# Sparse Polynomial Matrix Optimization

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#### Abstract

A polynomial matrix inequality (PMI) is a statement that a symmetric polynomial matrix is positive semidefinite over a given constraint set. Polynomial matrix optimization (PMO) concerns minimizing the smallest eigenvalue of a symmetric polynomial matrix subject to a tuple of PMIs. This work explores the use of sparsity methods in reducing the complexity of sum-of-squares based methods in verifying PMIs or solving PMO. In the unconstrained setting, Newton polytopes can be employed to sparsify the monomial basis, resulting in smaller semidefinite programs. In the general setting, we show how to exploit different types of sparsity (term sparsity, correlative sparsity, matrix sparsity) encoded in polynomial matrices to derive sparse semidefinite programming relaxations for PMO. For term sparsity, one intriguing phenomenon is that the related block structures do not necessarily converge to the one determined by sign symmetries, which is significantly distinguished from the scalar case. For correlative sparsity, unlike the scalar case, we provide a counterexample showing that asymptotic convergence does not hold under the Archimedean condition and the running intersection property. By employing the theory of matrix-valued measures, we establish several results on detecting global optimality and retrieving optimal solutions under correlative sparsity. The effectiveness of sparsity methods on reducing computational complexity is demonstrated on various examples of PMO.

# 1 Introduction

This paper is concerned with verification of polynomial matrix inequalities (PMI) and solving polynomial matrix optimization (PMO) problems. A PMI is a statement that a polynomially-defined symmetric matrix is positive semidefinite (PSD) over the locus of PSDness of other polynomially defined symmetric matrices [1]. PMIs are a generalization of (scalar) polynomial nonnegativity statements. Linear matrix inequalities are specific instances of PMIs restricted to degree 1 [2], but PMIs may describe nonconvex sets. Applications of PMIs include finding stability regions of autoregressive linear systems [3,4], sizing beams to minimize the cost of truss topologies under structural constraints [5], performing frequency-domain system identification of low-order linear systems under stability constraints [6], and simplifying optimal control tasks in the case where the applied input is constrained to lie in a semidefinite-representable set [7]. Refer to [8] for a survey of linear matrix inequality methods for solving polynomial optimization problems arising in control.

Polynomial optimization problems (POP) are programs where the objective and all constraints are defined by polynomials (forming a basic semialgebraic set). All POPs can be translated into equivalent programs with scalar linear objectives for which the constraint sets are described by polynomial inequality constraints. Checking nonnegativity of a polynomial over a basic semialgebraic set is generically an NP-hard problem, which extends (by reformulations in terms of membership oracles) to a generic NP-hardness of solving

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- J. Miller was partially supported by the Swiss National Science Foundation Grant 51NF40\_180545 under NCCR Automation. J. Wang was supported by National Key R&D Program of China under grant No. 2023YFA1009401, the Strategic Priority Research Program of the Chinese Academy of Sciences XDB0640000 & XDB0640200, and the National Natural Science Foundation of China under grant No. 12201618 & 12171324. F. Guo was supported by the Chinese National Natural Science Foundation under grant 12471478.

POPs [9]. Methods to verify polynomial nonnegativity include satisfiability solvers (e.g. dReal [10]) and sum of squares (SOS) methods [11,12].

If a real-valued polynomial with n variables can be represented as an SOS of other real-valued polynomials, then the original polynomial is certifiably nonnegative over the space  $\mathbb{R}^n$ . The set of SOS polynomials over  $\mathbb{R}^n$  is strictly contained in the set of nonnegative polynomials over  $\mathbb{R}^n$  [13]. Checking if a polynomial is an SOS over  $\mathbb{R}^n$  can be accomplished by solving a finite-dimensional convex optimization problem, which can be numerically treated using semidefinite program (SDP) or nonsymmetric interior point methods [11,12]. SOS methods can also be used in the constrained setting to verify nonnegativity over basic semialgebraic sets. If the constraint set is compact and its representing constraints satisfy a real-algebraic Archimedean structure, then every positive polynomial over the basic semialgebraic set can have its positivity verified using SOS methods [14] (though the polynomial degree needed to perform this verification could be exponential in n and d [15]).

These SOS methods for verifying polynomial nonnegativity have been extended to matrix SOS for PMIs [16,17], Hermitian SOS for complex polynomials [18,19], sums of Hermitian squares for noncommutative polynomials [20,21], and flag SOS for graph density polynomials [22]. The computational complexity of SOS implementation using SDP is determined by the size and multiplicity of the largest PSD matrix constraint [11]. In the context of a  $p \times p$  PMI with n variables where all polynomials are restricted to degree 2d, the size of the largest PSD matrix (under the dense monomial basis) is  $p\binom{n+d}{d}$ . This matrix size (and the corresponding time to solve SDPs) suffer in a jointly polynomial manner as p, n, and d grow. SOS decompositions can also be verified through nonsymmetric interior point methods [23] without the use of SDPs, but the same joint polynomial increase in scaling will hold (with exponential scaling in dimension if an interpolatory polynomial basis is used for fast Hessian inversion). Polynomial nonnegativity over sets admitting tractable Fourier analyses (e.g., ball, hypercube) can be accomplished in an optimization-free manner by checking a possibly exponential number of linear inequalities [24]. Other methods for SOS verification include using the Polya hierarchy of linear programs [25], trust-region optimization over a low-rank manifold [26], and search methods using tame geometry [27].

Existing knowledge of the problem structure can be used in order to reduce the computational expenditure of SOS-based verification [28]. This decrease in complexity can be accomplished by a combination of reducing the size of monomial basis used in formulating the polynomial representation and identifying opportunities for decomposing PSD matrix constraints in the SOS representation. Three dominant (and interlinked) approaches include correlative sparsity, term sparsity, and symmetry. Correlative sparsity structure ties together variables that appear in the same constraint or the same monomial term in the candidate polynomial [29]. Term sparsity structure pays attention to the monomials that appear in polynomials (commutative [30,31], noncommutative [32]). The Newton polytope method in the unconstrained setting uses the exponents of monomials found in the candidate polynomial to determine which monomials can categorically be ruled out of an SOS representation [33]. In the context of symmetry, enforcing that an SOS polynomial is additionally invariant/equivariant with respect to a given group action adds severe structural constraints to its SOS representation. The resultant SOS decomposition involves a block-diagonal PSD structure where the reduced monomial basis is comprised of primary and secondary invariants [34]. The term sparsity scheme in [30] can be interpreted as a refinement of symmetry reduction with respect to the class of sign symmetries [35]. Algebraic structure can be exploited if POPs are posed over regions described by polynomial equality constraints (in addition to polynomial inequality constraints), either by using Gröbner basis reduction over a quotient ring [36] or through the ideal-sparsity method by unfolding the separable equality constraints (e.g. x(x-1)=0). Multiple kinds of structure can be combined, such as the CS-TSSOS framework for correlative and term sparsity structures [37]. Term sparsity methods have also recently been used in sum-of-rational function optimization [38]. Term sparsity methods can also be used in the derivation of non-SOS certificates of polynomial nonnegativity. The sum of nonnegative circuit (SONC) framework decomposes a polynomial as the sum of 'circuit' polynomials that are verifiably nonnegative due to their coefficients' satisfaction of the AM/GM inequality [39]. The support and choice of these circuit polynomials are based on vertices of the Newton polytope (in the unconstrained setting). SONC verification therefore scales well when the candidate polynomial is sparse. SONC nonnegativity can be verified using relative entropy programs [40] or second-order cone programs [41, 42].

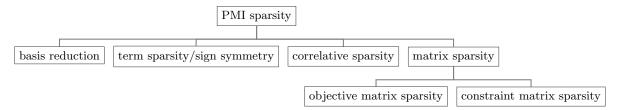


Figure 1: Different types of PMI sparsity.

A basic PMO problem is of form

$$\inf_{\boldsymbol{x} \in \mathbb{R}^n} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G_1(\boldsymbol{x}) \succeq 0, \dots, G_m(\boldsymbol{x}) \succeq 0, \tag{1}$$

where  $F, G_1, \ldots, G_m$  are symmetric polynomial matrices, and  $\lambda_{\min}(F(x))$  denotes the smallest eigenvalue of F(x). When F is a scalar polynomial (i.e., a  $1 \times 1$  polynomial matrix), Problem (1) is also known as a polynomial SDP which was extensively studied in the literature [43–47]. When both F and  $G_1, \ldots, G_m$  are polynomial matrices, a matrix Moment-SOS hierarchy for solving (1) was provided in [48]. SOS-simplifying structure can be extended to the matrix case. When F is a polynomial matrix and  $G_1, \ldots, G_m$  are polynomials, the work in [49] utilizes the matrix (chordal) sparsity of F to construct a sparse SOS representation for F. Note that matrix sparsity is independent of the presence of specific monomials in the nonzero entries. When F is a scalar polynomial, correlative sparsity was considered in [50] and constraint matrix sparsity was considered in [51]. More recently, the work in [52] extends the term sparsity method to the case of scalar F in the context of truss topology optimization. We summarize different types of PMI sparsity in Figure 1. General sparsity methods for Problem (1) have not previously been considered in the literature. This work fills this gap and studies sparsity reduction methods for PMO in full generality where F and  $G_1, \ldots, G_m$  are all polynomial matrices.

This work makes the following contributions:

- 1. In the unconstrained setting, we propose a method based on Newton polytopes for reducing monomial bases.
- 2. We provide an iterative procedure to exploit term sparsity, which yields a bilevel hierarchy of sparse Moment-SOS relaxations for Problem (1). Surprisingly, it turns out that the block structures produced by the iterative procedure with block closure do not necessarily converge to the one determined by sign symmetries of Problem (1), which is dramatically different from the scalar case.
- 3. We show how to exploit correlative sparsity for (1). When F is a scalar polynomial, it is known that asymptotic convergence of the correlatively sparse relaxations holds under the Archimedean condition and the running intersection property. However, when F is a polynomial matrix, we give a counterexample showing that asymptotic convergence does not hold under similar conditions. Moreover, by employing the theory of matrix-valued measures, we establish several results on detecting global optimality and retrieving optimal solutions in the correlatively sparse setting.
- 4. Decomposition methods based on the matrix sparsity structure of the objective matrix (extending the work of [49]) or PMI constraints are also provided.
- 5. Extensive numerical experiments are performed, which demonstrate the efficacy of our methods.

The rest of this paper is organized as follows. Section 2 introduces preliminaries such as notation, matrix SOS, matrix-valued measures, and graph theory. Section 3 applies the Newton polytope and term sparsity methods towards unconstrained PMIs. Section 4 concerns the term sparsity method for constrained PMO. Section 5 investigates correlative sparsity for PMO. Section 6 considers matrix sparsity methods for PMO. Section 7 demonstrates the effectiveness of these methods via various numerical examples. Section 8 concludes the paper.

## 2 Preliminaries

### 2.1 Notation

The n-dimensional real Euclidean vector space is  $\mathbb{R}^n$ . The set of natural numbers is  $\mathbb{N}$ , and the n-dimensional set of multi-indices is  $\mathbb{N}^n$ . The symbol [n] denotes the set  $\{1,\ldots,n\}$ . For a set  $\mathcal{A}$ , its cardinality is denoted by  $|\mathcal{A}|$ . The degree of a multi-index  $\alpha \in \mathbb{N}^n$  is  $|\alpha| := \max_{i \in [n]} \alpha_i$ . The associated monomial to an n-dimensional indeterminate  $\mathbf{x} := (x_1,\ldots,x_n)$  and a multi-index  $\alpha \in \mathbb{N}^n$  is  $\mathbf{x}^\alpha = \prod_{i=1}^n x_i^{\alpha_i}$ . Letting  $\mathcal{A} \subset \mathbb{N}^n$  be a finite-cardinality set of multi-indices and  $\{c_\alpha\}_{\alpha \in \mathcal{A}}$  be an associated set of real numbers, the polynomial formed by  $\mathcal{A}$  and  $\{c_\alpha\}_{\alpha \in \mathcal{A}}$  is  $f(\mathbf{x}) = \sum_{\alpha \in \mathcal{A}} c_\alpha \mathbf{x}^\alpha$ . The set of polynomials with real-valued coefficients is  $\mathbb{R}[\mathbf{x}]$ . The support of a polynomial  $f \in \mathbb{R}[\mathbf{x}]$ , denoted by  $\sup(f)$ , is the set of multi-indices  $\alpha$  such that  $c_\alpha \neq 0$ . The degree of a polynomial  $f \in \mathbb{R}[\mathbf{x}]$  is  $\deg f = \max_{\alpha \in \operatorname{supp}(f)} |\alpha|$ . The set of polynomials of degree at most d is denoted by  $\mathbb{R}[\mathbf{x}]_d$ .

The transpose of a matrix A is denoted by  $A^{\intercal}$ . The p-dimensional identity matrix is  $I_p$ . The Kronecker product between two matrices C and D is  $C \otimes D$ . The set of  $p \times p$  symmetric matrices is  $\mathbb{S}^p$ . The subset of  $p \times p$  PSD matrices is  $\mathbb{S}^p_+$ . Membership in the PSD set  $F \in \mathbb{S}^p_+$  will also be denoted as  $F \succeq 0$ , and the Loewner partial ordering will be used as  $F_1 \succeq F_2 \Leftrightarrow F_1 - F_2 \succeq 0$ .

The set of polynomial matrices of dimension  $p \times q$  is  $\mathbb{R}[\boldsymbol{x}]^{p \times q}$ . Given a polynomial matrix  $F(\boldsymbol{x}) = [F(\boldsymbol{x})_{ij}] \in \mathbb{R}[\boldsymbol{x}]^{p \times q}$ , we can write it as  $F(\boldsymbol{x}) = \sum_{\alpha} F_{\alpha} \boldsymbol{x}^{\alpha}$ ,  $F_{\alpha} \in \mathbb{R}^{p \times q}$ . The support of  $F(\boldsymbol{x})$ , denoted by  $\operatorname{supp}(F)$ , is the set of multi-indices  $\alpha$  such that  $F_{\alpha} \neq 0$ . The degree of  $F(\boldsymbol{x})$  is  $\deg F = \max_{i \in [p], \ j \in [q]} \deg F(\boldsymbol{x})_{ij}$ . The set of symmetric polynomial matrices of dimension p is  $\mathbb{S}^p[\boldsymbol{x}]$ . The set of p-dimensional symmetric polynomial matrices of degree at most d is denoted by  $\mathbb{S}^p[\boldsymbol{x}]_d$ .

## 2.2 Sum of Squares Polynomials

This subsection will review SOS methods for verifying nonnegativity of polynomials over  $\mathbb{R}^n$  and over constrained sets.

#### 2.2.1 Unconstrained

A polynomial  $f \in \mathbb{R}[x]_d$  is nonnegative over  $\mathbb{R}^n$  if  $f(x) \geq 0$  for any  $x \in \mathbb{R}^n$ . One method to verify polynomial nonnegativity is to use SOS certificates. A polynomial  $f \in \mathbb{R}[x]$  is SOS if there exist polynomials  $g_1, \ldots, g_s \in \mathbb{R}[x]$  such that  $f(x) = \sum_{i=1}^s g_i(x)^2$ . The set of SOS polynomials, denoted by  $\Sigma[x]$ , is contained inside the set of nonnegative polynomials over  $\mathbb{R}^n$ .

A polynomial matrix  $F(\mathbf{x}) \in \mathbb{S}^p[\mathbf{x}]$  is positive semidefinite (PSD) over  $\mathbb{R}^n$  if

$$\forall \boldsymbol{x} \in \mathbb{R}^n : \qquad F(\boldsymbol{x}) \succeq 0. \tag{2}$$

The statement in (2) is a PMI in  $\boldsymbol{x}$  over the unconstrained region  $\mathbb{R}^n$ . The matrix F is called an SOS matrix if there exists another polynomial matrix  $R(\boldsymbol{x}) \in \mathbb{R}[\boldsymbol{x}]^{s \times p}$  such that  $F(\boldsymbol{x}) = R(\boldsymbol{x})^{\mathsf{T}}R(\boldsymbol{x})$ . The set of n-dimensional SOS matrices is denoted by  $\Sigma^n[\boldsymbol{x}]$ . Note that the set of SOS (scalar) polynomials  $\Sigma[\boldsymbol{x}]$  is equivalent to the set  $\Sigma^1[\boldsymbol{x}]$  (the n=1 case of SOS matrices).

Checking if a polynomial matrix  $F(\boldsymbol{x}) \in \mathbb{S}^p[\boldsymbol{x}]_{2d}$  is inside the set  $\Sigma^p[\boldsymbol{x}]$  can be accomplished by solving an SDP. Letting  $\mathbf{m}_d(\boldsymbol{x})$  be the  $\binom{n+d}{d}$ -vector of monomials in  $\boldsymbol{x}$  up to degree d, the matrix F is an SOS matrix if there exists a PSD matrix  $Q \in \mathbb{S}_+^{p\binom{n+d}{d}}$  such that (Lemma 1 of [53])

$$F(\mathbf{x}) = (\mathbf{m}_d(\mathbf{x}) \otimes I_p)^{\mathsf{T}} Q(\mathbf{m}_d(\mathbf{x}) \otimes I_p). \tag{3}$$

Problem (3) is an SDP with respect to the PSD matrix constraint  $Q \in \mathbb{S}^{p\binom{n+d}{d}}_+$  and the affine equality (coefficient matching) constraints in (3). Note that (3) can also be written as

$$F(\boldsymbol{x}) = (I_p \otimes \mathbf{m}_d(\boldsymbol{x}))^{\mathsf{T}} \tilde{Q}(I_p \otimes \mathbf{m}_d(\boldsymbol{x})), \tag{4}$$

where  $\tilde{Q}$  is obtained from Q by certain row and column permutations.

