

On the Nesterov-Todd direction in semidefinite programming

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Abstract

Nesterov and Todd discuss several path-following and potential-reduction interior-point methods for certain convex programming problems. In the special case of semidefinite programming, we discuss how to compute the corresponding directions efficiently, how to view them as Newton directions, and how to take Mehrotra predictor-corrector steps in this framework. We also provide some computational results suggesting that our algorithm is more robust than alternative methods.

Key words: semidefinite programming, Newton direction, predictor-corrector.

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1 Introduction

This paper studies interior-point methods for the solution of the semidefinite programming problem (SDP) based on the search direction described by Nesterov and Todd [13, 14]. For simplicity, we call this direction the Nesterov-Todd (NT) direction. We consider the SDP given in the following standard form:

$$\begin{aligned} (SDP) \quad \min_X \quad & C \bullet X \\ & A_i \bullet X = b_i, \quad i = 1, \dots, m \\ & X \succeq 0, \end{aligned} \tag{1}$$

where $A_i \in \mathcal{S}\mathcal{R}^{n \times n}$, $b \in \mathbb{R}^m$, $C \in \mathcal{S}\mathcal{R}^{n \times n}$ are given, and $X \in \mathcal{S}\mathcal{R}^{n \times n}$. Here $\mathcal{S}\mathcal{R}^{n \times n}$ denotes the space of $n \times n$ symmetric matrices, and $X \succeq 0$ indicates that X is positive semidefinite. We assume that the A_i 's are linearly independent. The dual problem associated with (SDP) is:

$$\begin{aligned} (SDD) \quad \max_{y,S} \quad & b^T y \\ & \sum_{i=1}^m y_i A_i + S = C \\ & S \succeq 0, \end{aligned} \tag{2}$$

where $y \in \mathbb{R}^m$ and $S \in \mathcal{S}\mathcal{R}^{n \times n}$. Many interior-point algorithms for linear programming problems can be directly extended to solve SDPs, which have a wide range of applications in both continuous and combinatorial optimization (we refer the reader to [18] for an extensive list of applications).

In the study of interior-point methods for SDP, it is desirable to generate symmetric direction matrices. This can be achieved by symmetrizing (with respect to an invertible matrix P) the first order equation corresponding to the complementarity equation in the Newton system, as in Monteiro [12] and Y. Zhang [19]. This symmetrization of the Newton system gives rise to different search directions for different P . We give a simple proof that the symmetrized Newton system has a unique solution under certain conditions related to those appearing in the work of Shida, Shindoh and Kojima [15]. Based on this uniqueness result, we show that the NT direction can be expressed as the solution of a symmetrized Newton system. We note that very recently, independently of our work, Sturm and S. Zhang [16] described how to generate the NT direction as a Newton search direction for primal-dual path-following algorithms for SDP using

a symmetric primal-dual transformation, similar to Section 6 in [13]; this approach is very different from ours, and does not appear to lead directly to a Mehrotra-type predictor-corrector variant [10].

One of the main components of this paper is the implementation of such a predictor-corrector algorithm based on the NT direction where the direction is computed via a linear least squares problem. We discuss issues related to efficient implementation, which are briefly described in the following paragraphs. For simplicity, we will refer to this method as Algorithm NT-PC-LS.

In solving for the NT direction of an SDP, one needs to compute the scaling matrix $W := X^{1/2}(X^{1/2}SX^{1/2})^{-1/2}X^{1/2}$. A direct computation would involve two different matrix square roots. Here we show that W can be computed with two Cholesky factorizations and one singular value decomposition (SVD).

From the equation defining the NT direction in [13, 14], it is not clear how we can incorporate higher-order (quadratic) terms into a Mehrotra-type corrector. By regarding the NT direction as the solution to a symmetrized Newton system, we are able to derive the quadratic correction term as the solution of a Lyapunov equation. Remarkably, this correction term can be computed explicitly and simply by re-using the Cholesky factors and SVD already generated.

The search direction of a symmetrized Newton system is typically solved via a Schur complement equation. For some search directions, for example the NT and the H..K..M directions (see below), the Schur complement equation can be expressed as the normal equation of a linear least squares (LS) problem. We show how the coefficient matrix for the LS problem corresponding to the NT direction can readily be computed by using the Cholesky factors and SVD already generated in the computation of W .

For the purpose of comparison, we also implement three other methods using exactly the same algorithmic framework as Algorithm NT-PC-LS, but computing the search direction via a Schur complement equation. The first is based on the direction of Alizadeh, Haeberly, and Overton [1]; the second on one of the H..K..M directions; and the last on the NT direction. The second direction has a convoluted history: it apparently first appeared in a preprint of Helmberg, Rendl, Vanderbei, and Wolkowicz [5] in late 1993; was rediscovered independently as one member of a family of directions introduced in early 1994 by Kojima, Shindoh, and Hara [8]; and was most recently

derived (as well as a “dual” direction, also a member of the KSH family) in a different way by Monteiro [12] in 1995. This last derivation fits most conveniently with our discussions, but we have chosen a name that suggests all those who obtained it. These three methods are referred to as Algorithm AHO-PC-Sch, H..K..M-PC-Sch and NT-PC-Sch, respectively.

After the release of the first version of this paper, we observed that with careful implementations, the three algorithms that are based on the Schur complement approach can perform much better than what standard perturbation theory of solution of linear system of equations predicts. In particular, they can typically achieve a duality gap that is much better than the predicted limit of $\epsilon_{\text{mach}}^{1/2} \approx 10^{-8}$.

Our numerical results indicate that the methods (both the LS and Schur complement approaches) based on the NT direction are fast and robust. For most problems, the Schur complement approach is as stable as the LS approach. Nevertheless, the LS approach has the attractive feature that the condition number of the coefficient matrix involved in the LS problem is of the order of the square root of that of the Schur complement matrix. Conceivably, there may be problems where the LS approach can perform much better than the Schur complement approach because of this.

A brief summary on how the NT methods compare to the methods based on the AHO and H..K..M directions is as follows. The NT methods are almost as efficient as Algorithm AHO-PC-Sch in terms of the number of iterations required to attain a given accuracy, typically taking only one or two more iterations. On the other hand, each iteration of the NT methods is about 50% cheaper than those for Algorithm AHO-PC-Sch and only slightly more expensive than those of Algorithm H..K..M-PC-Sch. Overall, the NT methods seem to be more robust than the other two algorithms in the sense that problems of stagnation such as using very small step lengths appear less likely to occur. For the set of examples we consider in this paper, Algorithm H..K..M-PC-Sch often encounters such a stagnation problem for a class of SDPs known as the Educational Testing Problems, and Algorithm AHO-PC-Sch occasionally stagnates for the SDPs arising from Chebyshev approximation problems for matrices. Finally, we must mention that Algorithm AHO-PC-Sch seems to be the best of the tested methods in terms of reducing the duality gap, which it drives to a level smaller than 10^{-12} for many problems, whereas methods based on the H..K..M and NT directions can only

reach a level of about 10^{-10} or 10^{-11} for the same problems.

This paper is organized as follows. In Section 2, we introduce the NT direction for SDP and study some of its symmetry and invariance properties. In Section 3, we describe the symmetrized Newton system and prove that it has a unique solution under a certain positive semidefiniteness condition. Then we apply this uniqueness result to show that the NT direction can be viewed as the search direction of a certain symmetrized Newton system. We address implementation issues in Section 4: we give an efficient way to compute the scaling matrix W , show how the Schur complement equation can be expressed as a linear least squares problem, and derive the Mehrotra-type corrector for the NT direction. Results of numerical experiments are given in Section 5. Finally, we give an appendix containing some frequently used properties of the standard and symmetrized Kronecker products in the context of SDP.

Throughout this paper, \mathbb{R}^n denotes the n -dimensional Euclidean space and $\|\cdot\|$ denotes the Euclidean norm. The standard inner product between two real $n \times n$ matrices G and K is the number $G \bullet K := \mathbf{Tr} G^T K$, the trace of the matrix $G^T K$. A matrix $G \in \mathbb{R}^{n \times n}$ (not necessarily symmetric) is said to be positive definite (resp., positive semidefinite) if $v^T G v > 0$, ($v^T G v \geq 0$, resp.) for all $v \neq 0$. However, all positive (semi)definite matrices considered here are symmetric except in the statement and proof of Theorem 3.1, so we shall assume that positive (semi)definiteness implies symmetry unless explicitly stated otherwise. We write $G \succ 0$ ($G \succeq 0$) if G is symmetric and positive definite (positive semidefinite). For $G \succeq 0$, $G^{1/2}$ denotes the unique symmetric positive semidefinite square root of G . Finally, $\mathcal{N}(G)$ and $\mathcal{R}(G)$ denote the null space and range space of the matrix G , respectively,

2 The Nesterov-Todd direction and some symmetry and invariance issues

In their two recent papers [13, 14], Nesterov and Todd study interior-point methods for convex programming problems expressed in conic form. They develop efficient primal-dual algorithms for a class of problems for which the cone and its associated barrier are self-scaled. This class includes, among others, semidefinite programming. All the primal-dual methods in [13, 14] use directions that, for the case of SDP, are (up to a

scalar multiple) solutions for some σ to the following system of equations:

$$\begin{aligned} A_i \bullet \Delta X &= 0, \quad i = 1, \dots, m, \\ \sum_{i=1}^m \Delta y_i A_i + \Delta S &= 0, \\ W^{-1} \Delta X W^{-1} + \Delta S &= \sigma \mu X^{-1} - S, \end{aligned} \tag{3}$$

where $W := X^{1/2}(X^{1/2} S X^{1/2})^{-1/2} X^{1/2}$ and $\mu := X \bullet S/n$. The unique solution to (3) is an affine-scaling direction for $\sigma = 0$, and a centering direction for $\sigma = 1$ — see [14].

