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Solving sparse polynomial optimization problems with chordal structure using the sparse bounded-degree sum-of-squares hierarchy

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Abstract

The sparse bounded degree sum-of-squares (sparse-BSOS) hierarchy of Weisser, Lasserre and Toh [*Math Prog Compt:1-32, to appear*] constructs a sequence of lower bounds for a sparse polynomial optimization problem. Under some assumptions, it is proved by the authors that the sequence converges to the optimal value. In this paper, we modify the hierarchy to deal with problems containing equality constraints directly, without eliminating or replacing them by two inequalities. We also evaluate the sparse-BSOS hierarchy on a well-known bilinear programming problem, called the pooling problem, as well as a discrete-time optimal control problem.

Keywords: Polynomial optimization, Sparse sum-of-squares hierarchy, Semi-definite programming, Pooling problem, Chordal sparsity structure, Discrete-time optimal control

2010 MSC: 90C20, 90C22, 90C26, 90C30

1. Introduction

A polynomial optimization problem (POP) is a mathematical optimization problem in which all constraints and the objective function are multi-variate polynomials. POPs include non-convex quadratic programming problems, which were proved to be NP -hard by Pardalos and Vavasis [26].

5 Many approaches are available for constructing lower bounds for the optimal value of a POP (denoted by f^*). Kim, Kojima and Waki [18] proposed a relaxation of a POP using a generalized

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Lagrangian dual. Lasserre [21] introduced an LP hierarchy that constructs a sequence of lower bounds for f^* . Using the Krivine *positivstellensatz* [19], Lasserre showed that under some assumptions the sequence converges to f^* . In the hope of getting a tighter lower bound, Lasserre, Toh, and Yang [22] extended the LP hierarchy to an SDP one, called the bounded degree sum-of-squares (BSOS) hierarchy. The advantage of the BSOS hierarchy is that it contains one semi-definite matrix variable, which has a fixed size that is independent of the level of the hierarchy. A major drawback of the BSOS hierarchy lies in the fact that the number of linear variables grows quickly when the level of the hierarchy increases. Also, for a large problem, the size of the semi-definite matrix variable gets large, which makes the hierarchy inefficient. In an effort to resolve these issues, Weisser, Lasserre and Toh [32] introduced a modification of the BSOS hierarchy, called the sparse-BSOS hierarchy, for POPs with a particular structural sparsity, which satisfies the *running intersection property* (RIP).

The RIP is a well-known concept in graph theory. In the literature of positive semi-definite (PSD) matrices and polynomial optimization, exploiting a sparsity that satisfies the RIP is done by studying the corresponding chordal graphs, see [15] for PSD matrices and [31] for polynomial optimization. The results in [32] can be seen as a combination of the results in the papers [22] and [31].

POPs have many real-life applications. Some of these applications were studied in the recent paper by Ahmadi and Majumdar [1]. In this paper, we analyze the behavior of the sparse-BSOS hierarchy on a class of bilinear programming problems, called pooling problems, and a class of discrete-time optimal control problems.

Solving the pooling problem is attracting considerable interest due to their applications in many real-life optimization problems, like oil refinery planning, chemical process, and water-waste network design. There are many formulations for the pooling problem. Haverly [17] proposed a formulation, called the P-formulation. Even though it was shown by Alfaki and Haugland [3] that the P-formulation problem, in general, is *NP*-hard, recently Baltean-Lugojan and Misener [6] showed that the three well-known instances proposed by Haverly [17] belong to a subclass of polynomial-time solvable pooling problems. One way of finding a lower bound for the P-formulation problem is by using the McCormick relaxation of each bilinear term, which can be reformulated as a Mixed Integer Linear Programming problem. In order to tighten this relaxation, Tawarmalani and Sahinidis [29] proposed the *PQ-formulation*. Dey and Gupte [10] proved that even for the

PQ-formulation, using the McCormick relaxations of the bilinear terms might yield a lower bound that is far from the optimal value of the problem. There are other formulations with different characteristics for the pooling problem, like Q-, TP- formulations. Detailed discussion can be found in the surveys by Misener and Floudas [24] and Gupte et al. [16], and the Ph.D. thesis by Alfaki [2].

Recently, semi-definite programming (SDP) hierarchies have been used to find lower bounds for pooling problems. Frimannslund et al. [14] applied the hierarchy proposed by Lasserre [20] to pooling problems. As they pointed out, the fast increase in the sizes of the semi-definite matrix variables in the problem, which is related to the level of the hierarchy, prevents the hierarchy from being applicable for pooling problems. Recently, Marandi, Dahl, and De Klerk [23] evaluated the BSOS hierarchy on pooling problems. They found that the BSOS hierarchy is successful in acquiring the optimal values of small-sized instances, but because of the number of variables, the hierarchy does not work well on moderate and large-sized instances. In this paper, we evaluate the sparse-BSOS hierarchy on the P-formulation of the pooling problem and compare the results with BSOS.

Another class of problem that we consider in this paper is a class of optimal control problems. A continuous-time optimal control problem finds a control function for a dynamical system such that a certain objective function is optimized. A discrete-time optimal control (DTC) is a method of solving a continuous one by discretizing the time slot that is considered in it. There are different approaches to solve a DTC problem using a nonlinear optimization problem. In [13], the author provides necessary conditions to make the KKT solutions optimal for the problem. Also, the authors in [9, 11, 31] test their proposed method on a DTC problem. We refer the reader to the Ph.D. thesis by Nielsen [25] for a more detailed discussion. In this paper, we show how sparse-BSOS hierarchy works on a DTC problem.

The BSOS and sparse-BSOS hierarchies are applicable to POPs that do not contain any equality constraints. However, all pooling problem formulations and DTC problems contain many equality constraints. The standard way of dealing with equality constraints is elimination, or replacing them with two inequalities. A way of eliminating equality constraints in the P-formulation was proposed in [23]; however, the elimination may destroy the sparsity pattern. On the other hand, replacing any equality constraints with two inequalities keeps the sparsity pattern but increases the number of constraints in the problem, which is not desirable in the BSOS and sparse-BSOS hierarchies

because it makes each level harder to solve. In this paper, we show how the hierarchies can be
70 modified to deal with equality constraints directly so that the convergence results remain valid.

The remainder of the paper is organized as follows. Section 2 briefly defines the pooling problem and a formulations of it, namely the P-formulation. In Section 3, we describe continuous- and discrete-time optimal control problems. Section 4 describes the sparse-BSOS hierarchy proposed in [32]. Section 5 demonstrates the link between graph theory and polynomial optimization. In
75 particular, in Section 5.1 we mention some well-known results in graph theory, and in Section 5.2 we construct a graph corresponding to a POP and exploit a sparsity that satisfies the RIP. In Section 6, we show how to modify the BSOS and sparse-BSOS hierarchies to deal with equality constraints directly. A numerical evaluation of the results is provided in Section 7. This paper contains two appendices. In the first appendix, we construct a toy pooling problem instance to
80 show how eliminating equality constraints of the P-formulation, as proposed in [23], destroys the sparsity that satisfies the RIP. The second appendix contains a table with some extra information regarding our numerical experiments on some DTOC problems.

2. The P- formulation of the pooling problem

In this section, we describe the P-formulation of the pooling problem. The notation we are
85 using is the same as in [16]. A pooling problem is a generalization of a network flow problem in which the inputs possess different specifications. The goal is to minimize the cost of mixing the inputs such that the demand with restrictions over specifications is satisfied. In the pooling problem there are three types of units: ones that store the inputs, which we call *inputs* and denote by $\mathcal{I}$, ones that mix the incoming flows from *inputs*, which we call *pools* and denote by $\mathcal{L}$, and the
90 units that mix the incoming flows from *pools* and/or *inputs*, and store the outputs, which we call *output* and denote by $\mathcal{J}$. The pooling problem can be determined by an acyclic directed graph $G = (\mathcal{N}, \mathcal{A})$, where $\mathcal{N} = \mathcal{I} \cup \mathcal{L} \cup \mathcal{J}$, and $\mathcal{A}$ is the set of links between the units, which means $\mathcal{A} \subseteq (\mathcal{I} \times \mathcal{L}) \cup (\mathcal{I} \times \mathcal{J}) \cup (\mathcal{L} \times \mathcal{L}) \cup (\mathcal{L} \times \mathcal{J})$. In this paper, we consider the standard pooling problem, which has no link between the pools and hence $\mathcal{A} \cap \mathcal{L} \times \mathcal{L} = \emptyset$. Figure 1 shows an illustration of a
95 standard pooling problem.

