN** relaxation in (3.8), we use the symmetric alternating directions method of multipliers **sADMM** that has intermediate updates of dual multipliers Z_t: one dual update after the R-update and

then another after the Y-update. This approach has been used successfully in [6, 13]. Hence, both the R-update and the Y-update take into account newly updated dual variable information. (We include the details here for completeness.)

Let $Y_0 \in \mathbb{S}^{nk+1}, Z_0 \in \mathbb{S}^{nk+1}$. The updates for all nonnegative integers $k \in \mathbb{Z}_+$ are:

$$\begin{array}{rcl} R_{k+1} & = & \operatorname{argmin}_{R\in\mathbb{S}^{nk+1-k}} \mathcal{L}_\beta(Y_k, R, Z_k) \\ Z_{k+\frac{1}{2}} & = & Z_k + \beta(Y_k - VR_{k+1}V^T) \\ Y_{k+1} & = & \operatorname{argmin}_{Y\in\mathbb{S}^{nk+1}} \mathcal{L}_\beta(Y, R_{k+1}, Z_{k+\frac{1}{2}}) \\ Z_{k+1} & = & Z_{k+\frac{1}{2}} + \beta(Y_{k+1} - VR_{k+1}V^T). \end{array} \tag{4.2}$$

In our **DNN** model (3.8), the objective function is continuous and the feasible set is compact. By the Weierstrass theorem, an optimal primal pair (Y^*, R^*) always exists. As seen above, the constraint is linear and surjective and strong duality holds for the generalized **KKT** conditions. (See the optimality conditions in Subsection 3.2.3). In fact, in our application we modify the dual multiplier update using a projection, see Lemma 4.1 and Algorithm 4.1.

Explicit Primal updates for R, Y. The success of our splitting method is dependent on efficiently solving the subproblems. We start with using a spectral decomposition, implicitly defined below, to get the:

$$\begin{array}{rcll} R-\text{update} & = & \operatorname{argmin}_{R\in\mathbb{S}^{nk+1-k}} \mathcal{L}_\beta(R, Y_k, Z_k) & \\ & = & \operatorname{argmin}_{R\in\mathcal{R}} \|Y_k - VRV^T + \frac{1}{\beta}Z_k\|_F^2, & \text{by completing the square} \\ & = & \operatorname{argmin}_{R\in\mathcal{R}} \|V^TY_kV - R + \frac{1}{\beta}V^TZ_kV\|_F^2, & \text{since } V^TV = I \\ & = & \operatorname{argmin}_{R\in\mathcal{R}} \|R - V^T(Y_k + \frac{1}{\beta}Z_k)V\|_F^2 & \\ & = & \mathcal{P}_\mathcal{R}[V^T(Y_k + \frac{1}{\beta}Z_k)V] & \\ & = & U\operatorname{Diag}[\mathcal{P}_{\Delta_{k+1}}(\lambda)]U^T, & \text{spectral decomposition} \end{array}$$

where the $U\operatorname{Diag}(\lambda)U^T$ provides the spectral decomposition of $V^T(Y_k + \frac{1}{\beta}Z_k)V$ and then $\mathcal{P}_{\Delta_{k+1}}$ denotes the projection onto the *simplex* $\Delta_{k+1} := \{x \in \mathbb{R}^n_+ : \langle e, x\rangle = 1 + k\}$, see e.g., [7].

Next for the

$$\begin{array}{rcll} Y-\text{update} & = & \operatorname{argmin}_{Y\in\mathbb{S}^{nk+1}} \mathcal{L}_\beta(R_{k+1}, Y, Z_{k+\frac{1}{2}}) & \\ & = & \operatorname{argmin}_{Y\in\mathcal{Y}} \|Y - [VR_{k+1}V^T - \frac{1}{\beta}(\hat{D} + Z_{k+\frac{1}{2}})]\|_F^2 & \text{by completing the square} \\ & = & \mathcal{P}_\mathcal{Y}\left(VR_{k+1}V^T - \frac{1}{\beta}(\hat{D} + Z_{k+\frac{1}{2}})\right) & \\ & = & \mathcal{P}_{\text{arrowbox}}\left(\mathcal{P}_{\text{null}(\mathcal{G}_{\hat{\mathcal{J}}})}[VR_{k+1}V^T - \frac{1}{\beta}(\hat{D} + Z_{k+\frac{1}{2}})]\right), & \end{array}$$

where $\mathcal{G}_{\hat{\mathcal{J}}}$ is the gangster constraint linear transformation and $\mathcal{P}_{\text{arrowbox}}$ projects onto the polyhedral set $\{Y \in \mathbb{S}^{nk+1} : Y_{ij} \in [0, 1], \text{arrow}\,(Y) = e_0\}$.

Dual updates. The correct choice of the Lagrange dual multiplier Z is important in the progress of the algorithm and in obtaining strong lower bounds. In addition, if the set of dual multipliers for all iterations is compact, then it indicates the stability of the primal problem. Lagrange multipliers are used to replace constraints by adding the appropriate expression into the Lagrangian function. If an optimal Z^* for (3.8) is known in advance, then it makes sense that we do not need the corresponding primal feasibility constraint $Y = VRV^T$. Hence, following the idea of exploiting redundant constraints, we now aim to identify certain properties of an optimal dual multiplier and impose that property at each iteration of our algorithm.

