A Simplified/Improved HKM Direction for Certain Classes of Semidefinite Programming

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Abstract

Semidefinite Programming (SDP) provides strong bounds for many NP-hard combinatorial problems. Arguably the most popular/efficient search direction for solving SDPs using a primal-dual interior point (p-d i-p) framework is the *HKM direction.* This direction is a Newton direction found from the linearization of a symmetrized version of the optimality conditions. For many of the SDP relaxations of NP-hard problems, a simple primal-dual feasible starting point is available. In theory, the Newton type search directions maintain feasibility. However, in practice it is assumed that roundoff-error must be taken into account and the residuals are used to recover feasibility.

We introduce preprocessing for SDP to obtain a modified HKM direction. This direction attains *exact primal and dual feasibility* throughout the iterations while: setting the residuals to 0; reducing the arithmetic expense; maintaining the same iteration counts for well-conditioned problems; and reducing the iteration count for ill-conditioned problems. We apply the technique to the Max-Cut, Lovász Theta, and Quadratic Assignment problems. We include an illustration on an ill-conditioned two dimensional problem, a discussion on convergence, and a similar simplification for the Monteiro-Zhang family of search directions.

This paper can serve as an introduction to both the HKM search direction and preprocessing (presolve) for SDP.

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1 Introduction

The primal SDP we consider is

$$\text{(PSDP)} \qquad \begin{array}{rll} p^* := & \max & \operatorname{trace} CX \\ & \text{s.t.} & \mathcal{A}(X) = b \\ & & X \succeq 0. \end{array} \tag{1.1}$$

Its dual is

$$\text{(DSDP)} \qquad \begin{array}{rll} d^* := & \min & b^T y \\ & \text{s.t.} & \mathcal{A}^*(y) - Z = C \\ & & Z \succeq 0, \end{array} \tag{1.2}$$

where $C, X, Z \in \mathcal{S}^n$, $\mathcal{S}^n$ denotes the space of $n \times n$ real symmetric matrices, $y, b \in \Re^m$, and $\succeq$ ($\succ$) denotes positive semidefiniteness (resp. positive definiteness), known as the Löwner partial order; $\mathcal{A} : \mathcal{S}^n \to \Re^m$ is a linear operator and $\mathcal{A}^*$ is the adjoint operator. We assume that Slater's constraint qualification (strict feasibility) holds for both programs.

The SDP model has many applications and can be solved efficiently using primal-dual interior-point (p-d i-p) methods. In this paper we introduce a *preprocessing step* to reformulate the primal problem PSDP. We show that there are numerical advantages when deriving search directions for p-d i-p methods using this new formulation.

The HKM search direction was obtained independently by Helmberg, Rendl, Vanderbei, and Wolkowicz [7] and Kojima, Shindoh, and Hara [9]. Kojima et al. also described a dual

HKM direction. Later, Monteiro [14] gave another derivation of these directions. (See e.g. [13, Section 10.3],[23] for derivations and properties of these and other directions.) The HKM direction is, arguably, the most popular and efficient among the primal-dual interior-point (p-d i-p) directions for SDP. It is based on applying Newton's method to a symmetrized form of the optimality conditions for PSDP. Therefore, in theory, we get fast asymptotic and polynomial time algorithms; and, primal (resp. dual) feasibility is maintained throughout the iterations, if one starts with a primal (resp. dual) feasible point. However, in practice, roundoff error causes degradation in feasibility and the residuals are used to restore the feasibility, i.e. even though we start with a feasible point, an infeasible p-d i-p algorithm must be used.

In Linear Programming (LP), the nonnegativity constraints $x \geq 0$ is equivalent to $x \in \Re^n_+$, i.e. x is in the nonnegative orthant, a crossproduct of n 1-dimensional cones. Therefore, if a variable is fixed, it can be eliminated and the problem simplified. This is often done during the important preprocessing (or presolve) steps for LP, e.g. [12, 6]. Preprocessing for SDP is difficult and rarely done. (Some preprocessing is done in the matrix completion approach in e.g. [4, 15], where *free variable* that can be eliminated in the semidefinite constraints are identified.) But, SDP often includes simple constraints such as fixing certain components of matrix variables to given constants. However, the corresponding components cannot, in general, be eliminated since the matrix variables are restricted to be positive semidefinite. In this paper we take advantage of such simple constraints and show that a modified HKM search direction results in exact primal-dual feasibility throughout the iterations, for many classes of SDPs. In addition, the cost of the backsolve steps in each iteration is reduced, while the number of iterations is unchanged.

We provide three illustrations on SDP relaxations, each in increasing complexity. We include two simple $n = 2$ examples that illustrate the procedure and the stability benefits. The SDP relaxations are for
(i) Max-Cut: We simply fix the diagonal throughout all the iterations;
(ii) Lovász Theta function: We fix elements of the primal matrix to zero and project the diagonal to guarantee trace 1;
(iii) Quadratic Assignment problems: We project and rotate the problem and identify zeros in the primal matrix and then fix these elements to zero. In addition, we project other linear constraints.

1.1 Background

1.1.1 Optimality Conditions

The following characterization of optimality for PSDP is well known, see e.g. [20].

Theorem 1.1 *The primal-dual variables X, y, Z with $X \succeq 0, Z \succeq 0$ are optimal for (PSDP), (DSDP) if and only if the residuals satisfy*

$$\begin{array}{rclcll} R_D & := & \mathcal{A}^*(y) - Z - C & = & 0 & \textit{(dual feasibility)} \\ R_P & := & \mathcal{A}(X) - b & = & 0 & \textit{(primal feasibility)} \\ R_{ZX} & := & ZX & = & 0 & \textit{(complementary slackness).} \end{array} \qquad (1.3)$$

■

1.1.2 Derivation of Standard and Simplified HKM Directions

We now derive the HKM search direction $\Delta s = \begin{pmatrix} \Delta X \\ \Delta y \\ \Delta Z \end{pmatrix}$ from the following linearization of the optimality conditions (1.3) obtained after perturbing the complementarity conditions with barrier parameter $\mu > 0$

$$\begin{array}{rcl} \mathcal{A}^*(\Delta y) - \Delta Z & = & -R_D \\ \mathcal{A}(\Delta X) & = & -R_P \\ Z(\Delta X) + (\Delta Z)X & = & -R_C := \mu I - R_{ZX}. \end{array} \tag{1.4}$$

We get

$$\Delta Z = \mathcal{A}^*(\Delta y) + R_D \tag{1.5}$$

and

$$\Delta X = -Z^{-1}(\Delta Z)X - Z^{-1}R_C = -Z^{-1}(\mathcal{A}^*(\Delta y) + R_D)X + \mu Z^{-1} - X. \tag{1.6}$$

We substitute this into the second equation and solve for Δy using

$$\mathcal{A}(Z^{-1}\mathcal{A}^*(\Delta y)X) = \mathcal{A}(\mu Z^{-1} - X - Z^{-1}R_D X) + R_P = \mathcal{A}(\mu Z^{-1} - Z^{-1}R_D X) - b. \tag{1.7}$$

We can now backsubstitute to get the symmetric matrix ΔZ using (1.5). However, ΔX in (1.6) need not be symmetric. Therefore we *cheat* and symmetrize ΔX after backsubstition in (1.6), i.e. we solve for the system by assuming ΔX is a general matrix and then symmetrize by projecting the solution back into $\mathcal{S}^n$.

SUMMARY: Standard HKM Direction for General SDP

Solve for Δy in:	$\mathcal{A}(Z^{-1}\mathcal{A}^*(\Delta y)X) = \mathcal{A}(\mu Z^{-1} - Z^{-1}R_D X) - b$
Backsolve :	$\Delta X = \mu Z^{-1} - X$
	$\quad -.5\left(X(\mathcal{A}^*(\Delta y) + R_D)Z^{-1} + Z^{-1}(\mathcal{A}^*(\Delta y) + R_D)X\right)$
	$\Delta Z = \mathcal{A}^*(\Delta y) + R_D$

(1.8)

The above derivation uses dual feasibility to eliminate ΔZ in the linearized complementarity equation. Then this latter equation was used to eliminate ΔX in the primal feasibility equation. This resulted in the symmetric positive definite system in Δy, i.e. the first equation in (1.8). The solution was then used in the next two backsolve steps in (1.8).

The search direction is then used to find steplengths $\alpha_P > 0, \alpha_D > 0$ that maintain (sufficient) positive definiteness, $X + \alpha_P \Delta X \succ 0$, $Z + \alpha_D \Delta Z \succ 0$. Both X, Z are updated along with $y \leftarrow y + \alpha_D \Delta y$.

