Fast ADMM for sum-of-squares programs using partial orthogonality

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Abstract
Semidefinite programs (SDPs) arising from sum-of-squares (SOS) programming possess a structural property that we call partial orthogonality when they are formulated using the standard monomial basis. In this paper, we exploit a “diagonal plus low-rank” structure implied by partial orthogonality and develop a fast first-order method, based on the alternating direction method of multipliers (ADMM), to solve the homogeneous self-dual embedding of the SDPs describing SOS programs. Precisely, partial orthogonality is exploited to project more efficiently the iterates of a recent ADMM algorithm for generic conic programs onto the set defined by the affine constraints. Our method, implemented as a new package in the solver CDCS, is tested on a range of large-scale SOS programs arising from constrained polynomial optimization problems, and from Lyapunov stability analysis of polynomial dynamical systems. The results demonstrate the effectiveness of our approach compared to common state-of-the-art solvers.

Key words: Sum-of-Squares, ADMM, partial orthogonality, large-scale problems

1 Introduction
Optimizing the coefficients of a polynomial in \( n \) variables, subject to a non-negativity constraint on the entire space \( \mathbb{R}^n \) or on a semi-algebraic set \( S \subseteq \mathbb{R}^n \) (i.e., a set defined by a finite number of polynomial equations and inequalities), is a fundamental problem in many fields. For instance, linear, quadratic and mixed-integer optimization problems \cite{1}, as well as optimal power flow problems in power systems \cite{2}, can be rewritten as polynomial optimization problems (POPs) of the form

\[
\min \ p(x) \\
\text{subject to} \quad x \in S,
\]

where \( p(x) \) is a multivariate polynomial, and \( S \subseteq \mathbb{R}^n \) is a semi-algebraic set. Problem (1) is clearly equivalent to

\[
\max \ \gamma \\
\text{subject to} \quad p(x) - \gamma \geq 0 \ \forall x \in S,
\]

so the POP (1) can be solved globally if one can optimize over nonnegative polynomials on a semialgebraic set.

Another important example is the construction of a Lyapunov function in a neighborhood \( \mathcal{D} \) of an equilibrium point \( x^* \) of a dynamical system \( \dot{x}(t) = f(x(t)) \) to certify its local stability. A Lyapunov function \( V(x) \) must satisfy \cite{3}

\[
\begin{align}
V(x) > 0, & \quad \forall x \in \mathcal{D}\{x^*\}, \\
-\langle \nabla V(x), f(x) \rangle & \geq 0, \quad \forall x \in \mathcal{D}.
\end{align}
\]

(Here and in the rest of this paper, \( \langle \cdot, \cdot \rangle \) denotes the inner product in the appropriate Hilbert space.) Often \( f(x) \) is polynomial \cite{4}, and if one restricts the search to polynomial Lyapunov functions \( V(x) \), conditions (3a)-(3b) amount to a feasibility problem over nonnegative polynomials.

Testing for non-negativity is an NP-hard problem for polynomials of degree as low as 4 \cite{5}, and this difficulty is often resolved by requiring that the polynomials under consideration are sums of squares (SOS) of polynomials of lower degree. Such SOS relaxations have been successfully applied to polynomial optimization \cite{6} and systems analysis \cite{7}. Despite the tremendous impact of SOS techniques, the poor scalability to large-scale problems remains one of the fundamental challenges for the reasons outlined below.

The existence (or lack) of a SOS decomposition can be established using semidefinite programming \cite{5}. A semidefinite program (SDP) is an optimization problem for an \( N \times N \) symmetric matrix \( X \) (\( X \in \mathbb{S}^N \)) of the form (called standard primal form)

\[
\min \ X \quad \langle C, X \rangle \\
\text{subject to} \quad A(X) = b, \\
X \succeq 0,
\]

where \( X \succeq 0 \) denotes that \( X \) is positive semidefinite, \( C \in \mathbb{S}^N \) and \( A \in \mathbb{R}^{m \times N} \) are linear functions.

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Semidefinite programs can be solved up to any arbitrary precision in polynomial time using second-order interior-point methods [8, 9], and many efficient, open-source implementations are available [10, 11]. Interior-point methods generate a sequence \((X_k, y_k, Z_k)\), \(k = 1, 2, \ldots\), that converges to an optimal point \((X^*, y^*, Z^*)\) by updating the latest iterate along the search direction \((\Delta X, \Delta y, \Delta Z)\). In particular, \(\Delta y\) is found upon solving an \(m \times m\) linear system of equations, which requires \(O(m^3)\) flops in general.

Unfortunately, as we show subsequently, SDPs arising from SOS programming are characterised by \(m = O(N^3)\), so computing \(\Delta y\) requires \(O(N^6)\) flops — which is expensive even for moderate \(N\) (e.g., \(N = 500\)). Also, \(N\) typically grows in a combinatorial fashion as the number of variables and/or the degree of the polynomials in a SOS program increases. To see this, consider a polynomial of degree \(2d\) in \(n\) variables,

\[
p(x) = \sum_{\alpha \in \mathbb{N}^n, |\alpha| \leq 2d} p_{\alpha} x_1^{\alpha_1} \cdots x_n^{\alpha_n}.
\]