We start by describing how (3) arises. In fact, it is a special case for semidefinite programming of a system of equations defined for convex programming problems in conical form, where the cone, say K , has a *self-scaled* barrier function F . In our case, the cone K is the set of positive semidefinite matrices of order n , and the barrier function is defined by

$$F(X) := -\ln \det(X). \tag{4}$$

We will not give the definition of self-scaled barriers here, but note that a key consequence is that, for every X in the interior of the primal cone K and every S in the interior of the corresponding dual cone

$$K^* := \{S : \langle S, X \rangle \geq 0 \text{ for all } X \in K\},$$

there is a unique *scaling* point W in the interior of K with

$$F''(W)X = S. \tag{5}$$

The theory also implies that the dual function F_* , defined by

$$F_*(S) := \sup\{-\langle S, X \rangle - F(X) : X \in \text{int } K\},$$

is a self-scaled barrier for the dual cone K^* . In addition, we have $F''(W)F'_*(S) = F'(X)$. Further, $T := -F'(W)$ lies in the interior of K^* , with $F''_*(T) = [F''(W)]^{-1}$, so that (5) implies

$$F''_*(T)S = X,$$

and we have a dual scaling point also.

In the case of semidefinite programming, $F_*(S) = -\ln \det(S) - n$, $F'(X) = X^{-1}$ and similarly $F'_*(S) = S^{-1}$, and $F''(W)$ is the operator taking X to $W^{-1}XW^{-1}$ and similarly for $F''_*(T)$. The equation (5) then becomes

$$W^{-1}XW^{-1} = S, \tag{6}$$

from which we easily see that

$$(X^{1/2}W^{-1}X^{1/2})^2 = X^{1/2}SX^{1/2},$$

which gives $W = X^{1/2}(X^{1/2}SX^{1/2})^{-1/2}X^{1/2}$. Proceeding similarly from $WSW = X$, we get the other half of

$$W = X^{1/2}(X^{1/2}SX^{1/2})^{-1/2}X^{1/2} = S^{-1/2}(S^{1/2}XS^{1/2})^{1/2}S^{-1/2}. \quad (7)$$

The scaling matrix W is related to various notions of geometric mean for symmetric positive definite matrices. Indeed, (6) shows that W is the metric geometric mean of X and S^{-1} (and W^{-1} that of S and X^{-1}), and

$$W^{-1/2}XW^{-1/2} = W^{1/2}SW^{1/2} \quad (8)$$

is the spectral geometric mean of X and S [2, 6].

Thus system (3) amounts to feasibility equations for the primal and dual directions, together with the equation

$$F''(W)\Delta X + \Delta S = -S - \sigma\mu F'(X).$$

From the results above, this is equivalent to

$$\Delta X + F''_*(T)\Delta S = -X - \sigma\mu F'_*(S).$$

One nice feature of the Nesterov-Todd approach is that it provides general methods applying to any convex programming problem in conic form, as long as the cone is self-scaled; such cones include the nonnegative orthant and the second-order cone in addition to the cone of positive semidefinite matrices. Thus the convergence proofs and complexity estimates apply to this general class of problems. In contrast, the other methods considered here are specific to SDP, and require new convergence proofs.

In the literature on interior-point methods for semidefinite programming, one key point is the need for symmetric direction matrices, i.e., ΔX and ΔS must be symmetric. Indeed, this fails for the trial directions defined by certain rules (e.g., that in [5]), and a separate symmetrization step must be applied before continuing. We point out that the general development of [13, 14] leads to linear systems defined on the appropriate linear spaces, namely the set of symmetric matrices of order n in our case, so that the directions *must* lie in the correct spaces.

However, there is a second symmetry issue. Since (SDP) can be converted into (SDD) and vice versa, there is a natural symmetry between primal and dual. We would like our algorithms also to be symmetric between primal and dual. The equations above show that (apart from the lack of symmetry in the feasibility equations, which follows from the way in which the constraints are written) the Nesterov-Todd directions do possess this primal-dual symmetry. Some of the methods we discuss below do not share this property.

There is a third property which we believe is desirable for interior-point methods: scale invariance. For linear programming, it is well known that, if the primal variables are measured in different units, then the search directions scale appropriately. That is, if x is replaced by $D^{-1}x$ where D is diagonal and positive definite, and correspondingly A becomes AD , c becomes Dc , and s becomes Ds , then the search direction for any algorithm at the scaled trial point $(D^{-1}x, y, Ds)$ in the scaled problem is $(D^{-1}\Delta x, \Delta y, D\Delta s)$, where $(\Delta x, \Delta y, \Delta s)$ is the search direction at the unscaled point (x, y, s) in the original problem.

We will say that a search direction for semidefinite programming enjoys *scale invariance* if a similar property holds. Now we let U be any invertible $n \times n$ matrix, and consider the “scaling” where X is replaced by $\bar{X} := U^{-1}XU^{-T}$ and correspondingly each A_i by $\bar{A}_i := U^T A_i U$, C by $\bar{C} := U^T C U$ and S by $\bar{S} := U^T S U$. This defines a new, scaled problem: if (X, y, S) is feasible in the original problem and its dual, (\bar{X}, y, \bar{S}) is feasible in the scaled problem with the same objective function values. If the search direction at the unscaled point (X, y, S) in the original problem is $(\Delta X, \Delta y, \Delta S)$, we require the search direction at the scaled point (\bar{X}, y, \bar{S}) in the scaled problem to be $(\overline{\Delta X}, \Delta y, \overline{\Delta S}) := (U^{-1}\Delta XU^{-T}, \Delta y, U^T\Delta S U)$.

Proposition 2.1 *The Nesterov-Todd direction is scale-invariant.*

Proof:

In fact, this follows from the coordinate-free representation of the directions, but a direct proof is easy and instructive. From equation (6), it is easy to check that the scaling point corresponding to $U^{-1}XU^{-T}$ and $U^T S U$ is $U^{-1}WU^{-T}$ where W is that corresponding to X and S . Now it is merely a matter of substituting the scaled values of A_i , ΔX , ΔS and W into (3) to confirm that the solutions scale appropriately. \square

Note that if we choose U above to be $W^{1/2}$, then both X and S are scaled to the same point by (8). This is exactly parallel to the situation in linear programming. In this scaled space, the search directions are just Euclidean projections of the scaled right-hand side onto the appropriate orthogonal subspaces; see Section 6 of [13] for a general view of this. This scaling is the starting point for the development in Sturm and Zhang [16].

3 The central path and the Newton equation

3.1 The Newton equation and symmetric search directions

For the SDP problem, the central path is defined as the set of solutions to the following equations:

$$\begin{aligned} A_i \bullet X &= b_i, & \text{for } i = 1, \dots, m, \\ \sum_{i=1}^m y_i A_i &+ S &= C, \\ XS &= \mu I, \end{aligned} \tag{9}$$

for all $\mu > 0$ (together with the requirement that $X \succ 0, S \succ 0$). In [19], Zhang defines the following linear transformation for a given invertible matrix P :

$$H_P(M) := \frac{1}{2} [PMP^{-1} + P^{-T}M^T P^T], \tag{10}$$

and observes that if P is invertible and M is similar to a (symmetric) positive definite matrix, then

$$H_P(M) = \mu I \Leftrightarrow M = \mu I.$$

This observation indicates that the last equation in (9) can be replaced by

$$H_P(XS) = \mu I \tag{11}$$

without affecting the definition of the central path, since XS is similar to the positive definite matrix $S^{1/2}XS^{1/2}$.

Given an iterate (X, y, S) (not necessarily feasible) for the primal and dual semidefinite programming problems, many interior-point algorithms generate the next iterate

by taking a single Newton step applied to the nonlinear system of equations (9) or a related system. Much of the recent debate on interior-point methods for SDP has focused on the issue of the linearization of the third equation in this system. Suppose we try to approximate the point on the central path corresponding to a value $\sigma\mu$, where $\mu := X \bullet S/n$ and $\sigma \in [0, 1]$. If the solution is $(X + \Delta X, y + \Delta y, S + \Delta S)$, then we have

$$A_i \bullet \Delta X = b_i - A_i \bullet X, \quad \text{for } i = 1, \dots, m, \quad (12\text{-a})$$

$$\sum_{i=1}^m \Delta y_i A_i + \Delta S = C - S - \sum_{i=1}^m y_i A_i, \quad (12\text{-b})$$

$$\Delta X S + X \Delta S = \sigma\mu I - (X S + \Delta X \Delta S). \quad (12\text{-c})$$

The linearization of (12-c) gives:

$$\Delta X S + X \Delta S = \sigma\mu I - X S. \quad (12\text{-d})$$

As noted in Section 2, a key requirement for interior-point methods for semidefinite programming is to generate symmetric ΔX and ΔS matrices. By virtue of the equation (12-b), any ΔS that satisfies the above system has to be symmetric. However, this is not true in general for ΔX . Even when the system (12-a), (12-b), and (12-d) is feasible, there may not be any solutions with symmetric ΔX (see [8] for an example). Different recipes have been suggested to symmetrize equations (12-c) and (12-d). Zhang's characterization of the central path unifies these symmetrizations by viewing them as the transformation of the third equation for different values of the matrix P . In this case, (12-c) and (12-d) are replaced by

$$H_P(\Delta X S + X \Delta S) = \sigma\mu I - H_P(X S + \Delta X \Delta S) \quad (12\text{-c}')$$

and

$$H_P(\Delta X S + X \Delta S) = \sigma\mu I - H_P(X S), \quad (12\text{-d}')$$

and the resulting system can be viewed as defined by a linear transformation from $\mathbb{R}^m \times \mathcal{S}\mathbb{R}^{n \times n} \times \mathcal{S}\mathbb{R}^{n \times n}$ to itself, and thus under suitable conditions will produce a solution $(\Delta y, \Delta X, \Delta S)$ with symmetric ΔX and ΔS . Therefore, we will restrict ΔX to be symmetric in the rest of our discussion. Note that the equation (12-d') can then

be written in full detail as

$$\begin{aligned} P(\Delta X S + X \Delta S)P^{-1} + \\ P^{-T}(S \Delta X + \Delta S X)P^T = 2\sigma\mu I - PXS P^{-1} - P^{-T}SXP^T. \end{aligned} \quad (13)$$

Alizadeh, Haeberly, and Overton's linearization [1] corresponds to $P = I$, and Monteiro's two linearizations to $P = X^{-1/2}$ and $P = S^{1/2}$ [12]. In fact, the second of Monteiro's linearizations gives the same direction as that introduced by Helmborg, Rendl, Vanderbei, and Wolkowicz [5], and both give directions included in a class developed by Kojima, Shindoh, and Hara [8]; see also Lin and Saigal [9]. However, the motivation of [5, 8] is very different, and to view all these directions in a unified way, we follow Monteiro's approach. We denote these the AHO direction and the H..K..M directions. In Subsection 3.4, we shall see that the NT direction also results from such a linearization for a suitable P .