Note that if we first update $y \leftarrow y + \alpha_D \Delta y$ and then update $Z \leftarrow \mathcal{A}^*(y) - C$, then dual feasibility is exact in the sense that $Z - (\mathcal{A}^*(y) - C) = 0$. We can do this for primal feasibility as well using a reformulation of the constraints. Suppose that the matrix variable X is split into two vector variables $\begin{pmatrix} v \\ u \end{pmatrix}$, e.g. the diagonal elements in v and the strictly upper triangular off-diagonal elements in u (columnwise). We can write $X = X(v, u)$, $v = V(X), u = U(X)$ and $X = X(V(X), U(X))$. After an appropriate pivot operation we find linear operators $\mathcal{K}, \mathcal{L}$ such that

$$\mathcal{A}\left(X\begin{pmatrix} v \\ u \end{pmatrix}\right) = b \quad \text{iff} \quad \left\{ \begin{array}{rcl} [I\ \mathcal{K}]\begin{pmatrix} v \\ u \end{pmatrix} & = & c \\ \mathcal{L}\begin{pmatrix} v \\ u \end{pmatrix} & = & d \end{array} \right. \tag{1.9}$$

We can now substitute for X in the above derivation and eliminate v so that the backsolve in (1.8) is for the variable u only. i.e. this can ignore roundoff and simplify the backsubstitution steps, while maintaining exact primal-dual feasibility and fast convergence. We update as above using

$$y \leftarrow y + \alpha_D \Delta y \text{ then } Z \leftarrow \mathcal{A}^*(y) - C \tag{1.10}$$

i.e. the residual $R_D = 0$.

SUMMARY: Simplified HKM Direction for General SDP

$$\begin{array}{ll} \textbf{Solve} \text{ for } \Delta y \text{ in:} & \mathcal{A}\left(Z^{-1}\mathcal{A}^*(\Delta y)X\right) = \mathcal{A}\left(\mu Z^{-1}\right) - b \\ \textbf{Backsolve}: & \Delta u = U\left\{\mu Z^{-1} - X\right. \\ & \qquad \left. -.5\left(X(\mathcal{A}^*(\Delta y))Z^{-1} + Z^{-1}(\mathcal{A}^*(\Delta y))X\right)\right\} \\ & \Delta v = -\mathcal{K}(\Delta u) \\ & \Delta Z = \mathcal{A}^*(\Delta y) \end{array} \tag{1.11}$$

If the linear operator $\mathcal{K}$ is simple and/or the dimension of u is small relative to v, then the preprocessing has simplified the backsolve step as well as improved the accuracy after this backsolve. (We assume good accuracy in the reformulation.) Unlike the LP case, we show below that this is true for many classes of SDP.

1.2 Outline

In Sections 2.1, 2.2, 3, we illustrate the new simplified/improved direction on three relaxations of hard combinatorial problems: Max-Cut, Theta Function, and Quadratic Assignment, respectively. The examples in Section 2 are intuitive and based on the original structure of the matrix variables, i.e. for Max-Cut SDP we simply fix the diagonal to be all ones, while for the Theta Function SDP we fix appropriate zeros and provide a projection that guarantees the correct trace. In Section 3 we consider the SDP relaxation for the Quadratic Assignment Problem, QAP. The original relaxation does not satisfy Slater's constraint qualification. Therefore, a projection/regularization is applied. The new matrix variable does not have any obvious fixed elements or structure. We find a rotation of the matrix space so that the matrix variable has $O(n^3)$ fixed zeros and other special structure. Numerical tests were done to compare the two HKM directions. The tests illustrated that exact feasibility holds for the simplified direction, while the number of iterations were essentially the same.

The MATLAB programs are available with URL:
orion.math.uwaterloo.ca:80/˜hwolkowi/henry/software/imprhkm.d/readme.html

We include two illustrative $n = 2$ examples in Section 2.3. These examples show the benefits of maintaining exact feasibility for ill-conditioned problems. The MATLAB programs are available with URL:
orion.math.uwaterloo.ca:80/˜hwolkowi/henry/software/imprhkm.d/readme.html

We conclude in Section 4 with comments on: polynomial time convergence theorems; extension of the exact feasibility procedure to the Monteiro-Zhang family of search directions and to general SDPs.

2 Exact Primal-Dual Feasibility

In this section we look at two applications of the simplification technique and obtain exact primal-dual feasibility in each case. These applications follow intuitively from the special structure of the models and the choice of the operators $\mathcal{K}, \mathcal{L}$ in (1.9) are clear. These two examples serve as an introduction to the more subtle application to QAP in Section 3.

2.1 Max-Cut Problem

The Max-Cut problem (MC) consists in finding a partition of the set of vertices of a given undirected graph with weights on the edges so that the sum of the weights of the edges cut by the partition is maximized. Following is the well-known semidefinite relaxation of MC.

$$\text{(P)} \qquad \begin{array}{rll} \text{mc}^* \leq \nu^* := & \max & \operatorname{trace} QX \\ & \text{s.t.} & \operatorname{diag}(X) = e \\ & & X \succeq 0, \ X \in \mathcal{S}^n, \end{array} \tag{2.1}$$

where $\operatorname{diag}(X)$ denotes the vector formed from the diagonal elements of the matrix X and e denotes the (column) vector of all ones, of appropriate dimension. This relaxation has been extensively studied. It has been found to be surprisingly strong both in theory and in practice, e.g. [5, 10].

We use a preprocessing approach exploited in [24], i.e. we let v denote the diagonal elements of X and x denote the elements taken columnwise from the strict upper triangular part of X. The operators $\mathcal{K}, \mathcal{L}$ in (1.9) are both zero, we identify x with u, and $c = e$, the vector of all ones. This defines the operators U, V. Equivalently, we can define the operator $\operatorname{offDiag}(S) := S - \operatorname{Diag}(\operatorname{diag}(S))$, i.e. the operator sets the diagonal to 0. We use the well-known optimality conditions

Theorem 2.1 *The primal-dual variables X, y, Z with $X \succeq 0, Z \succeq 0$ are optimal for (P),(D) if and only if*

$$\begin{array}{ll} \operatorname{Diag}(y) - Z - Q = 0 & \textit{(dual feasibility)} \\ \operatorname{diag}(X) - e = 0 & \textit{(primal feasibility)} \\ ZX = 0 & \textit{(complementary slackness).} \end{array}$$

We assume that we start with a primal-dual strictly feasible pair, e.g. $\hat{X} = I$ and y chosen so that $Z = \mathrm{Diag}\,(y) - Q \succ 0$. We update y, Z using (1.10) so that the dual residual $R_D = 0$.

SUMMARY: Improved HKM Direction for Max-Cut Problem

Solve for Δy in :	$(Z^{-1} \circ X)\Delta y = \mu \mathrm{diag}\,(Z^{-1}) - e$
Backsolve :	$\mathrm{offDiag}\,(\Delta X) = \mathrm{offDiag}\,(\mu Z^{-1} - X)$
	$\quad -0.5\left(\mathrm{offDiag}\,(Z^{-1}\mathrm{Diag}\,(\Delta y) X) + \mathrm{offDiag}\,(X \mathrm{Diag}\,(\Delta y) Z^{-1})\right)$
	$\mathrm{diag}\,(\Delta X) = 0$
	$\Delta Z = \mathrm{Diag}\,(\Delta y)$

This simplified/modified HKM direction differs in an obvious way from the standard approach in that primal feasibility is maintained at each iteration, i.e. the diagonal of ΔX is fixed at zero at each iteration.

2.2 Lovász Theta Function Problem

Let $G = (\mathcal{V}, \mathcal{E})$ be an undirected graph; and let $n = |\mathcal{V}|$ and $m = |\mathcal{E}|$ be the number of nodes and edges, respectively. The Lovász theta number (defined in [11]) is the optimal value of the following SDP

$$
\text{(TP)} \qquad \begin{array}{rll} \theta(\mathcal{G}) := p^* := & \max & \mathrm{trace}\, EX \\ & \text{s.t.} & \mathrm{trace}\, X = 1 \\ & & \mathrm{trace}\, E_{ij} X = 0, \quad \forall (i,j) \in \mathcal{E} \\ & & X \succeq 0, \ X \in \mathcal{S}^n , \end{array} \tag{2.2}
$$

where $E_{ij} = (e_i e_j^T + e_j e_i^T)/\sqrt{2}$ is the ij unit matrix in $\mathcal{S}^n$, e_i is the i-th unit vector in $\Re^n$, and E is $n \times n$ matrix of all ones. The dual of (TP) is

$$
\text{(DTP)} \qquad \begin{array}{rll} d^* := & \min & z \\ & \text{s.t.} & zI + \sum\limits_{(i,j)\in\mathcal{E}} y_{ij} E_{ij} - Z = E \\ & & Z \succeq 0, \ Z \in \mathcal{S}^n , \end{array} \tag{2.3}
$$

where $z \in \Re$, $y = (y_{ij})_{(i,j)\in\mathcal{E}} \in \Re^m$. The theta number has important properties, e.g. it is tractable (can be computed in polynomial time) and it provides bounds for the stability and chromatic numbers of the graph, see e.g. [8, 10]. We use a preprocessing approach described in detail in [22]. This is similar to the approach used above for the Max-Cut problem, i.e. we find the linear operators $\mathcal{K}, \mathcal{L}$ in (1.9).