Lemma 4.1. Let

$$\mathcal{Z}_A := \left\{Z \in \mathbb{S}^{kn+1} : (Z + \hat{D})_{i,i} = 0, (Z + \hat{D})_{0,i} = 0, (Z + \hat{D})_{i,0} = 0, i = 1, ..., nk\right\}.$$

Let (Y^*, R^*, Z^*) be an optimal primal-dual pair for the **DNN** in (3.8). Then, $Z^* \in \mathcal{Z}_A$.

Proof. The proof of this fact uses the dual Y feasibility condition (3.9c) and a reformulation of the Y-feasible set. The details are in [11, Thm 2.1] and [6]. □

In view of Lemma 4.1 we propose the following modification of the symmetric **ADMM** algorithm, e.g., [12]. Our modification is in the way we update the multiplier. At every initial or intermediate update of the multiplier we project the dual variable onto $\mathcal{Z}_A$, i.e:

- $Z_{j+\frac{1}{2}} := Z_j + \gamma\beta\mathcal{P}_{\mathcal{Z}_A}(Y_j - VR_{j+1}V^T)$;
- $Z_{j+1} := Z_{j+\frac{1}{2}} + \gamma\beta\mathcal{P}_{\mathcal{Z}_A}(Y_{j+1} - VR_{j+1}V^T)$.

Note that a convergence proof using the modified updates is given in [11, Thm 3.2]. Therefore, in view of the **ADMM** updates (4.2) we propose the following Algorithm 4.1 with modified Z updates. The $\gamma \in (0,1)$ is the dual steplength.

Algorithm 4.1 sADMM, modified symmetric **ADMM**

Initialization: $j = 0, Y_j = 0 \in S^{nk+1}, Z_j = \mathcal{P}_{\mathcal{Z}_A}(0), \beta = \max(\lfloor\frac{nk+1}{k}\rfloor, 1), \gamma = 0.9$
while termination criteria are not met **do**
$R_{j+1} = U\,\mathrm{Diag}[\mathcal{P}_{\Delta_{j+1}}(d)]U^T$ where $U\,\mathrm{Diag}(d)U^T = \mathrm{eig}(V^T(Y_j + \frac{1}{\beta}Z_j)V)$
$Z_{j+\frac{1}{2}} = Z_j + \gamma\beta\mathcal{P}_{\mathcal{Z}_A}(Y_j - VR_{j+1}V^T)$
$Y_{j+1} = \mathcal{P}_{\mathrm{arrowbox}}[\mathcal{P}_{\mathrm{null}(\mathcal{G}_j)}(VR_{j+1}V^T - \frac{1}{\beta}(\hat{D} + Z_{j+\frac{1}{2}}))]$
$Z_{j+1} = Z_{j+\frac{1}{2}} + \gamma\beta\mathcal{P}_{\mathcal{Z}_A}(Y_{j+1} - VR_{j+1}V^T)$
$j = j + 1$
end while

Remark 4.2. In passing, we point out that we could choose any $\gamma \in (0,1)$ and $\beta > 0$. Theoretically this is all what we need. In our numerical experiments for Algorithm 4.1 we used an adaptive β based on the discussion in Subsection 4.3.1.

4.1. Bounding and duality gaps. Strong upper and lower bounds allow for early stopping conditions as well as proving optimality. We now provide provable upper and lower bounds to machine precision.

4.1.1. Provable lower bound to NP-hard problem. The Lagrangian dual function $g : \mathbb{S}^{nk+1} \to \mathbb{R}$ to the **DNN** model that we use is

$$\begin{array}{rcl} g(Z) & = & \min_{R\in\mathcal{R},Y\in\mathcal{Y}}\langle\hat{D},Y\rangle + \langle Z, Y - VRV^T\rangle \\ & = & \min_{Y\in\mathcal{Y},R\in\mathcal{R}}\langle\hat{D}+Z,Y\rangle - \langle Z, VRV^T\rangle \\ & = & \min_{Y\in\mathcal{Y}}\langle\hat{D}+Z,Y\rangle + \min_{R\in\mathcal{R}}(-\langle V^TZV, R\rangle) \\ & = & \min_{Y\in\mathcal{Y}}\langle\hat{D}+Z,Y\rangle - \max_{R\in\mathcal{R}}\langle V^TZV, R\rangle \\ & = & \min_{Y\in\mathcal{Y}}\langle\hat{D}+Z,Y\rangle - \max_{\|v\|^2=(k+1)} v^TV^TZVv \\ & = & \min_{Y\in\mathcal{Y}}\langle\hat{D}+Z,Y\rangle - (k+1)\lambda_{\max}(V^TZV). \end{array}$$

Hence, at iteration j, and applying weak duality, a lower bound to the optimal value of the **DNN** model (3.8) is

$$\begin{array}{rcl} p^*_{\mathbf{DNN}} & \geqslant & \max_Z g(Z) \\ & \geqslant & \min_{Y\in\mathcal{Y}}\langle\hat{D}+Z_j,Y\rangle - (k+1)\lambda_{\max}(V^TZ_jV). \end{array} \tag{4.3}$$

Note that from the definition of $\mathcal{Y}$ in (3.7), this bound is found from solving: an **LP** with a simplex type feasible set; and an eigenvalue problem. Thus both values can be found accurately and efficiently. Moreover, since **DNN** is a relaxation, weak duality implies that this lower bound is a *provable lower bound* for the original NP-hard Problem 2.1.