Let c_{ij} be the unit cost of sending one unit of flow from i to j . Also, let y_{ij} be the flow-rate between units i and j , where the link between the two units has the transmission capacity of at most u_{ij} . Also, each unit i may have a capacity C_i . Let $\mathcal{K}$ be the set of specifications, and let the

Figure 1: An example of a standard pooling problem with I inputs, L pools and J output.

concentration of the k th specification in input i be λ_{ik} , and in the pool l be p_{lk} . If the concentration
100 in the j th output has the lower and upper bounds restrictions of μ_{min} and μ_{max} , respectively, then
the P-formulation of the pooling problem is formulated as follows:

$$\min_{y,p} \quad \sum_{(i,j) \in \mathcal{A}} c_{ij} y_{ij} \quad (1a)$$

s.t.

$$\sum_{\substack{i \in \mathcal{I}: \\ (i,l) \in \mathcal{A}}} y_{il} = \sum_{\substack{j \in \mathcal{J}: \\ (l,j) \in \mathcal{A}}} y_{lj}, \quad l \in \mathcal{L}, \quad (1b)$$

$$\sum_{\substack{j \in \mathcal{L} \cup \mathcal{J}: \\ (i,j) \in \mathcal{A}}} y_{ij} \leq C_i, \quad i \in \mathcal{I}, \quad (1c)$$

$$\sum_{\substack{j \in \mathcal{J}: \\ (l,j) \in \mathcal{A}}} y_{lj} \leq C_l, \quad l \in \mathcal{L}, \quad (1d)$$

$$\sum_{\substack{i \in \mathcal{I} \cup \mathcal{L}: \\ (i,j) \in \mathcal{A}}} y_{ij} \leq C_j, \quad j \in \mathcal{J}, \quad (1e)$$

$$0 \leq y_{ij} \leq u_{ij}, \quad (i,j) \in \mathcal{A}, \quad (1f)$$

$$\sum_{\substack{i \in \mathcal{I}: \\ (i,l) \in \mathcal{A}}} \lambda_{ik} y_{il} = p_{lk} \sum_{\substack{j \in \mathcal{J}: \\ (l,j) \in \mathcal{A}}} y_{lj}, \quad l \in \mathcal{L}, \quad k \in \mathcal{K}, \quad (1g)$$

$$\sum_{\substack{i \in \mathcal{I}: \\ (i,j) \in \mathcal{A}}} \lambda_{ik} y_{ij} + \sum_{\substack{l \in \mathcal{L}: \\ (l,j) \in \mathcal{A}}} p_{lk} y_{lj} \leq \mu_{jk}^{max} \sum_{\substack{i \in \mathcal{I} \cup \mathcal{L}: \\ (i,j) \in \mathcal{A}}} y_{ij}, \quad j \in \mathcal{J}, \quad k \in \mathcal{K}, \quad (1h)$$

$$\sum_{\substack{i \in \mathcal{I}: \\ (i,j) \in \mathcal{A}}} \lambda_{ik} y_{ij} + \sum_{\substack{l \in \mathcal{L}: \\ (l,j) \in \mathcal{A}}} p_{lk} y_{lj} \geq \mu_{jk}^{min} \sum_{\substack{i \in \mathcal{I} \cup \mathcal{L}: \\ (i,j) \in \mathcal{A}}} y_{ij}, \quad j \in \mathcal{J}, \quad k \in \mathcal{K}. \quad (1i)$$

Here is a summarized interpretation of the constraints:

(1b): keeping the balance between the total incoming and outgoing flow-rates for each pool,

(1c),(1d),(1e): restricting the units' capacity,

105 **(1f):** restricting the capacity of the links between the units,

(1g): keeping the balance of the concentration of each specification in each pool for incoming and outgoing flows,

(1h),(1i): restricting the concentration of each specification in each output by the lower and upper bounds.

110 In this paper, we use a sparsity pattern and the sparse version of the bounded degree sum-of-squares hierarchy [32] to solve the P-formulation.

3. Discrete-time optimal control

In this section, we briefly describe continuous- and discrete-time optimal control (DIOC) problems. We borrow the notation from [27]. A continuous-time optimal control is the optimization problem

$$\begin{aligned} \min_{\substack{x(\cdot): \mathbb{R} \rightarrow \mathbb{R}^n \\ u(\cdot): \mathbb{R} \rightarrow \mathbb{R}^m}} & \int_0^T F[x(t), u(t), t] dt + S[x(T), T] \\ \text{s.t.} & \quad \dot{x}(t) = f[x(t), u(t), t], \quad \forall t \in [0, T] \\ & \quad x(t) \in \mathcal{X}, \quad u(t) \in \mathcal{U}, \quad \forall t \in [0, T] \\ & \quad x(0) = x_0, x(T) = x_T, \end{aligned} \quad (2)$$

where $F[.,.,.] : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R} \rightarrow \mathbb{R}$ is a function with continuous partial derivatives with respect to $x(t)$, $S[.,.] : \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}$ is a function with continuous partial derivatives with respect to $x(T)$,

115 $f : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R} \rightarrow \mathbb{R}^m$ is a function, $\mathcal{X} \subseteq \mathbb{R}^m$ and $\mathcal{U} \subseteq \mathbb{R}^n$ are given sets, and x_0, x_T are given vectors.

One of the methods for solving (2) is discretizing the problem and considering the discrete-time optimal control

$$\begin{aligned}
& \min_{\substack{x_k \in \mathbb{R}^n, k=1, \dots, N-1 \\ u_k \in \mathbb{R}^m, k=0, \dots, N-1}} \frac{1}{N} \sum_{k=0}^{N-1} F \left[x_k, u_k, \frac{kT}{N} \right] + S[x_N, T] \\
& \text{s.t. } x_{k+1} = x_k + \frac{1}{N} f \left[x_k, u_k, \frac{kT}{N} \right], k = 0, \dots, N-1 \\
& x_k \in \mathcal{X}, k = 1, \dots, N-1, \\
& u_k \in \mathcal{U}, k = 0, \dots, N-1,
\end{aligned} \tag{3}$$

where x_0, x_N are given. It is clear that when F and f are polynomials, and the sets $\mathcal{X}$ and $\mathcal{U}$ are semi-algebraic, then (3) is a polynomial optimization problem. The size of (3) is related to the number of intervals (N), which can be large. In Section 7.2, we show how one can apply the
120 sparse-BSOS hierarchy to solve (3).

4. Sparsity pattern in a polynomial problem

In this section, we briefly describe the sparse bounded degree sum-of-squares (sparse-BSOS) hierarchy in polynomial optimization introduced, by Weisser, Lasserre and Toh [32]. In what follows, for an integer $m \geq 0$,

$$[m] := \begin{cases} \{1, \dots, m\} & \text{if } m > 0, \\ \emptyset & \text{if } m = 0. \end{cases}$$

Also, we assume that $x \in \mathbb{R}^n$, and for a given $\mathcal{D} \subseteq [n]$, we denote by $\Sigma[x; \mathcal{D}]_\kappa$, the cone of sum-of-squares polynomials of degree at most 2κ , and by $\mathbb{R}[x; \mathcal{D}]$ the ring of all polynomials in the variables $\{x_i : i \in \mathcal{D}\}$.

For a general polynomial optimization problem

$$\begin{aligned}
f^* &= \min_x f(x) \\
&\text{s.t. } g_j(x) \geq 0, \quad j = 1, \dots, m,
\end{aligned} \tag{4}$$

125 where $x \in \mathbb{R}^n$, $n, m \in \mathbb{N}$ and all $f(x)$ and $g_j(x)$, $j = 1, \dots, m$ are n -variate polynomials, the *running intersection property* is defined as follows.

Definition 1. Problem (4) satisfies the running intersection property (RIP) if there exists $q \in \mathbb{N}$, $\mathcal{D}_\ell \subseteq [n]$ and $\mathcal{C}_\ell \subseteq [m]$ for all $\ell \in [q]$ such that

- $f = \sum_{\ell=1}^q f^\ell$, for some $f^\ell \in \mathbb{R}[x; \mathcal{D}_\ell]$, for all $\ell \in [q]$,
- $g_j \in \mathbb{R}[x; \mathcal{D}_\ell]$, for all $j \in \mathcal{C}_\ell$, and $\ell \in [q]$,
- $\bigcup_{\ell=1}^q \mathcal{D}_\ell = [n]$, and $\bigcup_{\ell=1}^q \mathcal{C}_\ell = [m]$,
- for all $\ell \in [q-1]$, there is an $s \leq \ell$ such that $(\mathcal{D}_{\ell+1} \cap \bigcup_{r=1}^\ell \mathcal{D}_r) \subseteq \mathcal{D}_s$. □

Assume that the running intersection property holds for (4). Let

$$\mathbb{N}_d^\ell := \left\{ (\alpha, \beta) \in \mathbb{N}^{2m} : \alpha_j = \beta_j = 0 \text{ if } j \notin \mathcal{C}_\ell, \sum_{j \in [m]} \alpha_j + \beta_j \leq d \right\},$$

and

$$h_{\alpha\beta}^\ell := \prod_{j \in [m]} g_j^{\alpha_j} (1 - g_j)^{\beta_j} \in \mathbb{R}[x; \mathcal{D}_\ell], \quad (\alpha, \beta) \in \mathbb{N}_d^\ell.$$

Then, we have the following result from [32].