3.2 Symmetrized Kronecker product notation

To compute the Newton step $(\Delta X, \Delta y, \Delta S)$, it is easier to express the linear systems of equations (12-a), (12-b) and (12-d') in the standard matrix-vector form by using symmetrized Kronecker products. First we define an operator taking symmetric matrices into vectors: if H is an $n \times n$ symmetric matrix, $\mathbf{svec}(H)$ is defined by

$$\mathbf{svec}(H) := (h_{11}, \sqrt{2} h_{21}, \dots, \sqrt{2} h_{n1}, h_{22}, \sqrt{2} h_{32}, \dots, \sqrt{2} h_{n2}, \dots, h_{nn})^T. \quad (14)$$

The factor $\sqrt{2}$ is introduced so that \mathbf{svec} is an isometry between $S\mathbb{R}^{n \times n}$ and $\mathbb{R}^{n(n+1)/2}$ with their respective standard inner products. We denote the inverse map of \mathbf{svec} by \mathbf{smat} .

The symmetrized Kronecker product of any two $n \times n$ matrices G and K (not necessarily symmetric) is a square matrix of order $n(n+1)/2$; its action on a vector $h := \mathbf{svec}(H)$, where $H \in S\mathbb{R}^{n \times n}$, is given by

$$(G \otimes_s K) \mathbf{svec}(H) := \frac{1}{2} \mathbf{svec}(KHG^T + GHK^T). \quad (15)$$

The operator \mathbf{svec} and the symmetrized Kronecker product were first used by Alizadeh et al. [1], but restricted to the case where G and K were both symmetric. In order to conform as much as possible with the standard Kronecker product, we have decided

to replace the notation they used, **skron**, by \otimes_s . We refer the reader to the appendix for some properties of the symmetrized Kronecker product, as well as corresponding properties for, and relations to, the standard Kronecker product.

Using (15) and (14), we now can write the system (12-a), (12-b) and (12-d') in a 3×3 block equation

$$\begin{pmatrix} 0 & \mathcal{A} & 0 \\ \mathcal{A}^T & 0 & \mathcal{I} \\ 0 & E & F \end{pmatrix} \begin{pmatrix} \Delta y \\ \mathbf{svec}(\Delta X) \\ \mathbf{svec}(\Delta S) \end{pmatrix} = \begin{pmatrix} r_p \\ \mathbf{svec}(R_d) \\ \mathbf{svec}(R_c) \end{pmatrix}, \quad (16)$$

where \mathcal{I} is the identity matrix of order $n(n+1)/2$,

$$E := P \otimes_s P^{-T} S, \quad F := PX \otimes_s P^{-T}, \quad (17)$$

$$r_p := b - \mathcal{A} \mathbf{svec}(X), \quad R_d := C - S - \sum_{i=1}^m y_i A_i, \quad R_c := \sigma \mu I - H_P(XS). \quad (18)$$

Here, \mathcal{A} is a matrix of dimension $m \times n(n+1)/2$ defined by

$$\mathcal{A}^T := [\mathbf{svec}(A_1) \cdots \mathbf{svec}(A_m)]. \quad (19)$$

The assumption that the A_i 's are linearly independent implies that \mathcal{A} has full row rank.

3.3 Uniqueness of symmetric search directions

For the rest of our presentation it is essential to understand the conditions under which the system (16) has a unique solution with symmetric ΔX and ΔS . In their recent paper [15], Shida, Shindoh, and Kojima established the existence and uniqueness of the solutions of (16) for some choices of the matrix P , as well as some other systems that may not be expressible in the form (16). When P is chosen to be $X^{-1/2}$, they show that the above system has a unique solution for all positive definite X and S ; however when $P = I$, the condition that $XS + SX$ is positive semidefinite is used to ensure the uniqueness of the solution. This last condition turns out to be sufficient but not necessary. Before generalizing their result to arbitrary invertible matrices P , we establish the invertibility of E and F .

Lemma 3.1 *Let P be invertible and let X and S be positive definite. Then the matrices $E := P \otimes_s P^{-T} S$ and $F := PX \otimes_s P^{-T}$ in (17) are invertible.*

Proof:

We only prove that E is invertible; the proof for F can be carried out similarly. The proof uses properties of the symmetrized Kronecker product that are listed in the appendix.

To show that E is invertible, we show that the condition $Ex = 0$ implies that $x = 0$. Let $R = \mathbf{smat}([P \otimes_s P]x)$. Noting that $E = (I \otimes_s P^{-T}SP^{-1})(P \otimes_s P)$, we have $(I \otimes_s P^{-T}SP^{-1})\mathbf{svec}(R) = 0$. This can be rewritten as

$$(P^{-T}SP^{-1})R + R(P^{-T}SP^{-1}) = 0. \quad (20)$$

Since $P^{-T}SP^{-1}$ is positive definite (because S is), $P^{-T}SP^{-1}$ and $-P^{-T}SP^{-1}$ have no eigenvalues in common. This implies that $R = 0$ is the only solution to the matrix equation (20) (see [4, p. 39]). Now $R = 0$ implies that $x = 0$, because $P \otimes_s P$ is invertible. \square

Theorem 3.1 *The system of equations (16) has a unique solution $(\Delta y, \Delta X, \Delta S) \in \mathbb{R}^m \times SR^{n \times n} \times SR^{n \times n}$ if $E^{-1}F$ is positive definite (not necessarily symmetric). In particular, this condition holds when $H_P(XS)$ is positive semidefinite.*

Proof:

For this proof, positive definiteness does not imply symmetry; if matrices are symmetric, we will explicitly say so.

It suffices to show that the 3×3 block system (with a square matrix)

$$\begin{pmatrix} 0 & \mathcal{A} & 0 \\ \mathcal{A}^T & 0 & \mathcal{I} \\ 0 & E & F \end{pmatrix} \begin{pmatrix} \Delta y \\ \mathbf{svec}(\Delta X) \\ \mathbf{svec}(\Delta S) \end{pmatrix} = 0 \quad (21)$$

only has the trivial solution.

Since E is invertible by Lemma 3.1, we can use block Gaussian elimination to reduce (21) to a Schur complement equation:

$$(\mathcal{A}E^{-1}F\mathcal{A}^T)\Delta y = 0. \quad (22)$$

Since $E^{-1}F$ is assumed to be positive definite and \mathcal{A} has full row rank, this implies that $\mathcal{A}E^{-1}F\mathcal{A}^T$ is positive definite and thus $\Delta y = 0$ is the only solution to (22).

Now the second block equation in (21) gives $\Delta S = -\mathbf{smat}(\mathcal{A}^T \Delta y) = 0$, and the third block equation gives $\Delta X = -E^{-1}F \Delta S = 0$. This shows that the solution to (16) exists and is unique.

To show that the condition $H_P(XS)$ is positive semidefinite implies that $E^{-1}F$ is positive definite, consider an arbitrary $n(n+1)/2$ -dimensional nonzero vector g . We shall prove that $g^T E^{-1}Fg > 0$. Let $k := E^{-T}g$ and $K := \mathbf{smat}(k)$, so that k is also nonzero. We have

$$\begin{aligned}
g^T E^{-1}Fg &= k^T F E^T k = k^T (PX \otimes_s P^{-T})(P^T \otimes_s SP^{-1}) k \\
&= \frac{1}{2} k^T (PXP^T \otimes_s P^{-T}SP^{-1}) k + \frac{1}{2} k^T (PXS P^{-1} \otimes_s I) k \\
&> \frac{1}{2} k^T (PXS P^{-1} \otimes_s I) k \\
&= \frac{1}{4} (\mathbf{svec}K)^T \mathbf{svec}(PXS P^{-1}K + KP^{-T}SXP^T) \\
&= \frac{1}{4} \mathbf{Tr} [K(PXS P^{-1} + P^{-T}SXP^T)K] \\
&= \frac{1}{2} \mathbf{Tr} [K H_P(XS) K] \geq 0.
\end{aligned}$$

The strict inequality above holds because $PXP^T \otimes_s P^{-T}SP^{-1}$ is positive definite, a consequence of the fact that PXP^T and $P^{-T}SP^{-1}$ are symmetric positive definite (see the appendix). The last inequality follows from the assumption that $H_P(XS)$ is positive semidefinite. This completes the proof. \square

We note that, if $P = X^{-1/2}$ or, more generally, $P = (X^{1/2}SX^{1/2})^\alpha X^{-1/2}$ for some α , then $H_P(XS) = X^{1/2}SX^{1/2}$, which is positive definite whenever X and S are positive definite. Similarly, when $P = S^{1/2}$, or $P = (S^{1/2}XS^{1/2})^\alpha S^{1/2}$, we have $H_P(XS) = S^{1/2}XS^{1/2}$, which again is positive definite whenever X and S are. When $P = I$, the sufficient condition given in Theorem 3.1 (i.e. that $H_P(XS)$ is positive semidefinite) coincides with the condition in [15]. So, as in [15], we see that the system (16) always has a unique solution with symmetric ΔX and ΔS for Monteiro's choices of P . This also holds for Alizadeh et al.'s choice of P if $XS + SX$ is positive semidefinite, but there are examples where the coefficient matrix in (16) is singular. One such example is given by

$$\mathcal{A} = [-1 \quad 2 \quad 0], \quad X = \begin{bmatrix} 1 & \sqrt{2} \\ \sqrt{2} & 3 \end{bmatrix}, \quad S = \begin{bmatrix} 1 & 0 \\ 0 & 11 \end{bmatrix}.$$

Indeed, in this case the Schur complement matrix in (22) is the 1×1 zero matrix.

The following proposition describes a class of matrices P that satisfy the sufficient condition of Theorem 3.1.

Proposition 3.1 *Let X and S be symmetric and positive definite matrices and let P be an invertible matrix. Let E and F be as in Lemma 3.1. Then the following are equivalent:*

- (a) PXP^T and $P^{-T}SP^{-1}$ commute;
- (b) $PXSP^{-1}$ is symmetric;
- (c) FE^T is symmetric; and
- (d) $E^{-1}F$ is symmetric.