4.1.2. Upper bounds. As for the upper bound, we consider two strategies for finding feasible solutions to the **BCQP** in (2.8). The 0-column approach is to take all but the first element of this 0-th column $Y(1\!:\!\mathrm{end}, 0)$ and compute its nearest feasible solution to **BCQP**. It is equivalent to the greedy approach of using only the maximum weight index for each consecutive block of length n, see [6, Section 3.2.2].

Alternatively, we use the eigenvector of Y corresponding to the largest eigenvalue. The Perron-Frobenius Theorem implies this eigenvector is nonnegative, as Y is nonnegative. We then compute the nearest feasible solution to **BCQP**. It is again equivalent to the greedy approach but with using the eigenvector.

Then, we compare the objective values for both approaches and select the upper bound with smaller magnitude. The relative duality gap at the current iterate j is defined to be $\frac{UB_j - LB_j}{|UB_j| + |LB_j| + 1}$ where UB_j, LB_j denote the current best upper, and lower bound, respectively.

4.2. Stopping criterion. By Proposition 3.6, we can define the primal and dual residuals of the **sADMM** algorithm at iterate j as follows:

- Primal residual $r_j := \|Y_j - V R_j V^T\|$;
- Dual-R residual $s_j^R := \|R_j - \mathcal{P}_{\mathcal{R}}\left(R_j + V^T Z_j V\right)\|$;
- Dual-Y residual $s_j^Y := \left\|Y_j - \mathcal{P}_{\mathcal{Y}}\left(Y_j - \hat{D} - Z_{j+\frac{1}{2}}\right)\right\|$.

We terminate the algorithm once one of the following conditions is satisfied:

- The maximum number of iterations (maxiter) $:= 10^4 + k(nk+1)$ is reached;
- The relative duality gap is less or equal to ϵ, a given tolerance;
- KKTres $:= \max\{r_j, s_j^R, s_j^Y\} < \eta$, a given tolerance.
- Both the least upper bound and the greatest lower bound have not changed for boundCounterMax $:=$ 200 times (stalling).

4.3. Heuristics for algorithm acceleration.

4.3.1. Adaptive step size. We apply the heuristic idea presented in [5], namely we bound the gap between the primal and dual residual norms within a factor of $\mu := 2$ as they converge to 0. This guarantees that they converge to 0 at about the same rate and one residual does not overshoot the other residual by too much. Since a large penalty β prioritizes primal feasibility over dual feasibility and a small penalty β prioritizes dual feasibility over primal feasibility, we scale β by a factor of $\tau^{\text{incr}} := 2$ if the primal residual overshoots the dual residual by a factor of μ and scale β down by a factor of $\tau^{\text{decr}} := 2$ if the dual residual overshoots the primal residual by a factor of μ. Otherwise, we keep β unchanged. Namely,

$$\beta_{j+1} := \begin{cases} \tau^{\text{incr}}\beta_j, & \|r_j\|_2 > \mu\|s_j\|_2; \\ \frac{\beta_j}{\tau^{\text{decr}}}, & \|s_j\|_2 > \mu\|r_j\|_2; \\ \beta_j, & \text{otherwise.} \end{cases}$$

4.3.2. Transformation and scaling. In this subsection, we consider translating and scaling the objective function, i.e., $\hat{D}$. Define the orthogonal projection map $P_V := VV^T$. Then,

$$\begin{aligned} \langle \hat{D}, Y\rangle &:= \langle \hat{D} + \alpha I, Y\rangle - (n+1)\alpha \\ &= \langle \hat{D} + \alpha I, P_V Y P_V\rangle - (n+1)\alpha \\ &= \langle (P_V \hat{D} P_V + \alpha I), Y\rangle - (n+1)\alpha. \end{aligned} \tag{4.4}$$

Hence, when finding the optimal Y,

$$\begin{aligned} \langle \hat{D}, Y\rangle \text{ is minimized} &\iff \delta\langle \hat{D}, Y\rangle = \langle \delta(P_V \hat{D} P_V + \alpha I), Y\rangle - (n+1)\delta\alpha \text{ is minimized} \\ &\iff \langle \delta(P_V \hat{D} P_V + \alpha I), Y\rangle \text{ is minimized.} \end{aligned}$$

This lets us transform $\hat{D}$ into $\delta(P_V \hat{D} P_V + \alpha I)$ without changing the optimal solutions. Numerical experiments show that once we scale $\hat{D}$ by some $\delta > 0$, the convergence becomes faster for the aforementioned input data distributions, e.g., providing a normalization for the objective function matrix.

4.4. Numerical tests. We now illustrate the efficiency of our algorithm on medium and large scale randomly generated problems. We observe that our **sADMM** approach finds the *exact* solution with relative duality gap $<$ 1e-13, i.e., in machine precision, in almost all of the instances we tried. Sometimes, our algorithm gets stuck at the relative duality gap $\approx$ 1e-13 and runs until it reaches the max iteration. These indeterminate cases appear as ourliers in the numerical tests. Further discussion about the nontrivial duality gap follows in Section 5.