Theorem 1. [32, Theorem 2] Consider the general polynomial optimization problem (4). Suppose that it satisfies the running intersection property, and $g_j(x) \leq 1$ for any feasible solution x , $j \in [m]$. Also, assume that for all $\ell \in [q]$, the ring of $\mathbb{R}[x; \mathcal{D}_\ell]$ is generated by $\{1, (g_j)_{j \in \mathcal{C}_\ell}\}$, and there exists $M_\ell > 0$ and $j \in \mathcal{C}_\ell$ such that $g_j = 1 - \frac{1}{M_\ell} (\sum_{i \in \mathcal{D}_\ell} x_i^2)$. Then, for any fixed $\kappa \in \mathbb{N}$, $\{q_d^\kappa\}$ is a non-decreasing sequence and $q_d^\kappa \rightarrow f^*$ as $d \rightarrow +\infty$, where

$$q_d^\kappa := \sup \left\{ t : \begin{array}{ll} f^\ell - \sum_{(\alpha, \beta) \in \mathbb{N}_d^\ell} \lambda_{\alpha\beta}^\ell h_{\alpha\beta}^\ell \in \Sigma[x; \mathcal{D}_\ell]_\kappa, & \ell \in [q] \\ f - t = \sum_{\ell \in [q]} f^\ell, \quad \lambda^\ell \geq 0, \quad t \in \mathbb{R}, \quad f^\ell \in \mathbb{R}[x; \mathcal{D}_\ell], \quad \ell \in [q] \end{array} \right\}. \quad (5)$$

□

Theorem 1 introduces a non-decreasing sequence that converges to the optimal value of (4) under some assumptions. Instead of (5), we consider the following equivalent problem where the f^ℓ , $\ell = 1, \dots, q$, have been eliminated,

$$q_d^\kappa = \sup \left\{ t : \begin{array}{l} f - t = \sum_{\ell \in [q]} \sum_{(\alpha, \beta) \in \mathbb{N}_d^\ell} \lambda_{\alpha\beta}^\ell h_{\alpha\beta}^\ell + \sum_{\ell \in [q]} \sigma_\ell \\ \sigma_\ell \in \Sigma[x; \mathcal{D}_\ell]_\kappa, \quad \lambda^\ell \geq 0, \quad t \in \mathbb{R}, \quad \ell \in [q] \end{array} \right\}. \quad (6)$$

The number of scalar variables in each level of (6) is smaller than the one in the same level of the BSOS hierarchy [22, equation (7)].

Definition 2. Given a vector $b \in \mathbb{R}^m$ ($m \leq n$) and a matrix $A \in \mathbb{R}^{m \times n}$, we call the system of linear constraints $Ax = b$ linearly (in)dependent, if the matrix $[A, b] \in \mathbb{R}^{m \times (n+1)}$ has linearly (in)dependent rows. □

In the next proposition we show that all constraints in (6) are linearly independent, when the degree of the sums of squares equals to the degree of the whole equality constraint, but before it, we need to emphasize on the following remark.

Remark 1. Let $x \in \mathbb{R}^n$ and $p(x) = \sum_{\alpha \in \bar{\mathbb{N}}_{2\omega}^{[n]}} p_\alpha x^\alpha$, where

$$\bar{\mathbb{N}}_\kappa^\mathcal{D} := \left\{ \alpha \in \mathbb{N}^n : \alpha_i = 0 \text{ if } i \notin \mathcal{D}, \sum_{i \in [n]} \alpha_i \leq \kappa \right\},$$

for a set $\mathcal{D} \subseteq [n]$. If $M \in \mathbb{R}^{\binom{n+\omega}{\omega} \times \binom{n+\omega}{\omega}}$ is a symmetric matrix variable whose rows (columns) are corresponding to the members of $\bar{\mathbb{N}}_\omega^{[n]}$, then linear constraints

$$p_\alpha = \sum_{\substack{\beta, \gamma \in \bar{\mathbb{N}}_\omega^{[n]} \\ \beta + \gamma = \alpha}} M_{\beta\gamma}, \quad \forall \alpha \in \bar{\mathbb{N}}_{2\omega}^{[n]}, \quad (7)$$

are linearly independent. This is because all the constraints in (7) involve different variables, i.e., no variable appears in two constraints in (7). To see this, let $\beta, \gamma \in \bar{\mathbb{N}}_\omega^{[n]}$ be fixed. Due to the construction of the constraints in (7), the variable $M_{\beta\gamma}$ appears only in the constraint corresponding to $\alpha = \beta + \gamma$, and no other constraints. □

Proposition 1. Consider problem (4). Let d be such that

$$2\kappa = \max\{d \max_{j=1, \dots, m} (\deg(g_j)), \deg(f), 2\kappa\}.$$

Then, all equality constraints in (6) are linearly independent, if the polynomial equality is modeled by equating the monomials coefficients.

Proof. For each $\ell \in [q]$, set $v^\ell = (x^\beta)_{\beta \in \bar{\mathbb{N}}_\kappa^{\mathcal{D}_\ell}}$. Also, let $\sigma_\ell = v^{\ell T} W^\ell v^\ell$, for each $\ell \in [q]$, where $W^\ell \in \mathbb{R}^{\binom{n_\ell + \kappa}{\kappa} \times \binom{n_\ell + \kappa}{\kappa}}$ is a positive semi-definite matrix variable, and $n_\ell = |\mathcal{D}_\ell|$. So, Remark 1 implies that the equality constraints in (6) are linearly independent, if the polynomial equality is modeled by equating the monomials coefficients. □

According to the proof of Proposition 1, if $2\kappa \neq \max\{d \max_{j=1,\dots,m} (\deg(g_j)), \deg(f), 2\kappa\}$, still
 155 the constraints corresponding to the monomials up to degree 2κ are linearly independent. If
 $\deg(f) > \max\{d \max_{j=1,\dots,m} (\deg(g_j)), 2\kappa\}$, then $\deg(f) = \max\{d \max_{j=1,\dots,m} (\deg(g_j)), \deg(f), 2\kappa\}$,
 and clearly the d th iteration of the hierarchy is infeasible, because there is no monomial with degree
 $\deg(f)$ in $\sum_{\ell \in [q]} \sum_{(\alpha, \beta) \in \mathbb{N}_d^\ell} \lambda_{\alpha\beta}^\ell h_{\alpha\beta}^\ell + \sum_{\ell \in [q]} \sigma_\ell$.

The main assumption in Theorem 1 is the existence of a splitting that satisfies the *running*
 160 *intersection property*. So, the question is how to exploit such sparsity for a polynomial optimization
 problem. In the next section we answer this question.

5. Polynomial optimization and chordal graphs

In this section, we study the relation between polynomial optimization and graph theory. Specif-
 ically, we mention some results on chordal graphs and use them to exploit sparsity for a polynomial
 165 optimization problem that satisfies the *running intersection property*.

5.1. Chordal graph and maximal cliques

In this subsection we recall some well-known results on chordal graphs and maximal cliques.
 The notation we are using in this section is the same as in [8].

Definition 3. Consider an undirected graph $G = (V, E)$, where V and E denote the sets of vertices
 170 and edges, respectively. A chord of a cycle is any edge joining two nonconsecutive vertices of the
 cycle. A graph G is called chordal, if every cycle of length greater than 3 has a chord. $\square$

Let $\text{adj}(v)$ denote the set of adjacent vertices to a vertex v . A vertex ordering ϕ of graph
 $G = (V, E)$ with n vertices is a bijection $\phi : V \rightarrow [n]$, and it can be denoted by indexing the vertex
 set, such that $V = \{v_1, \dots, v_n\}$, and $\phi(v_i) = i$, for $i \in [n]$. Let $v_1, \dots, v_n$ be a vertex ordering of G
 and set

$$\mathcal{L}_i := \{v_i, \dots, v_n\}, \quad i \in [n].$$

Definition 4. A vertex ordering ϕ is a perfect elimination ordering if for any $i \in [n]$ the subgraph
 of G induced by $\mathcal{L}_i \cap \text{adj}(v_i)$ is complete. $\square$

Theorem 2. (see, e.g., [8, Theorem 2.2]) A graph G is chordal if and only if G has a perfect
 175 *elimination ordering*.

Definition 5. Let $G = (V, E)$ be any graph. A clique of G is any subset of V for which the induced graph is complete in G . A maximal clique is a clique that is not properly contained in another clique. We denote by $\mathcal{K}_G$ the set of all maximal cliques of G . $\square$

Theorem 3. For a chordal graph G , assume that $|\mathcal{K}_G| = q$. Then, there is a labeling $\mathcal{K}_G = \{\mathcal{K}_1, \dots, \mathcal{K}_q\}$ such that

$$\forall \ell \in [q-1], \exists s \leq \ell : \left(\mathcal{K}_{\ell+1} \cap \bigcup_{r=1}^{\ell} \mathcal{K}_r \right) \subseteq \mathcal{K}_s.$$

Proof. By invoking [8, Theorem 3.1] and [8, Corollary 1], one can deduce the theorem. $\square$

180 For any vertex ordering ϕ of graph $G = (V, E)$, let us add extra edges to G in order to make all $\mathcal{L}_i \cap \text{adj}(v_i)$ complete, $i \in [n]$, and denote by E_ϕ^* the union of E with the extra edges. Then clearly $G^* = (V, E_\phi^*)$ is chordal, because ϕ is a *perfect elimination ordering* for G^* . The graph G^* is called a chordal extension (or triangulation) of G .

185 It is well-known that the Laplacian matrix of a graph $G = (V, E)$, denoted by L , is positive semi-definite. We denote the permuted Laplacian matrix of a graph G according to a vertex ordering ϕ by L_ϕ . As it is proved in [30, Section 9.1], using the Cholesky factorization $L_\phi = R^T R$, the nonzero entries of $R + R^T$ correspond to the edges in E_ϕ^* .

