An Introduction to Polynomial Optimization

Jie Wang

December 14, 2023

Contents

List of Acronyms

List of Symbols

$\mathbb{N}$	$\{0, 1, 2, \ldots\}$
$\mathbb{N}^*$	$\{1, 2, \ldots\}$
$\mathbb{Q}$	the field of rational numbers
$\mathbb{R}$	the field of real numbers
$\mathbb{C}$	the field of complex numbers
$\mathbf{0}$	the zero vector
$\mathbf{x} = (x_1, \ldots, x_n)$	a tuple of real variables
$\text{supp}(f)$	the support of the polynomial f
$[m]$	$\{1, 2, \ldots, m\}$
$\lvert \cdot \rvert$	the cardinality of a set or 1-norm of a vector
$\mathbb{R}^{n\times m}$	the set of $n \times m$ real matrices
$\mathbb{S}_n$	the set of real symmetric $n \times n$ matrices
$\mathbb{S}_n^+$	the set of $n \times n$ PSD matrices
$\langle \mathbf{A}, \mathbf{B} \rangle$	the trace of $\mathbf{AB}$ for $\mathbf{A}, \mathbf{B} \in \mathbb{S}_n$
$\mathbf{I}_n$	the $n \times n$ identity matrix
$\mathbf{M} \succcurlyeq 0$	$\mathbf{M}$ is a PSD matrix
F, G, H	graphs
$G(V, E)$	a graph with nodes V and edges E
$V(G)$ (resp. $E(G)$)	the node (resp. edge) set of the graph G
$\mathbf{B}_G$	the adjacency matrix of the graph G with unit diagonal
$G \subseteq H$	G is a subgraph of H
G'	a chordal extension of the graph G
$\mathbb{S}(G)$	the set of real symmetric matrices with sparsity pattern G
Π_G	the projection from $\mathbb{S}_{\lvert V(G)\rvert}$ to the subspace $\mathbb{S}(G)$
$\mathfrak{g} = \{g_1, \ldots, g_m\}$	a set of polynomials defining the constraints
$\mathbb{R}[\mathbf{x}]$	the ring of real n-variate polynomials
$\mathbb{R}[\mathbf{x}]_{2d}$	the set of real n-variate polynomials of degree at most $2d$
$\Sigma[\mathbf{x}]$	the set of SOS polynomials
$\Sigma[\mathbf{x}]_d$	the set of SOS polynomials of degree at most $2d$
$\mathcal{M}(\mathfrak{g})$	the quadratic module generated by $\mathfrak{g}$
$\mathcal{M}(\mathfrak{g})_r$	the r-truncated quadratic module generated by $\mathfrak{g}$
$\mathbf{S}$	a basic semialgebraic set
μ, ν	measures
$\mathbb{N}^n_r$	$\{\alpha \in \mathbb{N}^n \mid \sum_{j=1}^n \alpha_j \le r\}$
d_j	the ceil of half degree of $g_j \in \mathfrak{g}$
r	relaxation order
$r_{\min}$	minimum relaxation order
$\mathbf{y}$	a moment sequence
$L_{\mathbf{y}}$	the linear functional associated to $\mathbf{y}$
$\mathbf{M}_r(\mathbf{y})$	the r-th order moment matrix associated to $\mathbf{y}$

$\mathbf{M}_r(g\mathbf{y})$	the r-th order localizing matrix associated to $\mathbf{y}$ and g
$\delta_{\mathbf{a}}$	the Dirac measure centered at $\mathbf{a}$
p	number of variable cliques
s	sparse order
$\underline{x} = (x_1, \ldots, x_n)$	a tuple of noncommutating variables
$\mathbb{R}\langle \underline{x} \rangle$	the ring of real nc n-variate polynomials
$\mathbf{W}_r$	the vector of nc monomials of degree at most r
$\Sigma\langle \underline{x} \rangle$	the set of SOHS polynomials
$\mathcal{D}_{\mathfrak{g}}$	the nc semialgebraic set associated to $\mathfrak{g}$

Chapter 1

Semidefinite programming

1.1 Linear programming

The primal problem:

$$\begin{aligned} p_{\mathrm{lp}} := \inf_{\mathbf{x}\in\mathbb{R}^n} \quad & \mathbf{c}^\intercal \mathbf{x} \\ \text{s.t.} \quad & A\mathbf{x} = \mathbf{b}, \\ & \mathbf{x} \geq 0 \end{aligned} \tag{1.1}$$

The dual problem:

$$\begin{aligned} d_{\mathrm{lp}} := \sup_{\mathbf{y}\in\mathbb{R}^m} \quad & \mathbf{b}^\intercal \mathbf{y} \\ \text{s.t.} \quad & A^\intercal \mathbf{y} \leq \mathbf{c} \end{aligned} \tag{1.2}$$

- Weak duality: $p_{\mathrm{lp}} \geq d_{\mathrm{lp}}$.
- Strong duality: If both primal and dual problems are feasible, then $p_{\mathrm{lp}} = d_{\mathrm{lp}}$.
- Complementary slackness: $\mathbf{x}^* \circ (\mathbf{c} - A^\intercal \mathbf{y}^*) = \mathbf{0}$.

1.2 Semidefinite programming

First, we introduce some useful notations. We consider the vector space $\mathbb{S}_n$ of real symmetric $n \times n$ matrices, which is equipped with the usual inner product $\langle \mathbf{A}, \mathbf{B} \rangle = \mathrm{tr}(\mathbf{AB})$ for $\mathbf{A}, \mathbf{B} \in \mathbb{S}_n$. Let $\mathbf{I}_n$ be the $n \times n$ identity matrix. A matrix $\mathbf{M} \in \mathbb{S}_n$ is called *positive semidefinite (PSD)* (resp. *positive definite*) if $\mathbf{x}^\intercal \mathbf{M} \mathbf{x} \geq 0$ (resp. > 0), for all $\mathbf{x} \in \mathbb{R}^n$. In this case, we write $\mathbf{M} \succcurlyeq 0$ and define a partial order by writing $\mathbf{A} \succcurlyeq \mathbf{B}$ (resp. $\mathbf{A} \succ B$) if and only if $\mathbf{A} - \mathbf{B}$ is positive semidefinite (resp. positive definite). The set of $n \times n$ PSD matrices is denoted by $\mathbb{S}_n^+$.

The primal SDP:

$$\begin{aligned} p_{\mathrm{sdp}} := \inf \quad & \langle C, X \rangle \\ \text{s.t.} \quad & \langle A_i, X \rangle = b_i, \quad i = 1, \ldots, m, \\ & X \succeq 0 \end{aligned} \tag{1.3}$$

The dual SDP:

$$\begin{aligned} d_{\mathrm{sdp}} := \sup \quad & \mathbf{b}^\intercal \mathbf{y} \\ \text{s.t.} \quad & \sum_{i=1}^m A_i y_i \preceq C \end{aligned} \tag{1.4}$$

- Optimality condition: $X(C - \sum_{i=1}^m A_i y_i) = 0$.
- Weak duality: $p_{\mathrm{sdp}} \geq d_{\mathrm{sdp}}$.
- Strong duality: If the primal SDP or the dual SDP is strictly feasible, then $p_{\mathrm{sdp}} = d_{\mathrm{sdp}}$; if both primal and dual SDPs are feasible, then both SDPs have optimal solutions.

1.3 Binary quadratic optimization

The binary quadratic program:

$$\begin{aligned} \min \quad & \mathbf{x}^\intercal Q \mathbf{x} \\ \text{s.t.} \quad & x_i^2 = 1, \quad i = 1, \ldots, n \end{aligned} \tag{1.5}$$

The SDP relaxation:

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ \text{s.t.} \quad & X_{ii} = 1, \quad i = 1, \ldots, n, \\ & X \succeq 0 \end{aligned} \tag{1.6}$$

which provides a lower bound for (1.5).

• The Goemans and Williamson rounding:

Step 1: Factorize the SDP solution X as $X = V^\intercal V$, where $V = [v_1, \ldots, v_n] \in \mathbb{R}^{r \times n}$ and r is the rank of X.

Step 2: Since $X_{ij} = v_i^\intercal v_j$ and $X_{ii} = 1$, this factorization gives n vectors v_i on the unit sphere in $\mathbb{R}^r$.

Step 3: Now, choose a uniformly distributed random hyperplane in $\mathbb{R}^r$ (passing through the origin), and assign to each variable x_i either a $+1$ or a -1, depending on which side of the hyperplane the point v_i lies.

• Approximation ratios.

A symmetric matrix A is diagonally dominant if $a_{ii} \geq \sum_{j \neq i} |a_{ij}|$ for all i. This is an important case that corresponds, for instance, to the Max-Cut problem, where the cost function to be maximized is the Laplacian of a graph (V, E), given by $mc(\mathbf{x}) = \frac{1}{4} \sum_{(i,j) \in E} (x_i - x_j)^2$.

Theorem 1.1 *Suppose that $\mathbf{x}^{\text{sdp}}$ is a Goemans and Williamson rounding solution for the Max-Cut problem. Then $\mathbf{E}(mc(\mathbf{x}^{\text{sdp}})) \geq \alpha_{GW} \cdot opt$, where opt is the optimum of the Max-Cut problem.*

PROOF The probability of i and j getting a cut is

$$\frac{\theta}{\pi} = \frac{\arccos(v_i^\intercal v_j)}{\pi} = \frac{\arccos(X_{ij})}{\pi}.$$

So the expectation of the Max-Cut value is $\sum_{(i,j) \in E} \frac{\arccos(X_{ij})}{\pi}$. Now note that the SDP relaxation provides an upper bound $\sum_{(i,j) \in E} \frac{1}{2}(1 - X_{ij})$. Let

$$\alpha_{GW} := \min_{t \in [-1,1]} \frac{\frac{\arccos(t)}{\pi}}{\frac{1}{2}(1-t)} \approx 0.878.$$

Thus,

$$\mathbf{E}(mc(\mathbf{x}^{\text{sdp}})) \geq \alpha_{GW} \cdot opt.$$

□

1.4 Chordal graphs and sparse semidefinite programming

An *(undirected) graph* $G(V, E)$ or simply G consists of a set of nodes V and a set of edges $E \subseteq \{\{v_i, v_j\} \mid v_i \neq v_j, (v_i, v_j) \in V \times V\}$. For a graph G, we use $V(G)$ and $E(G)$ to indicate the node set of G and the edge set of G, respectively. The *adjacency matrix* of a graph G is denoted by $\mathbf{B}_G$ for which we put ones on its diagonal. For two graphs G, H, we say that G is a *subgraph* of H if $V(G) \subseteq V(H)$ and $E(G) \subseteq E(H)$, denoted by $G \subseteq H$. For a graph $G(V, E)$, a *cycle* of length k is a set of nodes $\{v_1, v_2, \ldots, v_k\} \subseteq V$ with $\{v_k, v_1\} \in E$ and $\{v_i, v_{i+1}\} \in E$, for $i \in [k-1]$. A *chord* in a cycle $\{v_1, v_2, \ldots, v_k\}$ is an edge $\{v_i, v_j\}$ that joins two nonconsecutive nodes in the cycle. A *clique* $C \subseteq V$ of G is a subset of nodes where $\{v_i, v_j\} \in E$ for any $v_i, v_j \in C$. If a clique is not a subset of any other clique, then it is called a *maximal clique*.

Definition 1.2 (chordal graph) *A graph is called a* chordal graph *if all its cycles of length at least four have a chord.*

The notion of chordal graphs plays an important role in sparse matrix theory. In particular, it is known that maximal cliques of a chordal graph can be enumerated efficiently in linear time in the number of nodes and edges of the graph. See e.g. [Gav72, VA+15] for the details.

The maximal cliques $I_1, \ldots, I_p$ of a chordal graph (possibly after some reordering) satisfy the so-called *running intersection property (RIP)*, i.e., for every $k \in [p-1]$, it holds

$$\left(I_{k+1} \cap \bigcup_{j \leq k} I_j \right) \subseteq I_i \quad \text{for some } i \leq k. \tag{1.7}$$

The RIP actually gives an equivalent characterization of chordal graphs.

Theorem 1.3 *A connected graph is chordal if and only if its maximal cliques after an appropriate ordering satisfy the RIP.*

Any non-chordal graph $G(V, E)$ can always be extended to a chordal graph $G'(V, E')$ by adding appropriate edges to E, which is called a *chordal extension* of $G(V, E)$. The chordal extension of G is usually not unique. We use the symbol G' to indicate a specific chordal extension of G. For graphs $G \subseteq H$, we assume that $G' \subseteq H'$ always holds for our purpose. For a graph G, among all chordal extensions of G, there is a particular one G' which makes every connected component of G to be a clique. Accordingly, a matrix with adjacency graph G' is block diagonal (after an appropriate permutation on rows and columns): each block corresponds to a connected component of G. We call this chordal extension the *maximal* chordal extension. Besides, we are also interested in smallest chordal extensions. By definition, a *smallest chordal extension* is a chordal extension with the smallest clique number (i.e., the maximal size of maximal cliques). However, computing a smallest chordal extension is generally NP-complete [ACP87]. Therefore in practice we compute approximately smallest chordal extensions instead with efficient heuristic algorithms; see [BK10] for more detailed discussions.

Example 1.4 *Let us consider the graph $G(V, E)$ represented in Figure 1.1, with the set of nodes $V = \{1, 2, 3, 4, 5, 6\}$ and*

$$E = \{\{1,2\}, \{1,3\}, \{1,4\}, \{1,5\}, \{1,6\}, \{2,3\}, \{2,5\}, \{3,6\}, \{5,6\}\}.$$

and the corresponding adjacency matrix

$$\mathbf{B}_G = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}.$$

One example of cycle of length 3 is $\{1, 5, 6\}$ and one example of cycle of length 4 is $\{6, 3, 2, 5\}$. Note that this graph is not chordal since there is no chord in this latter cycle. It is enough to add en edge between the nodes 2 and 6 (or alternatively between the nodes 3 and 5) to obtain a chordal extension of G.

Let $n \in \mathbb{N}^*$. Given a graph $G(V, E)$ with $V = [n]$, a symmetric matrix $\mathbf{Q}$ with rows and columns indexed by V is said to have sparsity pattern G if $\mathbf{Q}_{ij} = \mathbf{Q}_{ij} = 0$ whenever $i \neq j$ and $\{i, j\} \notin E$. Let $\mathbb{S}(G)$ be the set of real symmetric matrices with sparsity pattern G. The PSD matrices with sparsity pattern G form a convex cone

$$\mathbb{S}^+_{|V|} \cap \mathbb{S}(G) = \{\mathbf{Q} \in \mathbb{S}(G) \mid \mathbf{Q} \succeq 0\}. \tag{1.8}$$

A matrix in $\mathbb{S}(G)$ exhibits a block structure: each block corresponds to a maximal clique of G. Figure 1.2 depicts an instance of such block structures. Note that there might be overlaps between blocks because different maximal cliques may share nodes.