We use MATLAB version 2025a on (fastlinux in caption): Dell PowerEdge, Two Intel Xeon Gold 6244 8-core 3.6 GHz (Cascade Lake), 192 GB for the tests in Subsection 4.4.1 and Subsection 4.4.3. In Subsection 4.4.2, we use MATLAB version 2022a on two linux servers: (i) fastlinux: greyling22 Dell R840 4 Intel Xeon Gold 6254, with 3.10 GHz, 72 core and 384 GB for Table 4.1; and (ii) (biglinux in caption): Dell PowerEdge R6625, two AMD EPYC 9754 128-core 2.25 GHz, 1.5 TB for Table 4.2.

4.4.1. NP-hardness of WBP. To illustrate the difficulty in solving the original **NP**-hard problem, we solve **BCQP** in (2.8) using the commercial GUROBI solver, though total enumeration could be more competitive at times. We set $n = (2:1:8)$, $k = (2:1:8)$ for the tests, i.e., each of the k sets has the same n number of points. And we take the average of three tests for each problem size. For each test, a random **EDM** $D \in \mathbb{S}_+^{nk}$ is generated with embedding dimension $d = 2$. We can clearly see exponential growth in

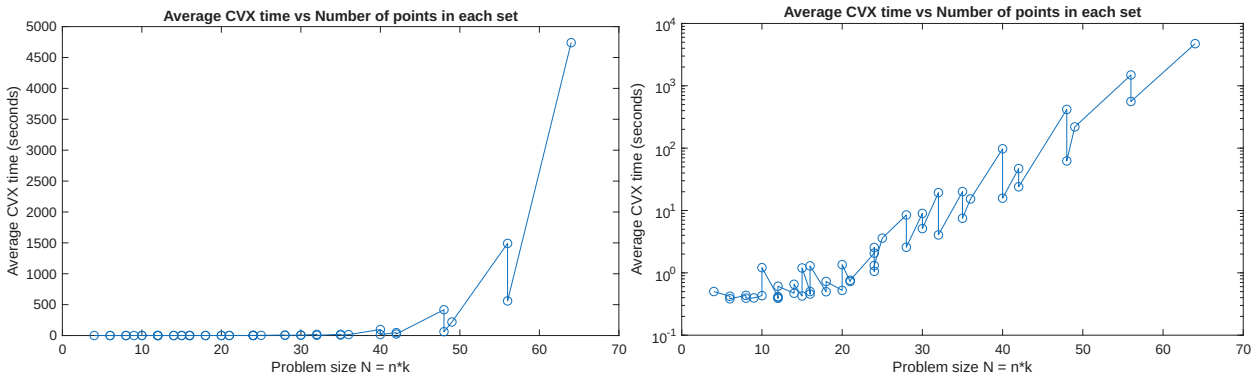

FIG. 4.1. GUROBI: *size $N = kn$ versus cpu time; illustrating exponential time*

time from Figure 4.1. Note that the CVX time is related to the number of feasible points, n^k. Hence, even if we have the same problem size, e.g., $(n, k) = (7, 8), (8, 7)$, the number of vertices, e.g., $n^k = 7^8, 8^7$, can be significantly different. Thus it appears in the figures that we have two values for the same problem size.

In contrast, we see the slow (linear) growth for **sADMM**, other than outliers, for the computation time versus the size $N = \sum_i n_i$, where n_i are the varying set sizes chosen randomly in the interval of width 5 about the given expected value n. See Figure 4.2, page 14. The figure on the right is log-log scale which reduces the effect of outliers, so we can clearly see the linear relation. (Note that an outlier is generally a result of one of five instances having a positive duality gap.) This was with $d = (3:3:6), k = (10:1:20), n = (20:1:30)$, and each set has the same size. We run five problems for each data instance and take the average time.

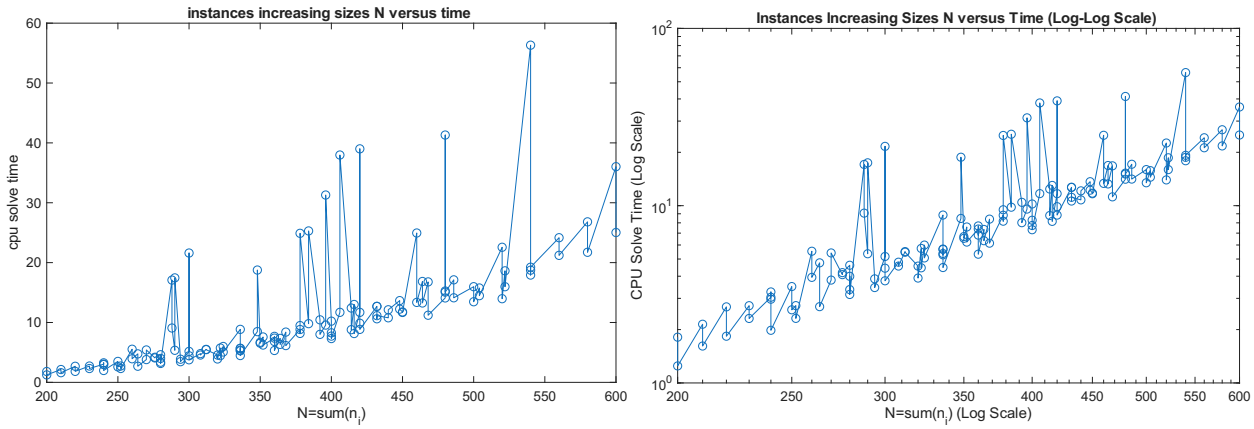

FIG. 4.2. ***sADMM**: size $N = kn$ versus cpu time; illustrating linear time*

4.4.2. Success of sADMM approach. The results below detail the efficiency and surprising success of our algorithm in finding the exact solution of the original NP-hard problem.