An SOS representation of \(p(x)\) exists if and only if there exists \(X \succeq 0\) such that \(p(x) = v_d(x)^T X v_d(x)\) [5], where

\[
v_d(x) = [1, x_1, x_2, \ldots, x_n, x_1^2, x_1 x_2, \ldots, x_n^d]^T
\]

is the standard monomial basis of degree \(d\). Upon equating coefficients, testing if \(p(x)\) is an SOS reduces to a feasibility SDP of the form

\[
\begin{align*}
\text{find } & X \\
\text{subject to } & \langle B_\alpha, X \rangle = p_\alpha, \quad \alpha \in \mathbb{N}^{2d}_n, \\
& X \succeq 0,
\end{align*}
\]

where \(\mathbb{N}^{2d}_n = \{\alpha \in \mathbb{N}^n : \sum_{i=1}^{n} \alpha_i \leq 2d\}\) (a precise definition of the matrices \(B_\alpha\) will be given in Section 2). When the full monomial basis (6) is used, the dimension of \(X\) and the number of constraints in (7) are \(N = \binom{n+2d}{d}\) and \(m = \binom{n+2d}{2d} = O(N^2)\), respectively. Consequently, solving SOS programs with interior point methods requires extensive computational resource: at the time of writing, testing the SOS decomposition for a generic polynomial in \(n = 30\) variables of degree \(2d = 6\) is impractical (if not impossible due to RAM limitations) on a regular PC.

Existing approaches to mitigate the scalability issue of SOS programs can be categorized into two classes.

1) Improved modeling. The first strategy is to replace the SDP obtained from an SOS relaxation with an optimization problem that is cheaper to solve using second-order interior-point methods. One method is to utilize techniques such as the Newton polytope [12], diagonal inconsistency [13], symmetry reduction [14], correlative sparsity [15], and facial reduction [16, 17] to eliminate the redundant monomials in the basis \(v_d(x)\). Another idea is to replace the positive semidefinite (PSD) constraint by the stronger condition that \(X\) be diagonally dominant or scaled diagonally dominant (see DSOS and SDSDS techniques in [18, 19]). These programs scale more favourably than SDPs because they can be solved using linear and second-order-cone programming, respectively. The conservativeness introduced by the requirement of diagonal dominance can be reduced with a basis pursuit algorithm [20], although it has recently emerged that it cannot be removed in general [21].

2) Computational improvements. The second strategy is to replace the computationally demanding interior-point methods with faster first-order methods, at the expense of reducing the accuracy of the solution. The design of efficient first-order algorithms for large-scale SDPs has recently received increasing attention: Wen et al. proposed an alternating direction augmented Lagrangian method for large-scale dual SDPs [22]; O’Donoghue et al. developed an operator-splitting method to solve the homogeneous self-dual embedding of conic programs [23], which has recently been extended by the authors to exploit aggregate sparsity via chordal decomposition [24–26]. Algorithms that specialize in SDPs from SOS programming also exist [27, 28], but can be applied only to unconstrained POPs with no free parameters — a small subset of SOS programs that does not include, among others, the SOS relaxations of (2) or the Lyapunov conditions (3a)-(3b). First-order regularization methods have also been applied to large-scale constrained POPs, but without taking into account any problem structure [29]. Finally, the sparsity of coefficient matching conditions was exploited in [30] to design an operator-splitting algorithm for general large-scale SOS programs, but that cannot detect infeasibility (at least in its current implementation; recent developments [31, 32] may obviate this issue).

In this paper, we develop a fast first-order algorithm based on the alternating direction method of multipliers (ADMM) to solve general large-scale SOS programs. Our contributions are:

1) At the modeling level, we highlight a basic structural property of SDPs arising from SOS programs represented using the standard monomial basis: the equality constraints are partially orthogonal by virtue of the orthogonality of the matching conditions. Notably, the SDPs formulated using the common SOS parsers SOSTOOLS [33], GloptiPoly [34], and YALMIP [35] satisfy this property.

2) At the computational level, we apply the concept of partial orthogonality to reveal a hidden “diagonal plus low-rank” structure in the ADMM algorithm of [23]. The projection of the iterates onto the affine constraints can therefore be simplified using the matrix inversion lemma, yielding substantial computational savings. Precisely, the factorization of a large \(m \times m\) matrix \((m = O(n^{2d}))\), see Table 1 for typical values) can be replaced with that of a \(t \times t\) matrix, where \(t\) is normally much smaller than \(m\).
We test our method—available as a new package in the MATLAB solver CDCS [36]—on a range of large-scale SOS programs. These include constrained polynomial optimizations and Lyapunov stability analysis for nonlinear polynomial systems. The results demonstrate significant computational savings compared to the state-of-the-art interior-point solvers SeDuMi [10], SDPT3 [11], SDPA [37], CSDP [38], and the first-order solver SCS [39].

The rest of this paper is organized as follows. Section 2 covers some preliminaries, and Section 3 presents the partial orthogonality in the equality constraints of SDPs arising in SOS programs. Section 4 shows how to exploit this orthogonal property to facilitate the solutions of large-scale SDPs using ADMM. Numerical experiments are presented in Section 5. Section 6 concludes the paper.