A vertex ordering that minimizes $|E_\phi^* \setminus E|$ over all possible vertex orderings of G is called a minimum ordering. Finding a minimum ordering is known to be NP-complete [30, Section 6.6]. There are many polynomial-time algorithms to find a “good” ordering, see [30, Section 6.6]. 190 *Minimum degree* ordering is such an algorithm, which finds the vertex v with the least degree, set $\phi(v) = i$ and delete v from the graph G in the i th iteration. Finding the vertex with the least degree in each iteration is time-consuming. Therefore, in our numerical results we use the *approximate minimum degree* ordering (AMD) introduced in [4], which finds upper bounds of the vertices’ degree in each iteration and use them to select the vertex v . 195

5.2. Exploiting sparsity in a polynomial optimization using chordal graphs

In this subsection, we construct a graph corresponding to problem (4) and use the results mentioned in Section 5.1 to exploit sparsity that satisfies the *running intersection property*. The graph is essentially the same as the one constructed in [31].

200 Consider a general polynomial problem (4). A graph $G = (V, E)$ associated to this problem can be constructed as follows:

- the vertex set $V := \{x_1, \dots, x_n\}$,
- $E_j := \{(x_i, x_k) : \text{variables } x_i, x_k \text{ are present in the definition of } g_j(x)\}, j \in [m]$,
- $E_0 := \{(x_i, x_k) : \text{product } x_i x_k \text{ is present in the definition of } f(x)\}$,
- the edge set $E := \bigcup_{j=0}^m E_j$.

Let L be the Laplacian matrix of $G = (V, E)$. Using the results in Section 5.1, in order to find the sparsity pattern for the polynomial optimization that satisfies the *running intersection property*, one can use Algorithm 1.

Algorithm 1 Exploit sparsity in the polynomial optimization (4) using chordal graphs

```

 $\phi \leftarrow$  get the ordering from AMD algorithm on graph  $G$ 
 $L_\phi \leftarrow$  reorder Laplacian matrix  $L$  according to  $\phi$ 
use Cholesky factorization of  $L_\phi$  to construct a chordal extension  $G^*$  of  $G$ 
 $\{\mathcal{D}_1, \dots, \mathcal{D}_q\} \leftarrow$  the maximal cliques of  $G^*$ 
for all  $l \in [q]$  do
     $\mathcal{C}_l \leftarrow$  all  $g_j$  in  $\mathbb{R}[x, \mathcal{D}_l]$ 
end for

```

Theorem 4. *There is a bijection $\Gamma : [q] \rightarrow [q]$, such that the index blocks $\mathcal{D}_{\Gamma(\ell)}$ and constraint blocks $\mathcal{C}_{\Gamma(\ell)}$, $\ell \in [q]$, constructed by Algorithm 1 satisfy the running intersection property.*

Proof. By Theorem 3, there is a bijection $\Gamma : [q] \rightarrow [q]$ such that

$$\forall \Gamma(\ell) \in [q-1], \exists \Gamma(s) \leq \Gamma(\ell) : \left(\mathcal{D}_{\Gamma(\ell)+1} \cap \bigcup_{r=1}^{\ell} \mathcal{D}_{\Gamma(r)} \right) \subseteq \mathcal{D}_{\Gamma(s)}.$$

Now, we show that $f = \sum_{\ell=1}^q f^\ell$, where $f^\ell \in \mathbb{R}[x; \mathcal{D}_{\Gamma(\ell)}]$, for all $\ell \in [q]$. Because f is a polynomial, it is sufficient to show that for each monomial in the definition of f there is an ℓ such that the monomial belongs to $\mathbb{R}[x; \mathcal{D}_\ell]$. Let x^β be a monomial in the definition of f , where $\beta \in \mathbb{N}^n$. Due to the structure of E_0 , the graph induced by the vertices corresponding to x^β is complete and hence contained in one of the maximal cliques of G^* . Therefore, there is an $\ell \in [q]$ such that $x^\beta \in \mathbb{R}[x; \mathcal{D}_\ell]$.

By the construction of $\mathcal{C}_l$, it is clear that $g_j \in \mathbb{R}[x, \mathcal{D}_\ell]$ for all $j \in \mathcal{C}_l$, $l \in [q]$, and $\bigcup_{\ell=1}^q \mathcal{C}_\ell = [m]$. Also, $\bigcup_{\ell=1}^q \mathcal{D}_\ell = [n]$, because $\{\mathcal{D}_1, \dots, \mathcal{D}_q\}$ is the set of all maximal cliques of G^* . $\square$

In Theorem 4, we showed that there is an ordering of $[q]$ with which the blocks $\mathcal{D}_\ell$ and $\mathcal{C}_\ell$, $\ell \in [q]$ satisfy the *running intersection property*. In the following lemma, we show that we do not need to know the ordering to solve problem (6). 220

Lemma 1. *Let $\Gamma : [q] \rightarrow [q]$ be a bijection for some $q \in \mathbb{N}$, $\mathcal{D}_\ell \subseteq [n]$ and $\mathcal{C}_\ell \subseteq [m]$ for all $\ell \in [q]$. Then for each $\kappa, d \in \mathbb{N}$, q_d^κ in (6) is given by*

$$q_d^\kappa = \sup \left\{ t : \begin{array}{l} f - t = \sum_{\ell \in [q]} \sum_{(\alpha, \beta) \in \mathbb{N}_d^{\Gamma(\ell)}} \lambda_{\alpha\beta}^{\Gamma(\ell)} h_{\alpha\beta}^{\Gamma(\ell)} + \sum_{\ell \in [q]} \sigma_{\Gamma(\ell)} \\ \sigma_\ell \in \Sigma[x; \mathcal{D}_\ell]_\kappa, \quad \lambda^\ell \geq 0, \quad t \in \mathbb{R}, \quad \ell \in [q] \end{array} \right\}. \quad (8)$$

Proof. The summations in (8) are over $\ell \in [q]$, and may change the order of summations. In other words:

$$\begin{aligned} \sum_{\ell \in [q]} \sum_{(\alpha, \beta) \in \mathbb{N}_d^{\Gamma(\ell)}} \lambda_{\alpha\beta}^{\Gamma(\ell)} h_{\alpha\beta}^{\Gamma(\ell)} &= \sum_{\ell \in [q]} \sum_{(\alpha, \beta) \in \mathbb{N}_d^\ell} \lambda_{\alpha\beta}^\ell h_{\alpha\beta}^\ell, \\ \sum_{\ell \in [q]} \sigma_{\Gamma(\ell)} &= \sum_{\ell \in [q]} \sigma_\ell. \end{aligned}$$

□

Theorems 1, 4 and Lemma 1 show that if:

- $g_j(x) \leq 1$ for any feasible solution x , $j \in [m]$,
 - for all $\ell \in [q]$, the ring of $\mathbb{R}[x; \mathcal{D}_\ell]$ is generated by $\{1, (g_j)_{j \in \mathcal{C}_\ell}\}$,
 - there exists $M_\ell > 0$ and $j \in \mathcal{C}_\ell$ such that $g_j = 1 - \frac{1}{M_\ell} (\sum_{i \in \mathcal{D}_\ell} x_i^2)$,
- 225

then for a fixed $\kappa \in \mathbb{N}$, $\{q_d^\kappa\}$ is a non-decreasing sequence that converges to the optimal value of (4), when $\mathcal{D}_\ell$ and $\mathcal{C}_\ell$ are the outputs of Algorithm 1.

The result of this section can be applied to the P-formulation (1) by elimination of equality constraints proposed in [23]. The following example shows how Algorithm 1 works for “Haverly1” and “Adhya1”, two pooling problem instances, after elimination of the equality constraints. 230

Example 1. “Haverly1” is a pooling problem instance with 3 inputs, 2 outputs and 1 pool, where the inputs are characterized with only 1 specification. The formulation of this instance after elimination of the equality constraints, proposed in [23, Section 3.2], is

$$\min \quad -200x_2(15x_1 - 12) - 200x_3(15x_1 - 6) + 200x_4 - 1000x_5$$

$$s.t. \quad 1 \geq -\frac{3}{4}(x_1 - 1)(x_2 + x_3) \geq 0 \quad (9a)$$

$$1 \geq \frac{1}{4}(3x_1 - 1)(x_2 + x_3) \geq 0 \quad (9b)$$

$$1 \geq 1 - 2(x_2 + x_4) \geq 0 \quad (9c)$$

$$1 \geq 1 - (x_3 + x_5) \geq 0 \quad (9d)$$

$$1 \geq \frac{1}{2}(x_4 + x_2) - \frac{2}{5}x_4 - \frac{3}{5}x_1x_2 \geq 0 \quad (9e)$$

$$1 \geq \frac{1}{2}(x_5 + x_3) - \frac{2}{3}x_5 - x_1x_3 \geq 0 \quad (9f)$$

$$1 \geq x_i \geq 0, \quad i = 1, \dots, 5. \quad (9g)$$

For this problem, the Laplacian matrix corresponding to its graph G (Figure 2a) is

$$L = \begin{bmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 & 0 \\ -1 & -1 & 3 & 0 & -1 \\ -1 & -1 & 0 & 2 & 0 \\ -1 & 0 & -1 & 0 & 2 \end{bmatrix}.$$

The output of the AMD algorithm is $\phi(\{x_1, x_2, x_3, x_4, x_5\}) = [5, 3, 1, 4, 2]$. Using the Cholesky factorization, one finds out that there is no need to add any extra edge, so G is chordal with the maximal cliques $\mathcal{D}_1 = \{x_1, x_2, x_3\}$, $\mathcal{D}_2 = \{x_1, x_2, x_4\}$, and $\mathcal{D}_3 = \{x_1, x_3, x_5\}$. Hence,

$$\mathcal{C}_1 = \{(9a), (9b), (9g)_1, (9g)_2, (9g)_3\},$$

$$\mathcal{C}_2 = \{(9c), (9e), (9g)_1, (9g)_2, (9g)_4\},$$

$$\mathcal{C}_3 = \{(9d), (9f), (9g)_1, (9g)_3, (9g)_5\},$$

where $(9g)_i$ is the constraint (9g) for x_i , $i = 1, \dots, 5$.