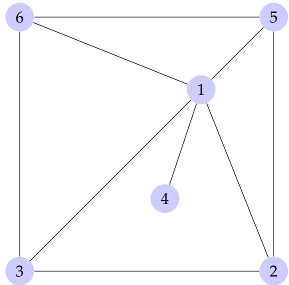

Figure 1.1: The graph from Example 1.4.

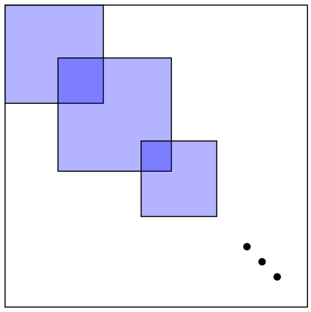

Figure 1.2: An instance of block structures for matrices in $\mathbb{S}(G)$. The blue area indicates the positions of possible nonzero entries.

Given a maximal clique C of $G(V, E)$, we define a matrix $\mathbf{R}_C \in \mathbb{R}^{|C|\times|V|}$ by

$$[\mathbf{R}_C]_{ij} = \begin{cases} 1, & \text{if } C(i) = j, \\ 0, & \text{otherwise,} \end{cases} \tag{1.9}$$

where $C(i)$ denotes the i-th node in C, sorted with respect to the ordering compatible with V. Note that $\mathbf{Q}_C = \mathbf{R}_C \mathbf{Q} \mathbf{R}_C^\mathsf{T} \in \mathbb{S}_{|C|}$ extracts a principal submatrix $\mathbf{Q}_C$ indexed by the clique C from a symmetry matrix $\mathbf{Q}$, and $\mathbf{Q} = \mathbf{R}_C^\mathsf{T} \mathbf{Q}_C \mathbf{R}_C$ inflates a $|C| \times |C|$ matrix $\mathbf{Q}_C$ into a sparse $|V| \times |V|$ matrix $\mathbf{Q}$.

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

Theorem 1.5 *Let $G(V, E)$ be a chordal graph and assume that $C_1, \ldots, C_p$ are the list of maximal cliques of G. Then a matrix $\mathbf{Q} \in \mathbb{S}_{|V|}^+ \cap \mathbb{S}(G)$ if and only if there exist $\mathbf{Q}_k \in \mathbb{S}_{|C_k|}^+$ for $k \in [p]$ such that $\mathbf{Q} = \sum_{k=1}^{p} \mathbf{R}_{C_k}^\mathsf{T} \mathbf{Q}_k \mathbf{R}_{C_k}$.*

Given a graph $G(V, E)$ with $V = [n]$, let Π_G be the projection from $\mathbb{S}_{|V|}$ to the subspace $\mathbb{S}(G)$, i.e., for $\mathbf{Q} \in \mathbb{S}_{|V|}$,

$$[\Pi_G(\mathbf{Q})]_{ij} = \begin{cases} \mathbf{Q}_{ij}, & \text{if } i = j \text{ or } \{i, j\} \in E, \\ 0, & \text{otherwise.} \end{cases} \tag{1.10}$$

We denote by $\Pi_G(\mathbb{S}_{|V|}^+)$ the set of matrices in $\mathbb{S}(G)$ that have a PSD completion, i.e.,

$$\Pi_G(\mathbb{S}_{|V|}^+) = \left\{ \Pi_G(\mathbf{Q}) \mid \mathbf{Q} \in \mathbb{S}_{|V|}^+ \right\}. \tag{1.11}$$

One can easily check that the PSD completable cone $\Pi_G(\mathbb{S}_{|V|}^+)$ and the PSD cone $\mathbb{S}_{|V|}^+ \cap \mathbb{S}(G)$ form a pair of dual cones in $\mathbb{S}(G)$. Moreover, for a chordal graph G, the decomposition result for the cone $\mathbb{S}^+_{|V|} \cap \mathbb{S}(G)$ in Theorem 1.5 leads to the following characterization of the PSD completable cone $\Pi_G(\mathbb{S}^+_{|V|})$.

Theorem 1.6 *Let $G(V, E)$ be a chordal graph and assume that $C_1, \ldots, C_p$ are the list of maximal cliques of G. Then a matrix $\mathbf{Q} \in \Pi_G(\mathbb{S}^+_{|V|})$ if and only if $\mathbf{Q}_k = \mathbf{R}_{C_k}\mathbf{Q}\mathbf{R}^\intercal_{C_k} \succeq 0$ for all $k \in [p]$.*

Theorem 1.5 and Theorem 1.6 play an important role in sparse semidefinite programming since they admit us to decompose an semidefinite programming (SDP) with chordal sparsity pattern into an SDP of smaller size, which yields significant computational improvement if the sizes of related maximal cliques are small.

Chapter 2

Polynomial nonnegativity, measures, and moments

2.1 Sums of squares and quadratic modules

Given a multivariate polynomial f, we want to decide whether it is nonnegative and if so, provide a certificate of its nonnegativity.

- A central problem in real algebraic geometry
- Widely appear in numerous fields
- Closely related to polynomial optimization
- NP-hard in general

Definition 2.1 *Sum of squares (SOS):* $f = f_1^2 + \cdots + f_t^2 \Rightarrow f$ *is nonnegative.*

Example 2.2 $f = 1 + 2x + 2x^2 + 2xy + y^2 = (1+x)^2 + (x+y)^2$.

Let $\Sigma[\mathbf{x}]$ stand for the cone of SOS polynomials and let $\Sigma[\mathbf{x}]_{n,2d}$ denote the cone of SOS polynomials of degree at most $2d$, namely $\Sigma[\mathbf{x}]_{n,2d} := \Sigma[\mathbf{x}] \cap \mathbb{R}[\mathbf{x}]_{n,2d}$. Let $P[\mathbf{x}]$ stand for the cone of nonnegative polynomials and let $P[\mathbf{x}]_{n,2d}$ denote the cone of nonnegative polynomials of degree at most $2d$.

- Hilbert, 1888: $\Sigma[\mathbf{x}]_{n,2d} = \mathbb{R}[\mathbf{x}]_{n,2d} \iff n = 1 \,||\, d = 2 \,||\, n = 2, d = 4$
- Artin, 1927: "nonnegative polynomials = rational SOS"
- Blekherman, 2006: "nonnegative polynomials $\gg$ SOS", $n \to \infty$ for fixed $2d \geq 4$

Example 2.3 *Motzkin's polynomial (1967):* $M(x,y) = x^4y^2 + x^2y^4 + 1 - 3x^2y^2$ *is nonnegative but is not an SOS.*

Theorem 2.4 (Reznick, 1995) *If* $\inf f(\mathbf{x}) > 0$*, then there exists* r *such that*

$$(1 + x_1^2 + \cdots + x_n^2)^r f(\mathbf{x}) \in \Sigma[\mathbf{x}].$$

Let $\deg(f) = 2d$ and $[\mathbf{x}]_d := [1, x_1, \ldots, x_n, x_1^d, \ldots, x_n^d]$. Then f is an SOS $\iff$ there exists a PSD matrix G such that

$$f = [\mathbf{x}]_d \cdot G \cdot [\mathbf{x}]_d^\intercal \quad \rightsquigarrow \quad \text{SDP}$$

G is called a Gram matrix of f, which is of size $\binom{n+d}{n} = \binom{n+d}{d}$.

Theorem 2.5 *If* f *has a positive definite Gram matrix with rational entries, then* f *admits a rational SOS decomposition.*

Definition 2.6 *The Newton polytope of a polynomial* $f = \sum_{\alpha \in \text{supp}(f)} c_\alpha \mathbf{x}^\alpha$*, denoted by* $\mathcal{N}(f)$*, is the convex hull of the set of exponents* α*, considered as vectors in* $\mathbb{R}^n$*.*

Theorem 2.7 *If* $f = \sum f_i^2$*, then* $\mathcal{N}(f_i) \subseteq \frac{1}{2}\mathcal{N}(f)$*.*

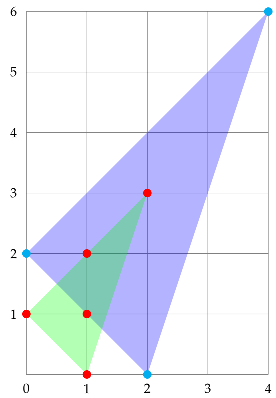

Figure 2.1: $f = 4x_1^4x_2^6 + x_1^2 - x_1x_2^2 + x_2^2$

Let $\mathbf{S} := \{\mathbf{x} \in \mathbb{R}^n \mid g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0\}$. For the ease of further notation, we set $g_0(\mathbf{x}) := 1$, and $d_j := \lceil \deg(g_j)/2 \rceil$, for all $j = 0, \ldots, m$. Given a basic compact semialgebraic set $\mathbf{S}$ and an integer $r \in \mathbb{N}^*$, let $\mathcal{M}(\mathfrak{g})$ be the quadratic module generated by $g_1, \ldots, g_m$:

$$\mathcal{M}(\mathfrak{g}) := \left\{ \sum_{j=0}^{m} \sigma_j(\mathbf{x}) g_j(\mathbf{x}) : \sigma_j \in \Sigma[\mathbf{x}], j = 0, \ldots, m \right\},$$

and let $\mathcal{M}(\mathfrak{g})_r$ be the r-truncated quadratic module:

$$\mathcal{M}(\mathfrak{g})_r := \left\{ \sum_{j=0}^{m} \sigma_j(\mathbf{x}) g_j(\mathbf{x}) : \sigma_j \in \Sigma[\mathbf{x}]_{r-d_j}, j = 0, \ldots, m \right\}.$$

A first important remark is that all polynomials belonging to $\mathcal{M}(\mathfrak{g})$ are positive on $\mathbf{S}$.

A second important remark is that $\mathcal{M}(\mathfrak{g})_r \subseteq \mathcal{M}(\mathfrak{g})_{r+1}$, for all $r \in \mathbb{N}^*$, since all SOS polynomials of degree $2r$ can be viewed as SOS polynomials of degree $2r + 2$.

Assumption 2.8 (Archimedean) *There exists $N > 0$ such that $N - \|\mathbf{x}\|_2^2 \in \mathcal{M}(\mathfrak{g})$.*

A quadratic module $\mathcal{M}(\mathfrak{g})$ for which Assumption 2.8 holds is said to be *Archimedean*. Assumption 2.8 is slightly stronger than compactness. Indeed, compactness of $\mathbf{S}$ already ensures that each variable has finite lower and upper bounds. One (easy) way to ensure that Assumption 2.8 holds is to add a redundant constraint involving a well-chosen N depending on these bounds, in the definition of $\mathbf{S}$.

Theorem 2.9 (Putinar's Positivstellensatz, 1993) *Let $\mathbf{S} := \{\mathbf{x} \in \mathbb{R}^n \mid g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0\}$. Assume that $\mathcal{M}(\mathfrak{g})$ satisfies Archimedean's condition. If f is positive on $\mathbf{S}$, then*

$$f = \sigma_0 + \sigma_1 g_1 + \cdots + \sigma_m g_m,$$

where $\sigma_0, \ldots, \sigma_m$ are SOS.

• **Quotient ring.** Suppose $\mathbf{S} := \{\mathbf{x} \in \mathbb{R}^n \mid g_1(\mathbf{x}) = 0, \ldots, g_m(\mathbf{x}) = 0\}$. Let $I = (g_1, \ldots, g_m) \subseteq \mathbb{R}[\mathbf{x}]$. Instead of writing $f = \sigma_0 + \tau_1 g_1 + \cdots + \tau_m g_m$ with $\tau_i \in \mathbb{R}[\mathbf{x}]$, we can consider

$$f \text{ is an SOS in the quotient ring } \mathbb{R}[\mathbf{x}]/I.$$

That means we can use the Gröbner basis of I to find a reduced monomial basis and to simplify the equality.

• **Symmetries.** Give rise to block diagonalization of SDP matrices. Please refer to [GP04].

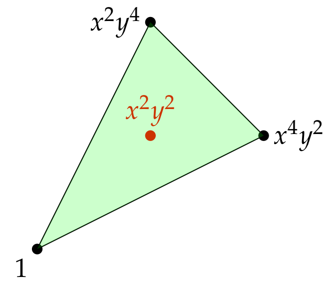

Figure 2.2

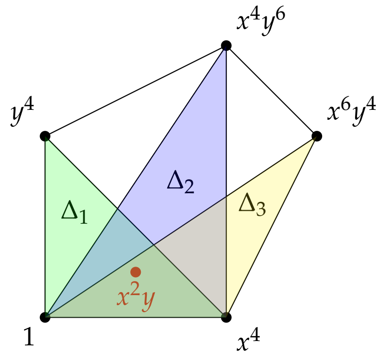

Figure 2.3

2.2 SONC polynomials

Example 2.10 *$M(x,y) = x^4y^2 + x^2y^4 + 1 - 3x^2y^2$ (arithmetic-geometric mean inequality $\Rightarrow$ nonnegativity)*

Definition 2.11 *circuit polynomial: $f = \sum_{\alpha\in\mathcal{A}} c_\alpha \mathbf{x}^\alpha - d_\beta \mathbf{x}^\beta$, $\alpha \in (2\mathbb{N})^n$, $c_\alpha > 0$, $\mathcal{A}$ is the vertex set of a simplex, $\beta \in \mathrm{conv}(\mathcal{A})^\circ$. SONC: $f = f_1 + \cdots + f_t$ with each f_i being a nonnegative circuit polynomial.*

Theorem 2.12 (Wang, 2022) *Suppose that f is a nonnegative polynomial with exactly one negative term. Then f is a SONC.*

Example 2.13 $f = 1 + x^4 + y^4 + x^6y^4 + x^4y^6 - x^2y$

Theorem 2.14 (Wang, 2022) *Suppose f is a SONC. Then f admits a SONC decomposition:*

$$f = \sum_{\mathrm{supp}(f_i)\subseteq \mathrm{supp}(f)} f_i,$$

where each f_i is a nonnegative circuit polynomial. Moreover, we can further assume that there is no cancellation occurring in the above decomposition.

For more details on SONC polynomials, please refer to [IDW16, Wan22].

2.3 Borel measures and moment matrices

Given a compact set $\mathbf{A} \subseteq \mathbb{R}^n$, we denote by $\mathscr{M}(\mathbf{A})$ the vector space of finite signed Borel measures supported on $\mathbf{A}$, namely real-valued functions from the Borel σ-algebra $\mathcal{B}(\mathbf{A})$. The support of a measure $\mu \in \mathscr{M}(\mathbf{A})$ is defined as the closure of the set of all points $\mathbf{x}$ such that $\mu(\mathbf{B}) \neq 0$ for any open neighborhood $\mathbf{B}$ of $\mathbf{x}$. Let $\mathscr{C}_+(\mathbf{A})$ (resp. $\mathscr{M}_+(\mathbf{A})$) stand for the cone of nonnegative elements of $\mathscr{C}(\mathbf{A})$ (resp. $\mathscr{M}(\mathbf{A})$).