2 Preliminaries

2.1 Notation

We use standard notation. The sets of nonnegative integers and real numbers are, respectively, \( \mathbb{N} \) and \( \mathbb{R} \). The cone of positive semidefinite matrices of size \( n \) is \( \mathbb{S}_+^n \). For \( x \in \mathbb{R}^n \) and \( \alpha \in \mathbb{N}^n \), \( x^\alpha = x_1^{\alpha_1}x_2^{\alpha_2} \cdots x_n^{\alpha_n} \) is a monomial in \( x \) of degree \( \|\alpha\| = \sum_{i=1}^{n} \alpha_i \). Given an integer \( d \in \mathbb{N} \), we let \( \mathbb{N}^n_d = \{ \alpha \in \mathbb{N}^n : \|\alpha\| \leq d \} \). Let \( \mathbb{R}[x]_{n,d} \) be the set of polynomials in \( n \) variables with real coefficients of degree no more than \( 2d \). A polynomial \( p(x) \in \mathbb{R}[x]_{n,d} \) is a sum of squares (SOS) if \( p(x) = \sum_{i=1}^{q} f_i^2(x) \), where \( f_i(x) \in \mathbb{R}[x]_{n,d} \), \( i = 1, \ldots , q \). The set of SOS polynomials is a cone, denoted \( \Sigma[x] \). The existence of an SOS representation clearly ensures that \( p(x) \geq 0 \) for all \( x \in \mathbb{R}^n \).

2.2 General SOS programs

A general SOS program takes the standard form

\[
\begin{align*}
\min_{u,s} \quad & u^T u \\
\text{subject to} \quad & s(x) = g_0(x) - \sum_{i=1}^{t} u_i g_i(x), \quad (8) \\
& s \in \Sigma[x],
\end{align*}
\]

where \( u \in \mathbb{R}^t \) and \( s \in \Sigma[x] \) are the decision variables, \( w \in \mathbb{R}^t \) defines a linear objective function, and \( g_i(x) \in \mathbb{R}[x]_{n,d}, i = 1, \ldots , t \) are given polynomials. Note that the SOS program (8) is general. For instance, when \( \mathcal{S} = \mathbb{R}^n \), the POP (2) can be relaxed into [5]:

\[
\begin{align*}
\min_{\gamma,s} \quad & -\gamma \\
\text{subject to} \quad & s(x) = p(x) - \gamma, \quad (9) \\
& s \in \Sigma[x]
\end{align*}
\]

Similarly, when \( D = \mathbb{R}^n \) and the vector field \( f(x) \) is polynomial, a Lyapunov function of the form \( V(x) = g_0(x) - \sum_{i=1}^{t} u_i g_i(x) \) with \( g_i(x), i = 1, \ldots , t \) given polynomials can be found by solving the feasibility SOS program [7]

\[
\begin{align*}
\text{find} \quad & u, r, s \\
\text{subject to} \quad & r(x) = g_0(x) - \sum_{i=1}^{t} u_i g_i(x), \quad (10) \\
& s(x) = \left( \sum_{i=1}^{t} u_i \nabla g_i(x) - \nabla g_0(x), f(x) \right), \\
& r, s \in \Sigma[x].
\end{align*}
\]

In addition, constrained POPs can be recast as SOS programs using Lasserre’s relaxation [6], and local stability of nonlinear polynomial systems can be established via SOS programming using the techniques in [3, 4].

2.3 SDP formulation

The SOS program (8) can be converted into an SDP upon fixing a polynomial basis to represent the SOS polynomial variables. The simplest and most common choice to represent a degree-2d SOS polynomial is the basis \( v_d(x) \) of monomials of degree no greater than \( d \), defined in (6). In fact, in (8) \( s(x) \) is SOS if and only if [5]

\[
\begin{align*}
& s(x) = v_d(x)^T X v_d(x) = \langle X, v_d(x)^T v_d(x) \rangle, \quad (11)
\end{align*}
\]

Let \( B_\alpha \) be the 0/1 indicator matrix for the monomial \( x^\alpha \) in \( v_d(x)^T v_d(x) \), i.e.,

\[
(B_\alpha)_{\beta,\gamma} = \begin{cases} 
1 & \text{if } \beta + \gamma = \alpha \\
0 & \text{otherwise} \end{cases} \quad (12)
\]

where the natural ordering of multi-indices \( \beta, \gamma \in \mathbb{N}_d^n \) is used to index the entries of \( B_\alpha \). Then,

\[
\begin{align*}
& v_d(x)^T v_d(x) = \sum_{\alpha \in \mathbb{N}_d^n} B_\alpha x^\alpha.
\end{align*}
\]

Upon writing \( g_i(x) = \sum_{\alpha \in \mathbb{N}_d^n} g_i,\alpha x^\alpha, i = 0, \ldots , t \), and representing \( s(x) \) as in (11), the equality constraint in (8) becomes

\[
\begin{align*}
& \sum_{\alpha \in \mathbb{N}_d^n} \left( g_0,\alpha - \sum_{i=1}^{t} u_i g_i,\alpha \right) x^\alpha = \langle X, v_d(x)^T v_d(x) \rangle \\
& = \sum_{\alpha \in \mathbb{N}_d^n} (B_\alpha, X) x^\alpha. \quad (13)
\end{align*}
\]

| \( n \) | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 |
|---|---|---|---|---|---|---|---|---|
| \( 2d = 2 \) | (5, 15) | (7, 28) | (9, 45) | (11, 66) | (13, 91) | (15, 120) | (17, 153) | (19, 190) |
| \( 2d = 4 \) | (15, 70) | (28, 210) | (45, 495) | (66, 1001) | (91, 1820) | (120, 3060) | (153, 4845) | (190, 7315) |
| \( 2d = 6 \) | (35, 210) | (84, 924) | (165, 3003) | (286, 8008) | (455, 18564) | (680, 38760) | (969, 74613) | (1330, 134596) |
Matching the coefficients on both sides yields the equality constraints

\[ g_{0,\alpha} - \sum_{i=1}^{t} u_{i} g_{i,\alpha} = \langle B_{\alpha}, X \rangle \quad \forall \alpha \in \mathbb{N}_{2d}^{n}. \tag{14} \]