Verification of the PMI in (2) can also be accomplished through *scalarization*. The scalarization approach introduces a new tuple of variables  $y \in \mathbb{R}^p$  to form the equivalent problem:

$$\forall (\boldsymbol{x}, \boldsymbol{y}) \in \mathbb{R}^{n+p} : \qquad \boldsymbol{y}^{\mathsf{T}} F(\boldsymbol{x}) \boldsymbol{y} \ge 0. \tag{5}$$

The SOS-restriction of the scalarized problem (5) is

$$\mathbf{y}^{\mathsf{T}}F(\mathbf{x})\mathbf{y} \in \Sigma[\mathbf{x}, \mathbf{y}].$$
 (6)

#### 2.2.2 Constrained

Let  $\mathbf{G} := \{G_k(\boldsymbol{x})\}_{k=1}^m$  be a set of symmetric polynomial matrices with  $G_k(\boldsymbol{x}) \in \mathbb{S}^{q_k}[\boldsymbol{x}]$  which defines a basic semialgebraic set as

$$\mathbf{K} := \{ \boldsymbol{x} \in \mathbb{R}^n \mid G_k(\boldsymbol{x}) \succeq 0, \quad \forall k \in [m] \}.$$
 (7)

A polynomial matrix  $F \in \mathbb{S}^p[x]$  satisfies a PMI over the constrained region **K** if

$$\forall \boldsymbol{x} \in \mathbf{K} : \qquad F(\boldsymbol{x}) \succeq 0. \tag{8}$$

The following exposition of SOS verification of PMIs originates from [53].

Let C be a a  $pq \times pq$  block matrix described as

$$C = \begin{bmatrix} C_{11} & C_{12} & \dots & C_{1p} \\ C_{21} & C_{22} & \dots & C_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ C_{p1} & C_{p2} & \dots & C_{pp} \end{bmatrix}$$
(9)

in which each block  $C_{ij}$  is of size  $q \times q$ . The p-product between  $C \in \mathbb{S}^{pq \times pq}$  and  $D \in \mathbb{S}^{q \times q}$  is defined by

$$\langle C, D \rangle_p := \begin{bmatrix} \operatorname{tr}(C_{11}^{\mathsf{T}}D) & \operatorname{tr}(C_{12}^{\mathsf{T}}D) & \dots & \operatorname{tr}(C_{1p}^{\mathsf{T}}D) \\ \operatorname{tr}(C_{21}^{\mathsf{T}}D) & \operatorname{tr}(C_{22}^{\mathsf{T}}D) & \dots & \operatorname{tr}(C_{2p}^{\mathsf{T}}D) \\ \vdots & \vdots & \ddots & \vdots \\ \operatorname{tr}(C_{p1}^{\mathsf{T}}D) & \operatorname{tr}(C_{p2}^{\mathsf{T}}D) & \dots & \operatorname{tr}(C_{pp}^{\mathsf{T}}D) \end{bmatrix}.$$

$$(10)$$

A sufficient SOS condition for (8) to hold is that there exist SOS matrices  $S_0 \in \Sigma^p[x], S_k \in \Sigma^{pq_k}[x], k \in [m]$  such that

$$F(\boldsymbol{x}) = S_0(\boldsymbol{x}) + \sum_{k=1}^{m} \langle S_k(\boldsymbol{x}), G_k(\boldsymbol{x}) \rangle_p.$$
(11)

The dimension-p set of weighted sum of squares (WSOS) polynomial matrices  $\Sigma^p[\mathbf{G}]$  is the subset of  $\mathbb{S}^p[\mathbf{x}]$  that have a representation in (11) (also referred to the quadratic module formed by  $\mathbf{G}$ ). The degree- $\leq 2d$  set of WSOS polynomials  $\Sigma^p[\mathbf{G}]_{2d}$  is the subset of  $\Sigma^p[\mathbf{G}]$  where deg  $S_0 \leq 2d$  and deg $\langle S_k(\mathbf{x}), G_k(\mathbf{x}) \rangle_p \leq 2d$  for all  $k \in [m]$ .

The quadratic module  $\Sigma^p[\mathbf{G}]$  formed by  $\mathbf{G}$  satisfies the *Archimedean* property if there exists an  $a \geq 0$  such that the scalar polynomial  $a - \|\mathbf{x}\|_2^2$  is a member of  $\Sigma^1[\mathbf{G}]$ . If  $\Sigma^p[\mathbf{G}]$  is Archimedean, then  $\mathbf{K}$  is compact, but not necessarily vice versa [54]. If there exists an  $\epsilon > 0$  such that  $F(\mathbf{x}) \succeq \epsilon I_p$  over  $\mathbf{K}$  and  $\Sigma^p[\mathbf{G}]$  is Archimedean, then Scherer and Hol's Positivestellensatz [53, Corollary 1] states that  $F(\mathbf{x})$  will have a representation in (11). However, the degrees of the S terms needed to form the (11) certification may be exponential in n and deg F (even for the p = 1 case) [15].

### 2.3 Matrix-Valued Measures and Moment Matrices

We recall some basics about the theory of matrix-valued measures and the associated moment matrices, which will be used to establish conditions for detecting global optimality and extracting optimal solutions from the Moment-SOS relaxations of PMO problems.

For the set **K** in (7), let  $B(\mathbf{K})$  be the smallest  $\sigma$ -algebra generated from the open subsets of **K** and  $\mathfrak{m}(\mathbf{K})$  the set of all finite Borel measures on **K**. A measure  $\phi \in \mathfrak{m}(\mathbf{K})$  is *positive* if  $\phi(\mathcal{A}) \geq 0$  for all  $\mathcal{A} \in B(\mathbf{K})$ . Denote by  $\mathfrak{m}_+(\mathbf{K})$  the set of all finite positive Borel measures on **K**. The support supp( $\phi$ ) of a Borel measure  $\phi \in \mathfrak{m}(\mathbf{K})$  is the (unique) smallest closed set  $\mathcal{A} \in B(\mathbf{K})$  such that  $\phi(\mathbf{K} \setminus \mathcal{A}) = 0$ .

Let  $\phi_{ij} \in \mathfrak{m}(\mathbf{K})$ , i, j = 1, ..., p. The  $p \times p$  matrix-valued measure  $\Phi$  on  $\mathbf{K}$  is defined as the matrix-valued function  $\Phi \colon B(\mathbf{K}) \to \mathbb{R}^{p \times p}$  with

$$\Phi(\mathcal{A}) := [\phi_{ij}(\mathcal{A})] \in \mathbb{R}^{p \times p}, \quad \forall \mathcal{A} \in B(\mathbf{K}).$$

If  $\phi_{ij} = \phi_{ji}$  for all i, j = 1, ..., p, we call  $\Phi$  a symmetric matrix-valued measure. If  $\mathbf{v}^{\intercal}\Phi(\mathcal{A})\mathbf{v} \geq 0$  holds for all  $\mathcal{A} \in B(\mathbf{K})$  and for all column vectors  $\mathbf{v} \in \mathbb{R}^p$ , we call  $\Phi$  a PSD matrix-valued measure. The set  $\sup (\Phi) := \bigcup_{i,j=1}^p \sup (\phi_{ij})$  is called the support of  $\Phi$ . We denote by  $\mathfrak{M}^p(\mathbf{K})$  (resp.  $\mathfrak{M}^p_+(\mathbf{K})$ ) the set of all  $p \times p$  (resp. PSD) symmetric matrix-valued measures on  $\mathbf{K}$ . A finitely atomic PSD matrix-valued measure  $\Phi \in \mathfrak{M}^p_+(\mathbf{K})$  is a matrix-valued measure of form  $\Phi = \sum_{i=1}^t W_i \delta_{\mathbf{x}^{(i)}}$  where  $W_i \in \mathbb{S}^p_+$ ,  $\mathbf{x}^{(i)}$ 's are distinct points in  $\mathbf{K}$ , and  $\delta_{\mathbf{x}^{(i)}}$  denotes the Dirac measure centered at  $\mathbf{x}^{(i)}$ , i = 1, ..., t.

For a given matrix-valued measure  $\Phi = [\phi_{ij}] \in \mathfrak{M}^p_+(\mathbf{K})$ , we define a linear functional  $\mathscr{L}_{\Phi} \colon \mathbb{S}[\mathbf{x}]^p \to \mathbb{R}$  as

$$\mathscr{L}_{\Phi}(F) = \int_{\mathbf{K}} \operatorname{tr}(F(\boldsymbol{x}) d\Phi(\boldsymbol{x})) = \sum_{i,j} \int_{\mathbf{K}} F_{ij}(\boldsymbol{x}) d\phi_{ij}(\boldsymbol{x}), \quad \forall F(\boldsymbol{x}) \in \mathbb{S}[\boldsymbol{x}]^{p}.$$
(12)

Let  $\mathbf{S} = (S_{\alpha})_{\alpha \in \mathbb{N}^n}$  be a multi-indexed sequence of symmetric matrices in  $\mathbb{S}^p$ . We define a linear functional  $\mathscr{L}_{\mathbf{S}} : \mathbb{S}[\mathbf{x}]^p \to \mathbb{R}$  in the following way:

$$\mathscr{L}_{\mathbf{S}}(F) \coloneqq \sum_{\boldsymbol{\alpha} \in \operatorname{supp}(F)} \operatorname{tr}\left(F_{\boldsymbol{\alpha}} S_{\boldsymbol{\alpha}}\right), \quad \forall F(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \operatorname{supp}(F)} F_{\boldsymbol{\alpha}} \boldsymbol{x}^{\boldsymbol{\alpha}} \in \mathbb{S}[\boldsymbol{x}]^p.$$

We call  $\mathcal{L}_{\mathbf{S}}$  the *Riesz functional* associated to the sequence **S**. The sequence **S** is called a matrix-valued **K**-moment sequence if there exists a matrix-valued measure  $\Phi = [\phi_{ij}] \in \mathfrak{M}^p_+(\mathbf{K})$  such that

$$\operatorname{supp}(\Phi) \subseteq \mathbf{K} \quad \text{and} \quad S_{\alpha} = \int_{\mathbf{K}} \boldsymbol{x}^{\alpha} d\Phi(\mathbf{K}) := \left[ \int_{\mathbf{K}} \boldsymbol{x}^{\alpha} d\phi_{ij}(\boldsymbol{x}) \right]_{i,j \in [p]}, \ \forall \alpha \in \mathbb{N}^{n}.$$
 (13)

The measure  $\Phi \in \mathfrak{M}^p_+(\mathbf{K})$  satisfying (13) is called a representing measure of **S**.

**Definition 2.1.** Given a sequence  $\mathbf{S} = (S_{\boldsymbol{\alpha}})_{\boldsymbol{\alpha} \in \mathbb{N}^n} \subseteq \mathbb{S}^p$ , the associated moment matrix  $M(\mathbf{S})$  is the block matrix whose block row and block column are indexed by  $\mathbb{N}^n$  and the  $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ -th block entry is  $S_{\boldsymbol{\alpha}+\boldsymbol{\beta}}$  for all  $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}^n$ . For  $G \in \mathbb{S}[\boldsymbol{x}]^q$ , the localizing matrix  $M(G\mathbf{S})$  associated to  $\mathbf{S}$  and G is the block matrix whose block row and block column are indexed by  $\mathbb{N}^n$  and the  $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ -th block entry is  $\sum_{\boldsymbol{\gamma} \in \text{supp}(G)} S_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}} \otimes G_{\boldsymbol{\gamma}}$  for all  $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}^n$ . For  $d \in \mathbb{N}$ , the d-th order moment matrix  $M_d(\mathbf{S})$  (resp. localizing matrix  $M_d(G\mathbf{S})$ ) is the submatrix of  $M(\mathbf{S})$  (resp.  $M(G\mathbf{S})$ ) whose block row and block column are both indexed by  $\mathbb{N}_d^n$ .

Let  $d_k := \lceil \deg G_k/2 \rceil$  for  $k \in [m]$  and  $d_{\mathbf{K}} := \max\{d_1, \ldots, d_m\}$ . As in the scalar case, the existence of a finitely atomic representing measure of a matrix-valued sequence can be guaranteed by the "flatness condition".

**Theorem 2.1** ( [48], Theorem 5). Given a truncated sequence  $\mathbf{S} = (S_{\boldsymbol{\alpha}})_{\boldsymbol{\alpha} \in \mathbb{N}_{2r}^n} \subseteq \mathbb{S}^p$ ,  $\mathbf{S}$  admits an atomic representing measure  $\Phi = \sum_{i=1}^t W_i \delta_{\boldsymbol{x}^{(i)}}$  with  $W_i \in \mathbb{S}_+^p$ ,  $\boldsymbol{x}^{(i)} \in \mathbf{K}$  and  $\sum_{i=1}^t \operatorname{rank}(W_i) = \operatorname{rank}(M_r(\mathbf{S}))$  if and only if  $M_r(\mathbf{S}) \succeq 0$ ,  $M_{r-d_k}(G\mathbf{S}) \succeq 0$  for  $k \in [m]$ , and  $\operatorname{rank}(M_r(\mathbf{S})) = \operatorname{rank}(M_{r-d_k}(\mathbf{S}))$ .

We refer the reader to [48] for more details on matrix-valued measures/moments.

# 2.4 Polynomial Matrix Optimization and the Moment-SOS Hierarchy

The SOS matrix can be used to solve PMO problems. Consider the problem of minimizing the smallest eigenvalue of  $F(x) \in \mathbb{S}^p[x]$  over all  $x \in \mathbf{K}$ :

$$\lambda^* := \sup_{\lambda \in \mathbb{R}} \lambda \quad \text{s.t.} \quad \forall \boldsymbol{x} \in \mathbf{K} : \ F(\boldsymbol{x}) \succeq \lambda I_p.$$
 (14)

The SOS-restriction of Problem (14) is

$$\sup_{\lambda \in \mathbb{R}} \lambda \quad \text{s.t.} \quad F(\boldsymbol{x}) - \lambda I_p \in \Sigma^p[\mathbf{G}], \tag{15}$$

and its r-th order  $(r \ge r_{\min} := \max\{\lceil \deg F/2 \rceil, d_1, \dots, d_m\})$  SOS restriction is

$$\lambda_r^* \coloneqq \sup_{\lambda \in \mathbb{R}} \lambda \quad \text{s.t.} \quad F(x) - \lambda I_p \in \Sigma^p[\mathbf{G}]_{2r}.$$
 (16)

The dual program of (16) (by convex duality) is an optimization problem posed over matrix-valued sequences  $\mathbf{S} = (S_{\alpha})_{\alpha \in \mathbb{N}_{2r}^n} \subseteq \mathbb{S}^p$  [48]:

$$\lambda_r := \begin{cases} \inf_{\mathbf{S}} & \mathcal{L}_{\mathbf{S}}(F) \\ \text{s.t.} & M_r(\mathbf{S}) \succeq 0, \\ & M_{r-d_k}(G_k \mathbf{S}) \succeq 0, \quad k \in [m], \\ & \mathcal{L}_{\mathbf{S}}(I_p) = 1. \end{cases}$$
 (17)

It is clear that  $\lambda_r^* \leq \lambda_r \leq \lambda^*$  for all  $r \geq r_{\min}$ . When  $\Sigma^p[\mathbf{G}]$  is Archimedean, Scherer and Hol's Positivestellensatz implies that  $\lim_{r\to\infty} \lambda_r^* = \lim_{r\to\infty} \lambda_r = \lambda^*$ . The relaxations (16) and (17) indexed by relaxation order r is called the matrix Moment-SOS hierarchy for Problem (14).

## 2.5 Graph Theory

The term-sparse, correlatively-sparse, and matrix-sparse decomposition methods for PMIs explored in this paper use graph theory to identify exploitable structure in the optimization problems. A graph  $\mathcal{G}(\mathcal{V}, \mathcal{E})$  is defined by a collection of nodes  $\mathcal{V}$  and edges  $\mathcal{E}$ . This paper will consider undirected graphs with self-loops. A complete graph is a graph in which every node is connected to every other node. A *clique* of  $\mathcal{G}$  is a subgraph of  $\mathcal{G}$  that is isomorphic to a complete graph. A *maximal clique* of  $\mathcal{G}$  is a clique that is not a subgraph of another clique of  $\mathcal{G}$ .

A path in  $\mathcal{G}$  exists between nodes  $v_i$  and  $v_j$  if there exists a sequence of nodes  $v_i, v_1, v_2, \ldots, v_q, v_j$  such that  $\{v_i, v_1\} \in \mathcal{E}, \{v_1, v_2\} \in \mathcal{E}, \ldots, \{v_q, v_j\} \in \mathcal{E}$ . The nodes  $v_i$  and  $v_j$  are thus path-connected. The block closure of a graph  $\mathcal{G}$  is the unique supergraph  $\mathcal{G}' \supseteq \mathcal{G}$  where an edge is added between every pair of nodes that are path-connected. The graph  $\mathcal{G}'$  is therefore isomorphic to a direct sum of complete graphs.