Condition (a) implies that $H_P(XS)$ is positive definite. Consequently, any of the conditions above imply that $E^{-1}F$ and FE^T are both positive definite.

Proof:

The equivalence of (a) and (b) is immediate: PXP^T and $P^{-T}SP^{-1}$ commute if and only if

$$PXSP^{-1} = (PXP^T)(P^{-T}SP^{-1}) = (P^{-T}SP^{-1})(PXP^T) = P^{-T}SX P^T. \quad (23)$$

On the other hand,

$$FE^T = (PX \otimes_s P^{-T})(P^T \otimes_s SP^{-1}) = \frac{1}{2}(PXP^T \otimes_s P^{-T}SP^{-1} + PXSP^{-1} \otimes_s I).$$

The first term in the last equality above is symmetric, since PXP^T and $P^{-T}SP^{-1}$ are. Therefore FE^T is symmetric if and only if the second term is. But this holds if and only if $PXSP^{-1}$ is symmetric. This shows the equivalence of (b) and (c). Finally, the equivalence of (c) and (d) is obvious: $E^{-1}F = E^{-1}(FE^T)E^{-T}$ is symmetric if and only if FE^T is.

Now suppose (a) holds (thus (b) holds). Then

$$H_P(XS) = PXSP^{-1} = (PXP^T)(P^{-T}SP^{-1}),$$

which is the product of two commuting positive definite matrices. This implies that $H_P(XS)$ is positive definite. Consequently, by Theorem 3.1, $E^{-1}F$ and hence FE^T are positive definite. \square

The first of the equivalent conditions of Proposition 3.1 holds for the two Monteiro choices for P (one of the two matrices is the identity), and also for $P = W^{-1/2}$ (the two matrices are equal from (8)), a choice we will see much more of.

Of the two H.K.M directions and the AHO direction, only the latter is primal-dual symmetric. Turning now to scale invariance, we see that the AHO direction is *not* scale-invariant; XS transforms to $U^{-1}XSU$ while SX transforms to $U^T SXU^{-T}$, and similarly for products involving directions.

To see that the other two directions are scale-invariant, we note first that the solution to (16) corresponding to P is the same as that corresponding to QP for any orthogonal Q ; indeed, the direction depends only on $P^T P$, as is easily seen by pre- and post-multiplying (13) by P^T and P^{-T} respectively. Next we use the following result:

Lemma 3.2 *Suppose $B = CC^T$ is positive definite. Then $Q := C^{-1}B^{1/2}$ is orthogonal.*

Proof:

We see that $QQ^T = C^{-1}BC^{-T} = C^{-1}CC^TC^{-T} = I$. □

Theorem 3.2 *Suppose P is defined from X and S in such a way that, if X becomes $\bar{X} := U^{-1}XU^{-T}$ and S becomes $\bar{S} := U^T SU$, then P becomes \bar{P} with $\bar{P}^T \bar{P} = U^T P^T P U$. Suppose also that $H_P(XS)$ is positive definite. Then the direction that solves (16) is scale-invariant. In particular this is true for the directions defined by $P = X^{-1/2}$, $P = S^{1/2}$, and $P = W^{-1/2}$.*

Proof:

By letting $B := \bar{P}^T \bar{P} = U^T P^T P U$ and applying the lemma twice, we find that $\bar{P} = QPU$ for some orthogonal Q . It is also easy to see that $H_{\bar{P}}(\bar{X}\bar{S})$ is positive definite too, so that the original and the scaled system both have unique solutions by Theorem 3.1. From our remarks above, the resulting search direction in the scaled problem is the same as if we used $\bar{P} = PU$; but it is easy to check that the scaled direction $(\overline{\Delta X}, \Delta y, \overline{\Delta S}) := (U^{-1}\Delta XU^{-T}, \Delta y, U^T \Delta SU)$ satisfy the resulting system (16). As noted above the three choices of P given satisfy condition (a) of Proposition 3.1 and therefore, the condition that $H_P(XS)$ is positive definite. □

This theorem implies that the two H.K.M directions as well as the direction corresponding to $P = W^{-1/2}$ are scale-invariant. In the next subsection we will show that

Direction	Primal-dual symmetry	Scale invariance	$E^{-1}F$ always p.d.
AHO ($P = I$) [1]	yes	no	no
H..K..M ($P = X^{-1/2}$ or $S^{1/2}$) [5, 8, 12]	no	yes	yes
NT ($P = W^{-1/2}$) [13, 14]	yes	yes	yes

Table 1: *Properties of the AHO, H..K..M, and NT directions*

this last direction is actually the Nesterov-Todd direction. Table 1 summarizes the symmetry properties of the aforementioned directions.

3.4 The Nesterov-Todd direction as a Newton direction

In this subsection, we show that the system (3) defining the NT direction is actually equivalent to (16) for some choices of P . These systems are not quite comparable: (16) allows for infeasible iterates, while (3) assumes that feasibility is maintained. Let us denote by (3') the system (3) where the two zeroes on the right-hand side are replaced by r_p and R_d respectively. We note that, independently of our work, Sturm and Zhang [16] recently derived the Nesterov-Todd direction as a Newton direction for path-following algorithms using the symmetric transformation given in (8).

We first note that if an invertible matrix P satisfies $P^T P = W^{-1}$, then

$$P^T P X S P^{-1} P^{-T} = W^{-1} X S W = S W W^{-1} X = S X. \quad (24)$$

Above we used the fact that

$$W^{-1} X = S W, \quad (25)$$

which follows from (6). Now, (24) indicates that

$$P X S P^{-1} = P^{-T} S X P^T.$$

Now using Proposition 3.1, we conclude that $H_P(XS)$ is positive definite.

There are several matrices P that satisfy $P^T P = W^{-1}$, for example $P = W^{-1/2}$ and $P = (X^{1/2} S X^{1/2})^{1/4} X^{-1/2}$. We will give another useful choice in the next subsection. Now, we are ready to show that the NT direction is a Newton direction.

Theorem 3.3 *Let P be a invertible matrix such that $P^T P = W^{-1}$. Then the solutions to (16) and (3') are identical.*

Proof:

It suffices to show the equivalence of the last equation in (3) and (13). We observe that (13) can be rewritten as

$$W^{-1}(X\Delta S + \Delta X S)W + \Delta S X + S\Delta X = 2\sigma\mu I - 2S X \quad (26)$$

by premultiplying it with P^T , postmultiplying it with P^{-T} , and using $P^T P = W^{-1}$. On the other hand, the last equation of (3) is equivalent to the following two equations:

$$W^{-1}\Delta X W^{-1}X + \Delta S X = \sigma\mu I - S X, \quad (27)$$

$$S\Delta X + S W \Delta S W = \sigma\mu S W X^{-1}W - S W S W. \quad (28)$$

For the first equality above, we postmultiplied the last equation of (3) by X , and for the second, we premultiplied it with $S W$, and postmultiplied it with W . Now adding up these two equations, observing that $S W X^{-1}W = I$, $S W S W = X$, and using (25), we get (26). This proves that the solution to (3') will also satisfy (16). However, (16) has a unique solution as indicated by the remarks above and Theorem 3.1, and therefore these two systems are equivalent. \square

4 Implementation

This section describes in detail how to perform the necessary computations at each iteration, and how to define and compute a Mehrotra predictor-corrector modification [10] of the Nesterov-Todd direction.

4.1 Computation of W

The main purpose here is to show that W can be computed using two Cholesky factorizations and one singular value decomposition (SVD).

Let the Cholesky factorizations of the positive definite matrices X and S be

$$X = LL^T, \quad S = RR^T, \quad (29)$$

and let $UDV^T = R^T L$ be the SVD of $R^T L$. Define Q to be the matrix $Q := L^{-1}X^{1/2}$. By Lemma 3.2, Q is an orthogonal matrix. It is easily seen that

$$X^{1/2}SX^{1/2} = Q^T(L^T R)(R^T L)Q = (Q^T V)D^2(V^T Q).$$

Note that VD^2V^T is the eigenvalue decomposition of $L^T R R^T L = L^T S R^T$, so we could use this instead of the SVD. But the condition number of this matrix is the square of that of $R^T L$, so the result is a less stable algorithm. Since $Q^T V$ is orthogonal, we have

$$(X^{1/2}SX^{1/2})^{-1/2} = (Q^T V)D^{-1}(V^T Q). \quad (30)$$

From (30), W can be computed easily:

$$W = LVD^{-1}V^T L^T = GG^T, \quad (31)$$

where

$$G := LVD^{-1/2}. \quad (32)$$

The matrix G is what we will use in the computation of the direction $(\Delta X, \Delta y, \Delta S)$. If X is not primal feasible, or if we wish to use the Mehrotra predictor-corrector modification, we will also need $G^{-1} = D^{1/2}V^T L^{-1}$, but this is easy to compute. For later use, note the following equation:

$$G^T S G = G^{-1} X G^{-T} = D, \quad (33)$$

i.e., G scales X and S to the same diagonal matrix, cf. (8).

We remark that $G^{-T}G^{-1} = W^{-1}$ from (31), so that $P := G^{-1}$ satisfies $P^T P = W^{-1}$ and hence is yet another choice for P that yields the NT direction. With this choice, (33) shows that $P^{-T}SP^{-1}$ and PXP^T are the same diagonal matrix. They commute both because they are equal and because they are diagonal; see Proposition 3.1.

Note that, if we use the “reverse” Cholesky factorization of S , so that L is lower but R upper triangular in (29), then we save work in computing the lower triangular matrix $R^T L$; moreover, the SVD of the latter may be less work. Also, we do not need to keep the orthogonal matrix U ; V and D are all we need.

4.2 Computation of the NT direction via a linear least squares problem

Using Theorem 3.3 and the choice $P = G^{-1}$, we can obtain the NT direction as the solution to

$$\begin{pmatrix} 0 & \mathcal{A} & 0 \\ \mathcal{A}^T & 0 & \mathcal{I} \\ 0 & E & F \end{pmatrix} \begin{pmatrix} \Delta y \\ \mathbf{svec}(\Delta X) \\ \mathbf{svec}(\Delta S) \end{pmatrix} = \begin{pmatrix} r_p \\ \mathbf{svec}(R_d) \\ \mathbf{svec}(R_c) \end{pmatrix}, \quad (34)$$

where \mathcal{I} is the identity matrix of order $n(n+1)/2$,

$$E = G^{-1} \otimes_s G^T S, \quad F = G^{-1} X \otimes_s G^T, \quad (35)$$

$$r_p := b - \mathcal{A} \mathbf{svec}(X), \quad R_d := C - S - \sum_{i=1}^m y_i A_i, \quad R_c := \sigma \mu I - D^2. \quad (36)$$

(We used $H_P(XS) = (G^{-1} X S G + G^T S X G^{-T})/2 = D^2$ from (33).) Here, \mathcal{A} is the matrix defined by (19).