We refer to these constraints as \textit{coefficient matching conditions} [30]. The SOS program (8) is then equivalent to the SDP

\[
\begin{align*}
\min_u & \quad w^T u \\
\text{subject to} & \quad \langle B_{\alpha}, X \rangle + \sum_{i=1}^{t} u_{i} g_{i,\alpha} = g_{0,\alpha} \quad \forall \alpha \in \mathbb{N}_{2d}^{n}, \\
& \quad X \succeq 0.
\end{align*}
\tag{15}
\]

As already mentioned in Section 1, when the full monomial basis \(v_d(x)\) is used to formulate the SDP (15), the size of the positive semidefinite matrix \(X\) and the number of constraints are, respectively,

\[
N = \begin{pmatrix} n+d \\ d \end{pmatrix}, \quad m = \begin{pmatrix} n+2d \\ 2d \end{pmatrix}
\tag{16}
\]

The size of the SDP (15) may be reduced (sometimes significantly) by eliminating redundant monomials based on certain structural properties of \(s(x)\); see [12–17].

\section{Partial orthogonality in SOS programs}

For simplicity, let us re-index the coefficient matching conditions (14) using integers \(i = 1, \ldots, m\) instead of the multi-indices \(\alpha\). Moreover, let \(\text{vec} : \mathbb{S}^{N} \rightarrow \mathbb{R}^{N^2}\) map a matrix to the stack of its columns and define \(A_1 \in \mathbb{R}^{m \times t}\) and \(A_2 \in \mathbb{R}^{m \times N^2}\) as

\[
A_1 := \begin{bmatrix} g_{1,1} & \cdots & g_{t,1} \\ \vdots & \ddots & \vdots \\ g_{1,m} & \cdots & g_{t,m} \end{bmatrix}, \quad A_2 := \begin{bmatrix} \text{vec}(B_1)^T \\ \vdots \\ \text{vec}(B_m)^T \end{bmatrix}.
\tag{17}
\]

In other words, \(A_1\) collects the coefficients of polynomials \(g_i(x)\), and \(A_2\) assembles the vectorized coefficients of the matrix \(X\) in (15). Finally, let \(S_+\) be the vectorized positive semidefinite cone, such that \(\text{vec}(X) \in S_+\) if and only if \(X \succeq 0\), and define

\[
A := [A_1 \ A_2] \in \mathbb{R}^{m \times (t+N^2)}, \\
b := [g_{0,1}, \ldots, g_{0,m}]^T \in \mathbb{R}^{m}, \\
c := [w^T \ 0, \ldots, 0]^T \in \mathbb{R}^{t+N^2}, \\
\xi := [u^T \ \text{vec}(X)^T]^T \in \mathbb{R}^{t+N^2}, \\
K := \mathbb{R}^{t} \times S_+.
\]

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{sparsity_patterns.png}
\caption{Sparsity patterns for (a) \(AA^T\), (b) \(A_1A_1^T\), and (c) \(A_2A_2^T\) for \texttt{sosdemo2} in SOSTOOLS [33].}
\end{figure}

We can then rewrite (15) as the primal-form conic problem

\[
\begin{align*}
\min_\xi & \quad c^T \xi \\
\text{subject to} & \quad A\xi = b, \\
& \quad \xi \in K.
\end{align*}
\tag{18}
\]

The key observation at this stage is that the rows of the constraint matrix \(A\) are partially orthogonal. More precisely, we have the following result.

\begin{proposition}
Let \(A = [A_1 \ A_2]\) be the constraint matrix of the conic formulation (17) of a SOS program modeled using the monomial basis. The \(m \times m\) matrix \(AA^T\) is of the "diagonal plus low rank" form. Precisely, \(D := A_2A_2^T\) is diagonal and \(AA^T = D + A_1A_1^T\).
\end{proposition}

\begin{proof}
The definition of \(A\) implies \(AA^T = A_1A_1^T + A_2A_2^T\), so we need to show that \(A_2A_2^T\) is diagonal. This is true by virtue of the definition (12) of the matrices \(B_i, i = 1, \ldots, m\): if an entry of \(B_i\) is nonzero, the corresponding entry of \(B_j\) must be zero for all \(j \neq i\). Consequently, if \(n_i\) denotes the number of nonzero entries in \(B_i\), we have \(\text{vec}(B_i)^T\text{vec}(B_j) = n_i\) if \(i = j\), and zero otherwise. Therefore \(A_2A_2^T = \text{diag}(n_1, \ldots, n_m)\).
\end{proof}

Note that, in essence, Proposition 1 simply restates that the constraint sub-matrices corresponding to the Gram matrix of the SOS decomposition are orthogonal. This almost trivial fact is a basic \textit{structural} property for any SOS program formulated using the usual monomial basis. Moreover, it is not difficult to check that Proposition 1 holds also when the full monomial basis is reduced using any of the techniques implemented in the commonly used parsers SOSTOOLS [33], GloptiPoly [34] and YALMIP [35].