First, we need the following definitions. Let $\mathcal{G}^c = (\mathcal{V}, \mathcal{E}^c)$ be the complement graph of $\mathcal{G}$, i.e. $\mathcal{E}^c$ is the edge set complement to $\mathcal{E}$. (We do not consider loops as edges.) Let $m_c = |\mathcal{E}^c| = \binom{n}{2} - m$. Define the linear operators $\mathrm{u2sMatEc} : \Re^{m_c} \to \mathcal{S}^n$ and $\mathrm{u2sMatE} : \Re^m \to \mathcal{S}^n$ as follows. (We identify the vector components for $x \in \Re^m$ or $x \in \Re^{m_c}$: x_{ij} with

$x_k,\ k = \binom{j-1}{2} + i$, if $i < j$ and with $x_k,\ k = \binom{i-1}{2} + j$, if $i > j$.)

$$
\begin{array}{rcl}
(\mathrm{u2sMatEc}\,(x))_{ij} & := & \begin{cases} 0 & \text{if } i = j, \text{ or } (i,j) \text{ or } (j,i) \in \mathcal{E} \\ x_{ij}/\sqrt{2} & \text{otherwise,} \end{cases} \\
(\mathrm{u2sMatE}\,(x))_{ij} & := & \begin{cases} x_{ij}/\sqrt{2} & \text{for } (i,j) \text{ or } (j,i) \in \mathcal{E} \\ 0 & \text{otherwise.} \end{cases}
\end{array}
$$

The division by $\sqrt{2}$ makes the mapping a partial isometry. Let $\mathrm{u2svecEc} := \mathrm{u2sMatEc}^{\dagger}$ denote the *Moore-Penrose generalized inverse* mapping onto $\Re^{m_c}$, i. e. $\sqrt{2}$ times the vector taken columnwise from the upper triangular part of X corresponding to the edge set E^c; similarly $\mathrm{u2svecE} := \mathrm{u2sMatE}^{\dagger}$ maps $\mathcal{S}^n$ onto $\Re^m$; u2svecEc (resp. u2svecE) is an inverse mapping if we restrict to the subspace of matrices with zero in positions corresponding to the edge set $\mathcal{E}$ (resp. $\mathcal{E}^c$). The adjoint operator $\mathrm{u2sMatEc}^* = \mathrm{u2svecEc}$, since

$$
\begin{array}{rcl}
\langle \mathrm{u2sMatEc}\,(v), S\rangle & = & \mathrm{trace}\,\mathrm{u2sMatEc}\,(v) S \\
& = & v^T \mathrm{u2svecEc}\,(S) = \langle v, \mathrm{u2svecEc}\,(S)\rangle\,,
\end{array}
$$

and similarly the adjoint operator $\mathrm{u2sMatE}^* = \mathrm{u2svecE}$. The composite mapping

$$
P_E := \mathrm{u2sMatE}\,\mathrm{u2sMatE}^* = \mathrm{u2sMatE}\,\mathrm{u2sMatE}^{\dagger} \tag{2.4}
$$

is the orthogonal projection onto the subspace of matrices with nonzeros only in positions corresponding to the edge set E. Similarly the following projection

$$
P_{E^c} := \mathrm{u2sMatEc}\,\mathrm{u2sMatEc}^* = \mathrm{u2sMatEc}\,\mathrm{u2sMatEc}^{\dagger}. \tag{2.5}
$$

We can represent feasible points in the following way. Let $\hat{X} \in \mathcal{S}^n$ be such that $\mathrm{trace}\,\hat{X} = 1$, $\mathrm{trace}\,E_{ij}\hat{X} = 0$, for all $(i,j) \in \mathcal{E}$. We let V denote a $n \times (n-1)$ matrix satisfying $V^T e = 0$. For stability, we choose V with orthogonal columns and set

$$
P_V := VV^T, \tag{2.6}
$$

to be the projection onto the set of vectors v with $v^T e = 0$. (Nonorthogonal choices of V that exploit sparsity can be used.) Then, $X \succeq 0$ is primal feasible if and only if

$$
X = \hat{X} + \mathrm{Diag}\,(Vd) + \mathrm{u2sMatEc}\,(x), \text{ for some } d \in \Re^{n-1},\ x \in \Re^{m_c}.
$$

Similarly, $Z \succeq 0$ is dual feasible if and only if

$$
Z = zI + \mathrm{u2sMatE}\,(y) - E, \text{ for some } z \in \Re,\ y \in \Re^m.
$$

To obtain optimality conditions we use the dual problem (DTP). Recall the primal (TP) given in (2.2). Slater's CQ (strict feasibility) holds for (TP) and (DTP), which implies that we have strong duality with the Lagrangian dual (e.g. [19]). Since Slater's condition is also satisfied for the dual program, we have primal attainment and get the following well-known characterization of optimality for (TP), (DTP). (See e.g. [25].)

Theorem 2.2 *Let $\hat{X}$ be feasible for (TP). The primal-dual variables d, x, z, y with*

$$X = \hat{X} + \mathrm{Diag}\,(Vd) + \mathrm{u2sMatEc}\,(x) \succeq 0, \;\; Z = zI + \mathrm{u2sMatE}\,(y) - E \succeq 0$$

are optimal for (TP),(DTP) if and only if

$$ZX = 0 \quad \textit{(complementary slackness).}$$

■

To apply the p-d i-p method, we use the perturbed complementary slackness equation. By multiplying the linearized perturbed complementary slackness equation from the left with Z^{-1} we obtain the following equation;

$$\mathrm{Diag}\,(V\Delta d) + \mathrm{u2sMatEc}\,(\Delta x) + Z^{-1}(\Delta z I + \mathrm{u2sMatE}\,(\Delta y))X = \mu Z^{-1} - X. \tag{2.7}$$

Applying the trace operator on (2.7) yields

$$\Delta z \mathrm{trace}\,(Z^{-1}X) + \mathrm{trace}\,(Z^{-1}\mathrm{u2sMatE}\,(\Delta y)X) = \mathrm{trace}\,(\mu Z^{-1} - X). \tag{2.8}$$

By acting with operator P_E (see (2.4)) onto (2.7) we obtain the following system

$$\Delta z P_E(Z^{-1}X) + P_E(Z^{-1}\mathrm{u2sMatE}\,(\Delta y)X) = P_E(\mu Z^{-1} - X). \tag{2.9}$$

The equation (2.8) and the system of equations (2.9) make the system of $m+1$ equations and $m+1$ unknowns that we first solve. There are two equivalent ways for finding Δx. First, by applying the operator u2svecEc onto (2.7), symmetrized, and second, by applying the projection P_{E^c} (see (2.5)) onto (2.7), symmetrized. Analogously, we can find the diagonal of $\Delta X = \mathrm{Diag}\,(V\Delta d) + \mathrm{u2sMatEc}\,(\Delta x)$ in two equivalent ways. For details see the following summary.