The system (34) involves $m + n(n+1)$ linear equations. A standard method to solve this large system efficiently is to use block Gaussian elimination to reduce it to a Schur complement equation involving only Δy :

$$\begin{aligned} (\mathcal{A} E^{-1} F \mathcal{A}^T) \Delta y &= r_p + \mathcal{A} E^{-1} F \mathbf{svec}(R_d) \\ &- \mathcal{A} E^{-1} \mathbf{svec}(R_c). \end{aligned} \quad (37)$$

In our case, E^{-1} is not easy to obtain, but we only need $E^{-1} F$ and $E^{-1} \mathbf{svec}(R_c)$. It is easy to check directly, by premultiplying by E , that

$$E^{-1} F = W \otimes_s W, \quad E^{-1} \mathbf{svec}(R_c) = \mathbf{svec}(\sigma \mu S^{-1} - X). \quad (38)$$

So $E^{-1} F$ is symmetric and positive definite, and its Cholesky-like factorization is $E^{-1} F = H H^T$, where $H = G \otimes_s G$, obtained from the identity $W \otimes_s W = (G \otimes_s G)(G \otimes_s G)^T$. Thus we can rewrite (37) as

$$\mathcal{A} H (\mathcal{A} H)^T \Delta y = \mathcal{A} H \left[H^T \mathbf{svec}(R_d) + H^{-1} [\mathbf{svec}(X_r) - E^{-1} \mathbf{svec}(R_c)] \right], \quad (39)$$

where X_r is an $n \times n$ symmetric matrix such that

$$\mathcal{A} \mathbf{svec}(X_r) = r_p = b - \mathcal{A} \mathbf{svec}(X). \quad (40)$$

Such a matrix always exists if \mathcal{A} has full row rank, as we have assumed. If X is primal feasible, we can simply take X_r to be the zero matrix. It is easily seen that (39) is the normal equation for the following linear least squares problem:

$$\min_{\Delta y} \|h - \mathcal{B}^T \Delta y\|, \quad (41)$$

where

$$\mathcal{B}^T := H^T \mathcal{A}^T = [\mathbf{svec}(G^T A_1 G) \cdots \mathbf{svec}(G^T A_m G)] \quad (42)$$

and

$$\begin{aligned} h &:= H^T \mathbf{svec}(R_d) + H^{-1}[\mathbf{svec}(X_r) - E^{-1} \mathbf{svec}(R_c)] \\ &= \mathbf{svec}(G^T R_d G + G^{-1} X_r G^{-T} - \sigma \mu D^{-1} + D). \end{aligned} \quad (43)$$

For the last expression, we used (38) and (33) to obtain

$$H^{-1} E^{-1} \mathbf{svec}(R_c) = (G^{-1} \otimes_s G^{-1}) \mathbf{svec}(\sigma \mu S^{-1} - X) = \mathbf{svec}(\sigma \mu D^{-1} - D).$$

Also observe that, if X is primal feasible so that X_r can be chosen as 0, then G^{-1} is not needed.

The step Δy can be obtained from (41) via QR factorization [3]; i.e., we use a QR factorization of \mathcal{B}^T rather than a Cholesky factorization of $\mathcal{B} \mathcal{B}^T$. Once Δy has been obtained, ΔS can be computed simply from the second block equation of (34), namely,

$$\Delta S = R_d - \mathbf{smat}(\mathcal{A}^T \Delta y). \quad (44)$$

There are two ways of computing ΔX . One is to compute it from the third block equation in (34):

$$\Delta X = \mathbf{smat}[E^{-1} \mathbf{svec}(R_c) - E^{-1} F \mathbf{svec}(\Delta S)] \quad (45)$$

using (38). Another way is to compute ΔX via the residual of the least squares problem (41):

$$\begin{aligned} \Delta X &= -H (h - \mathcal{B}^T \Delta y) + X_r \\ &= -G [\mathbf{smat}(h - \mathcal{B}^T \Delta y)] G^T + X_r. \end{aligned} \quad (46)$$

To see this, note that the linear system (34) implies that

$$d_X \in \mathcal{N}(\mathcal{B}), \quad d_S \in \mathcal{R}(\mathcal{B}^T),$$

$$d_X + d_S = -h,$$

where $d_X := H^{-1} \mathbf{svec}(\Delta X - X_r)$ and $d_S := H^T \mathbf{svec}(\Delta S - R_d)$. Both methods are unstable as μ approaches 0. Numerical experiments indicate that these two methods of computing ΔX have almost the same stability properties. In our computations, we compute ΔX via equation (46).

We have shown how the NT direction can be computed from a LS problem. The same can be done for the H..K..M direction corresponding to $P = S^{1/2}$, where now $E^{-1}F = X \otimes_s S^{-1}$. As before, the main task in the LS approach is getting a Cholesky-like factorization of $E^{-1}F$. By using (33), we have

$$\begin{aligned} E^{-1}F = X \otimes_s S^{-1} &= GDG^T \otimes_s GD^{-1}G^T \\ &= (G \otimes_s G)(D \otimes_s D^{-1})(G^T \otimes_s G^T). \end{aligned} \quad (47)$$

The middle term $D \otimes_s D^{-1}$ in (47) is a diagonal matrix with positive entries of the form $(d_i d_j^{-1} + d_j d_i^{-1})/2$, where the d_i 's are the diagonal entries of the matrix D . So the square root of $D \otimes_s D^{-1}$, say M , exists and can be computed trivially. It is now easy to see that we have the Cholesky-like factorization $E^{-1}F = HH^T$, where $H := (G \otimes_s G)M$.

In fact, the LS approach can be applied almost as easily to the direction that solves (16) whenever $E^{-1}F$ is symmetric. This is because $E^{-1}F$ can be expressed in the form

$$E^{-1}F = (P^{-1}Q \otimes_s P^{-1}Q) \tilde{D} (P^{-1}Q \otimes_s P^{-1}Q)^T,$$

where \tilde{D} is a positive definite diagonal matrix and Q is an orthogonal matrix whose columns form an orthonormal basis that simultaneously diagonalizes PXP^T and $P^{-T}SP^{-1}$ and \tilde{D} . Note that such a basis exists because by Proposition 3.1, the latter two matrices commute if $E^{-1}F$ is symmetric. (If $P = G^{-1}$, so that we have the NT direction, then Q and \tilde{D} turn out to be identity matrices.)

In the previous version of this paper, we claimed that the least squares approach is practical only for the computation of the NT direction. As the previous paragraphs show, this is not the case. Zhang [20] also observed that the LS approach can be

implemented practically for the H..K..M direction corresponding to $P = S^{1/2}$, and Kojima [7] noted this for the linear system involving Kronecker (rather than symmetric Kronecker) products where ΔX is explicitly symmetrized afterwards.

Finally, we note that the AHO direction cannot be computed from a least squares problem because the corresponding matrix $E^{-1}F$ is not symmetric.

4.3 A Mehrotra predictor-corrector modification of the NT direction

To derive the Mehrotra predictor-corrector direction, we suppose that we have approximations δX and δS to the search directions, and substitute them on the right-hand side of (12-c'). Then, using symmetrized Kronecker products, we get:

$$E \mathbf{svec}(\Delta X) + F \mathbf{svec}(\Delta S) = \mathbf{svec}(R_s), \quad (48)$$

where $E = P \otimes_s P^{-T} S$, $F = P X \otimes_s P^{-T}$ and

$$R_s = \sigma \mu I - H_P(XS + \delta X \delta S)$$

(subscript s for second-order). Then

$$R_s = R_c + R_q,$$

where R_q is the ‘‘quadratic correction’’ $-H_P(\delta X \delta S)$. It is easily seen that ΔX and ΔS depend on P only through the product $P^T P$. For the NT direction we can therefore again choose $P = G^{-1}$.

If we then proceed exactly as in the previous subsection, we see that we only have to replace $E^{-1} \mathbf{svec}(R_c)$ by $E^{-1} \mathbf{svec}(R_s)$ in (43) and (45). Thus in the second expression for h in (43), $-\sigma \mu D^{-1} + D$ must be replaced by $-\sigma \mu D^{-1} + D - R_{NT}$, where the correction R_{NT} for the NT direction is given by

$$\mathbf{svec}(R_{NT}) := H^{-1} E^{-1} \mathbf{svec}[-H_{G^{-1}}(\delta X \delta S)].$$

Thus R_{NT} is the solution to $EH \mathbf{svec}(R_{NT}) = \mathbf{svec}[-H_{G^{-1}}(\delta X \delta S)]$. But $H = G \otimes_s G$ and $E = G^{-1} \otimes_s G^T S$, so this simplifies to the Lyapunov equation

$$(G^T S G) R_{NT} + R_{NT} (G^T S G) = -G^{-1}(\delta X \delta S)G - G^T(\delta S \delta X)G^{-T}.$$

But by (33), $G^T S G$ is the diagonal matrix D , and we can therefore write down the solution explicitly:

$$R_{NT} = -(G^{-1}(\delta X \delta S)G + G^T(\delta S \delta X)G^{-T})./(de^T + ed^T), \quad (49)$$

where “./” means entrywise division, $d := \text{diag}(D)$, and $e := (1, \dots, 1)^T$. If we wished to use the Schur complement equation (37), the term $E^{-1} \mathbf{svec}(R_c)$ on the right-hand side would be replaced by

$$E^{-1} \mathbf{svec}(R_s) = \mathbf{svec}(\sigma \mu S^{-1} - X) + (G \otimes_s G) R_{NT}. \quad (50)$$

We also make this replacement in (45) since with the Schur complement approach this equation is used to compute ΔX .

4.4 A Mehrotra predictor-corrector algorithm based on the NT direction

The results derived in the previous subsections are the pieces involved in various steps of a Mehrotra-type predictor-corrector algorithm. Now we are ready to describe such a method based on the NT direction.