\begin{remark}
It is important to note that in general the product \(A_1A_1^T\) has no particular structure, and \(AA^T\) is not diagonal except for very special problem classes. For example, Figure 1 demonstrates the sparsity pattern of \(AA^T\), \(A_1A_1^T\), and \(A_2A_2^T\) for problem \texttt{sosdemo2} in SOSTOOLS [33], an SOS relaxation of a Lyapunov function search: \(A_2A_2^T\) is diagonal, but \(A_1A_1^T\) and \(AA^T\) are not. This makes the algorithms proposed in [27, 28] inapplicable, since they rely on full row-orthogonality of the constraint matrix \(A\).
\end{remark}

\begin{remark}
Using the monomial basis to formulate the coefficient matching conditions (14) makes the matrix \(A\) very sparse, because only a small subset of entries of the product \(v_d(x)v_d(x)^T\) are equal to a given monomial \(x^\alpha\). In particular, the density of the non-zero entries of \(A_2\) is \(O(n^{-2d})\) [30].
\end{remark}
However, sparsity cannot be easily exploited because the aggregate sparsity pattern of the SDP (18) is dense. Consequently, methods that take advantage of aggregate sparsity in SDPs [24–26, 40] are not useful in SOS programming. The algorithm proposed in [23] solves the homogeneous self-dual feasibility problem of (18) and (19) via the dual embedding [41] of a conic program in the form (18) and its dual,

\[
\max_{y, z} \, b^T y \\
\text{subject to} \quad A^T y + z = c, \quad z \in K^*, \tag{19}
\]

where the cone \(K^*\) is the dual of \(K\). In essence, when strong duality holds, optimal solutions for (18) and (19) (or a certificate of infeasibility) can be recovered from a non-zero solution of the homogeneous linear system

\[
\begin{bmatrix}
  z \\
  s \\
  \kappa \\
\end{bmatrix} =
\begin{bmatrix}
  0 & -A^T & c \\
  A & 0 & -b \\
  -c^T & b^T & 0 \\
\end{bmatrix}
\begin{bmatrix}
  \xi \\
  y \\
  \tau \\
\end{bmatrix} \tag{20}
\]

that satisfies \((\xi, y, \tau) \in K \times \mathbb{R}^m \times \mathbb{R}_+\) and \((z, s, \kappa) \in K^* \times \{0\}^m \times \mathbb{R}_+\). The interested reader is referred to [23] and references therein for more details; here, we simply note that when \(\tau = 1, \kappa = 0\), (20) reduces to the KKT conditions of (18) and (19),

\[
A\xi = b, \quad A^T y + z = c, \quad c^T x = b^T y, \quad (\xi, z) \in K \times K^*. \tag{19}
\]

Consequently, upon defining

\[
\begin{bmatrix}
  \xi \\
  y \\
  \tau \\
\end{bmatrix} =
\begin{bmatrix}
  z \\
  s \\
  \kappa \\
\end{bmatrix}, \quad \begin{bmatrix}
  0 & -A^T & c \\
  A & 0 & -b \\
  -c^T & b^T & 0
\end{bmatrix} =
\begin{bmatrix}
  u_1 \\
  u_2 \\
  u_3
\end{bmatrix} \tag{21}
\]

\(C := K \times \mathbb{R}^m \times \mathbb{R}_+, \) and \(C^* := K^* \times \{0\}^m \times \mathbb{R}_+\), to simplify the exposition, an optimal point for (18)-(19) (or a certificate of infeasibility) can be recovered from a non-zero solution of the homogeneous self-dual feasibility problem

\[
\begin{bmatrix}
  u_1 \\
  u_2 \\
  u_3
\end{bmatrix} \in C \times C^* \tag{22}
\]

It was shown in [23] that (22) can be solved using a simplified version of the classical ADMM algorithm (see e.g. [42]), whose \(k\)-th iteration consists of the following three steps (\(P_C\) denotes projection onto the cone \(C\), and the superscript \((k)\) indicates the value of a variable after the \(k\)-th iteration):

\[
\begin{align*}
\hat{u}^{(k)} &= (I + Q)^{-1} \left( u^{(k-1)} + v^{(k-1)} \right), \tag{23a} \\
u^{(k)} &= P_C \left( \hat{u}^{(k)} - v^{(k-1)} \right), \tag{23b} \\
v^{(k)} &= v^{(k-1)} - \hat{u}^{(k)} + u^{(k)}. \tag{23c}
\end{align*}
\]

Practical implementations of the algorithm rely on being able to carry out these steps cheaply. The next section describes an efficient implementation of (23a) when (22) represents an SOS program.

4.2 Application to SOS programming

Each iteration of the ADMM algorithm requires: 1) a projection onto a linear subspace in (23a) through the solution of a linear system with coefficient matrix \(I + Q\); 2) a projection onto the cone \(C\) in (23b); 3) the cheap update (23c).

The conic projection (23b) is relatively easy to compute when the cone size is not too large. However, recall that \(Q \in \mathbb{S}_p + \mathbb{N}^{2+m+1} + m = O(n^{2d})\) is very large in SDPs arising from SOS programs. As shown in Table 1, we have \(N = 969\) and \(m = 74,613\) for a polynomial in \(n = 16\) variables of degree \(2d = 6\), and it is computationally expensive to factorize a dense matrix of dimension over 50,000. Then, step (23a) may require extensive computational effort if we directly factorize \(I + Q\). Fortunately, \(Q\) is highly structured and, in the context of SOS programming, the block-entry \(A\) enjoys the property of partial orthogonality (cf. Proposition 1). As we will now show, this allows considerable simplifications and yields significant computational savings.