“Adhya1” is a pooling problem instance that has 5 inputs, 4 outputs, 2 pools where the inputs are characterized with 4 specifications. After elimination of the equality constraints, the problem contains 11 variables and 41 constraints. The graph in Figure 2b shows G where the red dashed arcs are corresponding to the components of $R + R^T$ that are zeros in L_ϕ . This means that the red dashed arcs are added to make the graph chordal. For G^* , the maximal cliques are

$$\mathcal{D}_1 = \{x_1, x_2, x_3, x_4, x_5, x_9, x_{10}, x_{11}\},$$

$$\mathcal{D}_2 = \{x_2, x_3, x_4, x_5, x_6, x_9, x_{10}, x_{11}\},$$

Figure 2: The graphs corresponding to “Haverly1” and “Adhya1” after elimination of the equality constraints. The red dashed arcs are added to make the graph chordal.

$$\begin{aligned}\mathcal{D}_3 &= \{x_3, x_4, x_5, x_6, x_7, x_9, x_{10}, x_{11}\}, \\ \mathcal{D}_4 &= \{x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}\}.\end{aligned}$$

□

Elimination of the equality constraints may destroy the sparsity pattern that satisfies the *running intersection property*. In Appendix A, we construct a toy pooling problem instance for which the elimination method proposed in [23] destroys the sparsity pattern of the P-formulation. Therefore, in the following section we study algebraic sets with equality constraints and prove a *positivstellensatz* that deals with equality constraints, and modify the BSOS and sparse-BSOS hierarchies accordingly.

250 6. Problems with equality constraints

Consider the following algebraic set:

$$\mathcal{F} := \{x \in \mathbb{R}^n : e_t(x) = 0, t \in [T], g_i(x) \geq 0, i \in [m]\}, \quad (10)$$

where $e_t, g_i \in \mathbb{R}[x, [n]]$, $t \in [T]$, $i \in [m]$. In the next theorem we show that one can slightly change the Krivine's *positivstellensatz* [19] in order to handle algebraic set $\mathcal{F}$.

Theorem 5. *Assume that $g_i(x) \leq 1$, for all $x \in \mathcal{F}$, $i \in [m]$. If a polynomial $f(x)$ is positive on $\mathcal{F}$ and the ring of polynomials $\mathbb{R}[x, [n]]$ is generated by $\{1, e_t(x), g_i(x)\}_{\substack{i \in [m] \\ t \in [T]}}$, then there is an integer d such that*

$$f(x) = \sum_{(\gamma, \alpha, \theta, \beta) \in \mathbb{N}_d^{2m+2T}} \lambda_{\gamma, \alpha, \theta, \beta} \prod_{t \in [T]} e_t(x)^{\gamma_t} (1 - e_t(x))^{\theta_t} \prod_{i \in [m]} g_i(x)^{\alpha_i} (1 - g_i(x))^{\beta_i},$$

for some λ such that

$$\begin{cases} \lambda_{\gamma, \alpha, \theta, \beta} \geq 0 & \text{if } \gamma = 0 \text{ or } T = 0, \\ \lambda_{\gamma, \alpha, \theta, \beta} \in \mathbb{R} & \text{otherwise.} \end{cases}$$

Proof. We prove this theorem by induction on T , the number of equality constraints. If $T = 0$, there is no equality constraints in $\mathcal{F}$. So, the result follows directly from Krivine's *positivstellensatz* [19]. Now, assume that the result holds for all sets in the form of (10) with T equality constraints and we prove it for a set $\mathcal{F}$ with $T + 1$ equality constraints.

Setting $g(x) := e_{T+1}(x)$, we can write $\mathcal{F}$ as follows:

$$\{x : g(x) \geq 0, -g(x) \geq 0, g_i(x) \geq 0, i = 1, \dots, m, e_t(x) = 0, t = 1, \dots, T\}.$$

So, by the induction hypothesis, there is an integer d such that

$$f(x) = \sum_{\substack{\bar{\alpha} = (a_0, a_1, \alpha, \gamma) \\ \bar{\beta} = (b_0, b_1, \beta, \theta) \\ \lambda_{\bar{\alpha}, \bar{\beta}} \in \mathbb{N}_d^{2m+2T+4}}} \lambda_{\bar{\alpha}, \bar{\beta}} g(x)^{a_0} (-g(x))^{a_1} (1 + g(x))^{b_1} h_{b_0 \alpha \beta \gamma \theta}(x),$$

where,

$$h_{b_0 \alpha \beta \gamma \theta}(x) = (1 - g(x))^{b_0} \prod_{i=1}^m g_i(x)^{\alpha_i} (1 - g_i(x))^{\beta_i} \prod_{t=1}^T e_t(x)^{\gamma_t} (1 - e_t(x))^{\theta_t},$$

and

$$\begin{cases} \lambda_{\bar{\alpha}, \bar{\beta}} \geq 0 & \gamma = 0 \text{ or } T = 0, \\ \lambda_{\bar{\alpha}, \bar{\beta}} \in \mathbb{R} & \text{otherwise.} \end{cases}$$

So, $f(x)$ can be written as

$$\sum_{\substack{\bar{\alpha} = (a_0, a_1, \alpha, \gamma) \\ \bar{\beta} = (b_0, b_1, \beta, \theta) \\ \lambda_{\bar{\alpha}, \bar{\beta}} \in \mathbb{N}_d^{2m+2T+4}}} (-1)^{a_1} \lambda_{\bar{\alpha}, \bar{\beta}} g(x)^{a_0+a_1} (1 + g(x))^{b_1} h_{b_0 \alpha \beta \gamma \theta}(x).$$

By using binomial theorem for $(1 + g(x))^{b_1}$, we have

$$f(x) = \sum_{\substack{\bar{\alpha} = (a_0, a_1, \alpha, \gamma) \\ \bar{\beta} = (b_0, b_1, \beta, \theta) \\ \lambda_{\bar{\alpha}, \bar{\beta}} \in \mathbb{N}_d^{2m+2T+4}}} (-1)^{a_1} \lambda_{\bar{\alpha}, \bar{\beta}} g(x)^{a_0+a_1} \left(\sum_{j=0}^{b_1} c_j g(x)^j \right) h_{b_0 \alpha \beta \gamma \theta}(x),$$

where c_j , $j = 0, \dots, b_1$, are the binomial coefficients and therefore positive. This means that

$$f(x) = \sum_{\substack{\bar{\alpha} = (a_0, a_1, \alpha, \gamma) \\ \bar{\beta} = (b_0, b_1, \beta, \theta) \\ \lambda_{\bar{\alpha}, \bar{\beta}} \in \mathbb{N}_d^{2m+2T+4}}} \sum_{j=0}^{b_1} (-1)^{a_1} c_j \lambda_{\bar{\alpha}, \bar{\beta}} g(x)^{a_0+a_1+j} h_{b_0 \alpha \beta \gamma \theta}(x).$$

Let us fix $b_0, \alpha, \beta, \gamma, \theta$ such that $k := b_0 + |\alpha| + |\beta| + |\gamma| + |\theta| \leq d$, and set

$$\chi_{b_0, \alpha, \beta, \gamma, \theta}(x) := \sum_{(a_0, a_1, b_1) \in \mathbb{N}_{d-k}^3} \sum_{j=0}^{b_1} (-1)^{a_1} c_j \lambda_{\bar{\alpha}, \bar{\beta}} g(x)^{a_0+a_1+j}.$$

The coefficient of $g(x)^l$, $l = 0, \dots, d-k$, in $\chi_{b_0, \alpha, \beta, \gamma, \theta}(x)$ is the summation of some $c_j \lambda_{\bar{\alpha}, \bar{\beta}}$ and $-c_j \lambda_{\bar{\alpha}, \bar{\beta}}$ corresponding to different $\bar{\beta}$ and j . If $l = 0$ and $\gamma = 0$, or $l = 0$ and $T = 0$, then, $a_0 = a_1 = j = 0$, which means the coefficient of $g(x)^0$ is nonnegative. Hence,

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$$\begin{aligned} f(x) &= \sum_{\substack{(b_0, \alpha, \beta, \gamma, \theta) \\ k \leq d}} \chi_{b_0, \alpha, \beta, \gamma, \theta}(x) h_{b_0, \alpha, \beta, \gamma, \theta}(x) \\ &= \sum_{\substack{(b_0, \alpha, \beta, \gamma, \theta) \\ k \leq d}} \sum_{l=0}^{d-k} \bar{\lambda}_{l, b_0, \alpha, \beta, \gamma, \theta} g(x)^l h_{b_0, \alpha, \beta, \gamma, \theta}(x), \end{aligned}$$

for some $\bar{\lambda}$ with real components such that $\bar{\lambda}_{l, b_0, \alpha, \beta, \gamma, \theta}$ is nonnegative if $l = 0$ and $\gamma = 0$ or $l = 0$ and $T = 0$. So, combining the two summations completes the proof. $\square$

Theorem 5 asserts that the coefficients corresponding to the polynomial-multiplications

$$\prod_{t \in [T]} e_t(x)^{\gamma_t} (1 - e_t(x))^{\theta_t} \prod_{i \in [m]} g_i(x)^{\alpha_i} (1 - g_i(x))^{\beta_i},$$

with $\gamma \neq 0$, are unrestricted.