SUMMARY: Improved HKM Direction for Lovász Theta Function Problem

Solve for $\Delta y, \Delta z$ in :

$$\begin{array}{rcl} \mathrm{trace}\,(\Delta z Z^{-1}X + Z^{-1}\mathrm{u2sMatE}\,(\Delta y)X) & = & \mathrm{trace}\,(\mu Z^{-1} - X) \\ P_E\,(\Delta z Z^{-1}X + Z^{-1}\mathrm{u2sMatE}\,(\Delta y)X) & = & P_E(\mu Z^{-1} - X) \end{array}$$

Backsolve :

$$\begin{array}{l} \Delta x = \mathrm{u2svecEc}\,(\mu Z^{-1} - X) \\ \qquad -0.5\mathrm{u2svecEc}\,(Z^{-1}(\Delta z I + \mathrm{u2sMatE}\,(\Delta y))X + X(\Delta z I + \mathrm{u2sMatE}\,(\Delta y))Z^{-1}) \\ \Delta d = V^T \mathrm{diag}\,(-\Delta z Z^{-1}X - Z^{-1}\mathrm{u2sMatE}\,(\Delta y)X + \mu Z^{-1} - X) \\ \Delta Z = \mathcal{A}^*(\Delta y) \end{array}$$

Equivalent backsolve :

$$\begin{array}{l} P_{E^c}(\Delta X) = P_{E^c}(\mu Z^{-1} - X) \\ \qquad -0.5 P_{E^c}(Z^{-1}(\Delta z I + \mathrm{u2sMatE}\,(\Delta y))X + X(\Delta z I + \mathrm{u2sMatE}\,(\Delta y))Z^{-1}) \\ P_E(\Delta X) = 0 \\ \mathrm{diag}\,(\Delta X) = P_V \mathrm{diag}\,(-\Delta z Z^{-1}X - Z^{-1}\mathrm{u2sMatE}\,(\Delta y)X + \mu Z^{-1} - X) \\ \Delta Z = \mathcal{A}^*(\Delta y) \end{array}$$

As for the Max-Cut we note that the direction is identical to the standard direction except that $P_E(\Delta X)$ is set to zero so need not be calculated; and, $\operatorname{diag}(\Delta X)$ is *centered*, equivalently if we denote with d the diagonal of the standard ΔX, then we reset the diagonal using $d - \frac{e^T d}{n} e$, i.e. we apply the orthogonal projection P_V that is defined in (2.6) onto d. These simple modifications guarantee exact primal feasibility throughout the iterations and also reduce the cost (number of multiplications in the backsolve) of an iteration.

2.3 Illustrative Two Dimensional Examples; Stability

We now consider a two dimensional primal-dual SDP pair (PSDP) and (DSDP). We compare the standard and simple HKM direction on problems where ill-conditioning arises and the HKM direction cannot be evaluated accurately.

2.3.1 Example Where Slater's CQ Fails

We use the data

$$C = \begin{pmatrix} -1 & -1 \\ -1 & 0 \end{pmatrix}, \quad A_1 = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix}, \quad b = \begin{pmatrix} \epsilon \\ -\epsilon \end{pmatrix}, \ \epsilon \geq 0.$$

Therefore the operator $\mathcal{A}$ and its adjoint are, respectively,

$$\mathcal{A}(X) = \begin{pmatrix} \operatorname{trace} A_1 X \\ \operatorname{trace} A_2 X \end{pmatrix}, \quad \mathcal{A}^*(y) = y_1 A_1 + y_2 A_2.$$

The primal constraints imply that $X \succeq 0$ is feasible if and only if

$$X = \hat{X} + \alpha \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1+\alpha & 0 \\ 0 & \epsilon \end{pmatrix}, \text{ with } \hat{X} = \begin{pmatrix} 1 & 0 \\ 0 & \epsilon \end{pmatrix}, 1+\alpha \geq 0. \tag{2.10}$$

Therefore, the optimal value is 0 and

$$X^* = \begin{pmatrix} 0 & 0 \\ 0 & \epsilon \end{pmatrix}$$

is the *unique optimal primal solution*. Slater's constraint qualification (strict feasibility) is satisfied for the primal if and only if $\epsilon > 0$; it is always satisfied for the dual. One dual optimal solution, independent of ϵ, is

$$y^* = -\frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \text{ with } Z^* = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

i.e.

$$Z^* = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix} - C \succeq 0, \quad Z^* X^* = 0.$$

For $\epsilon > 0$, this solution is unique and satisfies strict complementarity. Thus, the SDP is a *stable* program in this case, i.e. Slater's CQ holds for both primal and dual and the two primal constraints are linearly independent. However, for $\epsilon = 0$, the dual optimal set is unbounded, which can cause numerical difficulties. Difficulties also arise for ϵ close to zero. For example, in our tests with $\epsilon = 10^{-13}$ and a desired relative duality gap 10^{-12}, the standard HKM direction took 32 iterations, while the simplified direction took 16 iterations and it maintained exact primal-dual feasibility throughout the iterations. With $\epsilon = 10^{-13}$ and a desired relative duality gap 10^{-14}, the standard HKM direction took 42 iterations, while the simplified direction took 21 iterations. With $\epsilon = 0$ and a desired relative duality gap 10^{-14}, the algorithm converged with dual optimum $y^* = \begin{pmatrix} .5 \\ -1.5 \end{pmatrix}$; the standard HKM direction took 33 iterations, while the simplified direction took 18 iterations. For our line search we ensured that the minimum eigenvalue is nonnegative. (The customary line search uses a Cholesky factorization which fails since the feasible matrices X all have deficient rank if $\epsilon = 0$.)

2.3.2 Unstable Example

We use the same data as in Example 2.3.1 above except that we delete the second constraint and replace A_1 with $A_3 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$. Interestingly, even though the two constraints in Example 2.3.1 were linearly independent, the primal feasible set is unchanged with only one constraint, i.e. it is still the *ray* of the positive semidefinite cone $R = \left\{ \begin{pmatrix} \alpha & 0 \\ 0 & 0 \end{pmatrix} : \alpha \geq 0 \right\}$. Therefore the primal optimal value and optimum are unchanged. However, the dual optimal value is unattained. Numerical tests failed to find the optimal solution when starting from a primal feasible point.

2.3.3 Regularization Example

We use the same data as in Example 2.3.2 above. However, we now exploit the knowledge of the feasible set to change the dual, i.e. the dual constraint becomes

$$y_3 A_3 - C = Z + W, \text{ for some } Z \succeq 0, W = w_1 A_1 + w_2 A_2,$$

where A_1, A_2 are given in Example 2.3.1, see e.g. [2, 19]. This is equivalent to the dual in Example 2.3.1, since the matrix A_3 is linearly dependent on the two matrices A_1, A_2. We can derive an HKM type direction that finds $y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$ as the least squares solution of the underdetermined 1×3 system. This regularizes the problem and illustrates that identifying the feasible set in this way is useful.

3 Partial Exact Primal Feasibility for QAP

In this section we look at the Quadratic Assignment Problem, QAP, and its SDP relaxation given in [28] and modified in [21]. We find a rotation of the matrix space that identifies fixed elements so that we can apply our simplification technique for exact feasibility. We do this for a subset of the primal constraints and thus obtain only partial exact primal feasibility throughout the iterations.

This illustrates a procedure that could be applied to general SDPs once feasibility is attained for some of the constraints.

3.1 Background

The QAP in the trace formulation is

$$(QAP) \quad \mu^* := \min_{X\in\Pi} \ \operatorname{trace} AXBX^T - 2CX^T,$$

where A, B are real symmetric $n \times n$ matrices, C is a real $n \times n$ matrix, and Π denotes the set of permutation matrices. (We assume $n \geq 4$ to avoid trivialities.) One of the many applications of QAP is the modelling of the allocation of a set of n facilities to a set of n locations while minimizing the quadratic objective arising from the distance between the locations in combination with the flow between the facilities. See e.g. [18, 3].

We use the *Kronecker product*, or tensor product, of two matrices, $A \otimes B$, when discussing the quadratic assignment problem QAP; $\mathcal{M}^{n,k}$ is the space of $n \times k$ real matrices; $\mathcal{M}^n$ is the space of $n \times n$ real matrices; $\operatorname{vec}(X) \in \Re^{nk}$ denotes the vector formed from the columns of $X \in \mathcal{M}^{n,k}$; e_i is the ith unit vector, and here $E_{ij} := e_i e_j$ is a unit matrix in $\mathcal{M}^{n,k}$. We use the partition of a symmetric matrix $Y \in \mathcal{S}^{n^2+1}$ into blocks as follows.

$$Y = \left[\begin{array}{c|c} y_{00} & Y_0^T \\ \hline Y_0 & Z \end{array}\right] = \left[\begin{array}{c|ccc} y_{00} & Y^{01} & \dots & Y^{0n} \\ \hline Y^{10} & Y^{11} & \dots & Y^{1n} \\ \vdots & \vdots & \ddots & \vdots \\ Y^{n0} & Y^{n1} & \dots & Y^{nn} \end{array}\right], \tag{3.1}$$

where the index 0 refers to the first row and column. Hence $Y_0 \in \Re^{n^2}$, $Z \in \mathcal{S}^{n^2}$, $Y^{p0} \in \Re^n$, and $Y^{pq} \in \mathcal{M}^n$, $p, q \neq 0$. When referring to entry $r, s \in \{1, 2, \dots, n^2\}$ of Z, we use the pairs $(i, j), (k, l)$ with $i, j, k, l \in \{1, 2, \dots, n\}$. This identifies the element in row $r = (i-1)n + j$ and column $s = (k-1)n + l$ by $Y_{(i,j),(k,l)}$. This notation is going to simplify both the modeling and the presentation of properties of the relaxations. If we consider Z as a matrix consisting of $n \times n$ blocks Y^{ik}, then $Y_{(i,j),(k,l)}$ is just element (j, l) of block (i, k). We introduce more notation below as we need it.