We begin by noticing that (23a) requires the solution of a linear system of equations of the form

\[
\begin{bmatrix}
  I & -A^T & c \\
  A & I & -b \\
  -c^T & b^T & 1
\end{bmatrix}
\begin{bmatrix}
  u_1 \\
  u_2 \\
  u_3
\end{bmatrix} = \begin{bmatrix}
  \omega_1 \\
  \omega_2 \\
  \omega_3
\end{bmatrix}. \tag{24}
\]

After letting \(M := \begin{bmatrix} I - A^T \\ A \\ -c^T \end{bmatrix}, \zeta := \begin{bmatrix} c & b \end{bmatrix}\) and eliminating \(\hat{u}_3\) from the first and second block-equations in (24) we obtain

\[
\begin{bmatrix}
  M + \zeta^T \\
\end{bmatrix}
\begin{bmatrix}
  \hat{u}_1 \\
  \hat{u}_2
\end{bmatrix} = \begin{bmatrix}
  \omega_1 \\
  \omega_2
\end{bmatrix} - \omega_3 \zeta. \tag{25a}
\]

\[
\hat{u}_3 = \omega_3 + c^T \hat{u}_1 - b^T \hat{u}_2. \tag{25b}
\]

Applying the matrix inversion lemma [43] to (25a) yields

\[
\begin{bmatrix}
  \hat{u}_1 \\
  \hat{u}_2
\end{bmatrix} = \begin{bmatrix}
  I - (M^{-1} \zeta)^T M^{-1} \\
  \omega_1 - \omega_3 \omega_2 \\
  \omega_2 + b \omega_3
\end{bmatrix}. \tag{26}
\]

Note that the first matrix on the right-hand side of (26) only depends on problem data, and can be computed before
that I by Proposition 1, there exists a diagonal matrix

\[ A = \begin{bmatrix} I & -A^T \\ A & I \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \end{bmatrix} = \begin{bmatrix} \hat{\omega}_1 \\ \hat{\omega}_2 \end{bmatrix}. \] \tag{27}

Eliminating \( \sigma_1 \) from the second block-equation in (27) gives

\[ \begin{align*}
\sigma_1 &= \hat{\omega}_1 + A^T \sigma_2, \tag{28a} \\
(I + AA^T)\sigma_2 &= -A\hat{\omega}_1 + \hat{\omega}_2. \tag{28b}
\end{align*} \]

It is at this stage that partial orthogonality comes into play: by Proposition 1, there exists a diagonal matrix \( P \) such that \( I + AA^T = I + A_1A_1^T + A_2A_2^T = I + A_1A_1^T \). Recalling from Section 3 that \( A_1 \in \mathbb{R}^{n \times t} \) with \( t \ll m \) for typical SOS programs \((t = 3 \text{ and } m = 58 \text{ for problem sosdemo2 in SOSTOOLS})\), it is therefore convenient to apply the matrix inversion lemma to (28b) and write

\[ (I + AA^T)^{-1} = (P + A_1A_1^T)^{-1} = P^{-1} - P^{-1}A_1(I + A_1^TP^{-1}A_1)^{-1}A_1^TP^{-1}. \]

Since \( P \) is diagonal, its inverse is immediately computed. Then, \( \sigma_1 \) and \( \sigma_2 \) in (28) are found upon solving a \( t \times t \) linear system with coefficient matrix

\[ I + A_1^TP^{-1}A_1 \in \mathbb{R}^t, \tag{29} \]

plus relatively inexpensive matrix-vector, vector-vector, and scalar-vector operations. Moreover, since the matrix \( I + A_1^TP^{-1}A_1 \) depends only on the problem data and does not change at each iteration, its preferred factorization can be cached before iterating steps (23a)-(23c).

5 Numerical Experiments

We implemented the algorithm of [23], extended to take into account partial orthogonality in SOS programs, as a new package in the open-source solver CDCS [36]. Our implementation, which we refer to as CDCS-sos, solves step (23a) using a sparse permuted Cholesky factorization of the matrix in (29). The source code can be downloaded from https://github.com/oxfordcontrol/CDCS.

We tested CDCS-sos on a series of SOS programs, including constrained polynomial optimizations and Lyapunov stability analysis of polynomial systems (other SOS applications can be found in the Appendix). CPU times were compared to the direct and indirect implementations of the algorithm of [23] by the solver SCS [39], referred to as SCS-direct and SCS-indirect, respectively. In our experiments, the termination tolerance for CDCS-sos and SCS was set to \( 10^{-3} \), and the maximum number of iterations was \( 2 \times 10^5 \). Moreover, since first-order methods only aim at computing a solution of moderate accuracy, we assessed the suboptimality of the solution returned by CDCS-sos by comparing it to an accurate solution computed with the interior-point solver SeDuMi [10] (default parameters were used). Besides, to demonstrate the low memory requirements of first-order algorithms, we also run the interior-point solvers SDPT3 [11], SDPA [37], and CSDP [38] for comparison (default parameters were used). All experiments were run on a PC with a 2.8 GHz Intel® Core™ i7 CPU and 8GB of RAM.

5.1 Constrained polynomial optimization

As our first experiment, we consider the following constrained quartic polynomial minimization problem

\[
\min_x \sum_{1 \leq i < j \leq n} (x_ix_j + x_i^2x_j - x_i^3 - x_i^2x_j^2)
\]

subject to \( \sum_{i=1}^n x_i^2 \leq 1. \)

(30)

We used the second Lasserre relaxation, and the parser GloptiPoly [34] was used to recast (30) into an SDP.
We then tested the performance of CDCS-sos on the problem of minimizing a random polynomial $p(x)$ over the unit ball $\{x \in \mathbb{R}^n : \sum_{i=1}^n x_i^2 \leq 1\}$. Similar to [27, 30], we generated $p(x)$ according to

$$p(x) = p_0(x) + \sum_{i=1}^n x_i^{2d},$$

(31)

where $p_0(x)$ is a random polynomial (with no particular structure) of degree strictly less than $2d$. In the experiment, we chose $d = 2$, and used the second Lasserre relaxation.