Remark 2. Applying Theorem 5 to [32, Theorem 1], if a polynomial optimization problem with feasible region (10) satisfies the assumptions of Theorem 1, then the parts of linear variable λ^l in (5) associated with the polynomial-multiplications containing equality constraints are unrestricted, and all of the convergence results in [32] are valid.

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Remark 3. *Considering Theorem 5 and Remark 2, one can easily construct the corresponding graph to any polynomial optimization problem with some equality constraints, and exploit the sparsity that satisfies the running intersection property, as described in Section 5.*

For a pooling problem, let denote by G the graph of the P-formulation (1) constructed with the procedure in Section 5.2. All nodes in G are corresponding to a variable in the P-formulation (1). Because of the constraint (1c), nodes corresponding to $y_{il}, y_{ij}, (i, l), (i, j) \in \mathcal{A}$ are connected in G , for each $i \in \mathcal{I}$. We denote by $\mathcal{K}_i, i \in \mathcal{I}$, this type of cliques. The nodes corresponding to $y_{ij}, y_{lj}, (i, j), (l, j) \in \mathcal{A}$, for each $j \in \mathcal{J}$ are connected because of (1e), and we denote the cliques by $\mathcal{K}_j, j \in \mathcal{J}$. In the same way because of (1d), the nodes $y_{il}, y_{lj}, (i, l), (l, j) \in \mathcal{A}$, make the cliques $\mathcal{K}_l$ for each $l \in \mathcal{L}$. If there is an arc in $\mathcal{A}$ between two units, then their corresponding cliques have a node in common. This means that the overlaps between the cliques in G are related to the arcs in $\mathcal{A}$. Let denote by $\bar{G}$ the network (Figure 1) of the pooling problem. The latter discussion shows that the more sparse is $\bar{G}$, the fewer overlaps are between the cliques in G . This means that if $\bar{G}$ is sparse then the possibility that in the sparse-BSOS hierarchy the matrix variables have fewer overlaps is high and therefore in this case each level of the sparse-BSOS hierarchy can be solved faster than the same level of the BSOS one.

7. Numerical result

The results in Sections 5 and 6 have been implemented in a Julia 0.5 package called “*Polyopt*”, available on <https://github.com/MOSEK/Polyopt.jl>.

In the implementation of the BSOS hierarchy, we model the polynomial equality by equating the monomials coefficients. To construct problems that satisfy the assumptions of Theorem 1, we add to the problems the constraints

$$1 - \frac{1}{M_\ell} \left(\sum_{i \in \mathcal{D}_\ell} x_i^2 \right) \geq 0 \quad \ell \in [q].$$

All computations in this paper were carried out with Julia 0.5 on an Intel i7-4790 3.60GHz Windows computer with 16GB of RAM.

The rest of this section is split into two parts, each of which presents the evaluation of our results on a class of optimization problems. In all tables, #var., #const., and **bold** numbers refer to the number of linear variables, the number of constraints, and **the optimal values of the instances**

respectively. Furthermore, we use “ $\approx$ ” whenever MOSEK cannot solve the problem to optimality and provides us a near optimal solution.

7.1. The evaluation on the pooling problems using the P-formulation

295 In this subsection, we present the numerical evaluation of the sparse-BSOS hierarchy on the P-formulation of the pooling problem instances and compare it with the BSOS hierarchy [22].

Table 1: Detailed information of some pooling problem instances. # var. and # const. present the number of variables and constraints in the P-formulation (1), respectively.

* For this instance the exact optimal value is unknown, but the interval on which it lies is known to be $[-36233.40, -35812.33]$.

	optimal value	I	J	L	K	# var.	# const.
Haverly1	-400.00	3	2	1	1	7	13
Haverly2	-600.00	3	2	1	1	7	13
Haverly3	-750.00	3	2	1	1	7	13
Ben-Tal4	-450.00	4	2	1	1	8	15
Ben-Tal5	-3,500.00	5	5	3	2	38	63
DeyGupte4	-1.00	2	4	2	2	16	58
Foulds2	-1,100.00	6	4	2	1	22	42
Foulds3	-8.00	11	16	8	1	168	235
Foulds4	-8.00	11	16	8	1	168	235
Adhya1	-549.80	5	4	2	4	21	51
Adhya2	-549.80	5	4	2	6	25	67
Adhya3	-561.05	8	4	3	6	38	87
Adhya4	-877.60	8	5	2	4	26	61
RT2	-4,391.83	3	3	2	8	32	85
sppA0	Unknown *	20	15	10	24	411	1,066

The detailed information of the instances is presented in Table 1. The GAMS files of the instances except DeyGupte4 can be found in the website <http://www.ii.uib.no/~mohammeda/>

pooling/. The instance DeyGupte4 is constructed in [23], and the details can be found in that
 300 paper.

In the numerical experiments, we consider $\kappa = 1$ in (6). We compare the results of applying the BSOS and sparse-BSOS hierarchies to this formulation when the equality constraints are eliminated [23], and when they are handled directly using Theorem 5. The time in the tables contains the time of constructing the level of the hierarchy and solving it by MOSEK 8.0 [5] in second.

305 Table 2 presents the results of solving different pooling problem instances with the sparse-BSOS hierarchy (6) and BSOS hierarchy [22].

The comparison has been made in two ways: the columns that are denoted by “with elimination” contain the result of applying the corresponding hierarchy to the pooling problem instances using the elimination method proposed in [23]. In the other columns, we use Theorem 5 to handle the
 310 equality constraints directly. For a few instances, such as sppA0, the time that is mentioned in Table 2 is larger for the sparse-BSOS hierarchy than the one for the BSOS hierarchy. This is due to the overlap of the matrix variables in the sparse-BSOS hierarchy. The dash “-” in Table 2 means we cannot solve the corresponding level of the hierarchy, due to the size of the problem.

After elimination of equality constraints, the constraints and variables are reduced. This means
 315 that in this case, applying Theorem 5 is not worthwhile with respect to the time, because the solver needs to solve a larger problem. Comparing the columns in Tables 2 shows that using Theorem 5 does not necessarily result in better or worse lower bounds. For Adhya4, applying this theorem results in better lower bounds both in the sparse-BSOS and BSOS hierarchies, but this is not the case for Adhya1.

320 As it can be seen in Tables 2, the sparse-BSOS hierarchy may get worse lower bounds compared to the BSOS hierarchy, which can be seen on the second level of the sparse-BSOS hierarchy of Haverly1-3, Ben-Tal4, Adhya1-3. The advantage of the sparse-BSOS hierarchy is that each level of the hierarchy can be solved relatively faster than the BSOS one, if the problem is sparse. For Foulds2, the lower bounds from the BSOS and sparse-BSOS hierarchies are close but the time in
 325 the sparse-BSOS hierarchy is much less than in the BSOS one.

The intuition behind the sparse-BSOS hierarchy is to split the variables into some blocks that contain only some (and not all) variables. If the blocks have many variables in common, then it does not matter much if we merge them together. In Table 3 we present the results of solving the P-formulation of the pooling problem instances when two blocks are merged if the number of

330 variables in their intersection is greater than 75% of the size of the smallest one.

Table 2: Comparing the BSOS hierarchy and sparse-BSOS hierarchies with $\kappa = 1$ for the P-formulation. The columns denoted by “with elimination” apply the hierarchy after elimination of equality constraints. The number of maximal cliques (q) in each level is presented between parentheses. The time of the model construction and the solution time is presented between the brackets. Bold-faced entries indicate the (approximate) optimal value.