Let $\mathbf{S}$ be a basic compact semialgebraic set. The restriction of the Lebesgue measure on a subset $\mathbf{A} \subseteq \mathbf{S}$ is $\lambda_{\mathbf{A}}(\mathrm{d}\mathbf{x}) := \mathbf{1}_{\mathbf{A}}(\mathbf{x})\mathrm{d}\mathbf{x}$, where $\mathbf{1}_{\mathbf{A}} : \mathbf{S} \to \{0,1\}$ stands for the indicator function of $\mathbf{A}$, namely $\mathbf{1}_{\mathbf{A}}(\mathbf{x}) = 1$ if $\mathbf{x} \in \mathbf{A}$ and $\mathbf{1}_{\mathbf{A}}(\mathbf{x}) = 0$ otherwise. A sequence $\mathbf{y} := (y_\alpha)_{\alpha \in \mathbb{N}^n} \subseteq \mathbb{R}$ is said to have a representing measure on $\mathbf{S}$ if there exists $\mu \in \mathscr{M}(\mathbf{S})$ such that $y_\alpha = \int \mathbf{x}^\alpha \mu(\mathrm{d}\mathbf{x})$ for all $\alpha \in \mathbb{N}^n$, where we use the multinomial notation $\mathbf{x}^\alpha := x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}$.

Assume that $\mu, \nu \in \mathscr{M}_+(\mathbf{S})$ have the same moments $\mathbf{y}$, namely $y_\alpha = \int_S \mathbf{x}^\alpha \,\mathrm{d}\mu = \int_{\mathbf{S}} \mathbf{x}^\alpha \,\mathrm{d}\nu$, for all $\alpha \in \mathbb{N}^n$. Let us fix $f \in \mathscr{C}(\mathbf{S})$. Since $\mathbf{S}$ is compact, the Stone-Weierstrass theorem implies that the polynomials are dense in $\mathscr{C}(\mathbf{S})$, so $\int_S f \,\mathrm{d}\mu = \int_{\mathbf{S}} f \,\mathrm{d}\nu$. Since f was arbitrary, the above equality holds for any $f \in \mathscr{C}(\mathbf{S})$, which implies that $\mu = \nu$. Therefore, any finite Borel measures supported on $\mathbf{S}$ is *moment determinate*.

The moments of the Lebesgue measure on $\mathbf{A}$ are denoted by

$$y_\alpha^{\mathbf{A}} := \int \mathbf{x}^\alpha \lambda_{\mathbf{A}} \,\mathrm{d}\mathbf{x} \in \mathbb{R}, \quad \alpha \in \mathbb{N}^n. \tag{2.1}$$

The Lebesgue volume of $\mathbf{A}$ is $\operatorname{vol} \mathbf{A} := y_{\mathbf{0}}^{\mathbf{A}} = \int \lambda_{\mathbf{A}} \,\mathrm{d}\mathbf{x}$. For all $r \in \mathbb{N}$, let us define $\mathbb{N}_r^n := \{\alpha \in \mathbb{N}^n \mid \sum_{j=1}^n \alpha_j \leq r\}$, whose cardinality is $\binom{n+r}{r}$. Then a polynomial $f \in \mathbb{R}[\mathbf{x}]$ is written as follows:

$$\mathbf{x} \mapsto f(\mathbf{x}) = \sum_{\alpha \in \mathbb{N}^n} f_\alpha \mathbf{x}^\alpha,$$

and f is identified with its vector of coefficients $\mathbf{f} = (f_\alpha)_{\alpha \in \mathbb{N}^n}$ in the standard monomial basis $(\mathbf{x}^\alpha)_{\alpha \in \mathbb{N}^n}$.

Given a real sequence $\mathbf{y} = (y_\alpha)_{\alpha \in \mathbb{N}^n}$, let us define the linear functional $L_{\mathbf{y}} : \mathbb{R}[\mathbf{x}] \to \mathbb{R}$ by $L_{\mathbf{y}}(f) := \sum_\alpha f_\alpha y_\alpha$, for every polynomial $f = \sum_\alpha f_\alpha \mathbf{x}^\alpha$. Coming back to the previous 2-dimensional example from Chapter 2.1, with $f = x_1 x_2$, $g_1 = x_1 - x_1^2$ and $g_2 = x_2 - x_2^2$, we have $L_{\mathbf{y}}(f) = y_{11}$, $L_{\mathbf{y}}(g_1) = y_{10} - y_{20}$ and $L_{\mathbf{y}}(g_2) = y_{01} - y_{02}$.

Then, we associate to $\mathbf{y}$ the so-called *moment matrix* $\mathbf{M}_r(\mathbf{y})$ of order r, that is the real symmetric matrix with rows and columns indexed by $\mathbb{N}_r^n$ and the following entrywise definition:

$$[\mathbf{M}_r(\mathbf{y})]_{\beta,\gamma} := L_{\mathbf{y}}(\mathbf{x}^{\beta+\gamma}), \quad \forall \beta, \gamma \in \mathbb{N}_r^n.$$

Given $g \in \mathbb{R}[\mathbf{x}]$, we also associate to $\mathbf{y}$ and g the so-called *localizing matrix* of order r, that is the real symmetric matrix $\mathbf{M}_r(g\,\mathbf{y})$ with rows and columns indexed by $\mathbb{N}_r^n$ and the following entrywise definition:

$$[\mathbf{M}_r(g\,\mathbf{y})]_{\beta,\gamma} := L_{\mathbf{y}}(g(\mathbf{x})\,\mathbf{x}^{\beta+\gamma}), \quad \forall \beta, \gamma \in \mathbb{N}_r^n.$$

Let $\mathbf{S}$ be a basic compact semialgebraic set defined by $g_j \geq 0, j = 1, \ldots, m$. Then one can check that if $\mathbf{y}$ has a representing measure $\mu \in \mathscr{M}_+(\mathbf{S})$ then $\mathbf{M}_r(\mathbf{y}) \succeq 0$ and $\mathbf{M}_r(g_j\,\mathbf{y}) \succeq 0$, for $j = 1, \ldots, m$.

Let us give a simple example to illustrate the construction of moment and localizing matrices.

Example 2.15 *Let us take $n = 2$ and $r = 2$. The moment matrix $\mathbf{M}_2(\mathbf{y})$ is indexed by $\mathbb{N}_2^2$ and can be written as follows:*

$$\mathbf{M}_2(\mathbf{y}) = \left[\begin{array}{c|cc|ccc} 1 & y_{1,0} & y_{0,1} & y_{2,0} & y_{1,1} & y_{0,2} \\ \hline y_{1,0} & y_{2,0} & y_{1,1} & y_{3,0} & y_{2,1} & y_{1,2} \\ y_{0,1} & y_{1,1} & y_{0,2} & y_{2,1} & y_{1,2} & y_{0,3} \\ \hline y_{2,0} & y_{3,0} & y_{2,1} & y_{4,0} & y_{3,1} & y_{2,2} \\ y_{1,1} & y_{2,1} & y_{1,2} & y_{3,1} & y_{2,2} & y_{1,3} \\ y_{0,2} & y_{1,2} & y_{0,3} & y_{2,2} & y_{1,3} & y_{0,4} \end{array}\right].$$

Next, consider the polynomial $g_1(\mathbf{x}) = x_1 - x_1^2$ of degree 2. From the first-order moment matrix:

$$\mathbf{M}_1(\mathbf{y}) = \left[\begin{array}{c|cc} 1 & y_{1,0} & y_{0,1} \\ \hline y_{1,0} & y_{2,0} & y_{1,1} \\ y_{0,1} & y_{1,1} & y_{0,2} \end{array}\right],$$

we obtain the following localizing matrix:

$$\mathbf{M}_1(g_1\mathbf{y}) = \begin{bmatrix} y_{1,0} - y_{2,0} & y_{2,0} - y_{3,0} & y_{1,1} - y_{2,1} \\ y_{2,0} - y_{3,0} & y_{3,0} - y_{4,0} & y_{2,1} - y_{3,1} \\ y_{1,1} - y_{2,1} & y_{2,1} - y_{3,1} & y_{1,2} - y_{2,2} \end{bmatrix}.$$

For instance, the last entry $[\mathbf{M}_1(g_1\mathbf{y})]_{3,3}$ *is equal to* $L_{\mathbf{y}}(g_1(\mathbf{x}) \cdot x_2 \cdot x_2) = L_{\mathbf{y}}(x_1 x_2^2 - x_1^2 x_2^2) = y_{1,2} - y_{2,2}$.

Chapter 3

Polynomial optimization

3.1 The moment-SOS hierarchy

Let us consider the POP

$$\mathbf{P}: \quad f_{\min} = \inf_{\mathbf{x}} \{ f(\mathbf{x}) : \mathbf{x} \in \mathbf{S} \}, \tag{3.1}$$

where f is a polynomial and $\mathbf{S} := \{\mathbf{x} \in \mathbb{R}^n \mid g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0\}$. It happens that this problem can be cast as an LP over probability measures, namely,

$$f_{\text{meas}} := \inf_{\mu \in \mathscr{M}_+(\mathbf{S})} \left\{ \int_{\mathbf{S}} f \, \mathrm{d}\mu : \int_S \mathrm{d}\mu = 1 \right\}. \tag{3.2}$$

To see that $f_{\text{meas}} = f_{\min}$ holds, let us consider a global minimizer $\mathbf{x}^{\text{opt}} \in \mathbb{R}^n$ of f on $\mathbf{S}$ and consider the Dirac measure $\mu = \delta_{\mathbf{x}^{\text{opt}}}$ supported on this point. Note that this Dirac (probability) measure is feasible for the LP stated in (3.2), with value $\int_{\mathbf{S}} f \, \mathrm{d}\mu = f(\mathbf{x}^{\text{opt}}) = f_{\min}$, which implies that $\inf_{\mu \in \mathscr{M}_+(\mathbf{S})} \{ \int_{\mathbf{S}} f \, \mathrm{d}\mu : \int_S \mathrm{d}\mu = 1 \} \leq f_{\min}$. For the other direction, let us consider a measure μ feasible for LP (3.2). Then, simply observe that since $f(\mathbf{x}) \geq f_{\min}$, for all $\mathbf{x} \in \mathbf{S}$, the feasibility of μ implies that $\int_{\mathbf{S}} f \, \mathrm{d}\mu \geq \int_{\mathbf{S}} f_{\min} \, \mathrm{d}\mu = f_{\min} \int_{\mathbf{S}} \mathrm{d}\mu = f_{\min}$. Since it is true for any feasible solution, one has $\inf_{\mu \in \mathscr{M}_+(\mathbf{S})} \{ \int_{\mathbf{S}} f \, \mathrm{d}\mu : \int_S \mathrm{d}\mu = 1 \} \geq f_{\min}$. Another way to state this equality is to write

$$f_{\min} = \sup_b \{ b : f - b \geq 0 \text{ on } \mathbf{S} \}, \tag{3.3}$$

which is an LP over nonnegative polynomials, and to notice that the dual LP of (3.3) is LP (3.2). The equality then follows from the zero duality gap in infinite-dimensional LP.

After reformulating $\mathbf{P}$ as LP (3.2) over probability measures, one can then build a hierarchy of moment relaxations for the later problem. This is done by using the fact that the condition $\mu \in \mathscr{M}_+(\mathbf{S})$ can be relaxed as $\mathbf{M}_{r-d_j}(g_j \, \mathbf{y}) \succeq 0$, for all $j = 0, \ldots, m$, and all $r \geq d_j = \lceil \deg(g_j)/2 \rceil$.

Letting $r_{\min} := \max \{ \lceil \deg(f)/2 \rceil, d_1, \ldots, d_m \}$, at step $r \geq r_{\min}$ of the hierarchy, one considers the following primal SDP:

$$\mathbf{P}^r: \quad \begin{array}{rll} f^r := & \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ & \text{s.t.} & \mathbf{M}_r(\mathbf{y}) \succeq 0 \\ & & \mathbf{M}_{r-d_j}(g_j \, \mathbf{y}) \succeq 0, \quad j \in [m] \\ & & y_{\mathbf{0}} = 1 \end{array} \tag{3.4}$$

Before considering the corresponding dual SDP, let us remind that the moment and localizing matrices $\mathbf{M}_{r-d_j}(g_j \, \mathbf{y})$ have entries which are linear in $\mathbf{y}$. Namely, one has $\mathbf{M}_{r-d_j}(g_j \, \mathbf{y}) = \sum_{\alpha \in \mathbb{N}^n_{2r}} \mathbf{C}^j_\alpha \, y_\alpha$; the matrix $\mathbf{C}^j_\alpha$ has rows and columns indexed by $\mathbb{N}^n_{r-d_j}$ with (β, γ)-entry equal to $\sum_{\beta+\gamma+\delta=\alpha} g_{j,\delta}$. In particular for $m = 0$, one has $g_0 = 1$ and the matrix $\mathbf{B}_\alpha := \mathbf{C}^0_\alpha$ has (β, γ)-entry equal to $1_{\beta+\gamma=\alpha}$, where $1_{\alpha=\beta}$ stands for the function which returns 1 if $\alpha = \beta$ and 0 otherwise. With $t_j := \binom{n+r-d_j}{r-d_j}$, the dual of SDP (3.4) is then the following SDP:

$$\begin{cases} \sup\limits_{\mathbf{G}_j, b} & b \\ \text{s.t.} & f_\alpha - b 1_{\alpha=\mathbf{0}} = \sum\limits_{j=0}^{m} \langle \mathbf{C}_\alpha^j, \mathbf{G}_j \rangle, \quad \alpha \in \mathbb{N}_{2r}^n \\ & \mathbf{G}_j \in \mathbb{S}_{t_j}^+, \quad j = 0, \ldots, m \end{cases} \tag{3.5}$$

We can rewrite the equality constraints from SDP (3.5) in a more concise way, namely as $f - b \in \mathcal{M}(\mathfrak{g})_r$. To see this, let us first note that an SOS σ of degree $2r$ can be written as $\mathbf{v}^\intercal \mathbf{G} \mathbf{v}$, with

$$\mathbf{v} := (1, x_1, \ldots, x_n, x_1^2, x_1 x_2, \ldots, x_1^r, \ldots, x_n^r)$$

being the vectors of all monomials of degree at most r, and $\mathbf{G} \succeq 0$. The α-coefficient of $\sigma = \mathbf{v}^\intercal \mathbf{G} \mathbf{v}$ is equal to $\langle \mathbf{B}_\alpha, \mathbf{G} \rangle$. Similarly, for any $j \in [m]$ and SOS σ_j of degree at most $2(r - d_j)$, one can write $\sigma_j = \mathbf{v}_j^\intercal \mathbf{G}_j \mathbf{v}_j$, with $\mathbf{v}_j$ being the vector of all monomials of degree at most $r - d_j$, and $\mathbf{G}_j \succeq 0$. One can also check that the α-coefficient of $\sigma_j g_j$ is equal to $\langle \mathbf{C}_\alpha^j, \mathbf{G}_j \rangle$. Therefore, SDP (3.5) is equivalent to the following optimization problem over SOS polynomials:

$$\begin{cases} \sup\limits_{\sigma_j, b} & b \\ \text{s.t.} & f - b = \sum\limits_{j=0}^{m} \sigma_j g_j \\ & \sigma_j \in \Sigma[\mathbf{x}]_{r-d_j}, \quad j = 0, \ldots, m \end{cases} \tag{3.6}$$

or more concisely as

$$\sup_b \{ b : f - b \in \mathcal{M}(\mathfrak{g})_r \}. \tag{3.7}$$

The dual SDP (3.7) is obtained by replacing the nonnegativity condition $f - b \geq 0$ on $\mathbf{S}$ of the dual LP (3.3) by the more restrictive condition $f - b \in \mathcal{M}(\mathfrak{g})_r$. The sequences of SDPs 3.4 and (3.7) are called the moment hierarchy and the SOS hierarchy, respectively. In the sequel, we refer to the sequence of primal-dual programs (3.4)–(3.7) as the moment-SOS hierarchy.