In Table 4.1, page 15, we see a comparison between using the **sADMM** approach and CVX with the Sedumi solver. We can see the times for the CVXsolver increase dramatically. The relative duality gap from

CVX is *not* a provable gap as the lower bound is obtained using the dual optimal value minus the posted accuracy of the solve from CVX; we do not have accurate primal feasibility or dual feasibility from CVX. Thus the relative gap is essentially the posted accuracy from CVX. We do find a nearest feasible point to find the upper bound. In summary, we see that the dramatic difference in time and the improved accuracy with the guaranteed lower bound that verifies optimality.

dim/sets/size			Time (s)		rel. duality gap	
d	k	N	ADMM	CVXsolver	ADMM	CVXsolver
2	8	56	0.14	10.47	1.5e-14	1.3e-10
2	8	72	0.28	46.09	2.0e-14	9.1e-10
2	8	88	0.34	75.33	3.3e-15	5.2e-10
2	8	104	0.45	275.38	2.8e-14	6.1e-10
2	9	63	0.26	24.55	2.9e-15	3.2e-10
2	9	81	0.31	75.90	-1.5e-16	3.5e-10
2	9	99	0.30	373.53	1.6e-14	3.8e-10
2	9	117	0.67	809.28	-4.2e-14	5.9e-09
2	10	70	0.22	43.13	3.1e-14	1.2e-10
2	10	90	0.30	250.04	5.9e-16	3.0e-10
2	10	110	0.42	553.62	2.5e-14	4.4e-10
2	10	130	0.62	1555.54	3.4e-15	2.8e-09
3	8	56	0.10	9.55	4.6e-14	1.5e-10
3	8	72	0.38	46.60	2.6e-15	5.8e-10
3	8	88	0.21	77.41	-3.1e-15	6.6e-10
3	8	104	0.38	280.12	1.7e-14	7.6e-10
3	9	63	0.15	19.97	3.4e-15	1.6e-10
3	9	81	0.13	81.98	7.7e-15	3.3e-10
3	9	99	0.24	360.76	-2.8e-15	4.5e-10
3	9	117	0.62	803.72	4.7e-14	5.2e-09
3	10	70	0.21	39.18	5.2e-15	1.7e-10
3	10	90	0.23	236.75	9.1e-17	1.4e-10
3	10	110	0.29	562.02	3.0e-15	3.5e-10
3	10	130	0.76	1473.45	3.3e-14	4.7e-09

TABLE 4.1
Comparing ADMM with CVX Solver Sedumi

We include large problems in Table 4.2, page 16. Each set has a constant number of elements n. Other than outliers, the times are very reasonable.

4.4.3. Hidden embedding dimension. The embedding dimension d is *hidden* in our model as we only use the distances between the N points. This is why we do not see d in Figure 4.2. The size of the **DNN** model is $N + 1$ irrespective of d. The *hardness* of the problem is often hiding in the rank of the *optimal solution* Y of the **DNN** relaxation, i.e., if the rank is one, then we have solved the original NP-hard problem. However, if the rank of the optimal Y is large, then the heuristics for the upper and lower bounds may not be enough to find an optimal solution for the original NP-hard Problem 2.1. However, the rank of the objective matrix D that comes from d did not influence this at all. In the various tests that we have done we did not see any changes in the solution times or the ability to obtain a near zero duality gap for wide varying values of d.

Figure 4.3 in 16 shows cpu time for our **sADMM** method when we fix the problem size $N = nk$ and vary the embedding dimension d. Random problems are generated with $(n, k) \in \{10, 40\} \times \{30, 50\}$, and $d \in \{2, \ldots, 30\}$. The cpu time is dependent only on problem size and not on the embedding dimension.

5. Multiple optimal solutions and duality gaps. We now show that *multiple optimal* solutions for the original hard problem can lead to a duality gap between the optimal value of the original NP-hard

dim/sets/size			Time (s)	rel.duality gap
d	k	N	ADMM	ADMM
8	30	1200	104.81	-1.9e-15
8	30	1230	67.08	-3.2e-14
8	31	1240	94.90	-1.3e-14
8	31	1271	81.93	2.5e-14
8	32	1280	75.29	3.1e-14
8	32	1312	2025.42	1.8e-13
9	30	1200	4586.51	1.2e-13
9	30	1230	63.91	2.6e-14
9	31	1240	93.96	3.3e-14
9	31	1271	71.31	3.2e-14
9	32	1280	92.89	3.6e-14
9	32	1312	86.67	-2.2e-13