3.2 SDP Relaxation and HKM Direction

The following SDP relaxation is described in [28]:

$$(SDP_{\mathcal{O}}) \quad \begin{array}{lll} \min & \operatorname{trace} L_Q Y & \\ \text{s.t.} & \mathrm{b}^0\mathrm{diag}(Y) = I, & \mathrm{o}^0\mathrm{diag}(Y) = I \\ & \operatorname{arrow}(Y) = e_0, & \operatorname{trace} DY = 0 \\ & Y \succeq 0, \quad Y \in \mathcal{S}^{n^2+1}, & \end{array} \tag{3.2}$$

where

$$D := \begin{bmatrix} n & -e^T \otimes e^T \\ -e \otimes e & I \otimes E \end{bmatrix} + \begin{bmatrix} n & -e^T \otimes e^T \\ -e \otimes e & E \otimes I \end{bmatrix}.$$

Let $x = \mathrm{vec}\,(X)$ denote the vector obtained columnwise from $X \in \mathcal{M}^n$. The matrix $L_Q \in \mathcal{S}^{n^2+1}$ is motivated from

$$\mathrm{trace}\, AXBX^T - 2CX^T = \mathrm{trace}\, L_Q Y_x,$$

for

$$Y_x = \begin{bmatrix} 1 & x^T \\ x & xx^T \end{bmatrix}. \tag{3.3}$$

Thus

$$L_Q := \begin{bmatrix} 0 & -\mathrm{vec}\,(C)^T \\ -\mathrm{vec}\,(C) & B \otimes A \end{bmatrix}.$$

The operators acting on the matrix $Y \in \mathcal{S}^{n^2+1}$ are defined as follows.

$$\begin{array}{ll} \mathrm{b}^0\mathrm{diag}\,(Y) := \sum_{k=1}^{n} Y_{(k,\cdot),(k,\cdot)} & \text{(sum of diagonal blocks)} \\ \mathrm{o}^0\mathrm{diag}\,(Y) := \sum_{k=1}^{n} Y_{(\cdot,k),(\cdot,k)} & \text{(sum of diagonal elements)} \\ \mathrm{arrow}\,(Y) := \mathrm{diag}\,(Y) - \left(0, (Y_{0,1:n^2})^T\right) & \text{(diagonal minus 0 row).} \end{array}$$

For more details see [28]. Slater's condition fails for $(SDP_{\mathcal{O}})$, since $D \succeq 0$ and $\mathrm{trace}\, DY = 0$. The first step in the preprocessing is to satisfy Slater's condition. We can exploit the structure and project onto the minimal face to get a simpler SDP. The minimal face can be expressed as (see [28]).

$$\hat{V} \mathcal{S}_{(n-1)^2+1} \hat{V}^T,$$

where $\hat{V}$ is an $(n^2+1) \times ((n-1)^2+1)$ matrix,

$$\hat{V} := \left[\begin{array}{c|c} 1 & 0 \\ \hline \frac{1}{n}(e \otimes e) & V \otimes V \end{array}\right],$$

and V is an $n \times (n-1)$ matrix containing the basis of the orthogonal complement of e i.e., $V^T e = 0$; e.g.

$$V := \left[\begin{array}{c} I_{n-1} \\ \hline -e^T \end{array}\right].$$

Let us define the operator $\mathcal{G}_{\bar{J}} : \mathcal{S}^{n^2+1} \to \mathcal{S}^{n^2+1}$, called the *gangster operator*, as it *shoots holes in a matrix.* For matrix Y and $i, j = 1, \ldots, n^2+1$, the (i,j) component of the gangster operator is defined by

$$(\mathcal{G}_{\bar{J}}(Y))_{ij} := \begin{cases} Y_{ij} & \text{if } (i,j) \in \bar{J} \\ 0 & \text{otherwise.} \end{cases}$$

The set $\bar{J}$ is the union of two sets; $\bar{J} = \hat{J} \cup (0,0)$ where $\hat{J}$ is a set of indices of (up to symmetry) the off-diagonal elements of the diagonal blocks and the diagonal elements of the off-diagonal blocks.

$$\begin{array}{rcl} \hat{J} & := & \{(i,j) : i = (p-1)n + q, j = (p-1)n + r, q \neq r\} \;\cup \\ & & \{(i,j) : i = (p-1)n + q, j = (r-1)n + q, p \neq r, (p, r \neq n) \\ & & \quad ((r,p),(p,r) \neq (n-2, n-1), (n-1, n-2))\}. \end{array} \tag{3.4}$$

The off-diagonal block $(n-2, n-1)$ and the last column of off-diagonal blocks are redundant and so excluded (up to symmetry) from $\hat{J}$.

The projection onto the minimal face in conjunction with the gangster operator, helped in eliminating many redundant constraints and reduced the number of variables. The resulting equivalent relaxation is greatly simplified

$$
(QAP_{R2}) \qquad \begin{array}{rll} \mu_{R2} := & \min & \operatorname{trace} \bar{L}R := \operatorname{trace}(\hat{V}^T L_Q \hat{V})R \\ & \text{s.t.} & \mathcal{G}_{\bar{J}}(\hat{V}R\hat{V}^T) = E_{00} \\ & & R \succeq 0, \end{array} \tag{3.5}
$$

where $R, \bar{L} \in \mathcal{S}^{(n-1)^2+1}$. The constraint $\mathcal{G}_{\bar{J}}(\hat{V} \cdot \hat{V}^T)$ is full rank (onto).

The dual of (QAP_{R2}) is (we use S for the dual variable)

$$
(DQAP_{R2}) \qquad \begin{array}{rll} \nu_{R2} := & \max & S_{00} \\ & \text{s.t.} & \hat{V}^T(\mathcal{G}^*_{\bar{J}}(S))\hat{V} \preceq \bar{L}. \end{array} \tag{3.6}
$$

Note that the gangster operator is self–adjoint, i.e. $\mathcal{G}^*_{\bar{J}} = \mathcal{G}_{\bar{J}}$. Slater's CQ is satisfied for both primal and dual programs.

Theorem 3.1 *The primal-dual variables R, S, Z with $R \succeq 0, Z \succeq 0$ are optimal for (QAP_{R2}), $(DQAP_{R2})$ if and only if*

$$
\begin{array}{ll} \hat{V}^T\mathcal{G}^*_{\bar{J}}(S)\hat{V} + Z - \bar{L} = 0 & \textit{(dual feasibility)} \\ \mathcal{G}_{\bar{J}}(\hat{V}R\hat{V}^T) - E_{00} = 0 & \textit{(primal feasibility)} \\ ZR = 0 & \textit{(complementary slackness).} \end{array}
$$

■

After perturbing the complementarity conditions with barrier parameter $\mu > 0$, we obtain the following system

$$
\begin{array}{rcll} R_D & := & \hat{V}^T\mathcal{G}^*_{\bar{J}}(S)\hat{V} + Z - \bar{L} & = 0 \\ R_P & := & \mathcal{G}_{\bar{J}}(\hat{V}R\hat{V}^T) - E_{00} & = 0 \\ R_{ZR} & := & ZR - \mu I & = 0, \end{array} \tag{3.7}
$$

where $R, Z \in \mathcal{S}^{(n-1)^2+1}$, $R \succeq 0, Z \succeq 0$ and $S \in \mathcal{S}^{n^2+1}$. We now solve the following linearization;

$$
\begin{array}{rcl} \hat{V}^T\mathcal{G}^*{}_{\bar{J}}(\Delta S)\hat{V} + \Delta Z & = & -R_D \\ \mathcal{G}_{\bar{J}}(\hat{V}(\Delta R)\hat{V}^T) & = & -R_P \\ Z\Delta R + \Delta Z R & = & -R_{ZR}. \end{array}
$$

From dual feasibility we have

$$
\Delta Z = -\hat{V}^T\mathcal{G}^*{}_{\bar{J}}(\Delta S)\hat{V} - R_D.
$$

After substituting this into the third equation, we have

$$
\Delta R = Z^{-1}\hat{V}^T\mathcal{G}^*{}_{\bar{J}}(\Delta S)\hat{V}R + Z^{-1}R_D R - Z^{-1}R_{ZR}.
$$

(The above is symmetrized in the back substitution step.) After substituting for ΔR into the primal feasibility equation we obtain the following final positive definite system for ΔS.

$$\mathcal{G}_{\bar{J}}(\hat{V}Z^{-1}\hat{V}^T\mathcal{G}^*_{\bar{J}}(\Delta S)\hat{V}R\hat{V}^T) \;=\; \mathcal{G}_{\bar{J}}(\hat{V}(Z^{-1}R_{ZR} - Z^{-1}R_D R)\hat{V}^T) - R_P. \tag{3.8}$$

The size of the above linear system is $n^3 - 2n^2 + 1$.