Theorem 3.1 *Under Assumption 2.8, the hierarchy of primal-dual moment-SOS relaxations (3.4)–(3.7) provides nondecreasing sequences of lower bounds converging to the global optimum $f_{\min}$ of* $\mathbf{P}$ *(3.1).*

The above theorem provides the theoretical convergence guarantee of the moment-SOS hierarchy.

Remark 3.2 *Even though we only included inequality constraints in the definition of* $\mathbf{S}$ *for the sake of simplicity, equality constraints can be treated in a dedicated way. For each equality constraint $h(\mathbf{x}) = 0$, with $h \in \mathbb{R}[\mathbf{x}]$, one adds the localizing constraint $\mathbf{M}_{r-d_h}(h\,\mathbf{y}) = 0$, with $d_h := \lceil \deg(h)/2 \rceil$, in the primal moment program (3.4). Similarly, in the dual sum of squares (SOS) program (3.6), one adds a term τh to the sum $\sum_{j=0}^{m} \sigma_j g_j$, with $\tau \in \mathbb{R}[\mathbf{x}]_{2r-2d_h}$.*

In practice, it is possible to detect finite convergence of the hierarchy, which is the topic of the next section.

3.2 Minimizer extraction

Here we describe sufficient conditions to obtain finite convergence of the moment-sums of squares (moment-SOS) hierarchy and extract the global minimizers of the polynomial f on $\mathbf{S}$. For more details, please refer to [HL05b].

Theorem 3.3 *Consider the sequence of primal moment relaxations defined in* (3.4). *If for some* $r \geq r_{\mathbf{S}}$ *(*$r_{\mathbf{S}} := \max\{d_1, \ldots, d_m\}$*), SDP* (3.4) *has an optimal solution* $\mathbf{y}$ *which satisfies*

$$\operatorname{rank} \mathbf{M}_{r'}(\mathbf{y}) = \operatorname{rank} \mathbf{M}_{r'-r_{\mathbf{S}}}(\mathbf{y}) \text{ for some } r' \leq r, \tag{3.8}$$

then $f^r = f_{\min}$ *and the infinite-dimensional LP* (3.2) *has an optimal solution* $\mu \in \mathscr{M}(\mathbf{S})_+$*, which is finitely supported on* $t = \operatorname{rank} \mathbf{M}_{r'}(\mathbf{y})$ *points of* $\mathbf{S}$*, or equivalently* t *global minimizers of* f *on* $\mathbf{S}$.

If the rank stabilization (also called *flatness*) condition (3.8) is satisfied, then finite convergence occurs, namely the SDP relaxation (3.4) is exact with optimal value $f^r = f_{\min}$. In addition, one can extract $\operatorname{rank} \mathbf{M}_{r'}(\mathbf{y})$ global minimizers of f on $\mathbf{S}$ with the following algorithm.

Algorithm 1 `ExtractMinimizer`

Require: The moment matrix $\mathbf{M}_{r'}(\mathbf{y})$ of rank t satisfying the flatness condition (3.8)
Ensure: The t points $\mathbf{x}(i) \in \mathbf{S}$, $i \in [t]$, global minimizers of Problem $\mathbf{P}$ (3.1)
1: Compute the Cholesky factorization $\mathbf{C}\mathbf{C}^\intercal = \mathbf{M}_{r'}(\mathbf{y})$
2: Reduce $\mathbf{C}$ to a column echelon form $\mathbf{U}$
3: Compute from $\mathbf{U}$ the multiplication matrices $\mathbf{N}_i$, $i \in [n]$
4: Compute $\mathbf{N} := \sum_{i=1}^n \lambda_i \mathbf{N}_i$ with randomly generated coefficients λ_i
5: Compute the Schur decomposition $\mathbf{N} = \mathbf{Q}\mathbf{T}\mathbf{Q}^\intercal$
6: Compute the column vectors $\{\mathbf{q}_j\}_{1 \leq j \leq t}$ of $\mathbf{Q}$
7: Return $x_i(j) := \mathbf{q}_j^\intercal \mathbf{N}_i \mathbf{q}_j$, $i \in [n]$, $j \in [t]$

Proposition 3.4 *The procedure* `ExtractMinimizer` *described in Algorithm 1 is sound and returns* t *global optimizers of Problem* $\mathbf{P}$ (3.1).

PROOF Since the flatness condition (3.8) is satisfied, $\mathbf{y}$ is the moment sequence of a t-atomic Borel measure μ supported on $\mathbf{S}$. Namely, there are t points $\mathbf{x}(1), \ldots, \mathbf{x}(t) \in \mathbf{S}$ such that

$$\mu = \sum_{j=1}^{t} \kappa_j \delta_{\mathbf{x}(j)}, \quad \kappa_j > 0, \quad \sum_{j=1}^{t} \kappa_j = 1.$$

By construction of the moment matrix $\mathbf{M}_{r'}(\mathbf{y})$, one has

$$\mathbf{M}_{r'}(\mathbf{y}) = \sum_{j=1}^{r} \kappa_j \mathbf{v}_{r'}(\mathbf{x}(j)) \mathbf{v}_{r'}^\intercal(\mathbf{x}(j)) = \mathbf{V}\mathbf{D}\mathbf{V}^\intercal,$$

where the j-th column of $\mathbf{V}$ is $\mathbf{v}_{r'}(\mathbf{x}(j))$ and $\mathbf{D}$ is a $t \times t$ diagonal matrix with diagonal $(\kappa_j)_{1 \leq j \leq t}$. One can extract a Cholesky factor $\mathbf{C}$ as in Step 1, for instance via singular value decomposition. The following steps of the extraction algorithm consist of transforming $\mathbf{C}$ into $\mathbf{V}$ by suitable column operations. The reduction of $\mathbf{C}$ to a column echelon form in Step 2 is done by Gaussian elimination with column pivoting. By construction of the moment matrix, each row of $\mathbf{U}$ is indexed by a monomial $\mathbf{x}^\alpha$ involved in the vector $\mathbf{v}_{r'}$. Pivot elements in $\mathbf{U}$ correspond to monomials $\mathbf{x}^{\beta_j}$, $j \in [t]$ of the basis generating the t solutions. Namely, if $\mathbf{w} = (\mathbf{x}^{\beta_1}, \mathbf{x}^{\beta_2}, \ldots, \mathbf{x}^{\beta_t})$ denotes this generating basis, then

$$\mathbf{v}_{r'}(\mathbf{x}(j)) = \mathbf{U}\mathbf{w}(\mathbf{x}(j)), \quad j \in [t].$$

Overall, extracting the global minmizers boils down to solving the above systems of equations. To solve this system, we compute at Step 3 each multiplication matrix $\mathbf{N}_i$, $i \in [n]$, which contains the coefficients of the monomials $x_i \mathbf{x}^{\beta_j}$, $j \in [t]$, namely which satisfy

$$\mathbf{N}_i \mathbf{w}(\mathbf{x}) = x_i \mathbf{w}(\mathbf{x}).$$

The entries of the global minimizers are all eigenvalues of the multiplication matrices. Since $\mathbf{w}(\mathbf{x}(j))$ is an eigenvector common to all multuplication matrices, one builds the random combination $\mathbf{N}$ of Step 4, which ensures with probability 1 that its eigenvalues are all distinct and have 1-dimensional eigenspaces. The Shur decomposition of Step 5 gives the decomposition $\mathbf{N} = \mathbf{QTQ}^\intercal$ with an orthogonal matrix $\mathbf{Q}$ and an upper triangular matrix $\mathbf{T}$ with eigenvalues of $\mathbf{N}$ sorted in increasing order along the diagonal. □

Example 3.5 *Consider the polynomial optimization problem* $\mathbf{P}$ (3.1) *with* $f = -(x_1 - 1)^2 - (x_1 - x_2)^2 - (x_2 - 3)^2$ *and* $\mathbf{S} = \{\mathbf{x} \in \mathbb{R}^2 : 1 - (x_1 - 1)^2 \geq 0, 1 - (x_1 - x_2)^2 \geq 0, 1 - (x_1 - 3)^2 \geq 0\}$. *The first SDP relaxation outputs* $f^1 = -3$ *and* $\operatorname{rank} M_1(\mathbf{y}) = 3$, *while the second one outputs* $f^2 = -2$ *and the rank stabilizes with* $\operatorname{rank} M_1(\mathbf{y}) = \operatorname{rank} M_2(\mathbf{y}) = 3$. *Therefore the flatness condition holds, which implies that* $f_{\min} = f^2 = -2$. *The monomial basis is* $\mathbf{v}_2(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$. *The column echelon form* $\mathbf{U}$ *of the Cholesky factor of* $\mathbf{M}_2(\mathbf{y})$ *is given by*

$$\begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0 & 0 & 1 \\ -2 & 3 & 0 \\ -4 & 2 & 2 \\ -6 & 0 & 5 \end{bmatrix}.$$

Pivot entries correspond to the generating basis $\mathbf{w}(\mathbf{x}) = (1, x_1, x_2)$. *Therefore the entries of the 3 global minimizers satisfy the following system of polynomial equations:*

$$\begin{aligned} x_1^2 &= -2 + 3x_1 \\ x_1 x_2 &= -4 + 2x_1 + 2x_2 \\ x_2^2 &= -6 + 5x_2. \end{aligned}$$

The multiplication matrices by x_1 *and* x_2 *can be extracted from rows in* $\mathbf{U}$ *as follows:*

$$\mathbf{N}_1 = \begin{bmatrix} 0 & 1 & 0 \\ -2 & 3 & 0 \\ -4 & 2 & 2 \end{bmatrix}, \quad \mathbf{N}_2 = \begin{bmatrix} 0 & 0 & 1 \\ -4 & 2 & 2 \\ -6 & 0 & 5 \end{bmatrix}.$$

After selecting a random convex combination of $\mathbf{N}_1$ *and* $\mathbf{N}_2$ *and computing the orthogonal matrix in the corresponding Schur decomposition, we obtain the 3 minimizers* $\mathbf{x}(1) = (1, 2)$, $\mathbf{x}(2) = (2, 2)$ *and* $\mathbf{x}(3) = (2, 3)$.

3.3 Further topics

The extraction of minimizers in polynomial optimization is robust; see [KPV18].

Chapter 4

Exploiting structures in polynomial optimization

4.1 Correlative sparsity

Recall that a general POP is formulized as

$$\mathbf{P}: \quad f_{\min} = \inf_{\mathbf{x}} \{f(\mathbf{x}) : \mathbf{x} \in \mathbf{S}\}, \tag{4.1}$$

where $\mathbf{S} = \{\mathbf{x} \in \mathbb{R}^n : g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0\}$. Roughly speaking, the exploitation of CS in the moment-SOS hierarchy for $\mathbf{P}$ consists of two steps:

(1) decompose the variables $\mathbf{x}$ into a set of cliques according to the correlations between variables emerging in the input polynomial system;

(2) construct a sparse moment-SOS hierarchy with respect to the former decomposition of variables.

Let us proceed with more details. Recall $d_j := \lceil \deg(g_j)/2 \rceil$ for $j \in [m]$ and

$$r_{\min} := \max\{\lceil \deg(f)/2 \rceil, d_1, \ldots, d_m\}.$$

Fix from now on a relaxation order $r \geq r_{\min}$. Let $J' := \{j \in [m] \mid d_j = r\}$ which is possibly nonempty only when $r = r_{\min}$. We define the correlative sparsity pattern (csp) graph $G^{\mathrm{csp}}(V, E)$ associated to POP (4.1) whose node set is $V = \{1, 2, \ldots, n\}$ and whose edge set E satisfies $\{i, j\} \in E$ if one of following conditions holds:

(i) there exists $\alpha \in \mathrm{supp}(f) \cup \bigcup_{j \in J'} \mathrm{supp}(g_j)$ such that $\{i, j\} \subseteq \mathrm{supp}(\alpha)$;

(ii) there exists $k \in [m] \setminus J'$ such that $\{i, j\} \subseteq \bigcup_{\alpha \in \mathrm{supp}(g_k)} \mathrm{supp}(\alpha)$,

where $\mathrm{supp}(\alpha) := \{k \in [n] \mid \alpha_k \neq 0\}$ for $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$. Let $(G^{\mathrm{csp}})'$ be a chordal extension of G^{csp}[1] and $\{I_k\}_{k=1}^p$ be the list of maximal cliques of $(G^{\mathrm{csp}})'$ with $n_k := |I_k|$ so that the RIP (1.7) holds. Let $\mathbb{R}[\mathbf{x}, I_k]$ denote the ring of polynomials in the n_k variables $\{x_i\}_{i \in I_k}$ for $k \in [p]$. By construction, one can decompose the objective function f as $f = f_1 + \cdots + f_p$ with $f_k \in \mathbb{R}[\mathbf{x}, I_k]$ for all $k \in [p]$ (similarly for g_j with $j \in J'$). We then partition the constraint polynomials $g_j, j \in [m] \setminus J'$ into groups $\{g_j \mid j \in J_k\}, k \in [p]$ which satisfy

(i) $J_1, \ldots, J_p \subseteq [m] \setminus J'$ are pairwise disjoint and $\bigcup_{k=1}^p J_k = [m] \setminus J'$;

(ii) for any $k \in [p]$ and any $j \in J_k$, $\bigcup_{\alpha \in \mathrm{supp}(g_j)} \mathrm{supp}(\alpha) \subseteq I_k$,

[1] If G^{csp} is already a chordal graph, then we do not need the chordal extension.

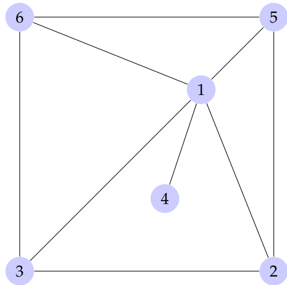

Figure 4.1: The csp graph for f over $\mathbf{S}$ from Example 4.9.

so that $g_j \in \mathbb{R}[\mathbf{x}, I_k]$ for all $k \in [p]$ and $j \in J_k$. In addition, suppose that Assumption 2.8 holds. Then all variables involved in POP (4.1) are bounded. To guarantee global convergence of the hierarchy that will be presented later, we need to add some redundant quadratic constraints to the description of the POP. We summarize all above in the following assumption.