TABLE 4.2
*Large problems with **sADMM** on biglinux server*

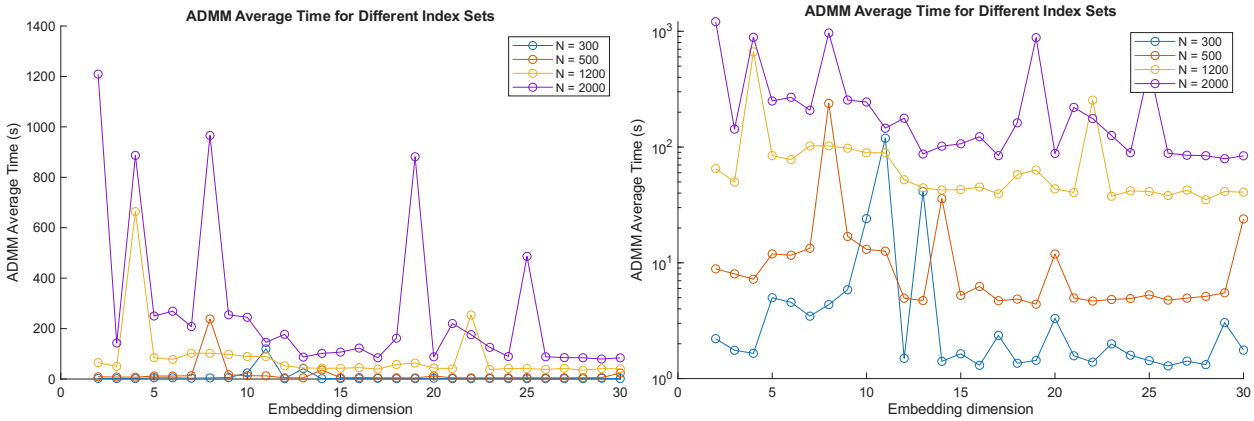

FIG. 4.3. ***sADMM**: Embedding dimension d versus cpu time in various sizes*

problem and the lower bound found from the **DNN** relaxation.

5.1. Criteria for duality gaps. To find duality gaps for SDP relaxations, we want to find optimal points for the relaxation that are not vertices, i.e., they are outside of the polyhedral set formed from the convex hull of the lifted vertices. The key for this is having multiple optimal solutions for the original problem. The following Lemma 5.1 and Corollary 5.2 provides a construction for obtaining a positive gap between the optimal values of a *general* hard problem with multiple optimal solutions and its **DNN** relaxation.

LEMMA 5.1. *Let $\{x_i\}_{i=1}^n \subset \mathbb{R}^n_+$ be a linearly independent set. Define the lifted vertices and barycenter, respectively,*

$$\left\{X_i = x_i x_i^T\right\}_{i=1}^n \subset \mathbb{S}^n, \quad \hat{X} := \frac{1}{n}\sum_{i=1}^n X_i.$$

Then $\hat{x} := \sum_i x_i > 0$, and

$$\hat{X} \in \mathbb{S}^n_{++} \cap \mathbb{R}^n_{++} \quad (= \operatorname{int} \boldsymbol{DNN}).$$

Proof. That $\hat{x} > 0$ follows by contradiction. That $\hat{X} \in \mathbb{R}^n_{++}$ now follows. Now note that $X_i \succeq 0, \forall i$, and

so $\hat{X} \succeq 0$ as well. Now suppose that $0 = \hat{X}v$, for some $0 \neq v \in \mathbb{R}^n$. Then

$$0 = v^T \hat{X} v = v^T \sum_i X_i v \implies 0 = v^T X_i v, \forall i \implies (v^T x_i)^2 = 0, \forall i \implies v = 0,$$

by the linear independence assumption; thus contradicting $v \neq 0$ and yielding $\hat{X} \succ 0$. □

Corollary 5.2. Suppose that the hypotheses of Lemma 5.1 hold. Let the points $x_i, i = 1, \ldots, n$ be given (multiple) optima for a given hard minimization problem, i.e.,

$$(P) \quad p^* = \min \left\{ x^T Q x \,:\, x \in \{0,1\}^n \right\} = x_i^T Q x_i,\ i = 1, \ldots, n.$$

Moreover, suppose that there exists a feasible y that is not optimal for (P),

$$y \in \{0,1\}^n, y^T Q y > p^*.$$

Then the **DNN** relaxation has feasible points $Y = yy^T, Z$ such that

$$\operatorname{tr} YQ > p^* > \operatorname{tr} ZQ,$$

i.e., Z yields a duality gap.

Proof. From Lemma 5.1 we have that the barycenter $\hat{X}$ of the $\{x_i\}$ satisfies $\hat{X} \in \operatorname{int} \mathbf{DNN}$. Note that $\operatorname{tr} YQ = y^T Q y > p^* = \operatorname{tr} \hat{X} Q$. Therefore, $\operatorname{tr}(\hat{X} - Y)Q < 0$, and for $\epsilon > 0$,

$$\operatorname{tr}(\hat{X} + \epsilon(\hat{X} - Y)Q = p^* + \epsilon \operatorname{tr}(X - Y)Q < p^*.$$

Moreover, the line segment $[Y, \hat{X} + \epsilon(\hat{X} - Y)]$ is feasible for the SDP relaxation for small enough $\epsilon > 0$ by $\hat{X} \in \operatorname{int} \mathbf{DNN}$. Therefore, we set $Z_\epsilon = \hat{X} + \epsilon(\hat{X} - Y), 0 < \epsilon << 1$ and obtain a duality gap for any such $Z = Z_\epsilon$. □

We can extend this theory to problems with general linear constraints $Ax = b$ by using **FR**. We now specifically extend it to our **BCQP** in (2.8). After **FR**, we need $nk + 1 - k$ linearly independent optimal points. This can be obtained when we choose $k >> n$. Recall the matrix K in (3.2) used for facial reduction and the facially reduced **DNN** relaxation in (3.8).