We now find strictly feasible (starting) points for (QAP_{R2}) and $(DQAP_{R2})$. The following two lemmas correct several typos in [28].

Lemma 3.2 *Define the* $((n-1)^2+1) \times ((n-1)^2+1)$ *matrix*

$$\hat{R} := \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \frac{1}{n^2(n-1)}(nI_{n-1} - E_{n-1}) \otimes (nI_{n-1} - E_{n-1}) \end{array}\right],$$

where E_{n-1} *is* $(n-1) \times (n-1)$ *matrix of all ones. Then* $\hat{R}$ *is positive definite and feasible for* (QAP_{R2}).

Proof. First, note that $\hat{R}$ is positive definite, since

$$x^T E_{n-1} x \leq \|E_{n-1}\| \|x\|^2 = (n-1)\|x\|^2 < n\|x\|^2$$

implies $nI_{n-1} - E_{n-1}$ is positive definite.

We complete the proof by showing that

$$\hat{V}\hat{R}\hat{V}^T = \hat{Y},$$

where $\hat{Y}$ is the barycenter for the unprojected QAP, i.e.

$$\hat{Y} = \frac{1}{n!}\sum_{X \in \Pi} Y_x, \quad x = \operatorname{vec} X,$$

and Y_x is defined in (3.3).

For simplicity, let us denote $I := I_{n-1}, E := E_{n-1}$.

$$\begin{aligned}
\hat{V}\hat{R}\hat{V}^T &= \left[\begin{array}{c|c} 1 & 0 \\ \hline \frac{1}{n}(e\otimes e) & V \otimes V \end{array}\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \frac{1}{n^2(n-1)}(nI - E)\otimes(nI-E) \end{array}\right] \left[\begin{array}{c|c} 1 & \frac{1}{n}(e^T\otimes e^T) \\ \hline 0 & V^T \otimes V^T \end{array}\right] \\
&= \left[\begin{array}{c|c} 1 & 0 \\ \hline \frac{1}{n}(e\otimes e) & V \otimes V \end{array}\right] \left[\begin{array}{c|c} 1 & \frac{1}{n}(e^T\otimes e^T) \\ \hline 0 & \frac{1}{n^2(n-1)}(nI - E)\otimes(nI-E)(V^T\otimes V^T) \end{array}\right] \\
&= \left[\begin{array}{c|c} 1 & \frac{1}{n}(e^T\otimes e^T) \\ \hline \frac{1}{n}(e\otimes e) & \frac{1}{n^2}E\otimes E + \frac{1}{n^2(n-1)}(nVV^T - VEV^T)\otimes(nVV^T - VEV^T) \end{array}\right].
\end{aligned}$$

Now it remains to show that $nVV^T - VE_{n-1}V^T = nI_n - E_n$. We have

$$\begin{aligned}
nVV^T - VE_{n-1}V^T &= n\left[\begin{array}{c|c} I_{n-1} & -e_{n-1} \\ \hline -e^T_{n-1} & (n-1) \end{array}\right] - \left[\begin{array}{c|c} E_{n-1} & -(n-1)e_{n-1} \\ \hline -(n-1)e^T_{n-1} & (n-1)^2 \end{array}\right] \\
&= \left[\begin{array}{c|c} nI_{n-1} - E_{n-1} & -e_{n-1} \\ \hline -e^T_{n-1} & n-1 \end{array}\right] \\
&= nI_n - E_n.
\end{aligned}$$

■

We now provide a strictly dual-feasible point.

Lemma 3.3 *Let*

$$\hat{Y} = \begin{bmatrix} M+n-1 & 0 \\ 0 & I_n \otimes (I_n - E_n) \end{bmatrix},$$

where E_n is $n \times n$ matrix of all ones. Then for $M \in \Re$ large enough, $\hat{Y}$ is positive definite and feasible for $(DQAP_{R2})$.

Proof. It is sufficient to show that $\hat{V}^T(\mathcal{G}_{\hat{J}}^*(\hat{Y}) + \hat{Y}_{00}e_0e_0^T)\hat{V}$ is positive definite.

$$\begin{aligned}
\hat{V}^T(\mathcal{G}_{\hat{J}}^*(\hat{Y}) + \hat{Y}_{00}e_0e_0^T)\hat{V} &= \begin{bmatrix} M & 0 \\ 0 & (V\otimes V)^T(I_n \otimes (I_n - E_n))(V \otimes V) \end{bmatrix} \\
&= \begin{bmatrix} M & 0 \\ 0 & (V^T I_n V) \otimes (V^T(I_n - E_n)V) \end{bmatrix} \\
&= \begin{bmatrix} M & 0 \\ 0 & V^TV \otimes V^TV \end{bmatrix} \\
&= \begin{bmatrix} M & 0 \\ 0 & (I_{n-1} + E_{n-1}) \otimes (I_{n-1} + E_{n-1}) \end{bmatrix}.
\end{aligned}$$

Since $I_{n-1} + E_{n-1}$ is positive definite we have that for $M \in \Re$ large enough,

$$\begin{bmatrix} M & 0 \\ 0 & (I_{n-1} + E_{n-1}) \otimes (I_{n-1} + E_{n-1}) \end{bmatrix}$$

is positive definite. ■

3.3 Preprocessing and Simplified HKM Direction

We continue preprocessing and use the approach described in [21]. This results in a reformulation of the primal constraints and the derivation of the modified HKM direction. More precisely, we use a particular solution and the general solution of the homogeneous equation to obtain the reformulation

$$R = \hat{R} + \mathcal{H}(r), \tag{3.9}$$

where $\mathcal{H}$ is a linear one-one (full column rank) operator.

Below we redefine $\hat{V}$ by subtracting the sum of all the columns except the first from the first column. This subtraction does not change the range space and the minimal cone, but results in an identity matrix being part of this new matrix and allows for simplification and elimination of many of the constraints. Thus, we set

$$\hat{V} \leftarrow \hat{V}M,$$

where the nonsingular $((n-1)^2+1) \times ((n-1)^2+1)$ matrix

$$M := \left[\begin{array}{c|c} 1 & 0 \\ \hline -\frac{1}{n}e & I \end{array} \right], \tag{3.10}$$

i.e. we subtract ($\frac{1}{n}$ times) all the columns from the first column but leave the other columns unchanged. The new $\hat{V}$ is now

$$\hat{V} = \left[\begin{array}{c|c|c||c|c} 1_1 & 0_{1\times n-1} & 0_{1\times n-1} & 0 & \dots \\ \hline\hline 0_{n-1\times 1} & I_{n-1} & 0_{n-1} & 0 & \dots \\ 1_1 & -e_{n-1}^T & 0_{1\times n-1} & 0 & \dots \\ \hline\hline 0_{n-1\times 1} & 0_{n-1} & I_{n-1} & 0 & \dots \\ 1_1 & 0 & -e_{n-1}^T & 0 & \dots \\ \hline \dots & \dots & \dots & & \\ \hline\hline e_{n-1} & -I_{n-1} & -I_{n-1} & \dots & \\ \hline\hline -(n-2) & e_{n-1}^T & e_{n-1}^T & \dots & \end{array} \right], \tag{3.11}$$

i.e. $\hat{V}$ is $(n^2+1) \times ((n-1)^2+1)$ and consists of one row and n blocks of rows with n rows in each block;

$$\hat{V}^T = \left[\begin{array}{c||cc|cc|c||c||c} 1_1 & 0_{1\times n-1} & 1_1 & 0_{1\times n-1} & 1_1 & \dots & e_{n-1}^T & -(n-2) \\ \hline 0_{n-1\times 1} & I_{n-1} & -e_{n-1} & 0_{n-1} & 0 & \dots & -I_{n-1} & e_{n-1} \\ 0_{n-1\times 1} & 0_{n-1} & 0_{n-1\times 1} & I_{n-1} & -e_{n-1} & \dots & -I_{n-1} & e_{n-1} \\ \hline 0 & 0 & 0 & 0 & 0 & & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{array} \right]. \tag{3.12}$$

Here e_{n-1} denotes the $(n-1) \times 1$ vector of all ones. We use that notation in the rest of the chapter, when there is no confusion.