Assumption 4.1 *Consider POP (4.1). The two index sets $[n]$ and $[m]$ are decomposed/partitioned into $\{I_1, \dots, I_p\}$ and $\{J', J_1, \dots, J_p\}$, respectively, such that*

(i) The objective function f can be decomposed as $f = f_1 + \cdots + f_p$ with $f_k \in \mathbb{R}[\mathbf{x}, I_k]$ for $k \in [p]$ and the same goes for the constraint polynomial g_j with $j \in J'$;

(ii) For all $k \in [p]$ and $j \in J_k$, $g_j \in \mathbb{R}[\mathbf{x}, I_k]$;

(iii) The RIP (1.7) holds for $I_1, \dots, I_p$ (possibly after some reordering);

(iv) For all $k \in [p]$, there exists $N_k > 0$ such that one of the constraint polynomials is $N_k - \sum_{i \in I_k} x_i^2$.

Example 4.2 *Consider an instance of POP (4.1) with $f(\mathbf{x}) = x_2x_5 + x_3x_6 - x_2x_3 - x_5x_6 + x_1(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6)$ and*

$$\mathbf{S} = \{\mathbf{x} \in \mathbb{R}^n : g(\mathbf{x}) \geq 0, \text{ for all } g \in \mathfrak{g}\},$$

with $\mathfrak{g} = \{(6.36 - x_1)(x_1 - 4), \dots, (6.36 - x_6)(x_6 - 4)\}$. Here, there are $n = 6$ variables and the number of constraints is $m = 6$. The related csp graph G^{csp} is depicted in Figure 4.1. After adding an edge between nodes 3 and 5, the resulting graph $(G^{\text{csp}})'$ is chordal with maximal cliques $I_1 = \{1, 4\}$, $I_2 = \{1, 2, 3, 5\}$, $I_3 = \{1, 3, 5, 6\}$. Here $p = 3$ and one can write $f = f_1 + f_2 + f_3$ with

$$\begin{aligned} f_1 &= -x_1x_4, \\ f_2 &= -x_1^2 + x_1x_2 + x_1x_3 - x_2x_3 + x_2x_5, \\ f_3 &= -x_5x_6 + x_1x_5 + x_1x_6 + x_3x_6. \end{aligned}$$

For the relaxation order $r = r_{\min} = 1$, let $J' = [6]$ and $J_k = \emptyset$ for $k \in [3]$; for the relaxation order $r \geq 2$, let $J' = \emptyset$ and $J_1 = \{1, 4\}$, $J_2 = \{2, 3, 5\}$, $J_3 = \{6\}$. Then Assumption 4.1(i)-(ii) hold. In addition, $I_1 \cap I_2 = \{1\} \subseteq I_3$, and so RIP (1.7), or equivalently Assumption 4.1 (iii), holds. For each $i \in [n]$, one has $6.36^2 - x_i^2 \geq 0$ for all $\mathbf{x} \in \mathbf{S}$, and so one can select $N_1 = 2 \cdot 6.36^2$, $N_2 = N_3 = 4 \cdot 6.36^2$ and add the redundant constraints $N_k - \sum_{i \in I_k} x_i^2 \geq 0$, $k \in [p]$ in the description of $\mathbf{S}$, so that Assumption 4.1 (iv) holds as well.

4.2 A sparse infinite-dimensional LP formulation

In this section, we assume $J' = \emptyset$. We now introduce a CS variant of the dense infinite-dimensional LP (3.2) formulation over probability measures stated in Chapter 3. The idea is to define a new measure for each subset I_k, $k \in [p]$, supported on a set S_k described by the constraints which only depend on the variables indexed by I_k, namely,

$$S_k := \{\mathbf{x} \in \mathbb{R}^{n_k} : g_j(\mathbf{x}) \geq 0, j \in J_k\}, \text{ for } k \in [p].$$

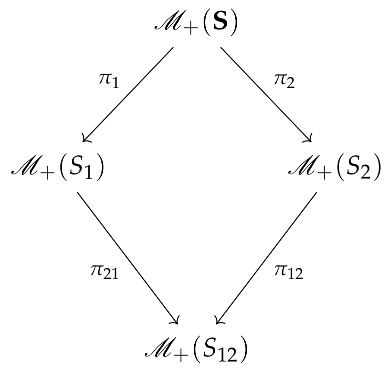

Figure 4.2: Illustration of Lemma 4.3 in the case $p = 2$.

So $\mathbf{S}$ can be equivalently described as

$$\mathbf{S} = \{\mathbf{x} \in \mathbb{R}^n : (x_i)_{i \in I_k} \in S_k, k \in [p]\}. \tag{4.2}$$

Similarly, for all $j, k \in [p]$ such that $I_j \cap I_k \neq \emptyset$, define

$$S_{jk} = S_{kj} := \{(x_i)_{i \in I_j \cap I_k} : (x_i)_{i \in I_j} \in S_j, (x_i)_{i \in I_k} \in S_k\}.$$

Afterwards, for each $k \in [p]$ we define the projection $\pi_k : \mathscr{M}_+(\mathbf{S}) \to \mathscr{M}_+(S_k)$ of the space of Borel measures supported on $\mathbf{S}$ on the space of Borel measures supported on S_k, namely, for all $\mu \in \mathscr{M}_+(\mathbf{S})$,

$$\pi_k \mu(\mathbf{B}) := \mu(\{\mathbf{x} : \mathbf{x} \in \mathbf{S}, (x_i)_{i \in I_k} \in \mathbf{B}\}),$$

for each Borel set $\mathbf{B} \in \mathcal{B}(S_k)$. We define similarly the projections π_{jk} for all $j, k \in [p]$ such that $I_j \cap I_k \neq \emptyset$. For each $k \in [p-1]$, we also rely on the set

$$U_k := \{j \in \{k+1, \dots, p\} : I_j \cap I_k \neq \emptyset\}.$$

Then the CS variant of (3.2) reads as follows:

$$\begin{array}{rll} f_{\text{cs}} := & \inf\limits_{\mu_k} & \sum\limits_{k=1}^{p} \int_{S_k} f_k(\mathbf{x}) \, \mathrm{d}\mu_k(\mathbf{x}) \\ & \text{s.t.} & \pi_{jk}\mu_j = \pi_{kj}\mu_k, \quad j \in U_k, k \in [p-1] \\ & & \int_{S_k} \mathrm{d}\mu_k(\mathbf{x}) = 1, \quad k \in [p] \\ & & \mu_k \in \mathscr{M}_+(S_k), \quad k \in [p] \end{array} \tag{4.3}$$

To prove $f_{\text{cs}} = f_{\min}$ under Assumption 4.1, we rely on the following auxiliary lemma, illustrated in Figure 4.2 in the case $p = 2$. This lemma uses the fact that one can disintegrate a probability measure on a product of Borel spaces into a marginal and a so-called *stochastic* kernel. Given two Borel spaces $\mathbf{S}$, $\mathbf{Z}$, a stochastic kernel $q(\mathrm{d}\mathbf{x}|\mathbf{z})$ on $\mathbf{S}$ given $\mathbf{Z}$ is defined by (1) $q(\mathrm{d}\mathbf{x}|\mathbf{z}) \in \mathscr{M}_+(\mathbf{S})$ for all $\mathbf{z} \in \mathbf{Z}$ and (2) the function $\mathbf{z} \mapsto q(\mathbf{B}|\mathbf{z})$ is $\mathcal{B}(\mathbf{Z})$-measurable for all $\mathbf{B} \in \mathcal{B}(\mathbf{Z})$.

Lemma 4.3 *Let $[n] = \cup_{k=1}^{p} I_k$ with $n_k = |I_k|$, $S_k \subseteq \mathbb{R}^{n_k}$ be given compact sets, and let $\mathbf{S} \subseteq \mathbb{R}^n$ be defined as in (4.2). Let $\mu_1 \in \mathscr{M}_+(S_1), \dots, \mu_p \in \mathscr{M}_+(S_p)$ be measures satisfying the equality constraints of LP (4.3). If RIP (1.7) holds for $I_1, \dots, I_p$, then there exists a probability measure $\mu \in \mathscr{M}_+(\mathbf{S})$ such that*

$$\pi_k \mu = \mu_k, \tag{4.4}$$

for all $k \in [p]$, that is, μ_k is the marginal of μ on $\mathbb{R}^{n_k}$, i.e., with respect to variables indexed by I_k.

PROOF The proof boils down to constructing μ by induction on p. If $p = 1$ and $I_1 = [n]$, the configuration corresponds exactly to the dense LP (3.2) formulation from Chapter 3, and one can simply take $\mu = \mu_1$. For the sake of conciseness, we only provide a proof for the case $p = 2$. Let $I_{12} := I_1 \cap I_2$ with cardinality n_{12}. If $I_{12} = \emptyset$, then one has $\mathbf{S} = \mathbf{S}_1 \times \mathbf{S}_2$ and we can simply define μ as the product measure of μ_1 and μ_2:

$$\mu(\mathbf{A} \times \mathbf{B}) := \mu_1(\mathbf{A}) \times \mu_2(\mathbf{B}),$$

for all $\mathbf{A} \in \mathcal{B}(\mathbb{R}^{n_1}), \mathbf{B} \in \mathcal{B}(\mathbb{R}^{n_2})$. This product measure μ satisfies (4.4).

Next, let us focus on the hardest case where $I_{12} \neq \emptyset$. Let $\overline{\pi}_k$ be the natural projection with respect to $I_k \backslash I_{12}$ and let us define the Borel set $\mathbf{Y}_k := \{\overline{\pi}_k(\mathbf{x}) : \mathbf{x} \in \mathbf{S}_k\} \in \mathcal{B}(\mathbb{R}^{n_k - n_{12}})$. It follows that μ_1, μ_2 can be seen as probability measures on the cartesian products $\mathbf{Y}_1 \times \mathbf{S}_{12} = \mathbf{S}_1$ and $\mathbf{S}_{12} \times \mathbf{Y}_2 = \mathbf{S}_2$, respectively. Let ν_1 and ν_2 be the stochastic kernels of μ_1 and μ_2, respectively. Since $\pi_{12}\mu_1 = \pi_{21}\mu_2 =: \nu$, one can disintegrate μ_1 and μ_2 as

$$\begin{aligned}
\mu_1(\mathbf{A} \times \mathbf{B}) &= \int_{\mathbf{B}} \nu_1(\mathbf{A}|\mathbf{x})\nu(\mathrm{d}\mathbf{x}), \quad \forall \mathbf{A} \in \mathcal{B}(\mathbf{Y}_1), \mathbf{B} \in \mathcal{B}(\mathbb{R}^{n_{12}}), \\
\mu_2(\mathbf{C} \times \mathbf{B}) &= \int_{\mathbf{B}} \nu_2(\mathbf{C}|\mathbf{x})\nu(\mathrm{d}\mathbf{x}), \quad \forall \mathbf{A} \in \mathcal{B}(\mathbf{Y}_2), \mathbf{B} \in \mathcal{B}(\mathbb{R}^{n_{12}}).
\end{aligned}$$

Then, one can define the measure $\mu \in \mathscr{M}_+(\mathbf{Y}_1 \times \mathbb{R}^{n_{12}} \times \mathbf{Y}_2)$ as follows:

$$\mu(\mathbf{A} \times \mathbf{B} \times \mathbf{C}) = \int_{\mathbf{B}} \nu_1(\mathbf{A}|\mathbf{x})\nu_2(\mathbf{C}|\mathbf{x})\nu(\mathrm{d}\mathbf{x}),$$

for every Borel rectangle $\mathbf{A} \times \mathbf{B} \times \mathbf{C} \in \mathcal{B}(\mathbf{Y}_1) \times \mathcal{B}(S_{12}) \times \mathcal{B}(\mathbf{Y}_2)$. In particular if $\mathbf{A} = \mathbf{Y}_1$, one has $\nu_1(\mathbf{A}|\mathbf{x}) = 1$ ν-a.e., and $\mu(\mathbf{Y}_1 \times \mathbf{B} \times \mathbf{C}) = \int_{\mathbf{B}} \nu_2(\mathbf{C}|\mathbf{x})\nu(\mathrm{d}\mathbf{x}) = \mu_2(\mathbf{B} \times \mathbf{C})$, implying that μ_2 is the marginal of μ on $\mathbf{S}_{12} \times \mathbf{Y}_2 = \mathbf{S}_2$. Similarly, μ_1 is the marginal of μ on $\mathbf{Y}_1 \times \mathbf{S}_{12} = \mathbf{S}_1$, yielding the desired result. □

Now, we are ready to prove that LP (4.3) is not just a relaxation of the dense LP (3.2).

Theorem 4.4 *Consider POP (4.1). If Assumption 4.1 holds, then* $f_{\mathrm{cs}} = f_{\min}$.

PROOF The first inequality $f_{\mathrm{cs}} \leq f_{\min}$ is easy to show: let $\mathbf{a}$ be a global minimizer of f on $\mathbf{S}$, assumed to exist thanks to the compactness hypothesis. Let $\mu = \delta_{\mathbf{a}}$ be the Dirac measure concentrated on $\mathbf{a}$, and $\mu_k := \pi_k\mu$ be its projection on $\mathscr{M}_+(S_k)$, for each $k \in [p]$. Namely, μ_k is the Dirac measure concentrated on $(a_i)_{i \in I_k} \in S_k$, and is in particular a probability measure supported on S_k. For each pair j, k such that $I_j \cap I_k \neq \emptyset$, the measure $\pi_{jk}\mu_j$ is the Dirac measure concentrated on $(a_i)_{i \in I_j \cap I_k} \in S_{jk}$, and so is $\pi_{kj}\mu_k$. Therefore, each measure μ_k is a feasible solution of (4.3). In addition, the objective value of LP (4.3) is equal to $\sum_{k=1}^{p} f_k(\mathbf{a}) = f_{\min}$, which proves the first inequality.