A cycle in a graph is a path that starts and ends with the same node. A graph is chordal if all its cycles of length at least four have a chord (i.e., an edge  $\{v_i, v_j\}$  that joins two nonconsecutive nodes in the cycle). A chordal extension of  $\mathcal{G}$  is a supergraph  $\mathcal{G}' \supseteq \mathcal{G}$  with  $\mathcal{G}'$  being a chordal graph. Determining if a graph is chordal can be done in linear time, but finding a chordal extension with a minimal number of edges is NP-hard [55]. Chordal extensions are typically not unique, and the block closure is a specific instance of a chordal extension. To distinguish from the block closure, we refer to an ordinary chordal extension by a chordal closure.

Figure 2 plots chordal and block closures for a graph with 10 nodes. The original graph structure is shown in the black edges. The blue edges in Figure 2a are a possible choice for a chordal closure; another admissible extension would adjoin the edges  $\{2,4\}$  and  $\{2,5\}$  to the original graph instead. The red edges 2b illustrate the block closure of the graph, transforming each connected component of the graph into a complete graph.

### 2.6 Sparse Semidefinite Programming

Chordal sparsity can be used to reduce the computational complexity needed to solve large-scale semidefinite programming problems. Given an undirected graph  $\mathcal{G}(\mathcal{V}, \mathcal{E})$  with nodes  $\mathcal{V} = \{1, \dots, p\}$ , we denote the set of sparse symmetric matrices by  $\mathbb{S}^p(\mathcal{G}, 0)$ , i.e.,

$$\mathbb{S}^p(\mathcal{G},0) := \{ A \in \mathbb{S}^p \mid A_{ij} = A_{ji} = 0, \text{ if } i \neq j \text{ and } \{i,j\} \notin \mathcal{E} \},$$

and let  $\Pi_{\mathcal{G}}: \mathbb{S}^p \to \mathbb{S}^p(\mathcal{G}, 0)$  be the projection defined by

$$[\Pi_{\mathcal{G}}(A)]_{ij} = \begin{cases} A_{ij}, & \text{if } i = j \text{ or } \{i, j\} \in \mathcal{E}, \\ 0, & \text{otherwise.} \end{cases}$$
(18)

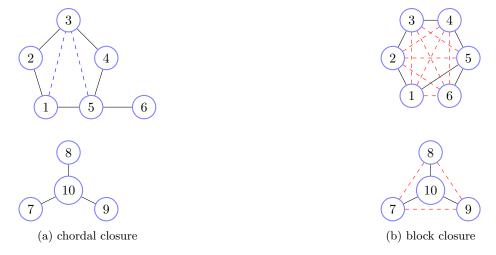


Figure 2: Example of chordal and block closures of a graph

We define the cone of sparse PSD matrices as  $\mathbb{S}^p_+(\mathcal{G},0) := \mathbb{S}^p_+ \cap \mathbb{S}^p(\mathcal{G},0)$  and the dual cone of completable PSD matrices is given by

$$\mathbb{S}_{+}^{p}(\mathcal{G},?) = \Pi_{\mathcal{G}}(\mathbb{S}_{+}^{p}) = \{\Pi_{\mathcal{G}}(A) \mid A \in \mathbb{S}_{+}^{p}\}.$$

For any maximal clique  $C_i$  of  $\mathcal{G}(\mathcal{V}, \mathcal{E})$ , we define the matrix  $E_{C_i} \in \mathbb{R}^{|C_i| \times p}$  by

$$[E_{\mathcal{C}_i}]_{jk} = \begin{cases} 1, & \text{if } \mathcal{C}_i(j) = k, \\ 0, & \text{otherwise,} \end{cases}$$

where  $C_i(j)$  denotes the *j*-th node in  $C_i$ , sorted in the natural ordering. Given  $A \in \mathbb{S}^p$ , the matrix  $E_{C_i}$  can be used to extract a principal submatrix indexed by  $C_i$ , i.e.,  $E_{C_i}AE_{C_i}^{\mathsf{T}} \in \mathbb{S}^{|C_i|}$ . Given  $A \in \mathbb{S}^{|C_i|}$ , the operation  $E_{C_i}^{\mathsf{T}}AE_{C_i}$  inflates A into a sparse  $p \times p$  matrix.

When the sparsity pattern graph  $\mathcal{G}$  is chordal, the cone  $\mathbb{S}^p_+(\mathcal{G},0)$  can be decomposed as a sum of simple convex cones, as stated in the following theorem.

**Theorem 2.2.** ( [56, Theorem 2.3]) Let  $\mathcal{G}(\mathcal{V}, \mathcal{E})$  be a chordal graph and let  $\{\mathcal{C}_1, \ldots, \mathcal{C}_t\}$  be the set of its maximal cliques. Then,  $A \in \mathbb{S}^p_+(\mathcal{G}, 0)$  if and only if there exist matrices  $A_i \in \mathbb{S}^{|\mathcal{C}_i|}_+$ ,  $i = 1, \ldots, t$ , such that  $A = \sum_{i=1}^t E_{\mathcal{C}_i}^{\mathcal{C}_i} A_i E_{\mathcal{C}_i}$ .

By duality, Theorem 2.2 leads to the following characterization of the PSD completable cone  $\mathbb{S}_{+}^{p}(\mathcal{G},?)$ .

**Theorem 2.3.** [57, Theorem 7] Let  $\mathcal{G}(\mathcal{V}, \mathcal{E})$  be a chordal graph and let  $\{\mathcal{C}_1, \dots, \mathcal{C}_t\}$  be the set of its maximal cliques. Then,  $A \in \mathbb{S}_+^p(\mathcal{G},?)$  if and only if  $E_{\mathcal{C}_i}AE_{\mathcal{C}_i}^{\mathsf{T}} \in \mathbb{S}_+^{|\mathcal{C}_i|}$  for all  $i \in [t]$ .

# 3 Term Sparsity for Unconstrained PMIs

This section will detail term sparsity methods for simplifying SOS verification of a single PMI  $F(x) \succeq 0$  in the fashion of Equation (3). The first subsection will discuss how to reduce the required monomial basis, thus setting some diagonal elements of the Gram matrix Q to zero. The second subsection will define matrix term sparsity patterns to impose a block structure on the matrix Q.

### 3.1 Selecting the Monomial Basis

Letting  $F(\mathbf{x}) \in \mathbb{S}^p[\mathbf{x}]_{2d}$  be a polynomial matrix, define  $\{\mathbf{v}^j(\mathbf{x})\}_{j=1}^p$  as a set of monomial (column) vectors such that

$$F(\boldsymbol{x}) = \operatorname{diag}(\boldsymbol{v}^{1}(\boldsymbol{x}), \boldsymbol{v}^{2}(\boldsymbol{x}), \dots, \boldsymbol{v}^{p}(\boldsymbol{x}))^{\mathsf{T}} \tilde{Q} \operatorname{diag}(\boldsymbol{v}^{1}(\boldsymbol{x}), \boldsymbol{v}^{2}(\boldsymbol{x}), \dots, \boldsymbol{v}^{p}(\boldsymbol{x})), \tag{19}$$

where diag( $\mathbf{v}^1(\mathbf{x})$ ,  $\mathbf{v}^2(\mathbf{x})$ , ...,  $\mathbf{v}^p(\mathbf{x})$ ) is the matrix formed by putting  $\mathbf{v}^j(\mathbf{x})$  at the j-th diagonal position and all other elements being zeros. The formulation in (4) is an instance where  $\forall k \in [p] : \mathbf{v}^j(\mathbf{x}) = \mathbf{m}_d(\mathbf{x})$  (the full monomial basis). The PMI  $\forall \mathbf{x} \in \mathbb{R}^n : F(\mathbf{x}) \succeq 0$  is verified if the Gram matrix satisfies  $\tilde{Q} \succeq 0$ . This subsection will use the monomial structure of  $F(\mathbf{x})$  to design bases  $\{\mathbf{v}^j(\mathbf{x})\}$  that may have a lower cardinality than the full basis  $\mathbf{m}_d(\mathbf{x})$ . The basis reduction will be accomplished by using Newton Polytope techniques on the scalarized PMI (6).

### 3.1.1 Newton Polytope Background

We first introduce background material on Newton Polytopes and their importance in sparse SOS representations.

**Definition 3.1.** The Newton polytope of a scalar polynomial  $f \in \mathbb{R}[x]$  is

$$New(f) = conv(supp(f)), \tag{20}$$

where  $conv(\cdot)$  means taking the convex hull.

**Example 3.1.** The Newton polytope of the Motzkin polynomial  $f = 1 + x_1^2 x_2^4 + x_1^4 x_2^2 - 3x_1^2 x_2^2$  is

$$New(f) = conv\left(\left\{\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}2\\4\end{bmatrix}, \begin{bmatrix}4\\2\end{bmatrix}\right\}\right). \tag{21}$$

Note that the point  $[2,2]^{\intercal}$  from the monomial  $x_1^2x_2^2$  is in the interior of the convex hull established by (21).

Newton polytopes can be used to reduce the number of active monomials in an SOS decomposition.

**Theorem 3.1** (Theorem 1 of [33]). Let f be a polynomial such that  $f \in \Sigma[x]_{2d}$ , and let  $g \in \mathbb{R}[x]^t$  be a vector of polynomials such that  $f(x) = \sum_{j=1}^t g_j(x)^2$ . The supports of each factor  $g_j$  are constrained by

$$\forall j \in [t]: \quad \text{New}(g_j) \subseteq \frac{1}{2} \text{New}(f).$$
 (22)

A Gram SOS representation  $f(\boldsymbol{x}) = \boldsymbol{v}(\boldsymbol{x})^{\intercal} \tilde{Q} \boldsymbol{v}(\boldsymbol{x})$  can therefore restrict the monomial vector  $\boldsymbol{v}(\boldsymbol{x})$  to all integer points of  $\frac{1}{2} \text{New}(f)$ , rather than choosing all  $\binom{n+d}{d}$  monomial elements in the full basis  $\mathbf{m}_d(\boldsymbol{x})$ . The size of the Gram matrix  $\tilde{Q}$  can therefore be reduced (ensuring that solving the SDP is more efficient), at the preprocessing cost of finding all integer points in the 1/2-scaled Newton polytope.

### 3.1.2 Newton Polytopes for Polynomial Matrix Inequalities

We now return to the PMI setting with a polynomial matrix  $F(\mathbf{x}) \in \mathbb{S}^p[\mathbf{x}]$ . Monomial bases  $\{\mathbf{v}^j(\mathbf{x})\}$  from (19) can be determined by virtue of Theorem 3.1 as follows.

**Theorem 3.2.** Let  $F(\mathbf{x}) \in \Sigma^p[\mathbf{x}]$  be a polynomial matrix and  $\mathcal{A}^j := \mathbb{N}^n \cap \frac{1}{2} \text{New}(F(\mathbf{x})_{jj})$ , where  $F(\mathbf{x})_{jj}$  is the j-th diagonal element of  $F(\mathbf{x})$ ,  $j \in [p]$ . Then the monomial basis  $\mathbf{v}^j(\mathbf{x})$  from (19) can be chosen without conservatism as  $\mathbf{v}^j(\mathbf{x}) = {\mathbf{x}^{\boldsymbol{\alpha}} \mid \boldsymbol{\alpha} \in \mathcal{A}^j}$ .

Proof. Consider the scalarization  $\mathbf{y}^{\mathsf{T}}F(\mathbf{x})\mathbf{y}$  of  $F(\mathbf{x})$  from (5). Since  $\mathbf{y}^{\mathsf{T}}F(\mathbf{x})\mathbf{y}$  is a quadratic form in  $\mathbf{y}$ , it holds that each integral point  $(\boldsymbol{\alpha}_{\boldsymbol{x}}, \boldsymbol{\alpha}_{\boldsymbol{y}}) \in \mathbb{N}^{n+p} \cap \frac{1}{2}\mathrm{New}(\mathbf{y}^{\mathsf{T}}F(\mathbf{x})\mathbf{y})$  satisfies  $|\boldsymbol{\alpha}_{\boldsymbol{y}}| = 1$ . For each  $j \in [p]$ , let  $\tilde{\mathcal{A}}^j := \{\boldsymbol{\alpha}_{\boldsymbol{x}} \in \mathbb{N}^n \mid (\boldsymbol{\alpha}_{\boldsymbol{x}}, \boldsymbol{\alpha}_{\boldsymbol{y}}) \in \mathbb{N}^{n+p} \cap \frac{1}{2}\mathrm{New}(\mathbf{y}^{\mathsf{T}}F(\mathbf{x})\mathbf{y}), \boldsymbol{\alpha}_{y_j} = 1\}$  corresponding to the set of  $\boldsymbol{x}$ -monomials multiplied by  $y_j$ . By Theorem 3.1, one can choose  $\mathbf{v}^j(\mathbf{x}) = \{\mathbf{x}^{\boldsymbol{\alpha}} \mid \boldsymbol{\alpha} \in \tilde{\mathcal{A}}^j\}$  without conservatism. Moreover, one can easily check that  $\tilde{\mathcal{A}}^j = \mathcal{A}^j$  from constructions.

The procedure in Theorem 3.2 will be outlined with an example.

**Example 3.2.** Let  $F(x) \in \mathbb{S}^3[x]$  be defined by

$$F(\mathbf{x}) = \begin{bmatrix} 1 + x_1^4 - 0.5x_1^2 + 0.25x_1 + x_2^2 + x_3^4 & -x_2 & x_1 + x_3 \\ -x_2 & 2 + 2x_2^4 + 2x_1^2 - x_1 & x_1 \\ x_1 + x_3 & x_1 & 2 + 3x_3^2 + x_1^2 x_2^2 \end{bmatrix}.$$
(23)

By respectively computing the Newton polytopes of the diagonal elements  $F(\mathbf{x})_{11}$ ,  $F(\mathbf{x})_{22}$ ,  $F(\mathbf{x})_{33}$ , the monomial bases  $\{\mathbf{v}^j(\mathbf{x})\}$  can be given as

$$\mathbf{v}^{1}(\mathbf{x}) = \{1, x_{1}^{2}, x_{1}, x_{1}x_{3}, x_{2}, x_{3}^{2}, x_{3}\}, \tag{24a}$$

$$\mathbf{v}^2(\mathbf{x}) = \{1, x_1, x_2, x_2^2\},\tag{24b}$$

$$\mathbf{v}^3(\mathbf{x}) = \{1, x_1 x_2, x_3\}. \tag{24c}$$

There are 14 monomials in total listed in (24). Verification that  $F(\mathbf{x})$  from (23) is an SOS matrix can therefore be accomplished by solving an SDP with a Gram matrix  $\tilde{Q} \in \mathbb{S}^{14}_+$  rather than in  $\mathbb{S}^{30}_+$  (as would be required with a full choice of all  $\binom{3+2}{3} = 10$  monomials for each of the three columns). An admissible SOS decomposition  $F(\mathbf{x}) = R(\mathbf{x})^{\mathsf{T}}R(\mathbf{x})$  found by the reduced bases in (24) is

$$R(\boldsymbol{x}) \approx \begin{bmatrix} 1 + 0.125x_1 - 0.517x_1^2 & 0.0864x_1 & x_3 \\ 0.0760x_1 + 0.8543x_1^2 & -0.617 + 0.0525x_1 & 0.608x_3 \\ 0.707x_1 & 0.707x_1 & 1.414 \\ x_2 & -1 & 0 \\ x_3^2 & 0 & 0 \\ -0.050x_1 & 0.787 - 0.594x_1 & 0.477x_3 \\ -0.016x_1 & 1.066x_1 & 0.155x_3 \\ 0 & 1.414x_2^2 & 0 \\ -0.1223x_1 & 0 & 1.174x_3 \\ 0 & 0 & x_1x_2 \end{bmatrix}.$$

$$(25)$$

## 3.2 Term Sparsity Patterns

The previous subsection concentrated on reducing the number of elements in the monomial bases  $\{v^j(x)\}$ . This subsection will focus on reducing the maximal size of PSD matrices involved in the SDP through the application of term sparsity.

**Definition 3.2.** Let  $\mathbf{B} := [\mathbf{v}^1(\mathbf{x}), \dots, \mathbf{v}^p(\mathbf{x})]$ . The term sparsity pattern (TSP) of a polynomial matrix  $F(\mathbf{x}) \in \mathbb{S}^p[\mathbf{x}]$  is an undirected graph including self-loops with nodes corresponding to entries of  $\mathbf{B}$ , and edges are drawn between nodes  $a \in \mathbf{v}^i(\mathbf{x})$  and  $b \in \mathbf{v}^j(\mathbf{x})$  if  $ab \in \{\mathbf{x}^\alpha \mid \alpha \in \operatorname{supp}(F_{ij})\}$  or if ab is a monomial square given that i = j.