	iteration	BSOS with elimination	BSOS	SBSOS with elimination	SBSOS
Haverly1	d=1	−600.00 [0.02]	−600.00 [0.03]	−600.00(3) [0.01]	−600.00(3) [0.03]
	d=2	−417.20 [0.04]	−417.20 [0.05]	−509.09(3) [0.02]	−505.00 [0.04]
	d=3	−400.00 [0.10]	−400.00 [0.15]	−400.00 (3) [0.06]	−400.00 (3) [0.07]
Haverly2	d=1	−1200.00 [0.03]	−1200.00 [0.03]	−1200.00(3) [0.02]	−1200.00(3) [0.03]
	d=2	−601.67 [0.05]	−600.00 [0.05]	−1,054.55(3) [0.05]	−1,054.55(3) [0.05]
	d=3	−600.00 [0.16]	−600.00 [0.21]	−634.65(3) [0.08]	−628.98(3) [0.09]
	d=4	−600.00 [2.63]	−600.00 [3.28]	−601.09(3) [0.44]	−600.51(3) [0.52]
Haverly3	d=1	−875.00 [0.03]	−875.00 [0.03]	−875.00(3) [0.03]	−875.00(3) [0.03]
	d=2	−750.00 [0.04]	−750.00 [0.05]	−811.98(3) [0.04]	−810.80(3) [0.05]
	d=3	−750.00 [0.10]	−750.00 [0.16]	−756.95(3) [0.06]	−754.01(3) [0.06]
	d=4	−750.00 [1.12]	−750.00 [1.91]	−750.00 (3) [0.20]	−750.00 (3) [0.31]
Ben-Tal4	d=1	−650.00 [0.03]	−650.00 [0.03]	−650.00(3) [0.03]	−650.00(3) [0.03]
	d=2	−467.20 [0.05]	−467.20 [0.05]	−558.29(3) [0.04]	−540.81(3) [0.04]
	d=3	−450.00 [0.18]	−450.00 [0.22]	−450.00 (3) [0.08]	−450.00 (3) [0.09]
Ben-Tal5	d=1	−3500.00 [0.06]	−3500.00 [0.15]	−3500.00 (9) [0.05]	−3500.00 (13) [0.09]
DeyGupte4	d=1	−4.00 [0.03]	−1.33 [0.04]	−4.00(1) [0.04]	−1.33(6) [0.05]
	d=2	−3.86 [0.19]	−1.33 [0.20]	−3.86(1) [0.19]	−1.33(6) [0.18]
	d=3	$\approx$ −0.99 [22.92]	−1.00 [36.77]	$\approx$ −0.99 (1) [23.15]	$\approx$ −1.30(6) [7.29]
Foulds2	d=1	−1,200.00 [0.03]	−1,200.00 [0.07]	−1,200.00(6) [0.05]	−1,200.00(8) [0.05]
	d=2	−1,191.30 [0.22]	−1,182.80 [0.34]	−1,193.92(6) [0.15]	−1,182.80(8) [0.16]
	d=3	−1,103.10 [26.45]	$\approx$ −1,102.34 [101.43]	−1,104.53(6) [3.79]	−1,103.96(8) [3.64]
Foulds3	d=1	−8.00 [62.26]	−8 [138.25]	−8 (20) [95.30]	−8 (33) [136.94]

Foulds4	d=1	-8.00 [61.77]	-8 [126.13]	-8(22) [194.33]	-8(33) [137.44]
Adhya1	d=1	-999.32 [0.03]	-999.32 [0.05]	-999.32(4) [0.04]	-999.32(4) [0.05]
	d=2	-721.12 [0.19]	-997.63 [0.40]	-957.02(4) [0.13]	$\approx$ -998.43(4) [0.22]
	d=3	-578.27 [36.50]	$\approx$ -669.86 [210.43]	-778.72(4) [3.42]	$\approx$ -860.91(4) [17.16]
Adhya2	d=1	-798.29 [0.01]	-854.10 [0.05]	-798.29(4) [0.01]	-854.10(4) [0.04]
	d=2	-577.00 [0.24]	-853.82 [0.89]	-686.60(4) [0.12]	-854.10(4) [0.44]
	d=3	-566.52 [39.02]	$\approx$ -575.81 [1,163.57]	-573.31(4) [8.42]	-749.44(4) [99.10]
Adhya3	d=1	-882.84 [0.02]	-882.84 [0.18]	-882.84(5) [0.03]	-882.84(7) [0.13]
	d=2	-805.08 [0.64]	-882.73 [9.28]	-870.55(5) [0.31]	-882.84(7) [3.20]
Adhya4	d=1	-1055.00 [0.01]	-1003.33 [0.05]	-1055.00(5) [0.02]	-1003.33(7) [0.05]
	d=2	-1,040.00 [0.33]	-1003.33 [0.90]	-1,040.00(5) [0.20]	-1003.33(7) [0.38]
	d=3	$\approx$ -908.13 [317.94]	-893.68 [1,343.85]	-1,012.16(5) [17.46]	-982.42(7) [40.42]
RT2	d=1	-45,420.50 [0.02]	-22,578.70 [0.20]	-45,420.49 [0.02]	-22,578.70(13) [0.22]
	d=2	$\approx$ -39,287.34 [0.54]	-22,153.45 [3.42]	$\approx$ -39,291.55(2) [0.56]	-22,153.48(13) [1.66]
sppA0	d=1	-47,675.00 [193.38]	—	-47,675.00(27) [413.88]	—

For Haverly1-3, and Ben-Tal4, there is no block merging. For DeyGupte4, Foulds3-4, Adhya2-3, RT2 and sppA0, all of the blocks get merged, which results in the BSOS hierarchy. Hence, we present the results for the rest of the instances in Table 3. In this table, we present the number of linear variables (the number of λ^ℓ , $\ell \in [q]$), the number of constraints, and the size of the semi-definite variables (**size of PSDs**) as well as the lower bounds that we get in each level of the hierarchies. As one can see, in all the instances in Table 3, the elimination of the equality constraints results in the high overlap in the maximal cliques of the associated graph to the P-formulation, and therefore we have merged all the maximal cliques. For the instances Foulds2 and Adhya4, even though the number of constraints in the first level of the sparse-BSOS hierarchy is less when the equality constraints are eliminated compared to the one when the equalities are handled directly, it is other way around in the third iteration. This is because, for each $\ell \in [q]$, the constraints in $\mathbb{R}[x; \mathcal{D}_\ell]$ are fewer than the ones in $\mathbb{R}[y]$, where x is the vector of variables in the P-formulation (1)

and y is the vector of variables in the P-formulation after eliminating equality constraints.

345 According to the discussion in Section 6, the overlaps in the matrix variables of the sparse-BSOS hierarchy corresponding to the P-formulation (1) is related to the sparsity of the network of the pooling problem, Figure 1, and the number of specifications. As one can see, for the four instances in Table 3, the networks of the instances are highly sparse, and therefore the possibility that each level of the sparse-BSOS hierarchy can be solved faster than the same level in the BSOS hierarchy is high. For Adhya2, the network is the same as Adhya1, but because the number of specifications
350 is much higher in Adhya2, the overlaps of the matrix variables in the sparse-BSOS hierarchy are much higher and more than 75% of their sizes.

Table 3: The result of solving the P-formulation of pooling problem instances with sparse-BSOS hierarchy when two maximal cliques are merged if the intersection size is larger than 75% of the size of smallest maximal clique (the size(s) of the positive semi-definite matrix variable(s) is (are) presented in the second row of each iteration).

	iteration	SBSOS with elimination			SBSOS		
		Value ([size of PSDs]) [time]	#const.	#var.	Value ([size of PSDs]) [time]	#const.	#var.
Ben-Tal5	d=1	-3,500.00 ([30]) [0.06]	465	112	-3,500.00 ([12, 22, 29]) [0.07]	601	169
Foulds2	d=1	-1,200.00 ([19]) [0.02]	190	80	-1,200.00 ([2 × 8, 19]) [0.02]	220	112
	d=2	-1,191.30 ([19]) [0.17]	973	3,161	-1,182.80 ([2 × 8, 19]) [0.16]	1,109	2,665
	d=3	-1,103.14 ([19]) [25.97]	13,601	85,321	≈-1,102.74 ([2 × 8, 19]) [20.61]	14,609	49,529
Adhya1	d=1	-999.32 ([12]) [0.01]	78	86	-999.32 ([12, 19]) [0.04]	223	114
	d=2	-721.12 ([12]) [0.13]	543	3,656	≈-998.09 ([12, 19]) [0.42]	2,317	4,035
	d=3	-578.27 ([12]) [38.18]	5,105	105,996	≈-776.44 ([12, 19]) [71.97]	41,127	107,300

Adhya4	d=1	-1,055.00 ([17]) [0.01]	153	106	-1,003.33 ([2 × 14, 19]) [0.03]	290	156
	d=2	-1,040.00 ([17]) [0.33]	1,730	5,566	-1,003.33 ([2 × 14, 19]) [0.31]	3,253	5,194
	d=3	≈-908.13 ([17]) [360.27]	27,922	198,486	-974.55 ([2 × 14, 19]) [62.54]	61,401	135,764

7.2. The evaluation on DTOC problems

Consider a DTOC problem (3). If F and f are polynomials, and $\mathcal{X}, \mathcal{U}$ are semi-algebraic sets, then it is easy to see that (3) satisfies the *RIP* with the maximal cliques

$$\mathcal{D}_k = \{x_{k+1}, x_k, u_k\}, \quad k = 0, \dots, N-1.$$

In the numerical experiments, we consider the following DTOC problem:

$$\begin{aligned}
& \min_{\substack{x_k \in \mathbb{R}, k=1, \dots, N-1 \\ u_k \in \mathbb{R}, k=0, \dots, N-1}} \frac{1}{N-1} \sum_{k=0}^{N-1} (x_k^2 + u_k^2) \\
& \text{s.t.} \quad x_{k+1} = x_k + \frac{1}{N} (x_k^2 - u_k), \quad k = 0, \dots, N-1, \\
& \quad x^\ell \leq x_k \leq x^u, \quad k = 1, \dots, N-1, \\
& \quad u^\ell \leq u_k \leq u^u, \quad k = 0, \dots, N-1,
\end{aligned} \tag{11}$$

355 for given $x^\ell, x^u, x_0, x_N, u^\ell, u^u$. Special cases of (11) were considered in [9, 11, 31].