Fig. 3 shows the total CPU time required by the interior-point and first-order solvers for this example, and Fig. 4 illustrates the average CPU time per 100 iterations of the first-order solvers. The data plotted in Figs. 3 and 4, are averaged over 5 random problem instances. It is evident that first-order methods (e.g., SCS) perform better than interior-point methods (e.g., SeDuMi), albeit at the cost of reduced accuracy (results similar to those in Table 3 are not reported for brevity, but the objective value returned by the first-order solvers was always within 0.8% of the high-accuracy optimal value computed using interior-point solvers when possible). As in the previous example, exploiting partial orthogonality in CDCS-sos gives the best improvements.

Table 3. Terminal objective value from interior-point solvers, SCS-direct, SCS-indirect and CDCS-sos for the SDP relaxation of (30).

| n  | SCS-direct | SCS-indirect | CDCS-sos |
|----|------------|--------------|----------|
| Objective | Objective | Accuracy | Objective | Accuracy | Objective | Accuracy |
| 10  | -9.914 | -9.124 | 0.10 % | -9.125 | 0.11 % | -9.090 | 0.27 % |
| 12  | -11.117 | -11.095 | 0.20 % | -11.095 | 0.19 % | -11.106 | 0.10 % |
| 14  | -13.118 | -13.089 | 0.22 % | -13.093 | 0.19 % | -13.155 | 0.29 % |
| 17  | -16.119 | -16.087 | 0.20 % | -16.088 | 0.19 % | -16.062 | 0.35 % |
| 20  | -19.120 | -19.165 | 0.24 % | -19.167 | 0.25 % | -19.078 | 0.22 % |
| 24  | -23.121 | -23.043 | 0.34 % | -23.038 | 0.36 % | -23.145 | 0.10 % |
| 29  | ** | -28.174 | — | -28.178 | — | -28.170 | — |
| 35  | ** | -34.054 | — | -34.052 | — | -34.075 | — |
| 42  | ** | -41.214 | — | -41.214 | — | -41.052 | — |

*: The objective values computed by SeDuMi, SDPT3, SDPA and CSDP (when available) differ by less than $10^{-8}$.

**: The problem could not be solved due to memory limitations.

—: No comparison is possible due to the lack of a reference accurate optimal value.

Table 2 reports the CPU time (in seconds) required by each of the solvers we tested to solve the SDP relaxations as the number of variables $n$ was increased. CDCS-sos is the fastest method for all the instances we tested. For large-scale POPs $(n \geq 29)$, the number of constraints in the resulting SDP is over 40,000, and all the interior-point solvers failed to find a solution due to memory limitations. In contrast, the number of non-orthogonal constraints $t$ is much smaller (shown in the table), reducing the cost of the affine projection step in the ADMM algorithm implemented in CDCS-sos. For the large-scale instances $(n \geq 29)$ in Table 2, CDCS-sos was approximately twice as fast as SCS. Fig. 2 illustrates that for all the cases we tested CDCS-sos was also faster than both SCS-direct and SCS-indirect in terms of average CPU time per 100 iterations (this metric is unaffected by possible small variations in the exact termination criteria of different solvers). Finally, Table 3 shows that although first-order methods only aim to provide solutions of moderate accuracy, the objective value returned by CDCS-sos and SCS was always within 0.5% of the high-accuracy optimal value computed using interior-point solvers. Such a small difference may be considered negligible in many applications.

We then tested the performance of CDCS-sos on the problem of minimizing a random polynomial $p(x)$ over the unit ball $\{x \in \mathbb{R}^n : \sum_{i=1}^n x_i^2 \leq 1\}$. Similar to [27, 30], we generated $p(x)$ according to

$$p(x) = p_0(x) + \sum_{i=1}^n x_i^{2d},$$

(31)

where $p_0(x)$ is a random polynomial (with no particular structure) of degree strictly less than $2d$. In the experiment, we chose $d = 2$, and used the second Lasserre relaxation.

Fig. 3 shows the total CPU time required by the interior-point and first-order solvers for this example, and Fig. 4 illustrates the average CPU time per 100 iterations of the first-order solvers. The data plotted in Figs. 3 and 4, are averaged over 5 random problem instances. It is evident that first-order methods (e.g., SCS) perform better than interior-point methods (e.g., SeDuMi), albeit at the cost of reduced accuracy (results similar to those in Table 3 are not reported for brevity, but the objective value returned by the first-order solvers was always within 0.8% of the high-accuracy optimal value computed with the interior-point solvers when possible). As in the previous example, exploiting partial orthogonality in CDCS-sos gives the best improvements.
Table 4. CPU time (in seconds) to solve the SDP relaxations of (10). \( N \) is the size of the largest PSD cone, \( m \) is the number of constraints, \( t \) is the size of the matrix factorized by CDCS-sos.