**Example 3.3.** Consider the bivariate matrix

$$F(\mathbf{x}) = \begin{bmatrix} 1 + x_1^2 + 2x_1^2x_2^2 + x_2^2 & x_1x_2 \\ x_1x_2 & 2 + x_1^2x_2^2 + x_2^4 \end{bmatrix}$$
(26)

admitting an SOS-matrix decomposition  $F(\mathbf{x}) = R(\mathbf{x})^{\intercal}R(\mathbf{x})$  with

$$R(\mathbf{x}) = \begin{bmatrix} x_1 & x_2 \\ \sqrt{2}x_1x_2 & 0 \\ x_2 & 0 \\ 1 & 0 \\ 0 & \sqrt{3/2} \\ 0 & x_1x_2 \\ 0 & x_2^2/\sqrt{2} \\ 0 & (x_2^2 - 1)/\sqrt{2} \end{bmatrix}.$$
 (27)

This example uses the standard full bases  $\mathbf{v}^1(\mathbf{x}) = \mathbf{v}^2(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_1 x_2, x_2^2]$ . The j-indices of a monomial  $a \in \mathbf{v}^j(\mathbf{x})$  for  $j \in \{1, 2\}$  will be indicated by a bracketed-superscript as  $[a]^j$ . The TSP of (26) is drawn in Figure 3. This graph has 5 connected components. As an example, the off-diagonal term  $F(\mathbf{x})_{12} = x_1 x_2$  could be created by multiplications of  $[1]^1, [x_1 x_2]^2$  or  $[x_1]^1, [x_2]^2$ .

The term sparsity method proceeds by the iterative repetition of two operations on the TSP graph [30]:

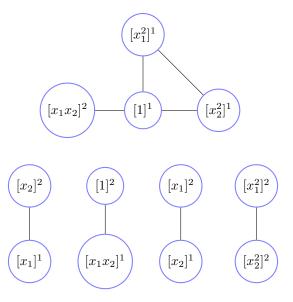


Figure 3: The TSP graph of F(x) in (26)

- Support Extension: Add edges to the graph based on the sets of active monomials;
- Chordal Extension: Add edges to the graph by performing a chordal extension.

More concretely, for each pair  $i, j \in [p]$ , define the initial support set associated to the (i, j)-position by

$$C_{i,j}^{(0)} := \begin{cases} \sup(F_{ii}) \cup \mathbf{v}^i(\mathbf{x})^{\circ 2}, & \text{if } i = j, \\ \sup(F_{ij}), & \text{otherwise,} \end{cases}$$
 (28)

where  $v^i(x)^{\circ 2}$  denotes the set of squares of monomials in  $v^i(x)$ . For  $s \geq 0$ , the support extension operation is defined as

SupportExtension(
$$\mathcal{E}^{(s)}$$
) :=  $\bigcup_{i,j=1}^{p} \left\{ \left\{ [a]^i, [b]^j \right\} \in \boldsymbol{v}^i(\boldsymbol{x}) \times \boldsymbol{v}^j(\boldsymbol{x}) \mid ab \in \mathcal{C}_{i,j}^{(s)} \right\}.$  (29)

Next, we perform a chordal extension on the graph with SupportExtension( $\mathcal{E}^{(s)}$ ) as its edges:

$$\mathcal{E}^{(s+1)} \leftarrow \text{ChordalExtension}(\text{SupportExtension}(\mathcal{E}^{(s)})), \tag{30}$$

and update the support set

$$C_{i,j}^{(s+1)} := \left\{ ab \,\middle|\, \left\{ [a]^i, [b]^j \right\} \in \mathcal{E}^{(s+1)} \right\}. \tag{31}$$

There are two typical choices for the chordal extension operation in (30): an (approximately) smallest chordal closure (i.e., chordal extension with the smallest tree-width) and the block closure. The block closure would offer a block-diagonal structure on the Gram matrix, whereas the sparser chordal closure could potentially contain overlaps among maximal cliques. Figure 4 compares the two types of chordal extensions for the TSP graph in Example 3.3.

The process in (30) is guaranteed to stabilize after a finite number of iterations, because the cardinality of the node set **B** is finite and both the support extension and chordal extension steps only add edges. After obtaining the graph  $\mathcal{G}^{(s)}(\mathbf{B}, \mathcal{E}^{(s)})$  at the s-th term sparsity step  $(s \ge 1)$ , we may consider the following sparse SDP to decompose  $F(\mathbf{x})$  as an SOS:

$$\begin{cases}
\operatorname{Find} & Q \in \mathbb{S}_{+}^{|\mathbf{B}|}(\mathcal{G}^{(s)}, 0) \\
\operatorname{s.t.} & F(\boldsymbol{x}) = \operatorname{diag}(\boldsymbol{v}^{1}(\boldsymbol{x}), \boldsymbol{v}^{2}(\boldsymbol{x}), \dots, \boldsymbol{v}^{p}(\boldsymbol{x}))^{\mathsf{T}} Q \operatorname{diag}(\boldsymbol{v}^{1}(\boldsymbol{x}), \boldsymbol{v}^{2}(\boldsymbol{x}), \dots, \boldsymbol{v}^{p}(\boldsymbol{x})).
\end{cases} (32)$$

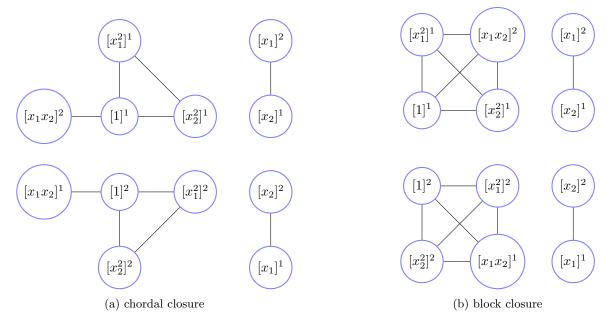


Figure 4: Chordal extensions of the TSP graph of F(x) in (26)

**Theorem 3.3.** Assume that the chordal extension in (30) is chosen to be the block closure and the process in (30) stabilizes at the s-th step. Then,  $F(\mathbf{x}) \in \Sigma^p[\mathbf{x}]$  if and only if (32) is feasible.

*Proof.* The proof is similar to the counterpart in [30, Theorem 3.3].

# 4 Term Sparsity for Constrained PMIs

This section will apply term sparsity techniques towards optimization over constrained PMIs. Specifically, we extend the iterative procedure on exploiting term sparsity for scalar polynomial optimization [30,31] to the situation of PMO. Just as in the unconstrained case of Section 3.2, the term sparsity decomposition will proceed based on alternating support extension and chordal extension steps.

Consider the PMO problem

$$\lambda^* := \inf_{\boldsymbol{x} \in \mathbb{R}^n} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G_1(\boldsymbol{x}) \succeq 0, \dots, G_m(\boldsymbol{x}) \succeq 0,$$
(33)

where  $F = [F_{ij}] \in \mathbb{S}^p[x]$  and  $G_k = [G_k^{i,j}] \in \mathbb{S}^{q_k}[x], k \in [m]$ . By abuse of notation, we denote a monomial basis  $\{x^{\alpha}\}_{\alpha \in \mathcal{B}}$  by its exponent set  $\mathcal{B}$  in the following. For a monomial basis  $\mathcal{B}$  and a positive integer k, we use  $\mathcal{B}^{(k)}$  to denote the vector of k-copies of  $\mathcal{B}$ , that is,

$$\mathcal{B}^{(k)} := (\underbrace{\alpha, \dots, \alpha}_{k \text{ copies}})_{\alpha \in \mathcal{B}}.$$
 (34)

For convenience, the k-copies of  $\alpha \in \mathcal{B}$  in  $\mathcal{B}^{(k)}$  is respectively referred to as  $[\alpha]^1, \dots, [\alpha]^k$ .

Recall that  $d_k := \lceil \deg G_k/2 \rceil$  for  $k \in [m]$  and  $r_{\min} := \max \{\lceil \deg F/2 \rceil, d_1, \dots, d_m \}$ . Fix a relaxation order  $r \ge r_{\min}$ . Set  $d_0 := 0$  and  $q_0 := 1$ . Let

$$\mathbf{B}_{r,k} := (\mathbb{N}_{r-d_k}^n)^{(pq_k)}, \quad k = 0, \dots, m, \tag{35}$$

and for each pair  $i, j \in [p]$ , let us define the initial support set

$$C_{i,j}^{(0)} := \begin{cases} \sup(F_{ii}) \cup (2\mathbb{N}_r^n), & \text{if } i = j, \\ \sup(F_{ij}), & \text{otherwise.} \end{cases}$$
(36)

Now for each  $k \in [m]$ , we iteratively define an ascending chain of graphs  $\left(\mathcal{G}_{r,k}^{(s)}\left(\mathbf{B}_{r,k},\mathcal{E}_{r,k}^{(s)}\right)\right)_{s\geq 1}$  via two successive operations:

1) **Support Extension.** Add edges to the graph  $\mathcal{G}_{r,k}^{(s)}$  according to the sets of activated supports  $\mathcal{C}_{i,j}^{(s)}$ :

$$\text{SupportExtension}(\mathcal{E}_{r,k}^{(s)}) \coloneqq \bigcup_{i,j=1}^{p} \bigg\{ \left\{ [\pmb{\alpha}]^i, [\pmb{\beta}]^j \right\} \in \mathbb{N}_{r-d_k}^n \times \mathbb{N}_{r-d_k}^n \, \bigg| \, \Big( \pmb{\alpha} + \pmb{\beta} + \text{supp}(G_k^{\bar{i},\bar{j}}) \Big) \cap \mathcal{C}_{\lceil i/q_k \rceil, \lceil j/q_k \rceil}^{(s)} \neq \emptyset \bigg\},$$

where for any  $i \in [pq_k]$ ,

$$\bar{i} \coloneqq \begin{cases} i \pmod{q_k}, & \text{if } q_k \nmid i, \\ q_k, & \text{otherwise.} \end{cases}$$

2) Chordal Extension. For each k, perform a chordal extension on the graph with SupportExtension( $\mathcal{E}_{r,k}^{(s)}$ ) as its edge set, i.e., let

$$\mathcal{E}_{r,k}^{(s+1)} \leftarrow \text{ChordalExtension}(\text{SupportExtension}(\mathcal{E}_{r,k}^{(s)})), \quad k = 0, \dots, m,$$
 (37)

and for each  $i, j \in [p]$ , update the sets of activated supports:

$$C_{i,j}^{(s+1)} := \bigcup_{k=0}^{m} \bigcup_{i',j'=1}^{q_k} \bigcup_{\{[\alpha]^{(i-1)q_k+i'}, [\beta]^{(j-1)q_k+j'}\} \in \mathcal{E}_{r,k}^{(s+1)}} \left(\alpha + \beta + \operatorname{supp}(G_k^{i',j'})\right).$$
(38)

Clearly, the process in (37) is guaranteed to stabilize after a finite number of iterations for all k, because the cardinality of each node set  $\mathbf{B}_{r,k}$  is finite and both the support extension and chordal extension steps only add edges.

Given an undirected graph  $\mathcal{G}(\mathcal{V}, \mathcal{E})$ , we use the symbol  $B_{\mathcal{G}} \in \{0,1\}^{|\mathcal{V}| \times |\mathcal{V}|}$  to refer to the adjacency matrix of  $\mathcal{G}$  whose diagonal are all ones. Then, for  $s \geq 1$ , the corresponding sparse moment relaxation for (33) is given by

$$\lambda_r^{(s)} := \begin{cases}
\inf & \mathcal{L}_{\mathbf{S}}(F) \\
\text{s.t.} & B_{\mathcal{G}_{r,0}^{(s)}} \circ M_r(\mathbf{S}) \in \mathbb{S}_+(\mathcal{G}_{r,0}^{(s)},?), \\
& B_{\mathcal{G}_{r,k}^{(s)}} \circ M_{r-d_k}(G_k\mathbf{S}) \in \mathbb{S}_+(\mathcal{G}_{r,k}^{(s)},?), \quad k \in [m], \\
& \mathcal{L}_{\mathbf{S}}(I_p) = 1.
\end{cases}$$
(39)

We call s the sparse order.

**Proposition 4.1.** The following statements are true:

- (i) Fixing a relaxation order  $r \ge r_{\min}$ , the sequence  $\left\{\lambda_r^{(s)}\right\}_{s \ge 1}$  is monotonically non-decreasing and  $\lambda_r^{(s)} \le \lambda^*$  for all  $s \ge 1$ .
- (ii) Fixing a sparse order  $s \ge 1$ , the sequence  $\left\{\lambda_r^{(s)}\right\}_{r \ge r_{\min}}$  is monotonically non-decreasing.
- (iii) Assume that the chordal extension in (37) is chosen to be the block closure. Then for any  $r \geq r_{\min}$ , the sequence  $\left\{\lambda_r^{(s)}\right\}_{s\geq 1}$  converges to  $\lambda_r$  in finitely many steps.

*Proof.* The proofs are similar to the counterparts in [30, 31].

Term sparse decompositions are intricately linked to sign symmetries of the underlying polynomial matrices:

**Definition 4.1.** A sign symmetry of a polynomial matrix  $P \in \mathbb{S}^p[x]$  is a binary vector  $\theta \in \{-1,1\}^n$  such that

$$\forall \boldsymbol{x} \in \mathbb{R}^n : P(\boldsymbol{x}) = P(\theta \circ \boldsymbol{x}), \tag{40}$$

where  $\circ$  means the entrywise product. The sign symmetries of P is the set of all such binary vectors.

Particular instances of sign symmetries include even symmetries (i.e.,  $F(\mathbf{x}) = F(-\mathbf{x})$ ) or coordinatewise symmetries (e.g.,  $F(x_1, x_2, x_3) = F(-x_1, x_2, x_3)$ ). Sign symmetries yield a block-diagonal structure for unconstrained matrix SOS decompositions [58], which can be extended to the constrained case as we shall do. Let R be the binary matrix whose columns consist of the common sign symmetries of  $F(\mathbf{x}), G_1(\mathbf{x}), \dots, G_m(\mathbf{x})$ . We define an equivalence relation  $\sim$  on  $\mathbf{B}_{r,k}$   $(k = 0, \dots, m)$  by

$$\alpha \sim \beta \iff R^{\mathsf{T}}(\alpha + \beta) \equiv 0 \pmod{2}.$$
 (41)

For each  $k \in \{0\} \cup [m]$ , the equivalence relation  $\sim$  gives rise to a partition of  $\mathbf{B}_{r,k}$ , and thus defines a block-diagonal structure on the moment matrix or localizing matrices (each block being indexed by an equivalence class in  $\mathbf{B}_{r,k}$ ).

**Theorem 4.2.** In (17), there is no loss of generality in assuming that the moment matrix and localizing matrices possess the block-diagonal structure provided by the common sign symmetries of  $F(\mathbf{x}), G_1(\mathbf{x}), \ldots, G_m(\mathbf{x})$ . Equivalently, if F has an SOS representation

$$F = S_0 + \sum_{k=1}^{m} \langle S_k, G_k \rangle_p, \tag{42}$$

for some SOS matrices  $S_0, \ldots, S_m$ , then there is no loss of generality in assuming that  $R^{\intercal} \boldsymbol{\alpha} \equiv 0 \pmod{2}$  for any  $\boldsymbol{\alpha} \in \operatorname{supp}(S_k), k = 0, \ldots, m$ .

Proof. Imposing the condition that  $R^{\mathsf{T}}\alpha \equiv 0 \pmod{2}$  for any  $\alpha \in \operatorname{supp}(S_k), k = 0, \dots, m$  boils down to removing the terms with exponents  $\alpha$  that do not satisfy  $R^{\mathsf{T}}\alpha \equiv 0 \pmod{2}$  from the right hand side of (42). Since any  $\alpha \in \operatorname{supp}(F)$  satisfies  $R^{\mathsf{T}}\alpha \equiv 0 \pmod{2}$ , doing so does not change the match of coefficients on both sides of (42) as desired.

As a corollary of Theorem 4.2, we immediately obtain the following sign symmetry adapted Positivstellensatz for polynomial matrices.

Corollary 4.3. Let R be the binary matrix whose columns consist of the common sign symmetries of the polynomial matrices  $F(\mathbf{x}), G_1(\mathbf{x}), \dots, G_m(\mathbf{x})$ . If F is positive definite on  $\mathbf{K}$  defined in (7), then F can be represented as

$$F = S_0 + \sum_{k=1}^{m} \langle S_k, G_k \rangle_p, \tag{43}$$

for some SOS matrices  $S_0, \ldots, S_m$  satisfying  $R^{\mathsf{T}} \alpha \equiv 0 \pmod{2}$  for any  $\alpha \in \operatorname{supp}(S_k), k = 0, \ldots, m$ .

*Proof.* It follows from Scherer and Hol's Positivestellensatz and Theorem 4.2.

It is easily seen from the construction that the block structure at any term sparsity iteration is a refinement of the one determined by sign symmetries. For scalar polynomial optimization, the block structures of the term sparsity iterations with block closures actually converge to the one determined by sign symmetries [30]. In contrast to the scalar case, such convergence may fail in the matrix setting. We illustrate this phenomenon in the following example.

Example 4.1. Consider the problem

$$\inf_{\boldsymbol{x} \in \mathbb{R}^2} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad 1 - x_1^2 - x_2^2 \ge 0$$
(44)

with

$$F(x) = \begin{bmatrix} x_1^2 & x_1 + x_2 \\ x_1 + x_2 & x_2^2 \end{bmatrix}.$$
 (45)

Note that (44) has only the trivial sign symmetry, which means that the related block structure is also trivial. On the other hand, with the relaxation order r=2, the procedure for exploiting term sparsity with block closures stabilizes at s=2, giving rise to two blocks for the moment matrix:  $\{[1]^1, [x_1]^2, [x_2]^2, [x_1^2]^1, [x_1x_2]^1, [x_2^2]^1\}$  and  $\{[1]^2, [x_1]^1, [x_2]^1, [x_1^2]^2, [x_1x_2]^2, [x_2^2]^2\}$ . The corresponding sparse relaxation (33) yields a lower bound -0.9142 which coincides with the bound given by the second order dense relaxation.