Algorithm NT-PC-LS. Suppose given an initial iterate (X^0, y^0, S^0) with X^0, S^0 positive definite. Choose $\tau \in (0, 1)$.

For $k = 0, 1, \dots$,

let the current and the next iterate be (X, y, S) and (X^+, y^+, S^+) respectively. Let $\mu := X \bullet S/n$.

- (Predictor step)

Compute the Newton step $(\delta X, \delta y, \delta S)$ from (41), (44) and (46), with $\sigma := 0$ in (43).

- Determine the parameter σ :

$$\sigma := \frac{[(X + \alpha \delta X) \bullet (S + \beta \delta S)]^2}{[X \bullet S]^2}. \quad (51)$$

Here

$$\alpha := \min \left(1, \frac{-\tau}{\lambda_{\min}(X^{-1} \delta X)} \right), \quad \beta := \min \left(1, \frac{-\tau}{\lambda_{\min}(S^{-1} \delta S)} \right), \quad (52)$$

are step lengths chosen to ensure that $X + \alpha\delta X$ and $S + \beta\delta S$ are positive definite (if the minimum eigenvalue in either expression is positive, we ignore the corresponding term).

- (Corrector step)

With σ and μ determined as above, compute the Newton step $(\Delta X, \Delta y, \Delta S)$ from (41), (44) and (46) with the matrix $-\sigma\mu D^{-1} + D$ in (43) replaced by the matrix

$$-\sigma\mu D^{-1} + D + (G^{-1}(\delta X \delta S)G + G^T(\delta S \delta X)G^{-T}) ./ (de^T + ed^T).$$

- Update (X, y, S) to (X^+, y^+, S^+) by

$$X^+ = X + \alpha \Delta X, \quad y^+ = y + \beta \Delta y, \quad S^+ = S + \beta \Delta S,$$

where α and β are determined from (52) with δX , δS replaced by ΔX , ΔS , so that X^+ and S^+ are positive definite.

Remarks.

- A typical value for τ will be very close to one. In our experiments, we use $\tau := .98$ (the typical linear programming value of .99995 seems to be too aggressive in the SDP case).
- Similarly, the exponent used for choosing σ in (51) is what we use in our experiments, but is more conservative than using an exponent of three, which is typical in linear programming. In our actual implementation, we also set a lower limit on σ depending on the step lengths taken in the predictor step, thus limiting how fast the barrier parameter can decrease. The rule is as follows:

$$\sigma_{\text{actual}} = \begin{cases} \max(0.05, \sigma) & \text{if } \alpha + \beta \geq 1.8, \\ \max(0.1, \sigma) & \text{if } 1.4 \leq \alpha + \beta < 1.8, \\ \max(0.2, \sigma) & \text{if } \alpha + \beta < 1.4. \end{cases}$$

A rule like this first appeared in [5].

- When solving the LS problem in the predictor step by Householder QR factorization, the Householder vectors are saved for later use in the corrector step, as is normally done for the LU factorization of the Schur complement matrix. In this way, the LS problem in the corrector step can be solved with just $O(mn^2)$ flops.

- In computing α in (52), it is cheaper to compute the minimum eigenvalue of the symmetric matrix $L^{-1}\delta XL^{-T}$, where $X = LL^T$ is the Cholesky factorization of X . This matrix has the same spectrum as that of the nonsymmetric matrix $X^{-1}\delta X$. We do the same when computing β .
- Actually, it is more efficient to do most of the computations with “ G ”-scaled quantities. At the beginning of the iteration, we compute G and hence \mathcal{B} and $\bar{R}_d := G^T R_d G$. We either compute $\bar{X}_r := G^{-1} X_r G^{-T}$ from X_r , or directly from $\mathcal{B} \mathbf{svec}(\bar{X}_r) = r_p$. Hence we calculate h from (43) and thus δy from (41). We then obtain

$$\bar{\delta S} := G^T \delta S G = \bar{R}_d - \mathbf{smat}(\mathcal{B}^T \delta y)$$

and

$$\bar{\delta X} := G^{-1} \delta X G^{-T} = \bar{X}_r - \mathbf{smat}(h - \mathcal{B}^T \delta y) = \sigma \mu D^{-1} - D - \bar{R}_d + \mathbf{smat}(\mathcal{B}^T \delta y).$$

Next we compute α and β from (52), but using $\lambda_{\min}(D^{-1/2} \bar{\delta X} D^{-1/2})$ and similarly for S ; note that in transformed space we want $D + \alpha \bar{\delta X} \succ 0$, since X and S both transform to $\bar{X} = \bar{S} = D$. Then we obtain σ from (51), but using barred quantities. For the corrector step, $-\sigma \mu D^{-1} + D$ in (43) is replaced by

$$-\sigma \mu D^{-1} + D + (\bar{\delta X} \bar{\delta S} + \bar{\delta S} \bar{\delta X}) / (de^T + ed^T).$$

Then proceed as above to obtain Δy , $\bar{\Delta X}$, and $\bar{\Delta S}$. Calculate new step lengths α and β . Finally we set

$$X^+ = G(D + \alpha \bar{\Delta X})G^T, \quad y^+ = y + \beta \Delta y, \quad S^+ = S + \beta \Delta S,$$

where ΔS is computed from (44) to maintain dual feasibility.

- The stopping criterion we use in our algorithm is as follows: we stop the iteration if $\sigma > 1$. This usually happens when the duality gap is in the range of the achievable accuracy of the algorithm. However, we note that more precise stopping criteria need to be devised. We also stop the iteration if the step lengths α and β in the corrector step are smaller than 10^{-8} (which implies that the iteration is not making any progress).
- Assuming that the Householder vectors are saved when solving the LS problem in the predictor step, the complexity of each iteration of this algorithm is $4mn^3 + m^2n^2 + O(n^3 + mn^2)$ floating point operations.

5 Numerical experiments

Our purpose here is to compare Algorithm NT-PC-LS with methods using the same algorithmic framework, but computing the directions via the Schur complement equation (37). In the latter methods, we consider three different search directions (we only consider one of the H..K..M directions, the one that coincides with the direction of Helmberg, Rendl, Vanderbei, and Wolkowicz [5] and the one that is easier to compute — see Zhang [19]):

1. AHO direction ($P = I$).
2. H..K..M direction ($P = S^{\frac{1}{2}}$).
3. NT direction ($P = G^{-1}$).

These three algorithms will be referred to as Algorithm AHO-PC-Sch, H..K..M-PC-Sch and NT-PC-Sch, respectively.

Our code is based on one of Alizadeh, Haeberly, and Overton for feasible iterates; we are grateful to them for making it available to us. We also mention here that they have had success with larger values of the step-length parameter τ , which we kept fixed at .98 for all our runs for comparison. Finally, the problems solved here appear to be larger than those solved by other authors, with n either 50 or 100.

We have already discussed how $(\Delta X, \Delta y, \Delta S)$ is computed for Algorithm NT-PC-LS. Now we briefly describe how it is computed for the other three methods. For simplicity, we only discuss the predictor step. The step δy is first computed from the Schur complement equation (37) via an LU or a Cholesky factorization of the $m \times m$ Schur complement matrix $\mathcal{A}E^{-1}F\mathcal{A}^T$, according to whether the matrix is symmetric positive definite. Once δy is obtained, δS is computed from (44) and δX from (45). It is clear that the main work involved in these methods is the computation of the coefficient matrix and the right-hand side vector of the Schur complement equation. In Table 2, we summarize some of the formulae that are needed in this computation. The complexity of each iteration of these methods is also included, ignoring lower order terms like $O(n^3 + mn^2)$.

For all the problems below, the starting points are feasible and so feasibility is maintained throughout in exact arithmetic. Our formulae for ΔS guarantee that dual feasibility is preserved to high accuracy, but the same is not true for primal feasi-

directions	AHO ($P = I$)	H..K..M ($P = S^{\frac{1}{2}}$)	NT ($P = G^{-1}$)
E	$I \otimes_s S$	$S^{\frac{1}{2}} \otimes_s S^{\frac{1}{2}}$	$G^{-1} \otimes_s G^T S$
F	$X \otimes_s I$	$S^{\frac{1}{2}} X \otimes_s S^{-\frac{1}{2}}$	$G^{-1} X \otimes_s G^T$
$E^{-1}F$	$(I \otimes_s S)^{-1}(X \otimes_s I)$	$X \otimes_s S^{-1}$	$W \otimes_s W$
R_c	$\sigma\mu I - (XS + SX)/2$	$\sigma\mu I - S^{\frac{1}{2}}XS^{\frac{1}{2}}$	$\sigma\mu I - D^2$
R_q	$-(\delta X \delta S + \delta S \delta X)/2$	$-H_{S^{\frac{1}{2}}}(\delta X \delta S)$	see (50)
complexity	$10mn^3 + m^2n^2$	$4mn^3 + m^2n^2$	$4mn^3 + m^2n^2$

Table 2: Summary of the formulae involved in the computation of the coefficient matrix and the right-hand side of the Schur complement equation for the AHO, H..K..M, and NT directions.

bility. Hence we adjust $\mathbf{svec}(\Delta X)$ (before updating to X^+) in each iteration to regain feasibility by projection onto the null space of \mathcal{A} , i.e, replacing $\mathbf{svec}(\Delta X)$ by $[I - \mathcal{A}^T(\mathcal{A}\mathcal{A}^T)^{-1}\mathcal{A}]\mathbf{svec}(\Delta X)$. This step is inexpensive. To compute the projection, we only need to compute the Cholesky factorization of the $m \times m$ matrix $\mathcal{A}\mathcal{A}^T$ once at the beginning of the algorithm. (We use the Cholesky factorization here instead of a QR factorization to avoid using the \mathbf{smat} and \mathbf{svec} operations, which are expensive in MATLAB, in the Schur complement methods; for Algorithm NT-PC-LS an alternative would be to use the QR factorization of $H^T\mathcal{A}^T$ obtained in the first iteration to do the primal feasibility correction in all iterations.)

We compare the performance of Algorithm NT-PC-LS and the three methods just mentioned on the following classes of semidefinite programming problems.