To prove the other inequality $f_{\mathrm{cs}} \geq f_{\min}$, let us fix a feasible solution (μ_k) of LP (4.3). By Lemma 4.3, there exists a probability measure $\mu \in \mathscr{M}_+(\mathbf{S})$ such that $\pi_k\mu = \mu_k$, for each $k \in [p]$. Then, one has

$$\sum_{k=1}^{p} \int_{S_k} f_k \, \mathrm{d}\mu_k = \sum_{k=1}^{p} \int_{S_k} f_k \, \mathrm{d}\mu = \int_{\mathbf{S}} \sum_{k=1}^{p} f_k \, \mathrm{d}\mu = \int_{\mathbf{S}} f \mathrm{d}\mu \geq f_{\min}.$$

□

4.3 The CS-adpated moment-SOS hierarchy

In this section, we continue assuming $J' = \emptyset$. For $k \in [p]$, a moment sequence $\mathbf{y} \subseteq \mathbb{R}$ and $g \in \mathbb{R}[\mathbf{x}, I_k]$, let $\mathbf{M}_r(\mathbf{y}, I_k)$ (resp. $\mathbf{M}_r(g\,\mathbf{y}, I_k)$) be the moment (resp. localizing) submatrix obtained from $\mathbf{M}_r(\mathbf{y})$ (resp. $\mathbf{M}_r(g\,\mathbf{y})$) by retaining only those rows and columns indexed by $\beta \in \mathbb{N}^n_r$ of $\mathbf{M}_r(\mathbf{y})$ (resp. $\mathbf{M}_r(g\mathbf{y})$) with $\mathrm{supp}(\beta) \subseteq I_k$.

Example 4.5 *Consider again Example 4.2. The moment matrix $\mathbf{M}_1(\mathbf{y}, I_1)$ is indexed by the support vectors $(0,0,0,0,0,0)$, $(1,0,0,0,0,0)$, $(0,0,0,1,0,0)$ (corresponding to the monomials 1, x_1 and x_4, respectively) and reads as follows:*

$$\mathbf{M}_1(\mathbf{y}, I_1) = \begin{bmatrix} 1 & | & y_{1,0,0,0,0,0} & y_{0,0,0,1,0,0} \\ & - & - & - \\ y_{1,0,0,0,0,0} & | & y_{2,0,0,0,0,0} & y_{1,0,0,1,0,0} \\ y_{0,0,0,1,0,0} & | & y_{1,0,0,1,0,0} & y_{0,0,0,2,0,0} \end{bmatrix}.$$

With $r \geq r_{\min}$, the moment hierarchy based on CS for POP (4.3) is defined as

$$\begin{cases} \inf\limits_{\mathbf{y}_k} & \sum_{k=1}^p L_{\mathbf{y}_k}(f_k) \\ \text{s.t.} & \mathbf{M}_r(\mathbf{y}_k, I_k) \succeq 0, \quad k \in [p] \\ & \mathbf{M}_{r-d_j}(g_j \mathbf{y}_k, I_k) \succeq 0, \quad j \in J_k, k \in [p] \\ & L_{\mathbf{y}_k}(\mathbf{x}^\alpha) = L_{\mathbf{y}_j}(\mathbf{x}^\alpha), \alpha \in \mathbb{N}^n_{2r}, \operatorname{supp}(\alpha) \subseteq I_k \cap I_j, j \in U_k, k \in [p] \\ & L_{\mathbf{y}_k}(1) = 1, \quad k \in [p] \end{cases} \tag{4.5}$$

Note that SDP (4.5) is equivalent to the following program:

$$\mathbf{P}^r_{\text{cs}} : \quad \begin{cases} \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & \mathbf{M}_r(\mathbf{y}, I_k) \succeq 0, \quad k \in [p] \\ & \mathbf{M}_{r-d_j}(g_j \mathbf{y}, I_k) \succeq 0, \quad j \in J_k, k \in [p] \\ & y_{\mathbf{0}} = 1 \end{cases} \tag{4.6}$$

with optimal value denoted by f^r_{cs}. Indeed, for any sequence $\mathbf{y} = (y_\alpha)_{\alpha \in \mathbb{N}^n_{2r}}$, one can define $\mathbf{y}_k := \{y_\alpha : \alpha \in \mathbb{N}^n_{2r}, \operatorname{supp}(\alpha) \subseteq I_k\}$, for all $k \in [p]$. One obviously has $L_{\mathbf{y}_k}(1) = 1$, and each moment matrix $\mathbf{M}_r(\mathbf{y}_k, I_k)$ is equal to $\mathbf{M}_r(\mathbf{y}, I_k)$ (and similarly for the localizing matrices). In addition, if $I_k \cap I_j \neq \emptyset$ and $\operatorname{supp}(\alpha) \subseteq I_k \cap I_j$, then

$$L_{\mathbf{y}_k}(\mathbf{x}^\alpha) = \{y_\alpha : \operatorname{supp}(\alpha) \subseteq I_k \cap I_j\} = L_{\mathbf{y}_j}(\mathbf{x}^\alpha).$$

Let $\Sigma[\mathbf{x}, I_k] \subseteq \mathbb{R}[\mathbf{x}, I_k]$ be the corresponding cone of SOS polynomials. Then the dual of (4.6) is

$$\begin{cases} \sup\limits_{b, \sigma_{k,j}} & b \\ \text{s.t.} & f - b = \sum_{k=1}^p \left(\sigma_{k,0} + \sum_{j \in J_k} \sigma_{k,j} g_j \right) \\ & \sigma_{k,0}, \sigma_{k,j} \in \Sigma[\mathbf{x}, I_k], \quad j \in J_k, k \in [p] \\ & \deg(\sigma_{k,0}), \deg(\sigma_{k,j} g_j) \leq 2r, \quad j \in J_k, k \in [p] \end{cases} \tag{4.7}$$

In the following, we refer to (4.6)–(4.7) as the CSSOS hierarchy. To prove that the sequence $(f^r_{\text{cs}})_{r \geq r_{\min}}$ converges to the global optimum $f_{\min}$ of the original POP (4.1), we rely on Lemma 4.3.

Theorem 4.6 *Consider POP (4.1). If Assumption 4.1 holds, then the CSSOS hierarchy (4.6)–(4.7) provides a nondecreasing sequence of lower bounds $(f^r_{\text{cs}})_{r \geq r_{\min}}$ converging to $f_{\min}$.*

Remark 4.7 *Despite the convergence guarantee stated in Theorem 4.6, note that SDP (4.6) is a relaxation of the dense SDP (3.4) in general, and one can have $f^r_{\text{cs}} < f^r$ for some relaxation order r. The underlying reason is that the situation here is different from the case of PSD matrix completion (Theorem 1.6). Namely, there is no guarantee that one can obtain a PSD matrix completion $\mathbf{M}_r(\mathbf{y})$ from the submatrices $\mathbf{M}_r(\mathbf{y}, I_k)$, $k \in [p]$ because of the specific Hankel structure of $\mathbf{M}_r(\mathbf{y})$.*

As a corollary of Theorem 4.6, we obtain the following representation result, which is a CS version of Putinar's Positivstellensatz.

Theorem 4.8 *Let $f \in \mathbb{R}[\mathbf{x}]$ be positive on a basic compact semialgebraic set $\mathbf{S}$. Let Assumption 4.1 hold. Then,*

$$f = \sum_{k=1}^{p} \left(\sigma_{k,0} + \sum_{j \in J_k} \sigma_{k,j} g_j \right), \tag{4.8}$$

for some polynomials $\sigma_{k,0}, \sigma_{k,j} \in \Sigma[\mathbf{x}, I_k]$, $j \in J_k$, $k \in [p]$.

Let us compare the computational cost of the CSSOS hierarchy (4.7) with the dense hierarchy (3.6). For this, we define $\tau := \max_{k\in[p]} |I_k| = \max_{k\in[p]} n_k$, that is, τ is the maximal size of the subsets $I_1, \ldots, I_p$.

(1) The dense SOS formulation (3.6) involves $m+1$ SOS polynomials in n variables of degree at most $2r$, yielding $m+1$ SDP matrices of size at most $\binom{n+r}{r}$ and $\binom{n+2r}{2r}$ equality constraints.

(2) The CSSOS formulation (4.7) involves $p+m$ SOS polynomials in at most τ variables and of degree at most $2r$, yielding $p+m$ SDP matrices of size at most $\binom{\tau+r}{r}$ and at most $p\binom{\tau+2r}{2r}$ equality constraints.

Overall, when n is fixed and r varies, the r-th step of the hierarchy involves $\mathcal{O}(r^{2n})$ equality constraints in the dense setting against $\mathcal{O}(pr^{2\tau})$ in the sparse setting. This allows one to handle POPs involving several hundred variables if the maximal subset size τ is small (say, $\tau \leq 10$). Furthermore, as shown in the following example, one can also benefit from the computational cost saving when r increases for POPs involving a small number of variables (say, $n \leq 10$).

Example 4.9 *Coming back to Example 4.2, let us compare the hierarchy of dense relaxations given in Chapter 3 with the CS variant. For $r=1$, the dense SDP relaxation (3.6) involves $\binom{n+2r}{2r} = \binom{6+2}{2} = 28$ equality constraints and provides a lower bound of $f^1 = 20.755$ for $f_{\min}$. The dense SDP relaxation (3.6) with $r=2$ involves $\binom{6+4}{4} = 210$ equality constraints and provides a tighter lower bound of $f^2 = 20.8608$. For $r=2$, the sparse SDP relaxation (4.7) involves $\binom{2+4}{4} + 2\binom{4+4}{4} = 155$ equality constraints and provides the same bound $f^2_{\text{cs}} = f^2 = 20.8608$. The dense SDP relaxation with $r=3$ involves 924 equality constraints against 448 for the sparse variant.*

As for the standard dense moment-SOS hierarchy stated in Chapter 3, one can also detect finite convergence of the CSSOS hierarchy and extract global minimizers with a dedicated extraction algorithm — the CS variant of Algorithm 1.

Theorem 4.10 *Consider POP (4.1). Let Assumption 4.1 (i)–(ii) hold and let us consider the hierarchy of moment relaxations $(\mathbf{P}^r_{\text{cs}})_{r\geq r_{\min}}$ defined in (4.6). Let $a_k := \max_{j\in J_k}\{d_j\}$ for all $k \in [p]$. If for some $r \geq r_{\min}$, $\mathbf{P}^r_{\text{cs}}$ has an optimal solution $\mathbf{y}$ which satisfies*

$$\operatorname{rank} \mathbf{M}_r(\mathbf{y}, I_k) = \operatorname{rank} \mathbf{M}_{r-a_k}(\mathbf{y}, I_k) \text{ for all } k \in [p], \tag{4.9}$$

and $\operatorname{rank} \mathbf{M}_r(\mathbf{y}, I_j \cap I_k) = 1$ for all pairs (j,k) with $I_j \cap I_k \neq \emptyset$, then the SDP relaxation (4.6) is exact, i.e., $f^r_{\text{cs}} = f_{\min}$. In addition, for each $k \in [p]$, let $\Delta_k := \{\mathbf{x}(k)\} \subseteq \mathbb{R}^{n_k}$ be a set of solutions obtained from the extraction procedure `Extract`*, stated in Algorithm 1 and applied to the moment matrix $\mathbf{M}_r(\mathbf{y}, I_k)$. Then every $\mathbf{x} \in \mathbb{R}^n$ obtained by $(x_i)_{i\in I_k} = \mathbf{x}(k)$ for some $\mathbf{x}(k) \in \Delta_k$ is a global minimizer of POP (4.1).*

Note that Assumption 4.1 (iii)–(iv) are not required in Theorem 4.10, as the rank conditions are strong enough to ensure finite convergence and extraction of a subset of global minimizers.

For more details on correlative sparsity, please refer to [WKKM06, Las06a].

4.4 Term sparsity

In this section, we describe an iterative procedure to exploit TS for the primal-dual moment-SOS relaxations of unconstrained POPs. Recall the formulation of an unconstrained POP:

$$\mathbf{P}: \quad f_{\min} := \inf\{f(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^n\} = \sup\{b : f - b \geq 0\}, \tag{4.10}$$

where $f = \sum_\alpha f_\alpha \mathbf{x}^\alpha \in \mathbb{R}[\mathbf{x}]$. Suppose that f is of degree $2d$ with $\operatorname{supp}(f) = \mathscr{A}$ (w.l.o.g. assuming $\mathbf{0} \in \mathscr{A}$) and $\mathbf{x}^{\mathscr{B}} := (\mathbf{x}^\beta)_{\beta\in\mathscr{B}}$ is a monomial basis arranged with resepct to any fixed ordering. For convenience, we slightly abuse notation in the sequel and denote by $\mathscr{B}$ (resp. β) instead of $\mathbf{x}^{\mathscr{B}}$ (resp. $\mathbf{x}^\beta$) a monomial basis (resp. a monomial). One may choose $\mathscr{B}$ to be the standard monomial basis $\mathbb{N}^n_d$. But when f is sparse, we may use a (possibly) smaller monomial basis by considering Newton polytopes.

Given a monomial basis $\mathscr{B}$ and a sequence $\mathbf{y} \subseteq \mathbb{R}$, the moment matrix $\mathbf{M}_{\mathscr{B}}(\mathbf{y})$ associated with $\mathscr{B}$ and $\mathbf{y}$ is the block of the moment matrix $\mathbf{M}_d(\mathbf{y})$ indexed by $\mathscr{B}$. Then the moment relaxation of $\mathbf{P}$ in the monomial basis $\mathscr{B}$ is given by

$$\mathbf{P}_{\text{mom}}: \quad \begin{array}{rll} f_{\text{mom}} := & \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ & \text{s.t.} & \mathbf{M}_{\mathscr{B}}(\mathbf{y}) \succeq 0 \\ & & y_{\mathbf{0}} = 1 \end{array} \tag{4.11}$$

For a graph $G(V,E)$ with $V \subseteq \mathbb{N}^n$, let the support of G be given by

$$\operatorname{supp}(G) := \{\beta + \gamma \mid \beta = \gamma \text{ or } \{\beta,\gamma\} \in E\}. \tag{4.12}$$

We define G^{tsp} to be the graph with nodes $V = \mathscr{B}$ and with edges

$$E(G^{\text{tsp}}) = \{\{\beta,\gamma\} \mid \beta \neq \gamma \in V, \beta + \gamma \in \mathscr{A} \cup (2\mathscr{B})\}, \tag{4.13}$$

which is called the tsp graph associated with f.

Starting with the initial graph $G^{(0)} = G^{\text{tsp}}$, we now define a sequence of graphs $(G^{(s)})_{s\geq 1}$ by iteratively performing two successive operations:

(1) **support extension**. Let $F^{(s)}$ be the graph with nodes V and with edges

$$E(F^{(s)}) = \left\{\{\beta,\gamma\} \mid \beta \neq \gamma \in V, \beta + \gamma \in \operatorname{supp}(G^{(s-1)})\right\}. \tag{4.14}$$

(2) **chordal extension**. Let $G^{(s)} = (F^{(s)})'$.

Example 4.11 *Let us consider the graph $G(V,E)$ with*

$$V = \{1, x_1, x_2, x_3, x_2x_3, x_1x_3, x_1x_2\} \text{ and } E = \{\{1, x_2x_3\}, \{x_2, x_1x_3\}\}.$$

Figure 4.3 illustrates the support extension of G.