# 5 Correlative Sparsity

The aim of this section is to explore the correlative sparsity of the PMO problem (33):

$$\lambda^* \coloneqq \inf_{\boldsymbol{x} \in \mathbb{R}^n} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G_1(\boldsymbol{x}) \succeq 0, \dots, G_m(\boldsymbol{x}) \succeq 0,$$

where  $F \in \mathbb{S}^p[\boldsymbol{x}]$  and  $G_k \in \mathbb{S}^{q_k}[\boldsymbol{x}], k \in [m]$ .

We define the *correlative sparsity pattern (CSP) graph* of (33), denoted by  $\mathcal{G}^{\text{csp}}$ , such that  $\mathcal{V}(\mathcal{G}^{\text{csp}}) = [n]$  and  $\{i, j\} \in \mathcal{E}(\mathcal{G}^{\text{csp}})$  if one of following conditions holds:

- (i) There exists  $\alpha \in \text{supp}(F)$  such that  $i, j \in \text{supp}(\alpha) := \{k \in [n] \mid \alpha_k \neq 0\};$
- (ii) There exists  $k \in [m]$  such that  $x_i, x_j \in \text{var}(G_k)$ , where  $\text{var}(G_k)$  is the subset of variables effectively involved in  $G_k$ .

Let  $\{\mathcal{I}_{\ell}\}_{\ell=1}^t$  be the list of maximal cliques of  $\mathcal{G}^{\text{csp}}$  with  $n_{\ell} := |\mathcal{I}_{\ell}|$ . For  $\ell \in [t]$ , let  $\mathbb{R}[\boldsymbol{x}(\mathcal{I}_{\ell})]$  denote the ring of polynomials in the  $n_{\ell}$  variables  $\boldsymbol{x}(\mathcal{I}_{\ell}) := \{x_i \mid i \in \mathcal{I}_{\ell}\}$ . We can partition the constraint polynomial matrices  $G_1, \ldots, G_m$  into groups  $\{G_k \mid k \in \mathcal{J}_{\ell}\}, \ell = 1, \ldots, t$  which satisfy

- (i)  $\mathcal{J}_1, \ldots, \mathcal{J}_t \subseteq [m]$  are pairwise disjoint and  $\bigcup_{\ell=1}^t \mathcal{J}_\ell = [m]$ ;
- (ii) For any  $k \in \mathcal{J}_{\ell}$ ,  $var(G_k) \subseteq \mathcal{I}_{\ell}$ ,  $\ell = 1, ..., t$ .

Given a sequence  $\mathbf{S} = (S_{\boldsymbol{\alpha}})_{\boldsymbol{\alpha} \in \mathbb{N}^n} \subseteq \mathbb{S}^p$  and  $\ell \in [t]$ , for  $d \in \mathbb{N}$  and  $G \in \mathbb{R}[\boldsymbol{x}(\mathcal{I}_\ell)]$ , let  $M_d(\mathbf{S}, \mathcal{I}_\ell)$  (resp.  $M_d(G\mathbf{S}, \mathcal{I}_\ell)$ ) be the moment (resp. localizing) submatrix obtained from  $M_d(\mathbf{S})$  (resp.  $M_d(G\mathbf{S})$ ) by retaining only those block rows and columns indexed by  $\boldsymbol{\alpha} \in \mathbb{N}_d^n$  with  $\operatorname{supp}(\boldsymbol{\alpha}) \subseteq \mathcal{I}_\ell$ .

Then with  $r \ge r_{\min}$ , the r-th order correlative sparsity adapted moment relaxation for (33) is given by

$$\lambda_r^{(\text{cs})} := \begin{cases}
\inf & \mathcal{L}_{\mathbf{S}}(F) \\
\text{s.t.} & M_r(\mathbf{S}, \mathcal{I}_{\ell}) \succeq 0, \quad \ell \in [t], \\
& M_{r-d_k}(G_k \mathbf{S}, \mathcal{I}_{\ell}) \succeq 0, \quad k \in \mathcal{J}_{\ell}, \ell \in [t], \\
& \mathcal{L}_{\mathbf{S}}(I_p) = 1,
\end{cases}$$
(46)

and its dual problem reads as

$$\begin{cases}
\sup \lambda \\
\text{s.t.} \quad F - \lambda I_p = \sum_{\ell=1}^t \left( S_{\ell,0} + \sum_{k \in \mathcal{J}_\ell} \left\langle S_{\ell,k}, G_k \right\rangle_p \right), \\
S_{\ell,0} \in \Sigma^p[\boldsymbol{x}(\mathcal{I}_\ell)]_{2r}, \quad S_{\ell,k} \in \Sigma^{pq_k}[\boldsymbol{x}(\mathcal{I}_\ell)]_{2(r-d_k)}, \quad k \in \mathcal{J}_\ell, \ell \in [t].
\end{cases} \tag{47}$$

Each  $\lambda_r^{(\text{cs})}$  therefore provides a lower bound on  $\lambda^*$  and the sequence  $\left\{\lambda_r^{(\text{cs})}\right\}_{r\geq r_{\min}}$  is monotonically non-decreasing. Moreover, asymptotic convergence to  $\lambda^*$  can be guaranteed under appropriate conditions when p=1.

**Theorem 5.1.** ([50, Theorem 1]) Let p = 1. Assume that the following conditions hold:

(i) The CSP  $\{\mathcal{I}_{\ell}\}_{\ell=1}^t$  satisfies the running intersection property, i.e., for every  $\ell \in [t-1]$ , there exists  $s \in [\ell]$  such that

$$\mathcal{I}_{\ell+1} \cap \bigcup_{j=1}^{\ell} \mathcal{I}_j \subseteq \mathcal{I}_s;$$

(ii) For each  $\ell \in [t]$ , there exists  $a_{\ell} > 0$  such that

$$a_{\ell} - \sum_{i \in \mathcal{I}_{\ell}} x_i^2 = \sigma_{\ell,0} + \sum_{k \in \mathcal{I}_{\ell}} \langle S_{\ell,k}, G_k \rangle,$$

where  $\sigma_{\ell,0} \in \Sigma^1[\boldsymbol{x}], \ S_{\ell,k} \in \Sigma^{q_k}[\boldsymbol{x}].$ 

Then  $\lim_{r\to\infty} \lambda_r^{(cs)} = \lambda^*$ .

In view of Theorem 5.1, one may expect that the asymptotic convergence also holds true when p > 1 under similar conditions. However, the following counterexample shows that this is not the case even when p = 2. In other words, the matrix counterpart (i.e., for p > 1) of Putinar's Positivstellensatz for polynomials with correlative sparsity studied in [50, 59, 60] does not hold in general.

### Example 5.1. Let

$$F(\mathbf{x}) = \begin{bmatrix} 2(x_1 - 1)^2 + (x_2 - 1)^2 + (x_2 - 2)^2 & 3 - 2x_2 \\ 3 - 2x_2 & 2(x_1 - 2)^2 + (x_2 - 1)^2 + (x_2 - 2)^2 \end{bmatrix}$$

and

$$\mathbf{K} = \{(x_1, x_2) \in \mathbb{R}^2 : 4 - x_1^2 \ge 0, 4 - x_2^2 \ge 0\}.$$

Let

$$Q = \begin{bmatrix} \frac{13}{2} & 3 & -2 & -3 & -3 & 2\\ 3 & \frac{25}{2} & 3 & -4 & -4 & -3\\ -2 & 3 & 2 & 0 & 0 & -2\\ -3 & -4 & 0 & 2 & 2 & 0\\ -3 & -4 & 0 & 2 & 2 & 0\\ 2 & -3 & -2 & 0 & 0 & 2 \end{bmatrix}.$$

The matrix Q has three eigenvalues: 0 and  $\frac{27}{2} \pm 3\sqrt{2}$  (so  $Q \succeq 0$ ), and

$$F(\boldsymbol{x}) - \frac{1}{2}I_2 = (\mathbf{m}_1(\boldsymbol{x}) \otimes I_2)^{\intercal}Q(\mathbf{m}_1(\boldsymbol{x}) \otimes I_2) \succeq 0.$$

Moreover, we have  $(\frac{3}{2},1) \in \mathbf{K}$  and  $\lambda_{\min}\left(F(\frac{3}{2},1)\right) = \frac{1}{2}$ . It implies that  $\inf_{\boldsymbol{x} \in \mathbf{K}} \lambda_{\min}(F(\boldsymbol{x})) = \frac{1}{2}$  (whose minimizers form a circle:  $(x_1 - \frac{3}{2})^2 + (x_2 - \frac{3}{2})^2 = \frac{1}{4}$ ). Hence, for any  $\varepsilon > 0$ ,

$$F(\boldsymbol{x}) - \left(\frac{1}{2} - \varepsilon\right) I_2 \succ 0, \quad \forall \boldsymbol{x} \in \mathbf{K}.$$

However, for any  $\varepsilon \in (0, \frac{1}{2})$ , we will show that the representation

$$F(\mathbf{x}) - \left(\frac{1}{2} - \varepsilon\right) I_2 = \sum_{i=1}^{2} \left( S_{i,0}(x_i) + (4 - x_i^2) S_{i,1}(x_i) \right), \tag{48}$$

where each  $S_{i,j} \in \Sigma^2[x_i]$ , does not hold. Suppose on the contrary that there exists a representation (48) for some  $\varepsilon \in (0, \frac{1}{2})$ . Let  $\Phi_1, \Phi_2$  be the following matrix-valued atomic measures defined in the  $x_1$ -space and  $x_2$ -space, respectively:

$$\Phi_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \delta_{(x_1=1)} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \delta_{(x_1=2)}, \quad \Phi_2 = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \delta_{(x_2=1)} + \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \delta_{(x_2=2)}.$$

Then, we define a linear functional  $\mathcal{L}: \mathbb{S}^2[x_1] + \mathbb{S}^2[x_2] \to \mathbb{R}$  by

$$\mathscr{L}(H_1(x_1) + H_2(x_2)) = \mathscr{L}_{\Phi_1}(H_1(x_1)) + \mathscr{L}_{\Phi_2}(H_2(x_2)), \quad \forall H_1(x_1) \in \mathbb{S}^2[x_1], H_2(x_2) \in \mathbb{S}^2[x_2].$$

Since  $\mathcal{L}_{\Phi_1}(I_2) = \mathcal{L}_{\Phi_2}(I_2) = 1$ , there is no ambiguity in the above definition. One can easily check that  $\mathcal{L}(F) = 0$ . Now applying  $\mathcal{L}$  to both sides of (48), we obtain

$$0 - \left(\frac{1}{2} - \varepsilon\right) = \mathcal{L}\left(F(\boldsymbol{x}) - \left(\frac{1}{2} - \varepsilon\right)I_2\right) = \mathcal{L}\left(\sum_{i=1}^2 \left(S_{i,0}(x_i) + (4 - x_i^2)S_{i,1}(x_i)\right)\right) \ge 0,$$

which is a contradiction.

Even though asymptotic convergence does not hold for PMO with correlative sparsity in general, finite convergence may still occur in practice, and this convergence could be detected by flatness conditions. For the rest of this section, we establish several results on detecting finite convergence and extracting optimal solutions when exploiting correlative sparsity. For each  $\ell \in [t]$ , let us define

$$\mathbf{K}_{\ell} := \left\{ \boldsymbol{x}(\ell) \in \mathbb{R}^{|\mathcal{I}_{\ell}|} \middle| G_{k}(\boldsymbol{x}) \succeq 0, \quad \forall k \in \mathcal{J}_{\ell} \right\}, \tag{49}$$

where  $\boldsymbol{x}(\ell) \coloneqq (x_i)_{i \in \mathcal{I}_{\ell}}$ .

**Theorem 5.2.** Let S be an optimal solution of (46). Assume that the following conditions hold:

- (i) For each  $\ell \in [t]$ ,  $\mathbf{S}^{\ell} \coloneqq (S_{\boldsymbol{\alpha}})_{\text{supp}(\boldsymbol{\alpha}) \subseteq \mathcal{I}_{\ell}}$  admits a representing measure  $\Phi_{\ell} = S_{\mathbf{0}} \left( \sum_{i=1}^{s_{\ell}} \xi_{i\ell} \delta_{\boldsymbol{x}^{i}(\ell)} \right)$  for some  $\xi_{i\ell} > 0$  with  $\sum_{i=1}^{s_{\ell}} \xi_{i\ell} = 1$  and  $\boldsymbol{x}^{1}(\ell), \dots, \boldsymbol{x}^{s_{\ell}}(\ell) \in \mathbf{K}_{\ell}$ ;
- (ii) For all pairs  $\{i, j\}$  with  $\mathcal{I}_i \cap \mathcal{I}_j \neq \emptyset$ , one has  $\operatorname{rank}(M_r(\mathbf{S}, \mathcal{I}_i \cap \mathcal{I}_j)) = 1$ .

Then  $\lambda_r^{(cs)} = \lambda^*$ . Moreover, each point  $\hat{\boldsymbol{x}} \in \mathbb{R}^n$  satisfying  $\hat{\boldsymbol{x}}(\ell) := (\hat{x}_i)_{i \in \mathcal{I}_\ell} = \boldsymbol{x}^{i_\ell}(\ell)$  for some  $i_\ell \in [s_\ell]$ ,  $\ell \in [t]$ , is an optimal solution of (33).

Proof. For each  $\ell \in [t]$ , let us pick a point  $\mathbf{x}^{i_{\ell}}(\ell)$ ,  $i_{\ell} \in [s_{\ell}]$ , and then define the point  $\hat{\mathbf{x}} \in \mathbb{R}^n$  such that  $\hat{\mathbf{x}}(\ell) \coloneqq (\hat{x})_{i \in \mathcal{I}_{\ell}} = \mathbf{x}^{i_{\ell}}(\ell)$ ,  $\ell \in [t]$ . Because  $\operatorname{rank}(M_r(\mathbf{S}, \mathcal{I}_i \cap \mathcal{I}_j)) = 1$  for all pairs  $\{i, j\}$  with  $\mathcal{I}_i \cap \mathcal{I}_j \neq \emptyset$ , the value of  $\hat{x}_k$  is unique for any  $k \in \mathcal{I}_i \cap \mathcal{I}_j \neq \emptyset$ . Therefore,  $\hat{\mathbf{x}}$  is well-defined and  $\hat{\mathbf{x}} \in \mathbf{K}$ . We can thus construct  $s = \prod_{j=1}^{\ell} s_{\ell}$  solutions  $\{\mathbf{x}^j\}_{j=1}^s \subseteq \mathbf{K}$ , each associated with the weight matrix  $W_j \coloneqq \prod_{\ell=1}^t \xi_{i_{\ell}\ell} S_{\mathbf{0}} \in \mathbb{S}_+^p$  if  $\hat{\mathbf{x}}(\ell) = \mathbf{x}^{i_{\ell}}(\ell)$  for some  $i_{\ell} \in [s_{\ell}]$ . We then define the following matrix measure

$$\Phi = \sum_{j=1}^{s} W_j \delta_{\boldsymbol{x}^j} \tag{50}$$

which is supported on  $\mathbf{K}$ , and its marginal measure on  $\mathbf{K}_{\ell}$  is  $\Phi_{\ell}$  for each  $\ell \in [t]$ . Moreover, it holds that

$$\sum_{j=1}^{s} W_j = \prod_{\ell=1}^{t} \left( \sum_{i=1}^{s_{\ell}} \xi_{i\ell} \right) S_{\mathbf{0}} = S_{\mathbf{0}}.$$
 (51)

Therefore, we have

$$\lambda^{\star} \ge \lambda_r^{(cs)} = \mathcal{L}_{\mathbf{S}}(F) = \sum_{j=1}^{s} \left\langle W_j, F(\boldsymbol{x}^j) \right\rangle \ge \sum_{j=1}^{s} \left\langle W_j, \lambda^{\star} I_p \right\rangle = \lambda^{\star} \left\langle \sum_{j=1}^{s} W_j, I_p \right\rangle = \lambda^{\star} \operatorname{tr}(S_{\mathbf{0}}) = \lambda^{\star}, \tag{52}$$

which implies  $\lambda_r^{(cs)} = \lambda^*$  and each  $x^j$  is an optimal solution of (33).