Remark 3.4 *Since $\hat{V}$ redefined, the feasible $\hat{R}$ for (QAP_{R2}) given in Lemma 3.2 must also be redefined. Namely, we set*

$$\hat{R} \leftarrow M^{-1}\hat{R}(M^{-1})^T,$$

where M is defined in (3.10). This new $\hat{R}$ satisfies all the properties in Lemma 3.5 below.

Note, that we can set zeros in the matrix $\bar{L}$ in the positions that correspond to gangster positions.

The primal has $n^3 - 2n^2 + 1$ equality constraints from the gangster operator and the matrix R has $t((n-1)^2+1)$ variables. Since the matrix $\hat{V}$ contains an identity matrix, we can move the gangster constraints onto the matrix R. This can be thought of as a pivot step and change of dictionary or representation of the problem. To simplifiy the calculations below, we recall that the minimal face (cone) is

$$\left\{ Y : Y = \hat{V}R\hat{V}^T, \quad R \succeq 0 \right\}. \tag{3.13}$$

Note that the redefined $\hat{V}$ does not change the range space and leaves the minimal cone unchanged. We now expand the expression for Y. We use superscripts to denote the block structure and subscripts to denote the block sizes. By abuse of notation, we have the same superscript for two different adjacent blocks that have different sizes. The block sizes correspond to the multiplication in (3.13). Then

$$Y = \left[\begin{array}{c||cc|c|cc}
Y^{00}_{1\times 1} & Y^{01}_{1\times n-1} & Y^{01}_{1\times 1} & \ldots & Y^{0n}_{1\times n-1} & Y^{0n}_{1\times 1} \\
\hline\hline
Y^{10}_{n-1\times 1} & Y^{11}_{n-1\times n-1} & Y^{11}_{n-1\times 1} & \ldots & & \\
Y^{10}_{1\times 1} & Y^{11}_{1\times n-1} & Y^{11}_{1\times 1} & \ldots & & \\
\hline
Y^{20}_{n-1\times 1} & Y^{21}_{n-1\times n-1} & Y^{21}_{n-1\times 1} & \ldots & & \\
Y^{20}_{1\times 1} & Y^{21}_{1\times n-1} & Y^{21}_{1\times 1} & \ldots & & \\
\hline
\ldots & \ldots & \ldots & \ldots & \ldots & \\
\hline
Y^{(n-1)0}_{n-1\times 1} & Y^{(n-1)1}_{n-1\times n-1} & Y^{(n-1)1}_{n-1\times 1} & \ldots & & \\
Y^{(n-1)0}_{1\times 1} & Y^{(n-1)1}_{1\times n-1} & Y^{(n-1)1}_{1\times 1} & \ldots & & \\
\hline\hline
Y^{n0}_{n-1\times 1} & Y^{n1}_{n-1\times n-1} & Y^{n1}_{n-1\times 1} & \ldots & & \\
\hline\hline
Y^{n0}_{1\times 1} & Y^{n1}_{1\times n-1} & Y^{n1}_{1\times 1} & \ldots & Y^{nn}_{1\times n-1} & Y^{nn}_{1\times 1}
\end{array}\right], \tag{3.14}$$

where the zeros in Y correspond to the off-diagonal elements of the diagonal blocks and the diagonal elements of the off-diagonal blocks. R is blocked appropriately corresponding to the column blocks of $\hat{V}$

$$R = \left[\begin{array}{c|ccc}
R^{00}_{1\times 1} & R^{01}_{1\times n-1} & \ldots & R^{0(n-1)}_{1\times n-1} \\
\hline
R^{10}_{n-1\times 1} & R^{11}_{n-1\times n-1} & \ldots & R^{1(n-1)}_{n-1\times n-1} \\
R^{20}_{n-1\times 1} & R^{21}_{n-1\times n-1} & \ldots & R^{2(n-1)}_{n-1\times n-1} \\
\ldots & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & R^{(n-1)(n-1)}_{n-1\times n-1}
\end{array}\right]. \tag{3.15}$$

We now look at the gangster constraints and move them onto R. (For more details see [21].) We will use conditions C1-C4 to simplify the backsolve for the HKM direction.

Lemma 3.5 *Let $R \in S^{(n-1)^2+1} \succeq 0$. Then R is feasible in (3.5) if and only if:*

$$\begin{cases}
\bullet\textit{C1:}\quad R_{00} = 1 \\
\bullet\textit{C2: the diagonal blocks are diagonal} \\
\bullet\textit{C3: the } \text{arrow } \textit{operator holds} \\
\bullet\textit{C4: the diagonals of the off-diagonal blocks are 0, i.e.} \\
\qquad 0_{n-1\times 1} = \left(-(n-2) + \sum_{j\geq 1} R^{0j}_{1\times n-1} e_{n-1} + \sum_{i\geq 1} R^{i0}_{n-1\times 1} - \sum_{i,j\geq 1} R^{ij}_{n-1\times n-1}\right) e_{n-1} \\
\bullet\textit{C5:}\quad E_{n-1\times n-1} - \sum_{j\geq 1} e_{n-1} R^{0j}_{1\times n-1} - \sum_{i\geq 1} R^{i0}_{n-1\times 1} e^T_{n-1} + \sum_{i,j\geq 1} R^{ij}_{n-1\times n-1} \textit{ is diagonal} \\
\bullet\textit{C6:}\quad 0 = 1 - \operatorname{trace}\left(R^{ii}_{n-1\times n-1} + R^{jj}_{n-1\times n-1}\right) + e^T\left(R^{ij}_{n-1\times n-1}\right)e, \quad \forall 1 \leq i < j \leq n-1 \\
\bullet\quad R \succeq 0.
\end{cases}$$

■

We now can define the operator $\mathcal{H}$ in (3.9). Let us denote with $\hat{J}_s$ the set of gangster indices defined as in (3.4) for $((n-1)^2+1) \times ((n-1)^2+1)$ matrices and with $\hat{J}_{s_c}$ the complement of $\hat{J}_s$. Let $s = |\hat{J}_s|$, $s_c = |\hat{J}_{s_c}|$ and $\bar{J}_s = \hat{J}_s \cup (0,0)$. Define the linear operator $\mathrm{u2sMatGs}_c : \Re^{s_c} \to \mathcal{S}^{(n-1)^2+1}$,

$$(\mathrm{u2sMatGs}_c(r))_{ij} := \begin{cases} r_{ij}/\sqrt{2} & \text{if } (i,j) \in \hat{J}_{s_c} \\ 0 & \text{otherwise.} \end{cases}$$

Here we identify the vector components $r = (r_k) \in \Re^{s_c}$, ordered columnwise from $R \in \mathcal{S}^n$, with r_{ij}, $(i,j) \in \bar{J}_{s_c}$. Let $\mathrm{u2svecGs}_c := \mathrm{u2sMatGs}_c^{\dagger}$ denote the *Moore-Penrose generalized inverse* mapping. This is an inverse mapping if we restrict to the subspace of matrices with zero on the gangster positions. The adjoint operator $\mathrm{u2sMatGs}_c^* = \mathrm{u2svecGs}_c$, since

$$\begin{aligned} \langle \mathrm{u2sMatGs}_c(v), S \rangle &= \operatorname{trace} \mathrm{u2sMatGs}_c(v) S \\ &= v^T \mathrm{u2svecGs}_c(S) = \langle v, \mathrm{u2svecGs}_c(S) \rangle . \end{aligned}$$

The linear operator

$$P_{\mathrm{arr}} := \operatorname{arrow} \operatorname{arrow}^{\dagger},$$

is the orthogonal projection of symmetric matrices with first element equal to zero onto matrices where the first row, first column, and diagonal are all equal. Let $\hat{R}$ be such that $\mathcal{G}_{\bar{J}_s}(\hat{R}) = E_{00}$ and $\operatorname{arrow}(\hat{R}) = e_0$. Then R is primal feasible if and only if

$$\begin{array}{c} R = \hat{R} + \mathrm{u2sMatGs}_c(r), \text{ where} \\ r \in \mathcal{R}^{s_c}, \text{ arrow}\,(\mathrm{u2sMatGs}_c(r)) = 0, \text{ and } C_5, C_6 \text{ from Lemma (3.5) are satisfied.} \end{array} \tag{3.16}$$

Thus $\mathcal{H}$ is defined in (3.16). By linearizing the perturbed complementary slackness from (3.7) and setting $R = \hat{R} + \mathrm{u2sMatGs}_c(r)$ and $Z = \bar{L} - \hat{V}^T \mathcal{G}_{\bar{J}}^*(S) \hat{V}$, we get

$$\mathrm{u2sMatGs}_c(\Delta r) - Z^{-1}(\hat{V}^T \mathcal{G}_{\bar{J}}^*(\Delta S) \hat{V}) R = -Z^{-1} R_{ZR}. \tag{3.17}$$