In our numerical experiments, we compare the sparse-BSOS hierarchy, when the equality constraints are replaced by two inequalities (which we will call SBSOS without Theorem 5), with the sparse-BSOS hierarchy after applying Theorem 5 (which we will call SBSOS with Theorem 5). To evaluate the lower bounds that we get from the SBSOS with and without Theorem 5, we compare
360 them with the bounds that we get from the global optimization solver BARON [28], and the objective value of the local solution obtained from CONOPT [12]. To pass the problems to the solvers, we use AIMMS 4.39 [7]. For a fair comparison, we report the times that MOSEK 8.0 needs to solve the level of the hierarchies, as well as the times taken by BARON and CONOPT to solve the

DTOC problems in seconds. We put a maximum time limit of 120 seconds for all methods. We emphasize that we do not report the result of using the BSOS hierarchy for this problem, since the number of variables in (11) is large and the size of the semi-definite matrix variable in the BSOS hierarchy makes the hierarchy inefficient for this type of problems.

Table 4: Numerical experiments on DTOC problems (11) with the input data $(x^\ell, x^u, x_0, x_N, u^\ell, u^u) = (0.9, 5, 1, 1, -10, 10)$, and different N , for $\kappa = 2, d = 2, .$

N	SBSOS with Theorem 5		SBSOS without Theorem 5		BARON[28]		CONOPT[12]	
	value	time	value	time	upper and lower bounds	time	Upper bound	time
50	1.6600	0.14	1.6600	0.19	[1.6600 , 1.6600]	1.06	1.6600	0.02
250	1.6569	0.78	1.6569	1.06	[1.6544, 1.6569]	120.00	1.6569	0.08
500	1.6566	1.65	1.6566	2.28	[1.6201, 1.6566]	120.00	1.6566	0.19
1000	1.6564	3.77	1.6564	4.88	[1.5932, 1.6564]	120.00	1.6564	0.80
2000	1.6563	9.14	1.6563	12.68	[1.5613, 1.6563]	120.00	1.6563	2.17
3000	1.6563	14.54	1.6563	22.14	[1.5611, 1.6563]	120.00	1.6563	5.23
4000	≈ 1.6563	25.12	≈ 1.6563	31.14	[0.8118, 1.6562]	120.00	1.6562	8.77
5000	≈ 1.6562	36.33	≈ 1.6562	54.83	[0.8118, 1.6562]	120.00	1.6562	42.20

Table 4 presents the results of applying the SBSOS with and without Theorem 5 to DTOC problems for fixed

$$(x^\ell, x^u, x_0, x_N, u^\ell, u^u) = (0.9, 5, 1, 1, -10, 10)$$

and different N , and demonstrates the advantage of applying Theorem 5 to the sparse-BSOS hierarchy. As one can see in the table, the lower bounds that we obtain from the SBSOS with and without Theorem 5 are the same but applying this theorem helps us to get the lower bounds much faster. Moreover, the lower bounds are equal to the objective values of the solutions found by both BARON and CONOPT. Therefore, even though the solvers can not guarantee optimality of the solutions, the lower bounds from the hierarchies assure us that the solutions are globally optimal for $N = 250, 1000, 2000, 3000$. For $N = 4000, 5000$ the lower bounds that we get from the hierarchies are not precise and hence we cannot deduce that the solution is optimal; however the lower bounds

are close to the objective values of the solutions.

Table 5 in Appendix B provides the number of variables, the number of constraints, and the size of the semi-definite variables in the SBSOS with and without Theorem 5.

8. Conclusion

In this paper, we studied the sparse-BSOS hierarchy introduced in [32]. We first showed how to find a splitting of variables for a general polynomial optimization problem that satisfies the *running intersection property*. Then, we modified this hierarchy to handle the problems with equality constraints. The results in this paper has been implemented in a Julia 0.5 package “Polyopt” to solve a polynomial optimization problem.

In the numerical results we compared the sparse-BSOS hierarchy with the BSOS one, when Theorem 5 is applied. For the P-formulation, the problems in each level of the sparse-BSOS hierarchy could be solved faster than the BSOS one if the network of the pooling problem is sparse enough and the number of specifications is small, like the instance Foulds2. The quality of the lower bounds we got from the sparse-BSOS hierarchy could sometimes be worse than the BSOS hierarchy. The modification we proposed to the BSOS and sparse-BSOS hierarchies to handle equality constraints could sometimes yield much better lower bounds than the original hierarchies, like the first and second levels of the hierarchies in the DeyGupte4 instance.

Applying the sparse-BSOS hierarchy to the discrete-time optimal control problems showed that the lower bounds we got from the sparse-BSOS hierarchy and the modified one using Theorem 5 were the same, but each level of the modified hierarchy could be solved faster. Also, the lower bounds guaranteed optimality of the solutions found by the solvers BARON and CONOPT.

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Appendices

475 A. New pooling problem instance

In this appendix, we construct a pooling problem instance with three inputs, two pools, and four outputs. Then, we show the elimination method proposed in [23] destroys the sparsity pattern

Figure 3: An example of a standard pooling problem for which the elimination method proposed in [23] destroys the sparsity pattern.

that exists in the P-formulation.

Consider the pooling problem instance with the diagram drawn in Figure 3. Assume that each
 480 input and pool has a capacity restriction of 600. The restriction of the capacities of the outputs 6, 7, 8, and 9 are 100, 200, 100, and 200, respectively. Also, assume that there is only one specification, which should be less than or equal to 2.5, 1.5, 3, and 2 in the outputs, respectively. The inputs contain 3, 1, and 2 unit(s) of the specification. The costs of buying one unit of the inputs are 6, 16, 10, respectively, and the price of selling the outputs are 9, 15, 6, and 12.

485 The P-formulation corresponding to this instance has fourteen variables. Using “Polyopt” package, the chordal extension of the associated graph to the P-formulation (1) has the following maximal cliques:

$$\begin{aligned}
 \mathcal{D}_1 &= \{3, 4, 10, 13, 14\}, \mathcal{D}_2 = \{1, 2, 9, 11, 12\}, \mathcal{D}_3 = \{1, 2, 6, 9, 12\}, \\
 \mathcal{D}_4 &= \{1, 5, 6, 9, 12\}, \mathcal{D}_5 = \{5, 6, 7, 12, 13\}, \mathcal{D}_6 = \{3, 7, 8, 10, 13\}, \\
 \mathcal{D}_7 &= \{3, 8, 10, 13, 14\}.
 \end{aligned} \tag{12}$$

As one can see, the overlap in the cliques are a bit high. For example $\{3, 8, 10, 13\}$ is a subset of both $\mathcal{D}_6$ and $\mathcal{D}_7$. Merging the cliques with the overlaps of larger than 3 results in the following sets
 490 of indexes:

$$\mathcal{D}_1 = \{3, 4, 7, 8, 10, 13, 14\}, \mathcal{D}_2 = \{1, 2, 5, 6, 9, 11, 12\}, \mathcal{D}_3 = \{5, 6, 7, 12, 13\}. \tag{13}$$

Now, for the chordal extension of the associated graph to the P-formulation after eliminating

the equality constraints, the maximal cliques are

$$\bar{\mathcal{D}}_1 = \{1, 2, 3, 4, 5, 6, 7, 9, 10\}, \bar{\mathcal{D}}_2 = \{3, 4, 7, 8, 10\},$$

where the only difference in them is 8. Therefore, merging them together results in $\{1, \dots, 10\}$. So, clearly eliminating the equality constraints destroyed the sparsity pattern of the P-formulation.

495 B. Additional information about the numerical results

In the following table, #var., #const., **size of PSDs**, and **bold** numbers mean the number of linear variables, the number of constraints, **the size of semi-definite matrix variable(s)**, and **the optimal value of the instance**, respectively. The time in the table contains the time of solving the level of the hierarchy by MOSEK 8.0 [5]. In this table, $n \times m$ in the column “**size of PSDs**”
500 means that the second level of the sparse-BSOS hierarchy has n semi-definite matrix variables with the size $m \times m$.

Table 5: Some extra information on the level of the sparse-BSOS hierarchy applied to the DTOC problem (11) with the input information $(x^\ell, x^u, x_0, x_N, u^\ell, u^u) = (0.9, 5, 1, 1, -10, 10)$, and $\kappa = 2, d = 2$. The column “SBSOS without Theorem 5” refers to the result of applying the sparse-BSOS hierarchy applied to the problem after replacing each equality by two inequalities.

N	SBSOS with Theorem 5					SBSOS without Theorem 5				
	value	time	#var.	#const.	size of PSDs	value	time	#var.	#const.	size of PSDs
50	1.6600	0.14	6,662	1,505	50×10	1.6600	0.19	9,452	1,505	50×10
250	1.6569	0.78	33,662	7,505	250×10	1.6569	1.06	47,252	7,505	250×10
500	1.6566	1.65	67,412	15,005	500×10	1.6566	2.28	94,502	15,005	500×10
1000	1.6564	3.77	134,912	30,005	1000×10	1.6564	4.88	189,002	30,005	1000×10
2000	1.6563	9.14	269,912	60,005	2000×10	1.6563	12.68	378,002	60,005	2000×10
3000	1.6563	14.54	404,912	90,005	3000×10	1.6563	22.14	567,002	90,005	3000×10
4000	≈ 1.6563	25.12	539,912	120,005	4000×10	≈ 1.6563	31.14	756,002	120,005	4000×10
5000	≈ 1.6562	36.33	674,912	150,005	5000×10	≈ 1.6562	54.83	945,002	150,005	5000×10