**Example 5.2.** Consider the PMO problem

$$\inf_{\boldsymbol{q} \in \mathbb{P}^3} \lambda_{\min} \left( (-x_1^2 + x_2)(\boldsymbol{q}_1 \boldsymbol{q}_1^{\mathsf{T}} + \boldsymbol{q}_2 \boldsymbol{q}_2^{\mathsf{T}}) + (x_2^2 + x_3^2) \boldsymbol{q}_3 \boldsymbol{q}_3^{\mathsf{T}} \right) \quad \text{s.t.} \quad 1 - x_1^2 - x_2^2 \ge 0, \ x_2^2 + x_3^2 = 1, \tag{53}$$

where  $q_1, q_2, q_3$  are the column vectors of the orthogonal matrix

$$Q = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} \end{bmatrix}.$$
 (54)

Problem (53) exhibits a CSP:  $\mathcal{I}_1 = \{1,2\}$  and  $\mathcal{I}_2 = \{2,3\}$ . Solving (46) with r = 2, we obtain  $\lambda_2^{(cs)} = -1.250$  and  $\operatorname{rank}(M_2(\mathbf{S},\mathcal{I}_1)) = \operatorname{rank}(M_1(\mathbf{S},\mathcal{I}_1)) = 4$ ,  $\operatorname{rank}(M_2(\mathbf{S},\mathcal{I}_2)) = \operatorname{rank}(M_1(\mathbf{S},\mathcal{I}_2)) = 4$ . Applying the extraction procedure in [48] to  $M_2(\mathbf{S},\mathcal{I}_1)$  and  $M_2(\mathbf{S},\mathcal{I}_2)$ , respectively, we retrieve the matrix measures:

$$\Phi_1 \approx W \left( \delta_{\boldsymbol{x}^1(1)} + \delta_{\boldsymbol{x}^2(1)} \right) \ \ and \ \Phi_2 \approx W \left( \delta_{\boldsymbol{x}^1(2)} + \delta_{\boldsymbol{x}^2(2)} \right) \tag{55}$$

with

$$W \approx \begin{bmatrix} 0.2083 & -0.0833 & 0.0416 \\ -0.0833 & 0.0833 & 0.0833 \\ 0.0416 & 0.0833 & 0.2083 \end{bmatrix}$$
 (56)

and

$$\boldsymbol{x}^{1}(1) \approx \begin{bmatrix} 0.8660 \\ -0.4999 \end{bmatrix}, \boldsymbol{x}^{2}(1) \approx \begin{bmatrix} -0.8660 \\ -0.4999 \end{bmatrix}, \boldsymbol{x}^{1}(2) \approx \begin{bmatrix} -0.4999 \\ 0.8660 \end{bmatrix}, \boldsymbol{x}^{2}(2) \approx \begin{bmatrix} -0.4999 \\ -0.8660 \end{bmatrix}. \tag{57}$$

We can merge  $\Phi_1$  and  $\Phi_2$  into

$$\Phi \approx W \left( \delta_{\hat{\boldsymbol{x}}^1} + \delta_{\hat{\boldsymbol{x}}^2} + \delta_{\hat{\boldsymbol{x}}^3} + \delta_{\hat{\boldsymbol{x}}^4} \right) \tag{58}$$

with

$$\hat{\boldsymbol{x}}^{1} \approx \begin{bmatrix} 0.8660 \\ -0.4999 \\ 0.8660 \end{bmatrix}, \hat{\boldsymbol{x}}^{2} \approx \begin{bmatrix} 0.8660 \\ -0.4999 \\ -0.8660 \end{bmatrix}, \hat{\boldsymbol{x}}^{3} \approx \begin{bmatrix} -0.8660 \\ -0.4999 \\ 0.8660 \end{bmatrix}, \hat{\boldsymbol{x}}^{4} \approx \begin{bmatrix} -0.8660 \\ -0.4999 \\ -0.8660 \end{bmatrix}.$$
 (59)

Thus, by Theorem (5.2), the optimum of (53) is -1.250 which is achieved at  $\hat{x}^1$ ,  $\hat{x}^2$ ,  $\hat{x}^3$ , and  $\hat{x}^4$ .

For each  $\ell \in [t]$ , let  $d_{\mathbf{K}_{\ell}} := \max_{j \in \mathcal{J}_{\ell}} \lceil \deg G_j/2 \rceil$ .

Corollary 5.3. Let S be an optimal solution of (46). Assume that the following conditions hold:

- (i)  $\operatorname{rank}(S_0) = 1$ ;
- (ii) For each  $\ell \in [t]$ , one has

$$\operatorname{rank}(M_r(\mathbf{S}, \mathcal{I}_\ell)) = \operatorname{rank}(M_{r-d_{\mathbf{K}_\ell}}(\mathbf{S}, \mathcal{I}_\ell)) (=: s_\ell); \tag{60}$$

(iii) For all pairs  $\{i, j\}$  with  $\mathcal{I}_i \cap \mathcal{I}_j \neq \emptyset$ , one has  $\operatorname{rank}(M_r(\mathbf{S}, \mathcal{I}_i \cap \mathcal{I}_j)) = 1$ .

Then  $\lambda_r^{(cs)} = \lambda^*$ . Moreover, let  $\Delta_\ell := \{ \boldsymbol{x}^i(\ell) \}_{i=1}^{s_\ell}$  be the set of points obtained by applying the extraction procedure in [48] to each moment matrix  $M_r(\mathbf{S}, \mathcal{I}_\ell)$ ,  $\ell \in [t]$ , and let  $S_0 = \boldsymbol{v} \boldsymbol{v}^\intercal$  for some  $\boldsymbol{v} \in \mathbb{R}^p$ . Then each point  $\hat{\boldsymbol{x}} \in \mathbb{R}^n$  satisfying  $\hat{\boldsymbol{x}}(\ell) := (\hat{x}_i)_{i \in \mathcal{I}_\ell} = \boldsymbol{x}^{i_\ell}(\ell)$  for some  $\boldsymbol{x}^{i_\ell}(\ell) \in \Delta_\ell$ ,  $\ell \in [t]$ , is an optimal solution of (33) and  $\boldsymbol{v}$  is the corresponding eigenvector.

*Proof.* By (60) and Theorem 2.1, for each  $\ell \in [t]$ , the sequence  $\mathbf{S}^{\ell} \coloneqq (S_{\alpha})_{|\alpha| \leq 2r, \text{supp}(\alpha) \subseteq \mathcal{I}_{\ell}}$  admits an  $s_{\ell}$ -atomic matrix measure  $\Phi_{\ell}$  supported on  $\mathbf{K}_{\ell}$ ,  $\ell \in [t]$  so that

$$\Phi_{\ell} = \sum_{i=1}^{s_{\ell}} W_{i\ell} \delta_{\boldsymbol{x}^{i}(\ell)} \text{ for some } W_{i\ell} \in \mathbb{S}_{+}^{p}.$$

$$(61)$$

Note that  $\sum_{i=1}^{s_{\ell}} W_{i\ell} = S_{\mathbf{0}}$  for each  $\ell \in [t]$ . The fact that  $\operatorname{rank}(S_{\mathbf{0}}) = 1$  together with  $W_{i\ell} \succeq 0$  implies that  $\operatorname{rank}(W_{i\ell}) = 1$  for all  $i, \ell$ , from which we deduce that there exists  $\xi_{i\ell} > 0$  such that  $W_{i\ell} = \xi_{i\ell} S_{\mathbf{0}}$  for all  $i, \ell$  and  $\sum_{i=1}^{s_{\ell}} \xi_{i\ell} = 1, \ell \in [t]$ . Then the conclusion follows from Theorem 5.2.

**Theorem 5.4.** Let S be an optimal solution of (46). Assume that the following conditions hold:

- (i) There exist weight matrices  $W_1, \ldots, W_s \in \mathbb{S}^p_+$  such that for each  $\ell \in [t]$ ,  $\mathbf{S}^\ell \coloneqq (S_{\alpha})_{\text{supp}(\alpha) \subseteq \mathcal{I}_\ell}$  admits a representing matrix measure  $\Phi_\ell = \sum_{i=1}^s W_i \delta_{\boldsymbol{x}^i(\ell)}$  for some points  $\boldsymbol{x}^1(\ell), \ldots, \boldsymbol{x}^s(\ell) \subseteq \mathbf{K}_\ell$ ;
- (ii) For each  $i \in [s]$ , the points  $\mathbf{x}^i(1), \ldots, \mathbf{x}^i(t)$  can be merged into a single point  $\hat{\mathbf{x}}^i \in \mathbb{R}^n$  such that  $\hat{\mathbf{x}}^i(\ell) = \mathbf{x}^i(\ell)$  for every  $\ell \in [t]$ .

Then  $\lambda_r^{(cs)} = \lambda^*$ . Moreover, each point  $\hat{x}^i, i \in [s]$  is an optimal solution of (33).

*Proof.* Let us define the matrix measure  $\Phi = \sum_{i=1}^{s} W_i \delta_{\hat{x}^i}$  which is supported on  $\mathbf{K}$ , and its marginal measure on  $\mathbf{K}_{\ell}$  is  $\Phi_{\ell}$  for each  $\ell \in [t]$ . Then,

$$\lambda^{\star} \ge \lambda_r^{(\text{cs})} = \mathcal{L}_{\mathbf{S}}(F) = \sum_{i=1}^s \left\langle W_i, F(\hat{\boldsymbol{x}}^i) \right\rangle \ge \sum_{i=1}^s \left\langle W_i, \lambda^{\star} I_p \right\rangle = \lambda^{\star} \left\langle \sum_{i=1}^s W_i, I_p \right\rangle = \lambda^{\star} \text{tr}\left(S_{\mathbf{0}}\right) = \lambda^{\star}, \tag{62}$$

which implies  $\lambda_r^{(cs)} = \lambda^*$  and each  $\hat{x}^i$  is an optimal solution of (33).

**Example 5.3.** Consider the PMO problem

$$\inf_{\boldsymbol{x} \in \mathbb{R}^3} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad 1 - x_1^2 - x_2^2 \ge 0, \ 1 - x_2^2 - x_3^2 \ge 0$$
 (63)

with

$$F(\mathbf{x}) = \begin{bmatrix} x_1^2 + x_2^2 & 2 + x_1 x_2 + x_3^2 \\ 2 + x_1 x_2 + x_3^2 & x_2 x_3 \end{bmatrix},$$
 (64)

which exhibits a CSP:  $\mathcal{I}_1 = \{1,2\}$  and  $\mathcal{I}_2 = \{2,3\}$ . Solving (46) with r = 2, we obtain  $\lambda_2^{(cs)} \approx -3.0643$  and  $\operatorname{rank}(M_2(\mathbf{S},\mathcal{I}_1)) = \operatorname{rank}(M_1(\mathbf{S},\mathcal{I}_1)) = 2$ ,  $\operatorname{rank}(M_2(\mathbf{S},\mathcal{I}_2)) = \operatorname{rank}(M_1(\mathbf{S},\mathcal{I}_2)) = 2$ . Applying the extraction procedure in [48] to  $M_2(\mathbf{S},\mathcal{I}_1)$  and  $M_2(\mathbf{S},\mathcal{I}_2)$ , respectively, we retrieve the matrix measures:

$$\Phi_1 \approx \begin{bmatrix} 0.2338 & -0.2494 \\ -0.2494 & 0.2661 \end{bmatrix} \delta_{\boldsymbol{x}^1(1)} + \begin{bmatrix} 0.2338 & -0.2494 \\ -0.2494 & 0.2661 \end{bmatrix} \delta_{\boldsymbol{x}^2(1)}, \tag{65}$$

$$\Phi_2 \approx \begin{bmatrix} 0.2338 & -0.2494 \\ -0.2494 & 0.2661 \end{bmatrix} \delta_{\boldsymbol{x}^1(2)} + \begin{bmatrix} 0.2338 & -0.2494 \\ -0.2494 & 0.2661 \end{bmatrix} \delta_{\boldsymbol{x}^2(2)}$$
(66)

with

$$x^{1}(1) \approx \begin{bmatrix} 0.2732 \\ 0.2561 \end{bmatrix}, x^{2}(1) \approx \begin{bmatrix} -0.2732 \\ -0.2561 \end{bmatrix}, x^{1}(2) \approx \begin{bmatrix} 0.2561 \\ -0.9666 \end{bmatrix}, x^{2}(2) \approx \begin{bmatrix} -0.2561 \\ 0.9666 \end{bmatrix}.$$
 (67)

We can merge  $\Phi_1$  and  $\Phi_2$  into

$$\Phi \approx \begin{bmatrix} 0.2338 & -0.2494 \\ -0.2494 & 0.2661 \end{bmatrix} \delta_{\hat{x}^1} + \begin{bmatrix} 0.2338 & -0.2494 \\ -0.2494 & 0.2661 \end{bmatrix} \delta_{\hat{x}^2}$$
(68)

with

$$\hat{\boldsymbol{x}}^{1} \approx \begin{bmatrix} 0.2732 \\ 0.2561 \\ -0.9666 \end{bmatrix}, \hat{\boldsymbol{x}}^{2} \approx \begin{bmatrix} -0.2732 \\ -0.2561 \\ 0.9666 \end{bmatrix}. \tag{69}$$

Thus, by Theorem (5.4), the optimum of (63) is -3.0643 which is achieved at  $\hat{x}^1$  and  $\hat{x}^2$ .

Corollary 5.5. Let **S** be an optimal solution of (46). If  $\operatorname{rank}(M_{r_{\min}}(\mathbf{S}, \mathcal{I}_{\ell})) = 1$  for each  $\ell \in [t]$ , then  $\lambda_r^{(cs)} = \lambda^*$ . Moreover, one can recover an optimal solution of (33).

Proof. Since rank $(M_{r_{\min}}(\mathbf{S}, \mathcal{I}_{\ell})) = 1$ , by [48, Theorem 5], each sequence  $\mathbf{S}^{\ell} := (S_{\alpha})_{|\alpha| \leq 2r_{\min}, \text{supp}(\alpha) \subseteq \mathcal{I}_{\ell}}$  admits a Dirac representing measure  $\Phi_{\ell} = S_{\mathbf{0}}\delta_{\boldsymbol{x}(\ell)}$  with  $\boldsymbol{x}(\ell) \in \mathbf{K}_{\ell}$ . Moreover, we can merge  $\boldsymbol{x}(1), \ldots, \boldsymbol{x}(t)$  into a point  $\hat{\boldsymbol{x}} \in \mathbb{R}^n$  by letting

$$\hat{\boldsymbol{x}}(\mathcal{I}_{\ell}) := (\hat{x}_i)_{i \in \mathcal{I}_{\ell}} = \boldsymbol{x}(\ell), \quad \forall \ell \in [t].$$

There is no ambiguity for  $\hat{x}_i$  when  $i \in \mathcal{I}_j \cap \mathcal{I}_k \neq \emptyset$  for some  $j, k \in [t]$ . In fact, denoting by  $e_i \in \mathbb{N}^n$  the vector whose *i*-th entry being 1 and the others being 0, we have  $S_{e_i} = S_0 x(j)_i = S_0 x(k)_i$ , which implies  $x(j)_i = x(k)_i$ . Then, the conclusion follows from Theorem 5.4.

# 6 Matrix Sparsity

In this section, we investigate how to exploit matrix sparsity (i.e., chordal sparsity pattern of objective or constraint polynomial matrices) to perform reductions on the SDP size for PMO (33). The cases for objective polynomial matrices and for constraint polynomial matrices will be addressed sequentially.

## 6.1 Objective matrix sparsity

To exploit chordal sparsity encoded in the objective matrix, we adapt Theorem 2.4, Theorem 2.5, and Corollary 2.2 in [49] dealing with scalar polynomial constraints to the case of PMI constraints. For the proofs, one only needs to replace the usual inner product  $\langle \cdot, \cdot \rangle$  in the corresponding proofs in [49] with the product  $\langle \cdot, \cdot \rangle_p$ . We thus omit the details.