Corollary 5.3. We consider the **BCQP** in (2.8) with optimal value p^*, and the **DNN** relaxation in (3.8). Let

$$\left\{ y_i = \begin{pmatrix} 1 \\ x_i \end{pmatrix} \right\}_{i=1}^{nk+1-k} \subset \mathbb{R}_+^{nk+1}$$

be a linearly independent set that are optimal for **BCQP** and with $\sum_i y_i > 0$. Define the lifted vertices and barycenter, respectively,

$$\left\{ Y_i = y_i y_i^T \right\}_i, \forall i, \quad \hat{Y} := \frac{1}{nk + 1 - k} \sum_{i=1}^{nk+1-k} Y_i.$$

Moreover, suppose that there exists a feasible $\bar{x}$ for **BCQP** that is not optimal. Then

$$\hat{Y} = V \hat{R} V^T \succeq 0,\ \hat{Y} > 0,\ \hat{R} > 0.$$

And there exists $Z = V R_Z V^T, R_Z \succ 0$ with optimal value $\operatorname{tr} DZ < p^*$, yielding a duality gap.

Proof. First note that incident vectors are feasible for the linear constraints and this guarantees that we have enough feasible points to guarantee that the barycenter satisfies $\hat{Y} > 0$. All lifted feasible points of the relaxation are in the minimal face and have a corresponding matrix $R \in \mathbb{S}^{nk+1-k}$ for the facial reduction $Y = VRV^T$. Since $R \succ 0$ after the **FR**, we can apply the same proof as in Corollary 5.2. In addition, note that the linear constraints, the arrow constraint and gangster constraints, remain satisfied in the line formed from any two feasible points. □

5.2. Wheel of wheels examples with a duality gap. We illustrate the above theory with some specific problems with special structure that have multiple optimal solutions for the original **NP**-hard problem. We see that a duality gap can exist between the optimal value of the original **NP**-hard problem and the optimal value of the **DNN** relaxation.

Example 5.4 (Wheel of wheels). We next present another input data distribution for which the duality gap between the optimal value of the **BCQP** formulation and the Lagrangian dual value is non-trivial. The issue is again the non-uniqueness of the optimal solutions and the **sADMM** algorithm fails to break ties among them.

The data distributions compose of a wheel of wheels, i.e., a wheel with an odd number of sets each of which is a wheel. Hence we call it an odd wheel. Given problem size parameters (k, n, d), define

- $\theta_k := \frac{2\pi}{k}$.
- a set of k centroids encoded by a matrix $C \in \mathbb{R}^{k\times 2}$ such that

$$C(i,:) = \begin{bmatrix}\cos(i\theta_k - \theta_k) & \sin(i\theta_k - \theta_k)\end{bmatrix}, i = 1, ..., k.$$

- the radius of each cluster $r_k := \frac{\sqrt{\cos(\theta_k - 1)^2 + \sin\theta_k^2}}{4}$.
- the set of input points encoded by a matrix $P := (C \otimes e_k) + r_k(e_k \otimes C) \in \mathbb{R}^{k^2\times 2}$.

When k is odd, there exists more than one optimal solution. A simple example with $k = 3 = n$ follows in Figure 5.1, page 19. We use the corresponding nine points in the configuration matrix ordered $1 - 9$ counter-clockwise in the triangles ordered counter-clockwise.

$$P = \begin{bmatrix} 1.7536 & 0.0137 \\ 0.6195 & 0.6362 \\ 0.6239 & -0.6643 \\ 0.2590 & 0.8609 \\ -0.8839 & 1.5449 \\ -0.8692 & 0.2201 \\ 0.2629 & -0.8740 \\ -0.8937 & -0.2100 \\ -0.8721 & -1.5275 \end{bmatrix}$$

The distances are ordered by choosing the points in lexicographic order:

$$(1,1), (1,2), \ldots (3,3).$$

The unique minimum distance is 11.1607 obtained from the points $2, 3, 2$ and with the primal optimal $x^* = \begin{pmatrix}0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0\end{pmatrix}^T$. The optimal value from CVX to 9 decimals precision is 10.8246, thus verifying an empirical duality gap of .3 to 9 decimals precision. The motivation for this counter-example is to have near optimal solutions. One could shrink triangle two to make point 4 equidistant to points $7, 8$ and move point 2 closer to point 3 and thus have a tie optimal solution.[7] Note that the maximum distance is 56.0227 obtained from points $(1, 2, 3)$.

However, when k is even, only one optimal solution clearly exists and the duality gap becomes trivial. An example with $k = 6 = n$ follows in Figure 5.2, page 20.

6. Conclusion. In this paper we presented a strategy for solving a class of **NP**-hard binary quadratic problems, the simple Wasserstein barycenter problem. This involves formulating a **DNN** relaxation, applying **FR** that gives rise to a natural splitting for a symmetric alternating directions method of multipliers **sADMM** with intermediate update of multipliers and strong upper and lower bounding techniques. In particular, the structure of both the primal and dual solutions is exploited in the updating steps of the **sADMM**. We applied this to the **NP**-hard computational problem called the simplified Wasserstein barycenter problem.