(1) Norm minimization problem:

$$\min_{x \in \mathbb{R}^m} \|A_0 + \sum_{k=1}^m x_k A_k\|, \quad (53)$$

where the A_k , $k = 0, \dots, m$, are real $N \times N$ matrices and the norm is the matrix 2-norm. It is well known that this problem can be expressed as an SDP involving $m + 2$ symmetric matrices of dimension $n \times n$, where $n = 2N$ [18]. For this problem, a feasible starting point is readily available, and we choose (X_0, y_0, S_0) to be feasible.

(2) Chebyshev approximation problem for a matrix:

$$\min_p \|p(A)\|, \tag{54}$$

where the minimization is over the class of monic polynomials of degree m and the norm is the matrix 2-norm. Here A is a real $N \times N$ matrix. The Chebyshev problem (54) is a special case of the norm minimization problem and thus can be expressed as an SDP.

We should note that since the power basis $\{I, A, \dots, A^m\}$ is highly ill-conditioned in general, it has to be replaced by a better conditioned alternative for numerical stability. In our actual computation, we use the orthonormal basis $\{Q_1, \dots, Q_{m+1}\}$, with respect to the inner product $A \bullet B$, obtained from the power basis via a modified Gram-Schmidt procedure. For details on how this change of basis transforms the original problem, see [17]. Again, we choose a feasible starting point for this problem.

(3) Max-Cut problem:

$$\begin{aligned} & - \min L \bullet X \\ \text{s.t. } & \text{diag}(X) = e/4, \quad X \succeq 0, \end{aligned} \tag{55}$$

where $L = A - \text{Diag}(Ae)$, e is the vector of all ones and A is the weighted adjacency matrix of a graph [5]. In our experiments, we only consider unweighted graphs where each edge is present independently with probability one half. We choose the following feasible starting point, where $\text{abs}(L)$ denotes the matrix of absolute values of the entries of L :

$$X_0 = \text{diag}(e/4), \quad y_0 = -1.1 \text{abs}(L) e, \quad S_0 = L - \text{diag}(y_0).$$

(4) ETP (Educational testing problem):

$$\begin{aligned} & \max e^T d \\ \text{s.t. } & A - \text{Diag}(d) \succeq 0, \quad d \geq 0, \end{aligned} \tag{56}$$

where A is an $N \times N$ positive definite matrix. This problem can readily be expressed as an SDP of the form (2), involving symmetric matrices of dimension $n \times n$, where $n = 2N$. Again, a feasible starting point is chosen for this problem.

In our experiments, the step-length parameter is fixed at $\tau = 0.98$ throughout, and all the computations are performed in MATLAB [11]. For each class, we solve two sets of problems. The first set consists of five instances with random data. That is, the given matrices are random, with entries chosen from the normal distribution with zero mean and unit variance. For the ETP problem, A is the matrix product of such a random matrix and its transpose so that the resulting matrix is symmetric positive definite. The second set consists of five instances of structured data. The given matrices are Toeplitz matrices, i.e., the entries are constant along each diagonal — thus we need only specify the first rows and columns. The entries in the first rows and columns are again chosen from the standard normal distribution. For the ETP problems, we do the same as before to ensure that A is symmetric positive definite.

For each of the two sets of problems, we plot the convergence curves of the duality gap of one of the instances. The plots are shown in Figures 1–4. The dashed curve corresponds to the AHO direction, the dotted curve corresponds to the H..K..M direction, and the solid curves correspond to the NT direction. For the most part, the two solid curves coincide with one another, indicating that the performances of Algorithm NT-PC-LS and NT-PC-Sch are about the same on most problems. This also shows that the Schur complement approach is as stable as the LS approach for the NT direction. Since the behavior of these two algorithms depends mainly on the properties of the NT direction rather than on how the direction is computed, we will not distinguish them in the subsequent discussion, but refer to them collectively as the NT methods.

In Tables 3 and 4, corresponding to the sets of instances with random and Toeplitz-structured data, respectively, we give the average CPU time and number of iterations for each method to reduce the duality gap by a factor of 10^{10} .

Our numerical results show that methods based on the Schur complement approach can perform much better than the predicted limit of $\epsilon_{\text{mach}}^{1/2}$ on many problems. We do not have any explanation for this at present. A summary of our observations is given below.

1. For Algorithm AHO-PC-Sch, the achievable accuracy in the duality gap can typically reach a level smaller than 10^{-12} for the first three classes of SDPs we consider here, whereas the methods that are based on the H..K..M and NT directions can only reach a level of about 10^{-10} or 10^{-11} for the same problems. It is surprising

that AHO-PC-Sch can achieve such an accuracy in the duality gap despite the fact that the condition number of the Schur complement matrix involved is of the order of the reciprocal of the duality gap. For the ETP problems, all the four algorithms reach the same level of accuracy of about 10^{-9} in the duality gap.

2. Besides being the most accurate, Algorithm AHO-PC-Sch is also the most efficient (in terms of the number of iterations) on the sets of problems we consider here, but the NT methods are almost as efficient, typically requiring only 1 or 2 more iterations to achieve a given precision in the duality gap. The H..K..M method is also almost as efficient as the AHO method, except on the ETP problems.
3. However, each iteration of Algorithm AHO-PC-Sch is about twice as expensive as each iteration of the H..K..M or the NT methods. Among the latter three methods, each iteration of NT-PC-LS is slightly more expensive than those of NT-PC-Sch (but not always), which in turn is slightly more expensive than those of H..K..M-PC-Sch.
4. Though the NT methods are not the best in achieving exceedingly high accuracy, they may be the most robust in the sense that problems of stagnation such as using very small step lengths seem less likely to occur. We have not observed stagnation problems with the NT methods in our numerical experiments, while the AHO method occasionally stagnates on the Chebyshev approximation problems for matrices, and the H..K..M method often encounters such difficulties on the ETP problems. This difficulty does not seem to be due to the Schur complement approach; using a least squares implementation of the H..K..M method yields similar results.

As we already mentioned in the introduction, the good performance of the methods that are based on the Schur complement approach was observed after the release of the first version of this paper, in which NT-PC-LS had been observed to be superior to the rest. We note that these improvements in the Schur-complement-based methods come from careful implementations; for example, the code now symmetrizes explicitly quantities that ought to be symmetric in exact arithmetic.

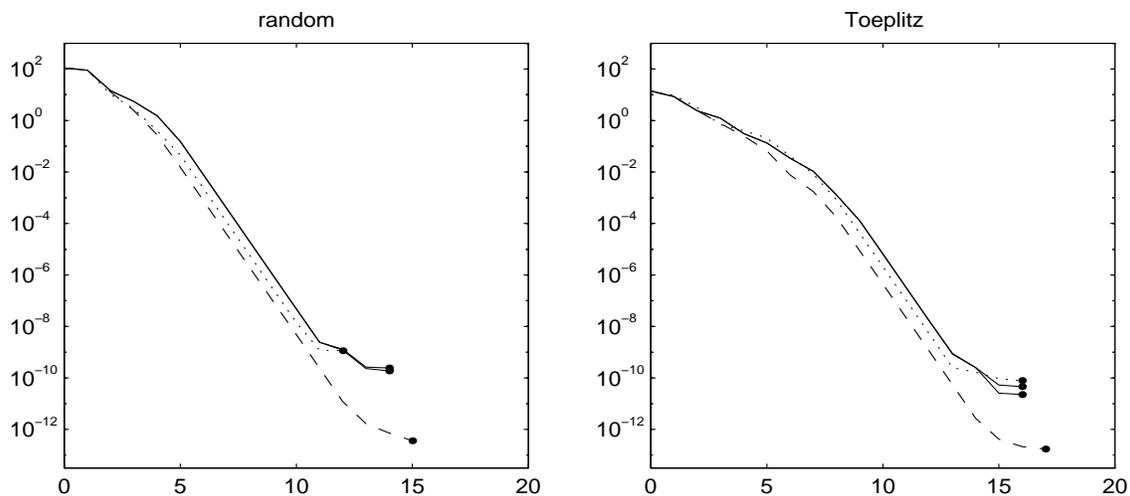


Figure 1: *Convergence curves of the duality gaps of a norm minimization problem for different methods. The dashed curve corresponds to the AHO direction, the dotted curve corresponds to the H.K.M direction, and the solid curves correspond to the NT direction.*