By construction, one has $G^{(s)} \subseteq G^{(s+1)}$ for $s \geq 1$ and therefore the sequence of graphs $(G^{(s)})_{s\geq 1}$ stabilizes after a finite number of steps. Following what we introduced in Chapter 1.4, we denote by $\Pi_{G^{(s)}}(\mathbb{S}^+_{|\mathscr{B}|})$ the set of matrices in $\mathbb{S}(G^{(s)})$ that have a PSD completion, and denote by $\mathbf{B}_{G^{(s)}}$ the adjacency matrix of $G^{(s)}$. If f is sparse, by replacing $\mathbf{M}_{\mathscr{B}}(\mathbf{y}) \succeq 0$ with the weaker condition $\mathbf{M}_{\mathscr{B}}(\mathbf{y}) \in \Pi_{G^{(s)}}(\mathbb{S}^+_{|\mathscr{B}|})$ in (4.11), we then obtain a sparse moment relaxation of (4.10) for each $s \geq 1$:

$$\mathbf{P}^s_{\text{ts}}: \quad \begin{cases} \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ \text{s.t.} & \mathbf{B}_{G^{(s)}} \circ \mathbf{M}_{\mathscr{B}}(\mathbf{y}) \in \Pi_{G^{(s)}}(\mathbb{S}^+_{|\mathscr{B}|}) \\ & y_{\mathbf{0}} = 1 \end{cases} \tag{4.15}$$

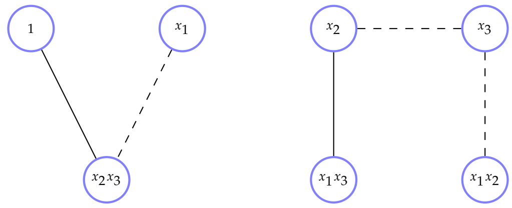

Figure 4.3: The support extension of G in Example 4.11. The dashed edges are added after support extension.

with optimum denoted by f_{ts}^s. We call $(\mathbf{P}_{\text{ts}}^s)_{s\geq 1}$ the TSSOS hierarchy for $\mathbf{P}$ and call s the *sparse order*.

Remark 4.12 *The intuition behind the support extension operation is that once one position related to y_α in the moment matrix $\mathbf{M}_{\mathscr{B}}(\mathbf{y})$ is "activated" in the sparsity pattern, then all positions related to y_α in $\mathbf{M}_{\mathscr{B}}(\mathbf{y})$ should be "activated". In addition, Theorems 1.5 and 1.6 provide the rationale behind the mechanism of the chordal extension operation.*

Theorem 4.13 *The sequence $(f_{\text{ts}}^s)_{s\geq 1}$ is monotonically nondecreasing and $f_{\text{ts}}^s \leq f_{mom}$ for all $s \geq 1$.*

PROOF The inclusion $G^{(k)} \subseteq G^{(k+1)}$ implies that each maximal clique of $G^{(k)}$ is a subset of some maximal clique of $G^{(k+1)}$. Thus by Theorem 1.6, we see that $\mathbf{P}_{\text{ts}}^s$ is a relaxation of $\mathbf{P}_{\text{ts}}^{s+1}$ (and also a relaxation of $\mathbf{P}_{\text{mom}}$). This yields the desired conclusions. □

As a consequence of Theorem 4.13, we obtain the following hierarchy of lower bounds for the optimum of $\mathbf{P}$:

$$f_{\text{ts}}^1 \leq f_{\text{ts}}^2 \leq \cdots \leq f_{\text{mom}} \leq f_{\text{min}}. \tag{4.16}$$

If the maximal chordal extension is chosen for the chordal extension operation, then we can show (see [WML21b] for more details) that the sequence $(f_{\text{ts}}^s)_{s\geq 1}$ converges to the global optimum f_{min}. Otherwise, there is no guarantee of such convergence as illustrated by the following example.

Example 4.14 *Consider*

$$\begin{aligned} f = & x_1^2 - 2x_1x_2 + 3x_2^2 - 2x_1^2x_2 + 2x_1^2x_2^2 - 2x_2x_3 + 6x_3^2 \\ & + 18x_2^2x_3 - 54x_2x_3^2 + 142x_2^2x_3^2. \end{aligned}$$

The monomial basis computed from the Newton polytope is $\{1, x_1, x_2, x_3, x_1x_2, x_2x_3\}$. Figure 4.4 shows the tsp graph G^{tsp} (without dashed edges) and its smallest chordal extension $G^{(1)}$ (with dashed edges) for f. The graph sequence $(G^{(s)})_{s\geq 1}$ stabilizes at $s = 1$. Solving $\mathbf{P}_{\text{ts}}^1$, we obtain $f_{\text{ts}}^1 \approx -0.00355$ while $f_{mom} = f_{\text{min}} = 0$. On the other hand, note that G^{tsp} has only one connected component. So with the maximal chordal extension, we immediately get the complete graph and it follows $f_{\text{ts}}^1 = f_{mom} = 0$ in this case.

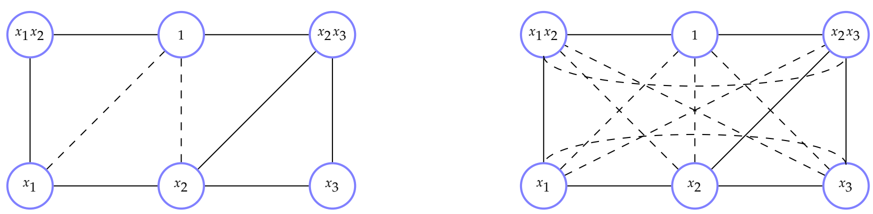

Figure 4.4: The tsp graph G^{tsp} and a smallest chordal extension (left) as well as the maximal chordal extension (right) for Example 4.14.

For each $s \geq 1$, the dual SDP of (4.15) is

$$\begin{cases} \sup\limits_{\mathbf{G},b} & b \\ \text{s.t.} & \langle \mathbf{G}, \mathbf{B}_\alpha \rangle = f_\alpha - b 1_{\alpha=\mathbf{0}}, \quad \forall \alpha \in \operatorname{supp}(G^{(s)}) \\ & \mathbf{G} \in \mathbb{S}^+_{|\mathscr{B}|} \cap \mathbb{S}(G^{(s)}) \end{cases} \tag{4.17}$$

where $\mathbf{B}_\alpha$ has been defined after (3.5).

Proposition 4.15 *For each $s \geq 1$, there is no duality gap between $\mathbf{P}^s_{\text{ts}}$ and its dual (4.17).*

PROOF This easily follows from the fact that $\mathbf{P}^s_{\text{ts}}$ satisfies Slater's condition by Proposition 3.1 of [Las01] and Theorem 1.6. □

4.5 The TSSOS hierarchy for constrained POPs

In this section, we describe an iterative procedure to exploit TS for the primal-dual moment-SOS hierarchy of constrained POPs:

$$\mathbf{P}: \quad f_{\min} := \inf \{ f(\mathbf{x}) : \mathbf{x} \in \mathbf{S} \}, \tag{4.18}$$

with

$$\mathbf{S} = \{ \mathbf{x} \in \mathbb{R}^n \mid g_1(\mathbf{x}) \geq 0, \ldots, g_m(\mathbf{x}) \geq 0 \}. \tag{4.19}$$

Let $\mathscr{A}$ denote the union of supports involved in $\mathbf{P}$, i.e.,

$$\mathscr{A} = \operatorname{supp}(f) \cup \bigcup_{j=1}^{m} \operatorname{supp}(g_j). \tag{4.20}$$

Let $r_{\min} := \max \{ \lceil \deg(f)/2 \rceil, d_1, \ldots, d_m \}$ with $d_j := \lceil \deg(g_j)/2 \rceil$ for $j \in [m]$. Fix a relaxation order $r \geq r_{\min}$. Let $g_0 = 1$, $d_0 = 0$ and $\mathscr{B}_{r,j} = \mathbb{N}^n_{r-d_j}$ be the standard monomial basis for $j = 0, 1, \ldots, m$. We define a graph G^{tsp} with nodes $\mathscr{B}_{r,0}$ and edges

$$E(G^{\text{tsp}}) = \{ \{\beta, \gamma\} \mid \beta \neq \gamma \in \mathscr{B}_{r,0}, \beta + \gamma \in \mathscr{A} \cup (2\mathscr{B}_{r,0}) \}, \tag{4.21}$$

which is called the tsp graph associated with $\mathbf{P}$ or essentially $\mathscr{A}$.

Now let us initialize with $G^{(0)}_{r,0} := G^{\text{tsp}}$ and $G^{(0)}_{r,j}$ being an empty graph for $j \in [m]$. Then for each $j \in \{0\} \cup [m]$, we define a sequence of graphs $(G^{(s)}_{r,j})_{s \geq 1}$ by iteratively performing two successive operations:

(1) **support extension**. Let $F^{(s)}_{r,j}$ be the graph with nodes $\mathscr{B}_{r,j}$ and edges

$$\begin{aligned} E(F^{(s)}_{r,j}) = \Big\{ & \{\beta, \gamma\} \mid \beta \neq \gamma \in \mathscr{B}_{r,j}, \\ & (\operatorname{supp}(g_j) + \beta + \gamma) \cap \bigcup_{i=0}^{m} (\operatorname{supp}(g_i) + \operatorname{supp}(G^{(s-1)}_{r,i})) \neq \emptyset \Big\}. \end{aligned} \tag{4.22}$$

(2) **chordal extension**. Let

$$G^{(s)}_{r,j} := (F^{(s)}_{r,j})', \quad j \in \{0\} \cup [m]. \tag{4.23}$$

Recall that the dense moment relaxation of order r for $\mathbf{P}$ is given by

$$\mathbf{P}^r: \quad \begin{aligned} f^r_{\text{mom}} := & \inf_{\mathbf{y}} & & L_{\mathbf{y}}(f) \\ & \text{s.t.} & & \mathbf{M}_{r-d_j}(g_j \mathbf{y}) \succeq 0, \quad j \in \{0\} \cup [m] \\ & & & y_{\mathbf{0}} = 1 \end{aligned} \tag{4.24}$$

Let $t_j := |\mathscr{B}_{r,j}| = \binom{n+r-d_j}{r-d_j}$. Therefore by replacing $\mathbf{M}_{r-d_j}(g_j\mathbf{y}) \succeq 0$ with the weaker condition $\mathbf{B}_{G_{r,j}^{(s)}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y}) \in \Pi_{G_{r,j}^{(s)}}(\mathbb{S}_{t_j}^+)$ for $j \in \{0\} \cup [m]$ in (4.24), we obtain the following sparse moment relaxation of $\mathbf{P}^r$ and $\mathbf{P}$ for each $s \geq 1$:

$$\mathbf{P}_{\text{ts}}^{r,s}: \quad \begin{array}{rll} f_{\text{ts}}^{r,s} := & \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ & \text{s.t.} & \mathbf{B}_{G_{r,0}^{(s)}} \circ \mathbf{M}_r(\mathbf{y}) \in \Pi_{G_{r,0}^{(s)}}(\mathbb{S}_{t_0}^+) \\ & & \mathbf{B}_{G_{r,j}^{(s)}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y}) \in \Pi_{G_{r,j}^{(s)}}(\mathbb{S}_{t_j}^+), \quad j \in [m] \\ & & y_{\mathbf{0}} = 1 \end{array} \tag{4.25}$$

As in the unconstrained case, we call s the sparse order. By construction, one has $G_{r,j}^{(s)} \subseteq G_{r,j}^{(s+1)}$ for all j,s. Therefore, for each $j \in \{0\} \cup [m]$, the sequence of graphs $(G_{r,j}^{(s)})_{s\geq 1}$ stabilizes after a finite number of steps. We denote the stabilized graph by $G_{r,j}^{(\bullet)}$ for all j and the corresponding moment relaxation by $\mathbf{P}_{\text{ts}}^{r,\bullet}$ with optimum $f_{\text{ts}}^{r,\bullet}$.

For each $s \geq 1$, the dual SDP of $\mathbf{P}_{\text{ts}}^{r,s}$ reads as

$$\begin{cases} \sup\limits_{\mathbf{G}_j, b} & b \\ \text{s.t.} & \sum_{j=0}^m \langle \mathbf{C}_\alpha^j, \mathbf{G}_j \rangle = f_\alpha - b\mathbf{1}_{\alpha=\mathbf{0}}, \quad \forall \alpha \in \bigcup_{j=0}^m (\text{supp}(g_j) + \text{supp}(G_{r,j}^{(s)})) \\ & \mathbf{G}_j \in \mathbb{S}_{t_j}^+ \cap \mathbb{S}(G_{r,j}^{(s)}), \quad j \in \{0\} \cup [m] \end{cases} \tag{4.26}$$

where $\mathbf{C}_\alpha^j$ is defined after (3.5). The primal-dual SDP relaxations (4.25)–(4.26) are called the TSSOS hierarchy associated with $\mathbf{P}$, which is indexed by two parameters: the relaxation order r and the sparse order s.

Theorem 4.16 *With the above notation, the following hold:*

(i) Assume that $\mathbf{S}$ has a nonempty interior. Then there is no duality gap between $\mathbf{P}_{\text{ts}}^{r,s}$ and its dual (4.26) for any $r \geq r_{\min}$ and $s \geq 1$.

(ii) Fixing a relaxation order $r \geq r_{\min}$, the sequence $(f_{\text{ts}}^{r,s})_{s\geq 1}$ is monotonically nondecreasing and $f_{\text{ts}}^{r,s} \leq f_{\text{mom}}^r$ for all $s \geq 1$.

(iii) When the maximal chordal extension is used for the chordal extension operation, the sequence $(f_{\text{ts}}^{r,s})_{s\geq 1}$ converges to f_{mom}^r in finitely many steps.

(iv) Fixing a sparse order $s \geq 1$, the sequence $(f_{\text{ts}}^{r,s})_{r\geq r_{\min}}$ is monotonically nondecreasing.

PROOF (i). This easily follows from the fact that $\mathbf{P}_{\text{ts}}^{r,s}$ satisfies Slater's condition by Theorem 4.2 of [Las01] and Theorem 1.6.

(ii). For all j,s, the inclusion $G_{r,j}^{(s)} \subseteq G_{r,j}^{(s+1)}$ implies that each maximal clique of $G_{r,j}^{(s)}$ is a subset of some maximal clique of $G_{r,j}^{(s+1)}$. Hence by Theorem 1.6, $\mathbf{P}_{\text{ts}}^{r,s}$ is a relaxation of $\mathbf{P}_{\text{ts}}^{r,s+1}$ (and also a relaxation of $\mathbf{P}^r$) from which we have that $(f_{\text{ts}}^{r,s})_{s\geq 1}$ is monotonically nondecreasing and $f_{\text{ts}}^{r,s} \leq f_{\text{mom}}^r$ for all $s \geq 1$.