[7] The wheel graph was used successfully to obtain duality gaps for the second lifting of the max-cut problem, see [4].

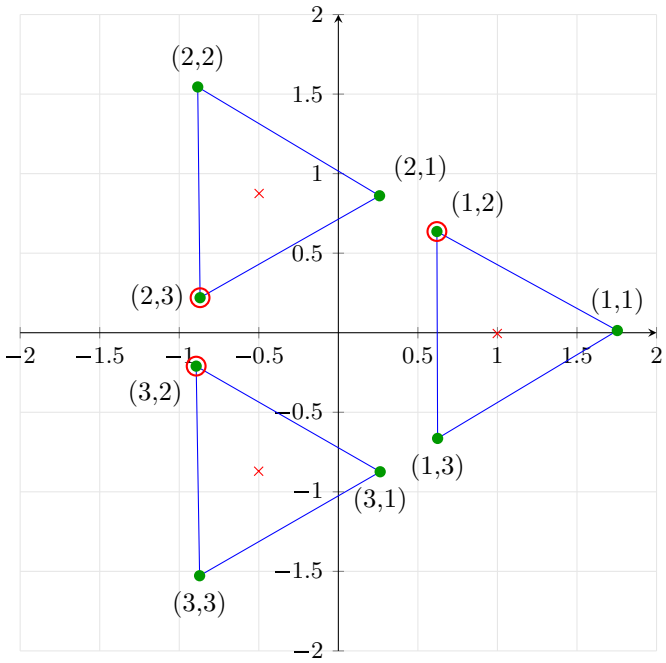

FIG. 5.1. *Duality gap for wheel of wheels: k=3=n*

Surprisingly, for the random problems we generated the gap between bounds was zero to machine precision and we were able to provably solve the original **NP**-hard optimization problem, i.e., if there were another optimal solution, then it would yield the same optimal value to machine precision. This coincided with $\text{rank}(Y^*) = 1$ for the optimal solution found for the **DNN** relaxation. We observed that the embedding dimension d is hidden in the **DNN** relaxation. However, for specially constructed input data that has near multiple optimal solutions, the algorithm had difficulty breaking ties and resulted in nontrivial gaps between lower and upper bounds coinciding with $\text{rank}(Y^*) > 1$, i.e., the original Wasserstein problem was not solved to optimality.

As for future research, we want to better understand the theoretical reasons for the positive duality gaps and find more classes of problems where this occurs. Does the lack of gaps correspond to large volumes for the normal cones at points on the boundary of the feasible set? In addition, we want to understand what happens under small perturbations to problems with duality gaps, i.e., if the gaps can be closed with perturbations.

Finally, we are gathering data about airports in North America by state and province in URL: ourairports.com/continents/NA/. We plan on solving the problem of finding the best hub in each state (or province) in order to find the location for the best hub for the country.

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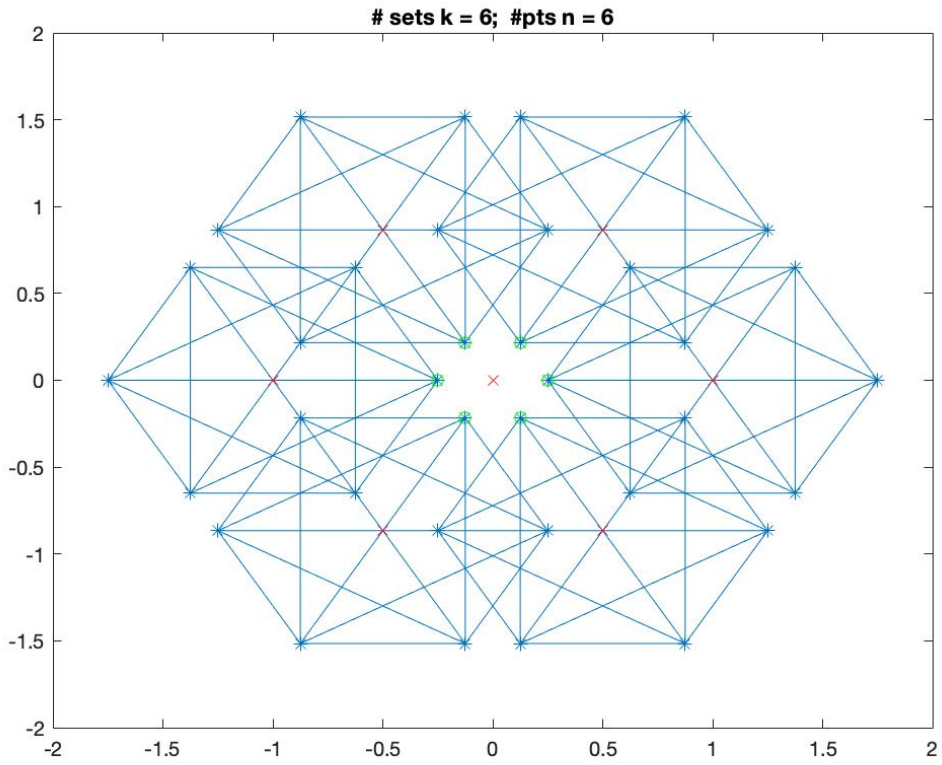

FIG. 5.2. *No duality gap for wheel of wheels: k=6=n*

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