**Theorem 6.1.** Let **K** be the semi-algebraic set defined in (7) and suppose that  $\Sigma^p[\mathbf{G}]$  is Archimedean. Let  $F(\mathbf{x})$  be a polynomial matrix whose sparsity graph is chordal and has maximal cliques  $C_1, \ldots, C_t$ . If  $F(\mathbf{x})$  is strictly positive definite on **K**, then there exist SOS matrices  $S_{k,i}(\mathbf{x})$  of size  $q_k|C_i| \times q_k|C_i|$  such that

$$F(\boldsymbol{x}) = \sum_{i=1}^{t} E_{\mathcal{C}_i}^{\intercal} \left( S_{0,i}(\boldsymbol{x}) + \sum_{k=1}^{m} \left\langle S_{k,i}(\boldsymbol{x}), G_k(\boldsymbol{x}) \right\rangle_p \right) E_{\mathcal{C}_i}.$$

**Theorem 6.2.** Let  $\mathbf{K}$  be a semi-algebraic set defined in (7) with homogeneous polynomial matrices  $G_1, \ldots, G_m$  of even degree and such that  $\mathbf{K} \setminus \{\mathbf{0}\}$  is nonempty. Let  $F(\mathbf{x})$  be a homogeneous polynomial matrix of even degree whose sparsity graph is chordal and has maximal cliques  $C_1, \ldots, C_t$ . If  $F(\mathbf{x})$  is strictly positive definite on  $\mathbf{K} \setminus \{\mathbf{0}\}$ , then there exists an integer  $\tau \geq 0$  and homogeneous SOS matrices  $S_{k,i}(\mathbf{x})$  of size  $q_k |C_i| \times q_k |C_i|$  such that

$$\|\boldsymbol{x}\|^{2\tau}F(\boldsymbol{x}) = \sum_{i=1}^t E_{\mathcal{C}_i}^{\mathsf{T}} \left( S_{0,i}(\boldsymbol{x}) + \sum_{k=1}^m \left\langle S_{k,i}(\boldsymbol{x}), G_k(\boldsymbol{x}) \right\rangle_p \right) E_{\mathcal{C}_i}.$$

Corollary 6.3. Let **K** be a semi-algebraic set defined in (7), and let  $F(\mathbf{x})$  be an inhomogeneous polynomial matrix of even degree whose sparsity graph is chordal and has maximal cliques  $C_1, \ldots, C_t$ . If  $F(\mathbf{x})$  is strictly positive definite on **K** and its highest-degree homogeneous part is strictly positive definite on  $\mathbb{R}^n \setminus \{\mathbf{0}\}$ , then there exists an integer  $\tau \geq 0$  and SOS matrices  $S_{k,i}(\mathbf{x})$  of size  $q_k|C_i| \times q_k|C_i|$  such that

$$(1+\|oldsymbol{x}\|)^{2 au}F(oldsymbol{x}) = \sum_{i=1}^t E_{\mathcal{C}_i}^\intercal \left(S_{0,i}(oldsymbol{x}) + \sum_{k=1}^m \left\langle S_{k,i}(oldsymbol{x}), G_k(oldsymbol{x}) 
ight
angle_p 
ight) E_{\mathcal{C}_i}.$$

Then, the decomposed optimization problem for (33) based on Theorems 6.1, 6.2, Corollary 6.3 reads as

$$\sup \lambda \quad \text{s.t.} \quad F(\boldsymbol{x}) - \lambda = \sum_{i=1}^{t} E_{\mathcal{C}_{i}}^{\mathsf{T}} \left( S_{0,i}(\boldsymbol{x}) + \sum_{k=1}^{m} \langle S_{k,i}(\boldsymbol{x}), G_{k}(\boldsymbol{x}) \rangle_{p} \right) E_{\mathcal{C}_{i}},$$

$$\sup \lambda \quad \text{s.t.} \quad \|\boldsymbol{x}\|^{2\tau} (F(\boldsymbol{x}) - \lambda) = \sum_{i=1}^{t} E_{\mathcal{C}_{i}}^{\mathsf{T}} \left( S_{0,i}(\boldsymbol{x}) + \sum_{k=1}^{m} \langle S_{k,i}(\boldsymbol{x}), G_{k}(\boldsymbol{x}) \rangle_{p} \right) E_{\mathcal{C}_{i}},$$

$$\sup \lambda \quad \text{s.t.} \quad (1 + \|\boldsymbol{x}\|)^{2\tau} (F(\boldsymbol{x}) - \lambda) = \sum_{i=1}^{t} E_{\mathcal{C}_{i}}^{\mathsf{T}} \left( S_{0,i}(\boldsymbol{x}) + \sum_{k=1}^{m} \langle S_{k,i}(\boldsymbol{x}), G_{k}(\boldsymbol{x}) \rangle_{p} \right) E_{\mathcal{C}_{i}},$$

respectively.

### 6.2 Constraint matrix sparsity

We now consider the case that the constraint matrix G(x) has a chordal sparsity graph  $\mathcal{G}$ . One way to exploit constraint matrix sparsity is decomposing a single PMI constraint into multiple ones of smaller sizes according to its sparsity pattern (by Theorem 2.2), which most often brings additional correlative sparsity to exploit. Let us illustrate this method by a concrete example.

**Example 6.1.** Consider the PMO problem

$$\inf_{\boldsymbol{x} \in \mathbb{R}^5} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G(\boldsymbol{x}) \succeq 0$$
 (70)

with

$$F(\mathbf{x}) = \begin{bmatrix} x_1 & x_2 & x_3 \\ x_2 & 1 & x_4 \\ x_3 & x_4 & x_5 \end{bmatrix} \text{ and } G(\mathbf{x}) = \begin{bmatrix} 1 - x_1^2 - x_2^2 - x_3^2 & x_1 x_2 x_3 & 0 \\ x_1 x_2 x_3 & x_3 & x_3 x_4 x_5 \\ 0 & x_3 x_4 x_5 & 1 - x_3^2 - x_4^2 - x_5^2 \end{bmatrix}.$$
(71)

By introducing an auxiliary variable  $x_6$  and Theorem 2.2, we can decompose the PMI constraint  $G(\mathbf{x}) \succeq 0$ 

$$G_1(x_1,x_2,x_3,x_6) = \begin{bmatrix} 1-x_1^2-x_2^2-x_3^2 & x_1x_2x_3 \\ x_1x_2x_3 & x_6^2 \end{bmatrix} \succeq 0, G_2(x_3,x_4,x_5,x_6) = \begin{bmatrix} x_3-x_6^2 & x_3x_4x_5 \\ x_3x_4x_5 & 1-x_3^2-x_4^2-x_5^2 \end{bmatrix} \succeq 0$$

such that  $G \succeq 0$  if and only if  $G_1 \succeq 0, G_2 \succeq 0$ . Then (70) becomes

$$\inf_{\boldsymbol{x} \in \mathbb{R}^6} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G_1(x_1, x_2, x_3, x_6) \succeq 0, \quad G_2(x_3, x_4, x_5, x_6) \succeq 0, \tag{72}$$

which exhibits a CSP:  $\mathcal{I}_1 = \{1, 2, 3, 6\}$  and  $\mathcal{I}_2 = \{3, 4, 5, 6\}$ .

In Appendix A, we provide another way to exploit constraint matrix sparsity.

# 7 Numerical Examples

The sparsity-adapted relaxations for PMO problems have been implemented in the Julia package TSSOS  $1.2.5^1$  [61]. In this section, we provide numerical examples to illustrate the efficiency of our approach with TSSOS where Mosek 10.0 [62] is employed as an SDP solver with default settings. When presenting the results in tables, the column labelled by 'mb' records the maximal PSD block size of SDP relaxations, the column labelled by 'bound' records lower bounds given by SDP relaxations, and the column labelled by 'time' records running time in seconds. Moreover, r stands for the relaxation order, s stands for the sparse order, and the symbol '-' indicates that Mosek runs out of memory. For brevity, TS denotes term sparsity, CS denotes correlative sparsity, and MS denotes matrix sparsity.

## 7.1 Term sparse examples

Our first example involves the objective matrix

$$F(\mathbf{x}) = \begin{bmatrix} x_1^4 & x_1^2 - x_2x_3 & x_3^2 - x_4x_5 & x_1x_4 & x_1x_5 \\ x_1^2 - x_2x_3 & x_2^4 & x_2^2 - x_3x_4 & x_2x_4 & x_2x_5 \\ x_3^2 - x_4x_5 & x_2^2 - x_3x_4 & x_3^4 & x_4^2 - x_1x_2 & x_5^2 - x_3x_5 \\ x_1x_4 & x_2x_4 & x_4^2 - x_1x_2 & x_4^4 & x_4^2 - x_1x_3 \\ x_1x_5 & x_2x_5 & x_5^2 - x_3x_5 & x_4^2 - x_1x_3 & x_5^4 \end{bmatrix}$$
(73)

and constraint matrices

$$G_1(\mathbf{x}) = \begin{bmatrix} 1 - x_1^2 - x_2^2 & x_2 x_3 \\ x_2 x_3 & 1 - x_3^2 \end{bmatrix}, \quad G_2(\mathbf{x}) = \begin{bmatrix} 1 - x_4^2 & x_4 x_5 \\ x_4 x_5 & 1 - x_5^2 \end{bmatrix}.$$
(74)

The considered optimization problem aims to minimize the minimum eigenvalue of F over the region defined by  $G_1, G_2$ :

$$\inf_{\boldsymbol{x} \in \mathbb{R}^5} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G_1(\boldsymbol{x}) \succeq 0, G_2(\boldsymbol{x}) \succeq 0.$$
 (75)

Table 1 reports the numerical results of this example, where we compare the dense approach with the sparse approach (exploiting term sparsity with block/chordal closures). It can be seen that except the case of performing chordal closures with s=2, the sparse approach is several times faster than the dense approach while yielding the same lower bound -2.2766 with one exception. The bound -2.2766 can be certified as the global optimum by checking the flatness condition. For this example, the term sparsity iteration with block closures stabilizes at s=2.

Next for a positive integer  $p \in \{20, 40, 60\}$ , we consider the problem

$$\inf_{\boldsymbol{x} \in \mathbb{R}^3} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G(\boldsymbol{x}) \succeq 0$$
 (76)

with

$$F(\mathbf{x}) = (1 - x_1^2 - x_2^2)I_p + (x_1^2 - x_3^2)A + (x_1^2 x_3^2 - 2x_2^2)B,$$
(77)

and

$$G(\mathbf{x}) = \begin{bmatrix} 1 - x_1^2 - x_2^2 & x_2 x_3 \\ x_2 x_3 & 1 - x_3^2 \end{bmatrix}.$$
 (78)

<sup>&</sup>lt;sup>1</sup>TSSOS is freely available at https://github.com/wangjie212/TSSOS.

Table 1: Results for Problem (75).

		r=2			r = 3			r=4	
	mb	bound	time	mb	bound	time	mb	bound	time
Dense	105	-2.2766	0.47	280	-2.2766	6.55	630	-2.2766	137
TS (block, $s = 1$ )	50	-2.2766	0.18	118	-2.2766	2.68	330	-2.2766	28.5
TS (block, $s = 2$ )	80	-2.2766	0.22	200	-2.2766	3.64	430	-2.2766	40.9
TS (chordal, $s = 1$ )	35	-2.3781	0.08	80	-2.2766	1.20	160	-2.2766	9.39
TS (chordal, $s = 2$ )	71	-2.2766	0.38	200	-2.2766	12.6	430	-2.2766	218

The matrices  $A, B \in \mathbb{S}^p$  are generated with entries being drawn randomly from the uniform distribution on (0,1). Table 2 reports the numerical results of this problem, where we compare the dense approach with the sparse approach (exploiting term sparsity with block or chordal closures). It can be seen that the sparse approach is significantly faster and more scalable than the dense approach while yielding the same lower bounds. For this problem, the term sparsity iteration with block closures stabilizes at s = 2.

Table 2: Results for Problem (76) with r = 2.

		p = 20				p = 40		p = 60			
	mb	bound	time		mb	bound	time	 mb	bound	$_{ m time}$	
Dense	200	-20.533	7.91		400	-39.786	217	600	-	-	
TS (block, $s = 1$ )	80	-20.533	0.54		160	-39.786	11.5	240	-61.079	64.1	
TS (block, $s = 2$ )	80	-20.533	0.50		160	-39.786	10.1	240	-61.079	64.4	
TS (chordal, $s = 1$ )	75	-20.533	0.81		150	-39.786	18.2	225	-61.079	133	
TS (chordal, $s = 2$ )	80	-20.533	0.50		160	-39.786	10.3	240	-61.079	64.7	

## 7.2 Correlatively sparse examples

Consider the problem

$$\inf_{\boldsymbol{x} \in \mathbb{R}^5} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G_1(\boldsymbol{x}) \succeq 0, G_2(\boldsymbol{x}) \succeq 0$$
 (79)

with

$$F(\mathbf{x}) = \begin{bmatrix} x_1^4 & x_1^2 - x_2 x_3 & x_3^2 - x_4 x_5 & 0.5 & 0.5 \\ x_1^2 - x_2 x_3 & x_2^4 & x_2^2 - x_3 x_4 & 0.5 & 0.5 \\ x_3^2 - x_4 x_5 & x_2^2 - x_3 x_4 & x_3^4 & x_4^2 - x_1 x_2 & x_5^2 - x_3 x_4 \\ 0.5 & 0.5 & x_4^2 - x_1 x_2 & x_4^4 & x_4^2 - x_1 x_3 \\ 0.5 & 0.5 & x_5^2 - x_3 x_4 & x_4^2 - x_1 x_3 & x_5^4 \end{bmatrix}$$
(80)

and

$$G_1(\mathbf{x}) = \begin{bmatrix} 1 - x_1^2 - x_2^2 & x_2 x_3 \\ x_2 x_3 & 1 - x_3^2 \end{bmatrix}, \quad G_2(\mathbf{x}) = \begin{bmatrix} 1 - x_4^2 & x_4 x_5 \\ x_4 x_5 & 1 - x_5^2 \end{bmatrix}, \tag{81}$$

which exhibits a CSP:  $\mathcal{I}_1 = \{1, 2, 3\}, \mathcal{I}_2 = \{3, 4\}, \text{ and } \mathcal{I}_3 = \{4, 5\}.$ 

Table 3 reports the numerical results of this example, where we compare the dense approach with three sparse approaches: exploiting correlative sparsity, exploiting both correlative sparsity and term sparsity with block or chordal closures. It can be seen that the approach exploiting correlative sparsity runs much faster than the dense approach without sacrificing the accuracy, and taking term sparsity into account brings some extra speed-up.

The next example involves a PMO problem with an increasing number of variables. For a given integer  $n \geq 3$ , let

$$F(\mathbf{x}) = \begin{bmatrix} \sum_{k=1}^{n-2} x_k^2 & \sum_{k=1}^{n-1} x_k x_{k+1} & 1\\ \sum_{k=1}^{n-1} x_k x_{k+1} & \sum_{k=2}^{n-1} x_k^2 & \sum_{k=1}^{n-2} x_k x_{k+2}\\ 1 & \sum_{k=1}^{n-2} x_k x_{k+2} & \sum_{k=3}^{n} x_k^2 \end{bmatrix}$$
(82)

Table 3: Results for Problem (79).

r	Dense				CS			(	CS + Bloc	ck	(	CS + Chordal		
T	mb	bound	time	$\overline{\mathrm{mb}}$	bound	time	_	mb	bound	time	mb	bound	time	
2	105	-2.4131	0.59	50	-2.4131	0.06		23	-2.4131	0.03	23	-2.4413	0.03	
3	280	-2.4131	6.77	100	-2.4131	0.38		62	-2.4131	0.12	23	-2.4131	0.08	
4	630	-2.4131	156	200	-2.4131	1.92		74	-2.4131	0.28	62	-2.4131	0.27	

and

$$G_k(\mathbf{x}) = \begin{bmatrix} 1 - x_k^2 - x_{k+1}^2 & x_{k+1} + 0.5 \\ x_{k+1} + 0.5 & 1 - x_{k+2}^2 \end{bmatrix}, \quad k \in [n-2],$$
(83)

and consider the optimization problem

$$\inf_{\boldsymbol{x} \in \mathbb{R}^n} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G_k(\boldsymbol{x}) \succeq 0, \ k \in [n-2].$$
(84)

Problem (84) possesses a CSP:  $\mathcal{I}_k = \{k, k+1, k+2\}, k \in [n-2]$ . Table 4 reports the related numerical results with r=2 as n increases. As for the previous example, we compare the dense approach with three sparse approaches: exploiting correlative sparsity, exploiting both correlative sparsity and term sparsity with block or chordal closures. It can be seen that the approach exploiting correlative sparsity yields the same bounds as the dense approach but in much less time (especially when the number of variables n is large). Taking term sparsity into account can further reduce the running time but provides looser bounds.

Table 4: Results for Problem (84) with r = 2.

m	n Dense				CS				CS + Blo	ck		CS + Chordal		
n	mb	bound	time	mb	bound	time		mb	bound	time	_	mb	bound	time
5	63	-1.0247	0.09	30	-1.0247	0.05		16	-1.3461	0.02		10	-1.5894	0.02
7	108	-1.1157	0.58	30	-1.1157	0.07		16	-1.5573	0.05		10	-1.9640	0.04
9	165	-1.3891	3.68	30	-1.3891	0.10		16	-1.7754	0.06		10	-2.3446	0.05
11	234	-1.7620	13.0	30	-1.7620	0.12		16	-2.0065	0.08		10	-2.7280	0.06
13	315	-2.1403	53.6	30	-2.1403	0.15		16	-2.2547	0.11		10	-3.1129	0.09

### 7.3 Matrix sparse examples

In this subsection, we solve four PMO problems with matrix sparsity. The first problem is

$$\inf_{\boldsymbol{x} \in \mathbb{R}^5} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G_1(\boldsymbol{x}) \succeq 0, G_2(\boldsymbol{x}) \succeq 0$$
(85)

with

and

$$G_1(\mathbf{x}) = \begin{bmatrix} 1 - x_1^2 - x_2^2 & x_2 x_3 \\ x_2 x_3 & 1 - x_3^2 \end{bmatrix}, \quad G_2(\mathbf{x}) = \begin{bmatrix} 1 - x_4^2 & x_4 x_5 \\ x_4 x_5 & 1 - x_5^2 \end{bmatrix}.$$
(87)

Table 5 reports the related numerical results of Problem (85), where we compare the dense approach with three sparse approaches: exploiting matrix sparsity, exploiting both matrix sparsity and term sparsity

Table 5: Results for Problem (85).

r	Dense				MS			MS + Blo	ck	M	MS + Chordal			
,	mb	bound	time	mb	bound	time	mb	bound	time	mb	bound	time		
2	105	-2.4180	0.42	63	-2.4180	0.13	33	-2.4180	0.08	33	-2.4180	0.06		
3	280	-2.4180	7.25	168	-2.4180	2.59	90	-2.4180	0.92	90	-2.4180	1.00		
4	630	-2.4180	151	378	-2.4180	28.3	198	-2.4180	8.38	153	-2.4180	4.87		

with block or chordal closures. It can be seen that the three sparse approaches all yield the same bound as the dense approach but in much less time. In addition, exploiting term sparsity brings some extra speed-up.