Acting with operator $\mathcal{G}_{\bar{J}_s}$ onto the previous equation we obtain the following (positive definite) linear system in ΔS

$$\mathcal{G}_{\bar{J}_s}(Z^{-1} \hat{V}^T \mathcal{G}_{\bar{J}}^*(\Delta S) \hat{V} R) = -\mathcal{G}_{\bar{J}_s}(\mu Z^{-1} - R).$$

By acting with the operator $\mathrm{u2svecGs}_c$ onto the symmetrized equation (3.17), we get

$$\Delta r = \frac{1}{2} \mathrm{u2svecGs}_c(Z^{-1} \hat{V}^T \mathcal{G}_{\bar{J}}^*(\Delta S) \hat{V} R + R \hat{V}^T \mathcal{G}_{\bar{J}}^*(\Delta S) \hat{V} Z^{-1}) + \mathrm{u2svecGs}_c(\mu Z^{-1} - R).$$

For $\Delta R = \mathrm{u2sMatGs}_c(\Delta r)$ we set $(\Delta R)(0,0) = 0$. Since the diagonal, first row, and first column of ΔR should be equal, we apply the operator P_{arr} onto ΔR. Namely, if Δd is the diagonal and Δr is the first row of ΔR, then we reset the diagonal using

$$\Delta d \leftarrow \frac{1}{2}(\Delta d + \Delta r).$$

Now, for ΔR we set first row to be equal to the first column that is equal to the diagonal Δd.

SUMMARY: Improved HKM Direction for QAP

$$\begin{array}{ll}
\textbf{Solve} \text{ for } \Delta S \text{ in}: & \mathcal{G}_{\bar{J}_s}(Z^{-1}\hat{V}^T\mathcal{G}^*_{\bar{J}}(\Delta S)\hat{V}R) = \mathcal{G}_{\bar{J}_s}(R-\mu Z^{-1}) \\
\textbf{Backsolve}: & \Delta r = 0.5\text{u2svecGs}_c(Z^{-1}\hat{V}^T\mathcal{G}^*_{\bar{J}}(\Delta S)\hat{V}R + R\hat{V}^T\mathcal{G}^*_{\bar{J}}(\Delta S)\hat{V}Z^{-1}) \\
& \quad +\text{u2svecGs}_c(\mu Z^{-1} - R) \\
& (\Delta R)(0,0) = 0 \\
& \Delta R = P_{\text{arr}}(\Delta R) \\
& \Delta Z = -\hat{V}^T\mathcal{G}^*_{\bar{J}}(\Delta S)\hat{V}
\end{array}$$

Therefore, in each iteration, conditions $C1$–$C4$ in Lemma 3.5 are satisfied exactly.

Remark 3.6 *The conditions $C5$ and $C6$ from Lemma 3.5 should also be used for for improving the HKM direction, but they are overly complicated for practical use. For instance, let us look closely to the condition $C5$*

$$E_{n-1\times n-1} - \sum_{j\geq 1} e_{n-1}R^{0j}_{1\times n-1} - \sum_{i\geq 1} R^{i0}_{n-1\times 1}e^T_{n-1} + \sum_{i,j\geq 1} R^{ij}_{n-1\times n-1}$$

is diagonal. For $s,t \in \{1,\ldots,n-1\}, s \leq t$ this reduces to

$$\sum_{j\geq 1}\Delta R^{0j}_t + \sum_{i\geq 1}\Delta R^{i0}_s - \sum_{i,j\geq 1}\Delta R^{ij}_{st} = 0, \tag{3.18}$$

which is equivalent to

$$\sum_{j\geq 1}(\Delta R^{0j}_t + \Delta R^{0j}_s) - \sum_{i<j}(\Delta R^{ij}_{st} + \Delta R^{ij}_{ts}) = 0.$$

Thus in each step ΔR should be fixed such that (3.18) is satisfied, $\forall s,t \in \{1,\ldots,n-1\}, s \leq t$.

4 Concluding Remarks

In this paper we have presented a preprocessing approach for SDPs that provides a simplification (improvement) for the HKM search direction. The simplification exploits the structure of individual SDPs and changes the backsolve steps to reduce the arithmetic while maintaining exact primal (and dual) feasibility. The method is illustrated on three problem instances: Max-Cut; Lovász theta function; and Quadratic Assignment. Similar techniques can be applied to many other relaxations of hard combinatorial problems, e.g. to the SDP relaxation of the graph partitioning problem presented in [26]. These problems all contain binary constraints which implies that all feasible points of the relaxation have either fixed elements and/or zeros.

We also included two 2 dimensional examples that illustrated the stability benefits of maintaining exact feasibility.

Convergence analysis for the new direction is exactly the same as for the standard HKM direction, since this is an 'exact' Newton step that ignores the roundoff, i.e. existing convergence theorems hold.

We note that the simplification can be applied to the complete MZ family of search directions. Following [13, Section 10.3], define the symmetrization operator

$$\mathcal{S}_P(U) := \frac{1}{2}\left[PUP^{-1} + (PUP^{-1})^T\right], \qquad \mathcal{S}_P : \mathcal{M}^n \rightarrow \mathcal{S}^n,$$

where P is a given nonsingular matrix. If $P = Z^{1/2}$, then the standard HKM direction is the Newton direction for the system (1.3), where the last equation is replaced by the symmetrized perturbed equation $\mathcal{S}_P(XZ) = \mu I$. (Using XZ rather than ZX is a minor modification.) The dual HKM direction uses $P = X^{-1/2}$. Using $P = I$ yields the so-called *AHO direction*, see [1]; while $P = W^{-1/2}, W = Z^{-1/2}(Z^{1/2}XZ^{1/2})^{1/2}Z^{-1/2}$ is the *NT direction* studied in [16, 17]. Arbitrary choices for nonsingular P yield the MZ family of search directions, see [27]. Thus we consider the symmetrization of (1.4)

$$\begin{array}{lcl} \mathcal{A}^*(\Delta y) - \Delta Z & = & -R_D \\ \mathcal{A}(\Delta X) & = & -R_P \\ \mathcal{S}_P(Z(\Delta X) + (\Delta Z)X) & = & = \mu I - \mathcal{S}_P(R_{ZX}). \end{array} \tag{4.1}$$

The solution to this linearization (under existence assumptions) is given by:

$$\begin{array}{l} \textbf{Solve} \text{ for } \Delta y \text{ in :} \\ \quad \mathcal{A}\left[(\mathcal{S}_P Z\cdot)^{-1}(\mathcal{A}^*(\Delta y)X)\right] = R_P - \mathcal{A}\left[(\mathcal{S}_P Z\cdot)^{-1}((R_{ZX} - R_D X\right] \\ \textbf{Backsolve} : \\ \quad \Delta Z = R_D + \mathcal{A}^*(\Delta y) \\ \quad \Delta X = (\mathcal{S}_P Z\cdot)^{-1}\left[\mu I - \mathcal{S}_P(R_{ZX} - \Delta Z X)\right]. \end{array} \tag{4.2}$$

Therefore the backsolve steps for both ΔZ and ΔX can be simplified/improved under the appropriate special structure assumptions.

One can generalize this approach to preprocessing for general SDPs. For an LP constraint $Ax = b$, we find permutation matrices P, Q so that the equivalent constraint $PAQ(Q^T x) = Pb$ yields an equivalent constraint of form

$$(PAQ)y = \begin{pmatrix} \bar{A} & 0 \\ C & D \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} \bar{b} \\ d \end{pmatrix}$$

with $\bar{A}$ nonsingular or full row rank with relatively low dimensional null space. For example, in the nonsingular case, we get $v = \bar{A}^{-1}\bar{b}$ and the variables Qv can be eliminated. Thus we have to identify submatrices of type $\bar{A}$. The situation in the SDP case is similar, since we can express the primal SDP constraint $\mathcal{A}X = b$ using $(\operatorname{trace} A_i X) = b_i$, for appropriate symmetric matrices A_i. We then use $x = \operatorname{svec} X$, the vector formed from the diagonal and upper triangular part of X (columnwise), with the upper triangular part multiplied by $\sqrt{2}$, i.e. $\operatorname{trace} XY = \operatorname{svec} X^T \operatorname{svec} Y$. If we let the rows of A be $a_i = (\operatorname{svec} A_i)^T$, then we get the equivalent constraint $Ax = b$ and we have the equivalent problem of identifying submatrices $\bar{A}$ of A.

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