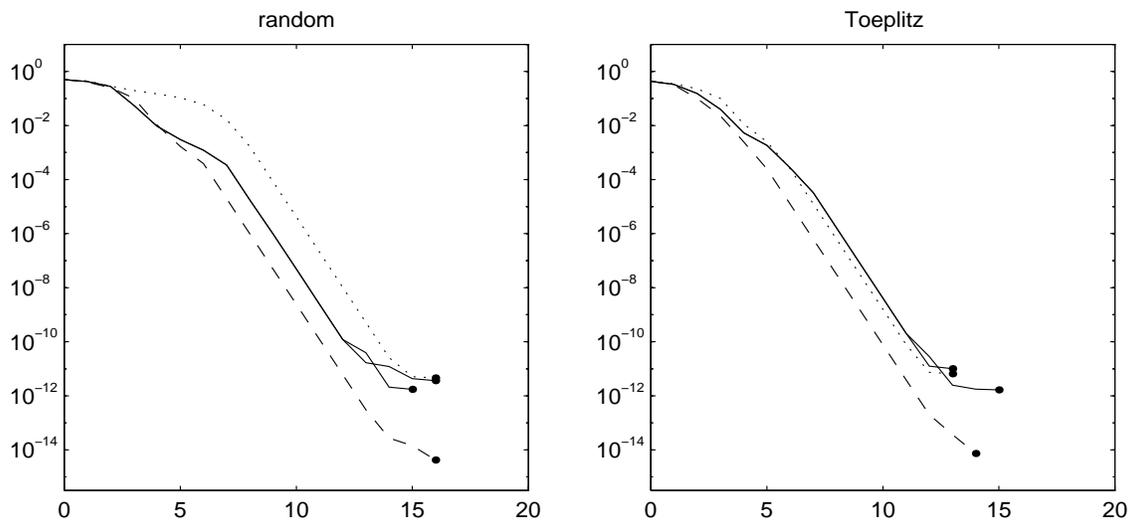


Figure 2: *Same as Figure 1 but for a Chebyshev problem.*

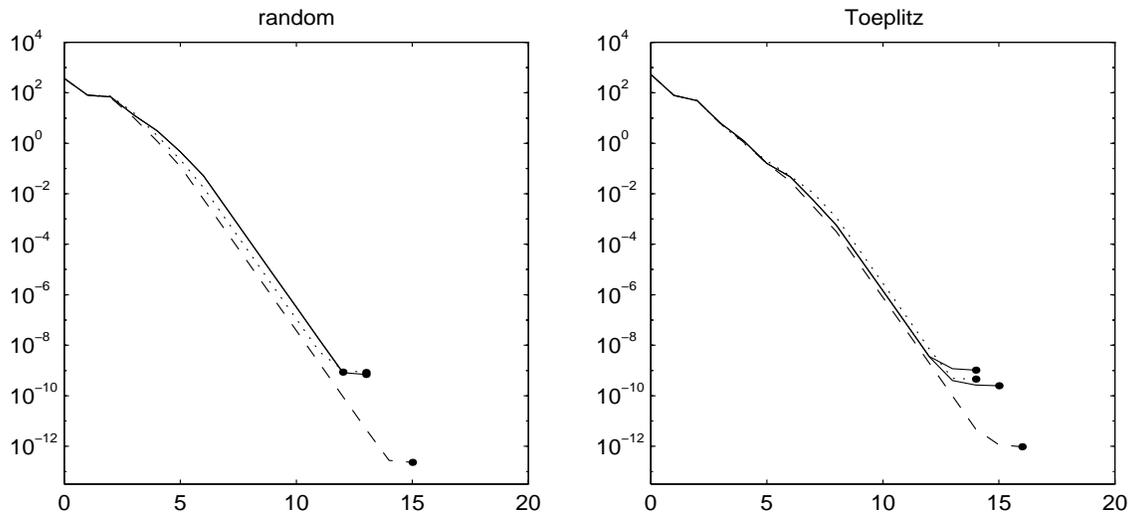


Figure 3: Same as Figure 1 but for a Max-Cut problem.

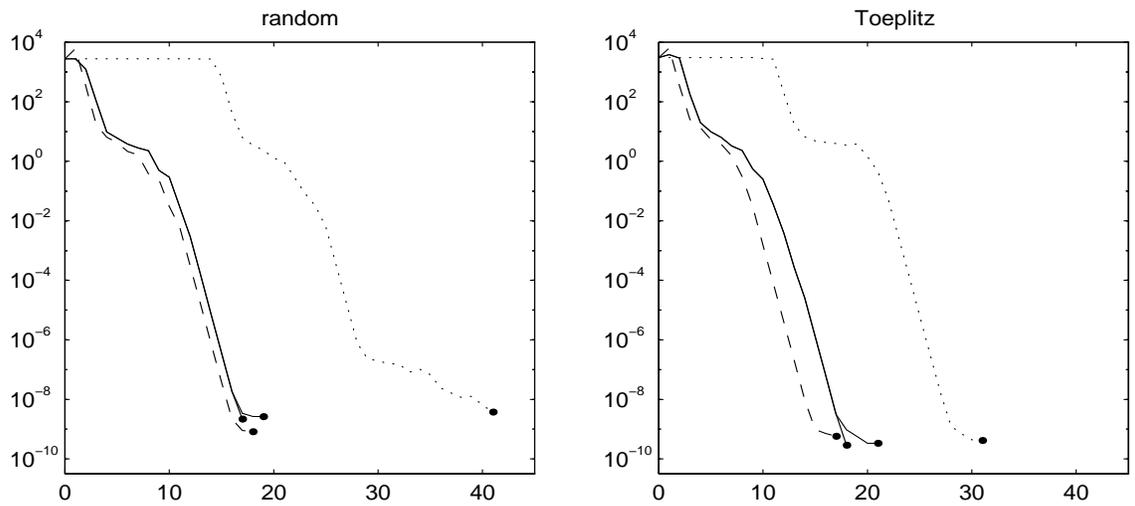


Figure 4: Same as Figure 1 but for an ETP problem. This class of SDP problems proves to be more difficult for the H..K..M direction.

Random examples		Average CPU time (secs.) to reduce the duality gap by 10^{10}				Average no. of iterations to reduce the duality gap by 10^{10}			
		AHO	H..K..M	NT(Schur)	NT(LS)	AHO	H..K..M	NT(Schur)	NT(LS)
Norm Minimization	$n = 100$ $m = 25$	145.8	73.7	87.3	84.0	10.8	11.0	11.2	11.2
Chebyshev	$n = 100$ $m = 25$	157.3	93.8	97.9	93.0	11.0	13.8	12.4	12.4
Max-Cut	$n = 50$ $m = 50$	35.7	17.7	19.4	27.0	10.2	10.4	10.8	10.8
ETP	$n = 100$ $m = 100$	65.3	52.4	37.4	44.2	14.2	22.8	15.6	15.8

Table 3: Computational results on different classes of SDPs. Five instances with random data are considered for each class of the SDP. The computations were done on a Sun Ultra Sparc Station.

Toeplitz examples		Average CPU time (secs.) to reduce the duality gap by 10^{10}				Average no. of iterations to reduce the duality gap by 10^{10}			
		AHO	H..K..M	NT(Schur)	NT(LS)	AHO	H..K..M	NT(Schur)	NT(LS)
Norm Minimization	$n = 100$ $m = 25$	153.9	85.6	98.0	94.2	11.4	12.4	12.4	12.4
Chebyshev	$n = 100$ $m = 25$	146.6*	87.0	99.5	94.5	10.4*	12.8	12.6	12.6
Max-Cut	$n = 50$ $m = 50$	36.0	17.3	20.5	27.3	10.6	10.8	11.4	11.4
ETP	$n = 100$ $m = 100$	68.1	65.3	44.2	51.0	14.8	27.2	17.0	17.0

Table 4: Same as Table 3 but for Toeplitz-structured data.

* The method based on the AHO direction fails on one of the instances due to step lengths going below 10^{-8} . The number reported here is based on the other 4 successful instances.

Appendix

We present some useful properties of the standard and symmetrized Kronecker products.

- Standard Kronecker product:
 1. $G \otimes K = [g_{ij}K]$.
 2. $(G \otimes K)\mathbf{vec}(H) = \mathbf{vec}(KHG^T)$ (where \mathbf{vec} is defined below).
 3. $(G \otimes K)^T = G^T \otimes K^T$.
 4. $G \otimes I$ is symmetric iff G is.
 5. $(G \otimes K)^{-1} = G^{-1} \otimes K^{-1}$.
 6. $(G \otimes K)(H \otimes L) = GH \otimes KL$.
 7. If $\Lambda(G) = \{\lambda_i\}$ and $\Lambda(K) = \{\mu_j\}$, then $\Lambda(G \otimes K) = \{\lambda_i\mu_j\}$. If x_i and y_j are the eigenvectors corresponding to the eigenvalues λ_i and μ_j of G and K , then $\mathbf{vec}(y_jx_i^T)$ is the eigenvector corresponding to the eigenvalue $\lambda_i\mu_j$ of $G \otimes K$.
 8. $\mathbf{vec}(G)^T\mathbf{vec}(K) = G \bullet K$.
- Symmetrized Kronecker product:
 1. $(G \otimes_s K)\mathbf{svec}(H) = \frac{1}{2}\mathbf{svec}(KHG^T + GHK^T)$.
 2. $G \otimes_s K = K \otimes_s G$.
 3. $(G \otimes_s K)^T = G^T \otimes_s K^T$.
 4. $G \otimes_s I$ is symmetric iff G is.
 5. $(G \otimes_s G)^{-1} = G^{-1} \otimes_s G^{-1}$.
 6. $(G \otimes_s K)(H \otimes_s L) = \frac{1}{2}(GH \otimes_s KL + GL \otimes_s KH)$.
 7. $(G \otimes_s K)(H \otimes_s H) = (GH \otimes_s KH)$ and $(H \otimes_s H)(G \otimes_s K) = (HG \otimes_s HK)$.
 8. If $\Lambda(G) = \{\lambda_i\}$, then $\Lambda(G \otimes_s G) = \{\lambda_i\lambda_j\}$. If x_i and x_j are the eigenvectors corresponding to the eigenvalues λ_i, λ_j of G , then $\mathbf{svec}(\frac{1}{2}(x_ix_j^T + x_jx_i^T))$ is the eigenvector corresponding to the eigenvalue $\lambda_i\lambda_j$ of $G \otimes_s G$.
 9. $\mathbf{svec}(G)^T\mathbf{svec}(K) = G \bullet K$.
 10. If G and K are symmetric and positive definite, then so is $G \otimes_s K$.

The properties of the symmetrized Kronecker product can be verified by relating it to the standard Kronecker product, and then using its properties. To this end, consider

the $n(n+1)/2 \times n^2$ matrix U such that $U \mathbf{vec}(H) = \mathbf{svec}(H)$ and $U^T \mathbf{svec}(H) = \mathbf{vec}(H)$ for all $n \times n$ symmetric matrices H . Here

$$\mathbf{vec}(H) := (h_{11}, h_{21}, \dots, h_{n1}, h_{12}, \dots, h_{nn})^T.$$

If we label the rows of U in the order $(1, 1), (2, 1), \dots, (n, 1), (2, 2), (3, 2), \dots, (n, 2), (3, 3), \dots, (n, n)$ and its columns in the order $(1, 1), (2, 1), \dots, (n, 1), (1, 2), \dots, (n, 2), (1, 3), \dots, (n, n)$, then

$$U_{(i,j),(k,l)} = \begin{cases} 1 & \text{if } i = j = k = l, \\ 1/\sqrt{2} & \text{if } i = k \neq j = l, \text{ or } i = l \neq j = k, \\ 0 & \text{otherwise.} \end{cases}$$

For example, for $n = 3$,

$$U = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 & 0 & 0 & 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Note that $UU^T = I_{n(n+1)/2}$. Although $U^T U \neq I_{n^2}$, we have that $U^T U \mathbf{vec}(H) = \mathbf{vec}(H)$ for every $n \times n$ symmetric matrix H ,

With the matrix U , $G \otimes_s K$ can be expressed in terms of the standard Kronecker products of G and K as follows:

$$G \otimes_s K = \frac{1}{2} U(G \otimes K + K \otimes G)U^T.$$

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