| \( n \) | \( N \) | \( m \) | \( t \) | SeDuMi | SDPT3 | SDPA | CSDP | SCS-direct | SCS-indirect | CDCS-sos |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 65 | 1100 | 110 | 2.8 | 1.8 | 2.0 | 2.6 | 0.2 | 0.2 | 0.3 |
| 12 | 90 | 1963 | 156 | 6.3 | 4.9 | 3.5 | 1.0 | 0.3 | 0.3 | 0.4 |
| 14 | 119 | 3255 | 210 | 36.2 | 16.3 | 44.8 | 2.6 | 0.8 | 0.7 | 0.6 |
| 17 | 170 | 6273 | 306 | 265.1 | 78.0 | 204.7 | 9.5 | 1.3 | 1.3 | 1.1 |
| 20 | 230 | 11025 | 420 | 1346.0 | 361.3 | 940.5 | 40.4 | 3.1 | 3.0 | 2.4 |
| 24 | 324 | 21050 | 600 | ** | ** | 8775.5 | 238.4 | 15.1 | 6.6 | 5.1 |
| 29 | 464 | 41760 | 870 | ** | ** | ** | ** | 17.1 | 16.9 | 14.3 |
| 35 | 665 | 83475 | 1260 | ** | ** | ** | ** | 67.6 | 57.1 | 37.4 |
| 42 | 945 | 164948 | 1806 | ** | ** | ** | ** | 133.7 | 129.2 | 92.8 |

**: The problem could not be solved due to memory limitations.

Figure 4. Average CPU time per 100 iterations for the SOS program for the minimization of the random polynomial (31).

5.2 Finding Lyapunov functions

As our next experiment, we considered the problem of constructing Lyapunov functions to verify local stability of polynomial systems, i.e., we solve the SOS program (10) for different system instances. We used SOSTOOLS [33] to generate the corresponding SDPs.

In the experiment, we randomly generated polynomial dynamical systems \( \dot{x} = f(x) \) of degree three with a locally asymptotically stable equilibrium at the origin, and then checked for local stability in the ball \( D = \{ x \in \mathbb{R}^n : \sum_{i=1}^n x_i^2 \leq 1 \} \). We used a complete quadratic polynomial as the candidate Lyapunov function. The total CPU times required by the solvers we tested to solve the SDP relaxations are reported in Table 4. Fig. 5 shows the average CPU times per 100 iterations for SCS and CDCS-sos. The results clearly show that the iterations in CDCS-sos are faster than in SCS (both direct and indirect implementations) for all our random problem instances. Once again, first-order methods require much less memory than interior point methods, and both CDCS-sos and SCS are able to solve large-scale problems \( (n \geq 29) \) that are beyond the reach of common interior-point solvers (SeDuMi, SDPT3, SDPA, and CSDP).

5.3 CPU times for the affine projection (23a)

The results in Sections 5.1 and 5.2 show the overall efficiency of our implementation of the ADMM-based algorithm (23a)–(23c) for large-scale SOS programs, compared to common state-of-the-art solvers. Analysing the CPU time for each of steps (23a)–(23c) reveals that (23b) sometimes requires the most computational effort, and we observed that our MATLAB implementation carries out this step more efficiently than SCS. In order to assess the unique advantages of exploiting partial orthogonality when solving the affine projection (23a), we re-ran our numerical experiments using two additional methods for this step (also available in CDCS-sos). The first one uses a cached sparse permuted LDL\(^T\) factorization of the coefficient matrix in (27), which is similar to the direct method implemented in SCS. The second approach applies a sparse Cholesky decomposition to (28b), without exploiting partial orthogonality. Figure 6 compares the average CPU time required by these two alternative approaches to solve 100 instances of the linear system (23a) when solving the problems in Sections 5.1 and 5.2. For all tested problem instances, exploiting partial orthogonality as described in Section 4 is the most efficient method, and in particular it is more than twice as fast as the LDL\(^T\) factorization strategy implemented in SCS.

6 Conclusion

In this paper, we highlighted the partial orthogonality in the SDPs arising from SOS programs formulated using the standard monomial basis. We then revealed a hidden “diagonal plus low-rank” structure at the computational level, which was exploited to develop a fast ADMM algorithm. Precisely, we showed that the cost of projecting the iterates of the algorithm in [23] onto a set defined by the affine con-
Table A.1. CPU time (in seconds) and number of iterations required to solve the demo problems in SOSTOOLS [33]. $N$ is the size of the largest PSD cone, $m$ is the number of constraints, $t$ is the size of the matrix factorized by CDCS-sos.

| Demo | $N$ | $m$ | $t$ | Time (s) | Iter. |
|------|-----|-----|-----|----------|-------|
| 1    | 3   | 5   | 0   | 0.058    | 51    |
| 2    | 13  | 58  | 3   | 0.226    | 145   |
| 3    | 15  | 45  | 1   | 2.601‡   | 2000  |
| 4    | 35  | 210 | 0   | 0.155    | 64    |
| 5    | 36  | 330 | 150 | 0.977‡   | 331   |
| 6    | 21  | 126 | 126 | 0.139‡   | 57    |
| 7    | 5   | 18  | 9   | 3.554‡   | 2000  |
| 8    | 2   | 6   | 3   | 0.277    | 186   |
| 9    | 12  | 60  | 78  | 0.090    | 43    |
| 10   | 20  | 84  | 22  | 0.135‡   | 60    |

‡: Maximum number of iterations reached.
†: Case of $t \geq m$, for which CDCS-sos would be worse than SCS.
*: The upper bound of this instance was modified as 0.88 in our experiment, while the original one was 0.8724 in SOSTOOLS.

maximum number of interactions when solving the Demos 3 and 7, since the resulting SDPs are not well-conditioned. For these instances of small size, CDCS-sos returned a solution in a few seconds. Similar to the cases of constrained POPs and finding Lyapunov functions in Section 5, we can expect that CDCS-sos is able to offer more computational advantages when the sizes of these SOS applications increase.

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