Now we consider

$$\inf_{\boldsymbol{x} \in \mathbb{R}^5} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G(\boldsymbol{x}) \succeq 0$$
(88)

with

$$F(\mathbf{x}) = \begin{bmatrix} x_1^4 + x_2^4 + 1 & x_1 x_3 \\ x_1 x_3 & x_3^4 + x_4^4 + x_5^4 + 0.5 \end{bmatrix}$$
(89)

and

$$G(\boldsymbol{x}) = \begin{bmatrix} 1 - x_1^2 & x_1 x_2 & x_1 x_3 & & & \\ x_1 x_2 & 1 - x_2^2 & x_2 x_3 & & & \\ x_1 x_3 & x_2 x_3 & 1 - x_3^2 & x_3 x_4 & x_3 x_5 & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & & \\ & & &$$

By introducing a new variable  $x_6$ , the PMI constraint  $G(x) \succeq 0$  can be decomposed as

$$G_1(x_1, x_2, x_3, x_6) = \begin{bmatrix} 1 - x_1^2 & x_1 x_2 & x_1 x_3 \\ x_1 x_2 & 1 - x_2^2 & x_2 x_3 \\ x_1 x_3 & x_2 x_3 & x_6^2 \end{bmatrix} \succeq 0, G_2(x_3, x_4, x_5, x_6) = \begin{bmatrix} 1 - x_3^2 - x_6^2 & x_3 x_4 & x_3 x_5 \\ x_3 x_4 & 1 - x_4^2 & x_4 x_5 \\ x_3 x_5 & x_4 x_5 & 1 - x_5^2 \end{bmatrix} \succeq 0$$

such that  $G \succeq 0$  if and only if  $G_1 \succeq 0$ ,  $G_2 \succeq 0$ . Note that after the decomposition, the PMO problem exhibits a CSP:  $\mathcal{I}_1 = \{1, 2, 3, 6\}, \mathcal{I}_2 = \{3, 4, 5, 6\}.$ 

Table 6 reports the related numerical results of Problem (88), where we compare the dense approach with three sparse approaches: exploiting both matrix sparsity and correlative sparsity, exploiting matrix sparsity, correlative sparsity, and term sparsity with block or chordal closures. It can be seen that the three sparse approaches all yield the same bound as the dense approach but in much less time (especially when  $r \geq 3$ ). In addition, exploiting term sparsity brings extra sizable speed-up.

Table 6: Results for Problem (88).

r	Dense				MS+CS			M	S+CS+B	lock	M	MS+CS+Chordal		
,	mb	bound	time	mb	bound	$_{ m time}$		mb	bound	time	mb	bound	time	
2	60	0.3977	0.06	30	0.3977	0.04		6	0.3977	0.01	6	0.3977	0.01	
3	210	0.3977	1.20	90	0.3977	0.24		14	0.3977	0.02	10	0.3977	0.02	
4	560	0.3977	10.1	210	0.3977	1.88		26	0.3977	0.08	20	0.3977	0.07	

We next consider a PMO problem adapted from [51, Sec. 6]:

$$\inf_{\boldsymbol{x} \in \mathbb{R}^n} \lambda_{\min}(F(\boldsymbol{x})) \quad \text{s.t.} \quad G(\boldsymbol{x}) \succeq 0$$
(91)

with

$$F(\boldsymbol{x}) = \begin{bmatrix} 1 & x_1 x_2 \\ x_1 x_2 & 1 + x_n^2 \end{bmatrix}$$

$$\tag{92}$$

and

$$G(\mathbf{x}) = \begin{bmatrix} 1 - x_1^4 & 0 & 0 & \cdots & 0 & x_1 x_2 \\ 0 & 1 - x_2^4 & 0 & \cdots & 0 & x_2 x_3 \\ 0 & 0 & 0 & \cdots & 0 & x_3 x_4 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 - x_{n-1}^4 & x_{n-1} x_n \\ x_1 x_2 & x_2 x_3 & x_3 x_4 & \cdots & x_{n-1} x_n & 1 - x_n^4 \end{bmatrix} \succeq 0.$$
(93)

By introducing n-2 new variables  $\{x_{n+1},\ldots,x_{2n-2}\}$ , the PMI constraint  $G(x) \succeq 0$  can be decomposed as

$$G_1(x_1, x_2, x_{n+1}) = \begin{bmatrix} 1 - x_1^4 & x_1 x_2 \\ x_1 x_2 & x_{n+1}^2 \end{bmatrix} \succeq 0, \quad G_{n-1}(x_{n-1}, x_n, x_{2n-2}) = \begin{bmatrix} 1 - x_{n-1}^4 & x_{n-1} x_n \\ x_{n-1} x_n & 1 - x_n^4 - x_{2n-2}^2 \end{bmatrix} \succeq 0,$$

and

$$G_i(x_i, x_{i+1}, x_{n+i-1}, x_{n+i}) = \begin{bmatrix} 1 - x_i^4 & x_i x_{i+1} \\ x_i x_{i+1} & x_{n+i}^2 - x_{n+i-1}^2 \end{bmatrix} \succeq 0, \quad i = 2, \dots, n-2,$$

such that  $G \succeq 0$  if and only if  $G_i \succeq 0, i \in [n-1]$ . Note that after the decomposition, the PMO problem exhibits a CSP:  $\mathcal{I}_1 = \{1, 2, n+1\}, \mathcal{I}_i = \{i, i+1, n+i-1, n+i\} (i=2, \ldots, n-2), \mathcal{I}_{n-1} = \{n-1, n, 2n-2\}.$ 

Table 7 reports the related numerical results of Problem (91) with  $n \in \{5, 7, 9, 11, 13\}$ , where we compare the dense approach with three sparse approaches: exploiting both matrix sparsity and correlative sparsity, exploiting matrix sparsity, correlative sparsity, and term sparsity with block or chordal closures. It can be seen that the three sparse approaches all yield the same bound as the dense approach but in much less time (when  $n \in \{5, 7\}$ ) and scale much better with n. In addition, exploiting term sparsity brings extra sizable speed-up.

m		Dense			MS+CS			M	S+CS+B	lock	MS-	+CS+Ch	ordal
n	mb	bound	time	mb	bound	time		mb	bound	time	 mb	bound	time
5	252	0.2138	4.07	140	0.2138	1.27		15	0.2138	0.05	15	0.2138	0.05
7	660	0.2138	185	140	0.2138	1.86		15	0.2138	0.08	15	0.2138	0.09
9	1430	-	-	140	0.2138	2.50		15	0.2138	0.13	15	0.2138	0.16
11	2730	-	-	140	0.2138	3.43		15	0.2138	0.19	15	0.2138	0.23
13	4760	-	-	140	0.2138	4.57		15	0.2138	0.26	15	0.2138	0.27

Table 7: Results for Problem (91) with r = 4.

Let  $\omega$  be an even positive integer and consider the following optimization problem with a PMI constraint:

$$\begin{cases}
\inf_{\lambda_{1},\lambda_{2}} \quad \lambda_{2} - 10\lambda_{1} \\
\\
\text{s.t.} \quad P_{\omega}(\boldsymbol{x}) = \begin{bmatrix}
\lambda_{2}x_{1}^{4} + x_{2}^{4} & \lambda_{1}x_{1}^{2}x_{2}^{2} \\
\lambda_{1}x_{1}^{2}x_{2}^{2} & \lambda_{2}x_{2}^{4} + x_{3}^{4} & \lambda_{2}x_{2}^{2}x_{3}^{2} \\
& \lambda_{2}x_{2}^{2}x_{3}^{2} & \lambda_{2}x_{3}^{4} + x_{1}^{4} & \lambda_{1}x_{1}^{2}x_{3}^{2} \\
& \lambda_{1}x_{1}^{2}x_{3}^{2} & \lambda_{2}x_{1}^{4} + x_{2}^{4} & \lambda_{2}x_{1}^{2}x_{2}^{2} \\
& & \lambda_{2}x_{1}^{2}x_{2}^{2} & \lambda_{2}x_{2}^{4} + x_{3}^{4} & \ddots \\
& & \ddots & \ddots & \lambda_{1}x_{2}^{2}x_{3}^{2} \\
& & \lambda_{1}x_{2}^{2}x_{3}^{2} & \lambda_{2}x_{3}^{4} + x_{1}^{4}
\end{bmatrix} \succeq 0,$$

$$(94)$$

where  $P_{\omega}(\boldsymbol{x})$  is a  $3\omega \times 3\omega$  tridiagonal polynomial matrix. The sparsity graph of  $P_{\omega}(\boldsymbol{x})$  has maximal cliques:  $\mathcal{C}_i = \{i, i+1\}, i \in [3\omega - 1]$ . By Theorem 6.2, Problem (94) can be reformulated as ([49])

$$\begin{cases}
\inf_{\lambda_{1},\lambda_{2}} \quad \lambda_{2} - 10\lambda_{1} \\
\text{s.t.} \quad \|\boldsymbol{x}\|^{2\tau} P_{\omega}(\boldsymbol{x}) = \sum_{i=1}^{3\omega-1} E_{\mathcal{C}_{i}}^{\mathsf{T}} S_{i}(\boldsymbol{x}) E_{\mathcal{C}_{i}}, \\
S_{i}(\boldsymbol{x}) \text{ is an SOS matrix,} \quad \forall i \in [3\omega - 1].
\end{cases} \tag{95}$$

Table 8 reports the related numerical results of Problem (94) with  $\tau = 3, r = 5$  and  $\omega \in \{10, 20, 30, 40, 50\}$ , where we compare two sparse approaches: exploiting matrix sparsity and exploiting both matrix sparsity and term sparsity with block closures. It can be seen that the two sparse approaches always yield the same bounds. Additionally exploiting term sparsity speeds up computation by several times.

Table 8: Results for Problem (94) with  $\tau = 3, r = 5$ .

/·1		MS			MS+TS	
$\omega$	mb	bound	time	mb	bound	time
10	112	-9.0933	5.27	20	-9.0933	0.74
20	112	-9.0240	11.1	20	-9.0240	1.62
30	112	-9.0108	15.1	20	-9.0108	3.12
40	112	-9.0061	18.4	20	-9.0061	4.27
50	112	-9.0039	23.8	20	-9.0039	5.99

# 8 Conclusions

This paper have explored the use of various sparsity methods in reducing the size of matrix Moment-SOS relaxations for verification of PMIs and solving PMO. Multiple sparsity structures can be exploited in a combined way to maximize the amount of dimension reductions. Those methods make the matrix Moment-SOS hierarchy more capable of tackling practical applications as illustrated via diverse numerical examples. The sparsity routines introduced in this paper were incorporated into the TSSOS package, and are thus available to interested practitioners in fields such as optimization, control, and operations research.

# Acknowledgements

The authors thank Yang Zheng, Mareike Dressler, and Timo de Wolff for discussions about term sparsity patterns in PMIs, and thank Roy S. Smith for his advice, support, and funding.

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# A An alternative exploitation of constraint matrix sparsity

We first extend Theorem 2.3 towards block-partitioned matrices. Suppose that  $A \in \mathbb{R}^{pq \times pq}$  is a block matrix of form

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1p} \\ A_{21} & A_{22} & \cdots & A_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ A_{p1} & A_{p2} & \cdots & A_{pp} \end{bmatrix},$$

where each block  $A_{ij} \in \mathbb{R}^{q \times q}$ , i, j = 1, ..., p. Given an undirected graph  $\mathcal{G}(\mathcal{V}, \mathcal{E})$  with nodes  $\mathcal{V} = \{1, ..., p\}$ , we define the set of q-partitioned sparse symmetric matrices as

$$\mathbb{S}_q^{pq}(\mathcal{G},0) := \{ A \in \mathbb{S}^{pq} \mid A_{ij} = A_{ii}^{\mathsf{T}} = 0, \text{ if } i \neq j \text{ and } \{i,j\} \notin \mathcal{E} \},$$

and define the cone of q-partitioned completable PSD matrices as

$$\mathbb{S}_{q,+}^{pq}(\mathcal{G},?) \coloneqq \Pi_{\mathcal{G}}^{q}(\mathbb{S}_{+}^{pq}) = \{\Pi_{\mathcal{G}}^{q}(A) \mid A \in \mathbb{S}_{+}^{pq}\},\$$

where  $\Pi^q_{\mathcal{G}}: \mathbb{S}^{pq} \to \mathbb{S}^{pq}_q(\mathcal{G},0)$  is the projection given by

$$[\Pi_{\mathcal{G}}(A)]_{ij} = \begin{cases} A_{ij}, & \text{if } i = j \text{ or } \{i, j\} \in \mathcal{E}, \\ 0, & \text{otherwise.} \end{cases}$$
(96)

Given any maximal clique  $C_i$  of G, define the block-wise index matrix  $E_{C_i,q} \in \mathbb{R}^{|C_i|q \times pq}$  by

$$[E_{\mathcal{C}_i,q}]_{jk} = \begin{cases} I_q, & \text{if } \mathcal{C}_i(j) = k, \\ 0, & \text{otherwise.} \end{cases}$$

The following theorem extends Theorem 2.3 to the case of block matrices.

**Theorem A.1.** ( [63, Theorem 2.18]) Let  $\mathcal{G}(\mathcal{V}, \mathcal{E})$  be a chordal graph and let  $\{\mathcal{C}_1, \dots, \mathcal{C}_t\}$  be the set of its maximal cliques. Then  $A \in \mathbb{S}_{q,+}^{pq}(\mathcal{G},?)$  if and only if  $E_{\mathcal{C}_i,q}AE_{\mathcal{C}_i,q}^{\intercal} \in \mathbb{S}_+^{|\mathcal{C}_i|q}$  for all  $i \in [t]$ .

The following proposition allows us to consider an appropriate PSD completable matrix for representing  $\langle S(\boldsymbol{x}), G(\boldsymbol{x}) \rangle_p$  when  $G(\boldsymbol{x})$  is sparse.

**Proposition A.2.** Let  $G(x) \in \mathbb{S}^q[x]$  be a polynomial matrix that has a chordal sparsity graph  $\mathcal{G}$ , and let  $S(x) \in \mathbb{S}^{pq}[x]$  be an SOS matrix of degree 2d. Then there exists  $Q \in \mathbb{S}^{pq|\mathbf{m}_d(x)|}_{p|\mathbf{m}_d(x)|,+}(\mathcal{G},?)$  such that

$$\langle S(\boldsymbol{x}), G(\boldsymbol{x}) \rangle_p = \left\langle (I_{pq} \otimes \mathbf{m}_d(\boldsymbol{x}))^{\mathsf{T}} \tilde{Q}(I_{pq} \otimes \mathbf{m}_d(\boldsymbol{x})), G(\boldsymbol{x}) \right\rangle_p,$$
 (97)

where  $\tilde{Q}$  is obtained from Q by certain row and column permutations.

*Proof.* By (4), there exists  $Q \in \mathbb{S}^{pq|\mathbf{m}_d(\boldsymbol{x})|}_+$  such that

$$S(\boldsymbol{x}) = (I_{pq} \otimes \mathbf{m}_d(\boldsymbol{x}))^{\intercal} Q(I_{pq} \otimes \mathbf{m}_d(\boldsymbol{x})).$$

Let  $Q = [Q_{ij}]_{i,j \in [p]}$  with blocks  $Q_{ij} = Q_{ji}^{\intercal} \in \mathbb{R}^{q|\mathbf{m}_d(\boldsymbol{x})| \times q|\mathbf{m}_d(\boldsymbol{x})|}$ . By definition, we have

$$\langle S(\boldsymbol{x}), G(\boldsymbol{x}) \rangle_p = \begin{bmatrix} \langle S_{11}(\boldsymbol{x}), G(\boldsymbol{x}) \rangle & \dots & \langle S_{1p}(\boldsymbol{x}), G(\boldsymbol{x}) \rangle \\ \vdots & \ddots & \vdots \\ \langle S_{p1}(\boldsymbol{x}), G(\boldsymbol{x}) \rangle & \dots & \langle S_{pp}(\boldsymbol{x}), G(\boldsymbol{x}) \rangle \end{bmatrix}$$

$$= \begin{bmatrix} \langle G(\boldsymbol{x}) \otimes (\mathbf{m}_d(\boldsymbol{x}) \cdot \mathbf{m}_d(\boldsymbol{x})^\intercal), Q_{11} \rangle & \dots & \langle G(\boldsymbol{x}) \otimes (\mathbf{m}_d(\boldsymbol{x}) \cdot \mathbf{m}_d(\boldsymbol{x})^\intercal), Q_{1p} \rangle \\ \vdots & \ddots & \vdots \\ \langle G(\boldsymbol{x}) \otimes (\mathbf{m}_d(\boldsymbol{x}) \cdot \mathbf{m}_d(\boldsymbol{x})^\intercal), Q_{p1} \rangle & \dots & \langle G(\boldsymbol{x}) \otimes (\mathbf{m}_d(\boldsymbol{x}) \cdot \mathbf{m}_d(\boldsymbol{x})^\intercal), Q_{pp} \rangle \end{bmatrix}.$$

Note that  $G(\boldsymbol{x}) \otimes (\mathbf{m}_d(\boldsymbol{x}) \cdot \mathbf{m}_d(\boldsymbol{x})^{\mathsf{T}})$  has a block sparse structure induced by the chordal sparsity of  $G(\boldsymbol{x})$ . Therefore, up to certain row and column permutations, we may assume that  $Q \in \mathbb{S}^{pq|\mathbf{m}_d(\boldsymbol{x})|}_{p|\mathbf{m}_d(\boldsymbol{x})|,+}(\mathcal{G},?)$ .