(iii). Let $\mathbf{y} = (y_\alpha)$ be an arbitrary feasible solution of $\mathbf{P}_{\text{ts}}^{r,\bullet}$. We note that $\{y_\alpha \mid \alpha \in \bigcup_{j\in\{0\}\cup[m]}(\text{supp}(g_j) + \text{supp}(G_{r,j}^{(\bullet)}))\}$ is the set of decision variables involved in $\mathbf{P}_{\text{ts}}^{r,\bullet}$, and $\{y_\alpha \mid \alpha \in \mathbb{N}_{2r}^n\}$ is the set of decision variables involved in $\mathbf{P}^r$ (4.24). We then define a vector $\overline{\mathbf{y}} = (\overline{y}_\alpha)_{\alpha\in\mathbb{N}_{2r}^n}$ as follows:

$$\overline{y}_\alpha = \begin{cases} y_\alpha, & \text{if } \alpha \in \bigcup_{j\in\{0\}\cup[m]}(\text{supp}(g_j) + \text{supp}(G_{r,j}^{(\bullet)})), \\ 0, & \text{otherwise.} \end{cases}$$

By construction and since $G_{r,j}^{(\bullet)}$ stabilizes under support extension for all j, we immediately have $\mathbf{M}_{r-d_j}(g_j\overline{\mathbf{y}}) = \mathbf{B}_{G_{r,j}^{(\bullet)}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y})$. As we use the maximal chordal extension for the chordal extension operation, the matrix $\mathbf{B}_{G_{r,j}^{(\bullet)}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y})$ is block-diagonal up to permutation. So from $\mathbf{B}_{G_{r,j}^{(\bullet)}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y}) \in \Pi_{G_{r,j}^{(\bullet)}}(\mathbb{S}_+^{t_j})$ it follows $\mathbf{M}_{r-d_j}(g_j\overline{\mathbf{y}}) \succeq 0$ for $j \in \{0\} \cup [m]$. Therefore $\overline{\mathbf{y}}$ is a feasible solution of $\mathbf{P}^r$ and so $L_{\mathbf{y}}(f) = L_{\overline{\mathbf{y}}}(f) \geq f_{\mathrm{mom}}^r$. Hence $f_{\mathrm{ts}}^{r,\bullet} \geq f_{\mathrm{mom}}^r$ as $\mathbf{y}$ is an arbitrary feasible solution of $\mathbf{P}_{\mathrm{ts}}^{r,\bullet}$. By (ii), we already have $f_{\mathrm{ts}}^{r,\bullet} \leq f_{\mathrm{mom}}^r$. Therefore, $f_{\mathrm{ts}}^{r,\bullet} = f_{\mathrm{mom}}^r$ as desired.

(iv). The conclusion follows if we can show that $G_{r,j}^{(s)} \subseteq G_{r+1,j}^{(s)}$ for all j, r since by Theorem 1.6 this implies that $\mathbf{P}_{\mathrm{ts}}^{r,s}$ is a relaxation of $\mathbf{P}_{\mathrm{ts}}^{r+1,s}$. Let us prove $G_{r,j}^{(s)} \subseteq G_{r+1,j}^{(s)}$ by induction on s. For $s = 1$, from (4.21), we have $G_{r,0}^{(0)} \subseteq G_{r+1,0}^{(0)}$, which implies $G_{r,j}^{(1)} \subseteq G_{r+1,j}^{(1)}$ for $j \in \{0\} \cup [m]$. Now assume that $G_{r,j}^{(s)} \subseteq G_{r+1,j}^{(s)}$, $j \in \{0\} \cup [m]$ hold for a given $s \geq 1$. Then from (4.22) and by the induction hypothesis, we have $G_{r,j}^{(s+1)} \subseteq G_{r+1,j}^{(s+1)}$ for $j \in \{0\} \cup [m]$, which completes the induction and also completes the proof. □

By Theorem 4.16, we have the following two-level hierarchy of lower bounds for the optimum $f_{\min}$ of $\mathbf{P}$:

$$\begin{array}{ccccccc}
f_{\mathrm{ts}}^{r_{\min},1} & \leq & f_{\mathrm{ts}}^{r_{\min},2} & \leq & \cdots & \leq & f_{\mathrm{mom}}^{r_{\min}} \\
\wedge| & & \wedge| & & & & \wedge| \\
f_{\mathrm{ts}}^{r_{\min}+1,1} & \leq & f_{\mathrm{ts}}^{r_{\min}+1,2} & \leq & \cdots & \leq & f_{\mathrm{mom}}^{r_{\min}+1} \\
\wedge| & & \wedge| & & & & \wedge| \\
\vdots & & \vdots & & \vdots & & \vdots \\
\wedge| & & \wedge| & & & & \wedge| \\
f_{\mathrm{ts}}^{r,1} & \leq & f_{\mathrm{ts}}^{r,2} & \leq & \cdots & \leq & f_{\mathrm{mom}}^{r} \\
\wedge| & & \wedge| & & & & \wedge| \\
\vdots & & \vdots & & \vdots & & \vdots
\end{array} \tag{4.27}$$

The TSSOS hierarchy entails a trade-off between the computational cost and the quality of the obtained lower bound via the two tunable parameters r and s. Besides, one has the freedom to choose a specific chordal extension in (4.23) (e.g., maximal chordal extensions, approximately smallest chordal extensions and so on). This choice could affect the resulting sizes of PSD blocks and the quality of the related lower bound. Intuitively, chordal extensions with smaller clique numbers would lead to PSD blocks of smaller sizes and lower bounds of (possibly) lower quality while chordal extensions with larger clique numbers would lead to PSD blocks with larger sizes and lower bounds of (possibly) higher quality.

Remark 4.17 *If $\mathbf{P}$ is a QCQP, then $\mathbf{P}_{ts}^{1,1}$ and $\mathbf{P}^1$ yield the same lower bound, i.e., $f_{\mathrm{ts}}^{1,1} = f_{\mathrm{mom}}^1$. Indeed, for a QCQP, the moment relaxation $\mathbf{P}^1$ reads as*

$$\begin{cases}
\inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\
\text{s.t.} & \mathbf{M}_1(\mathbf{y}) \succeq 0 \\
& L_{\mathbf{y}}(g_j) \geq 0, \quad j \in [m] \\
& y_{\mathbf{0}} = 1
\end{cases}$$

Note that the objective function and the affine constraints of $\mathbf{P}^1$ involve only the decision variables $\{y_{\mathbf{0}}\} \cup \{y_\alpha\}_{\alpha \in \mathscr{A}}$ with $\mathscr{A} = \mathrm{supp}(f) \cup \bigcup_{j=1}^m \mathrm{supp}(g_j)$. Hence there is no discrepancy of optima in replacing $\mathbf{P}^1$ with $\mathbf{P}_{\mathrm{ts}}^{1,1}$ by construction.

4.6 Sign symmetries and a sparse representation theorem for positive polynomials

The exploitation of TS developed in the previous sections is closely related to *sign symmetries*. Intuitively, a polynomial is said to have sign symmetries if it is invariant when we change signs of some variables. For instance, the polynomial $f(x_1, x_2) = x_1^2 + x_2^2 + x_1x_2$ has the sign symmetry associated to $(x_1, x_2) \mapsto (-x_1, -x_2)$ as $f(-x_1, -x_2) = f(x_1, x_2)$. To be more precise, we give the following definition of sign symmetries in terms of support sets.

Definition 4.18 (sign symmetry) *Given a finite set $\mathscr{A} \subseteq \mathbb{N}^n$, the* sign symmetries *of $\mathscr{A}$ are defined by all vectors $\mathbf{s} \in \mathbb{Z}_2^n := \{0,1\}^n$ such that $\mathbf{s}^\intercal \alpha \equiv 0 \pmod 2$ for all $\alpha \in \mathscr{A}$.*

Assume that the maximal chordal extension is chosen for the chordal extension operation in Chapter 4.5. As mentioned earlier, for any j the sequence of graphs $(G_{r,j}^{(s)})_{s\geq 1}$ ends up with $G_{r,j}^{(\bullet)}$ in finitely many steps. Note that the graph $G_{r,j}^{(\bullet)}$ induces a partition of the monomial basis $\mathbb{N}^n_{r-d_j}$: two monomials $\beta, \gamma \in \mathbb{N}^n_{r-d_j}$ belong to the same block if and only if they belong to the same connected component of $G_{r,j}^{(\bullet)}$. The following theorem provides an interpretation of this partition in terms of sign symmetries.

Theorem 4.19 *Notations are as in the previous sections. Fix the relaxation order $r \geq r_{\min}$. Assume that the maximal chordal extension is chosen for the chordal extension operation and the sign symmetries of $\mathscr{A}$ are given by the columns of a binary matrix denoted by $\mathbf{R}$. Then for each $j \in \{0\} \cup [m]$, β, γ belong to the same block in the partition of $\mathbb{N}^n_{r-d_j}$ induced by $G_{r,j}^{(\bullet)}$ if and only if $\mathbf{R}^\intercal(\beta + \gamma) \equiv 0 \pmod 2$. In other words, for a fixed relaxation order the block structures arising from the TSSOS hierarchy converge to the block structure determined by the sign symmetries of the POP assuming that the maximal chordal extension is used for the chordal extension operation.*

Theorem 4.19 is applied for the standard monomial basis $\mathbb{N}^n_{r-d_j}$. If a smaller monomial basis is chosen, then we only have the "only if" part of the conclusion in Theorem 4.19.

Example 4.20 *Let $f = 1 + x_1^2x_2^4 + x_1^4x_2^2 + x_1^4x_2^4 - x_1x_2^2 - 3x_1^2x_2^2$ and $\mathscr{A} = \operatorname{supp}(f)$. The monomial basis given by the Newton polytope method is $\mathscr{B} = \{1, x_1x_2, x_1x_2^2, x_1^2x_2, x_1^2x_2^2\}$. The sign symmetries of $\mathscr{A}$ consist of two elements: $(0,0)$ and $(0,1)$. According to the sign symmetries, $\mathscr{B}$ is partitioned into $\{1, x_1x_2^2, x_1^2x_2^2\}$ and $\{x_1x_2, x_1^2x_2\}$. On the other hand, the partition of $\mathscr{B}$ induced by $G^{(\bullet)}$ is $\{1, x_1x_2^2, x_1^2x_2^2\}$, $\{x_1x_2\}$ and $\{x_1^2x_2\}$, which is a refinement of the partition determined by the sign symmetries.*

As a corollary of Theorem 4.19, we can prove a sparse representation theorem for positive polynomials on compact basic semialgebraic sets.

Theorem 4.21 *Let $\mathbf{S}$ be defined as in (4.19). Assume that the quadratic module $\mathcal{M}(\mathfrak{g})$ is Archimedean and that the polynomial f is positive on $\mathbf{S}$. Let $\mathscr{A} = \operatorname{supp}(f) \cup \bigcup_{j=1}^m \operatorname{supp}(g_j)$ and let the sign symmetries of $\mathscr{A}$ be given by the columns of the binary matrix R. Then f can be decomposed as*

$$f = \sigma_0 + \sum_{j=1}^m \sigma_j g_j,$$

for some SOS polynomials $\sigma_0, \sigma_1, \ldots, \sigma_m$ satisfying $R^\intercal \alpha \equiv 0 \pmod 2$ for any $\alpha \in \operatorname{supp}(\sigma_j)$, $j = 0, \ldots, m$.

PROOF By Putinar's Positivstellensatz (Theorem 2.9), there exist SOS polynomials $\sigma_0', \sigma_1', \ldots, \sigma_m'$ such that

$$f = \sigma_0' + \sum_{j=1}^{m} \sigma_j' g_j. \tag{4.28}$$

Let $d_j = \lceil \deg(g_j)/2 \rceil, j = 0, 1, \ldots, m$ and

$$r = \max\{\lceil \deg(\sigma_j' g_j)/2 \rceil : j = 0, 1, \ldots, m\}$$

with $g_0 = 1$. Let $\mathbf{G}_j$ be a Gram matrix associated with σ_j' and indexed by the monomial basis $\mathbb{N}^n_{r-d_j}, j = 0, 1, \ldots, m$. Then define $\sigma_j = (\mathbf{x}^{\mathbb{N}^n_{r-d_j}})^\intercal (\mathbf{B}_{G^{(\bullet)}_{r,j}} \circ \mathbf{G}_j) \mathbf{x}^{\mathbb{N}^n_{r-d_j}}$ for $j = 0, 1, \ldots, m$, where $G^{(\bullet)}_{r,j}$ is defined in Chapter 4.5. For any $j \in \{0\} \cup [m]$, since $\mathbf{B}_{G^{(\bullet)}_{r,j}} \circ \mathbf{G}_j$ is block-diagonal (up to permutation) and $\mathbf{G}_j$ is positive semidefinite, we see that σ_j is an SOS polynomial.

Suppose $\alpha \in \mathrm{supp}(\sigma_j)$ with $j \in \{0\} \cup [m]$. Then we can write $\alpha = \alpha' + \beta + \gamma$ for some $\alpha' \in \mathrm{supp}(g_j)$ and some β, γ belonging to the same connected component of $G^{(\bullet)}_{r,j}$. By Theorem 4.19, we have $\mathbf{R}^\intercal(\beta + \gamma) \equiv 0 \pmod 2$ and therefore, $\mathbf{R}^\intercal \alpha \equiv 0 \pmod 2$. Moreover, for any $\alpha' \in \mathrm{supp}(g_j)$ and β, γ not belonging to the same connected component of $G^{(\bullet)}_{r,j}$, we have $\mathbf{R}^\intercal(\beta + \gamma) \not\equiv 0 \pmod 2$ by Theorem 4.19 and so $\mathbf{R}^\intercal(\alpha' + \beta + \gamma) \not\equiv 0 \pmod 2$. From these facts we deduce that substituting σ_j' with σ_j in (4.28) is just removing the terms whose exponents α do not satisfy $\mathbf{R}^\intercal \alpha \equiv 0 \pmod 2$ from the right-hand side of (4.28). Doing so, one does not change the match of coefficients on both sides of the equality. Thus we have

$$f = \sigma_0 + \sum_{j=1}^{m} \sigma_j g_j,$$

with the desired property. □

4.7 The CS-TSSOS hierarchy

The underlying idea to exploit CS and TS simultaneously in the moment-SOS hierarchy consists of the following two steps:

(1) decomposing the set of variables into a tuple of cliques $\{I_k\}_{k \in [p]}$ by exploiting CS;

(2) applying the iterative procedure for exploiting TS to each decoupled subsystem involving variables $\mathbf{x}(I_k)$.

More concretely, let us fix a relaxation order $r \geq r_{\min}$. Suppose that G^{csp} is the csp graph associated to POP (3.1) defined as in Chapter 4.1, $(G^{\mathrm{csp}})'$ is a chordal extension of G^{csp}, and $I_k, k \in [p]$ are the maximal cliques of $(G^{\mathrm{csp}})'$ with cardinality being denoted by $n_k, k \in [p]$. As in Chapter 4.1, the set of variables $\mathbf{x}$ is decomposed into $\mathbf{x}(I_1), \mathbf{x}(I_2), \ldots, \mathbf{x}(I_p)$ by exploiting CS. In addition, assume that the constraints are assigned to the variable cliques according to $J_1, \ldots, J_p, J'$ as defined in Chapter 4.1.

Now we apply the iterative procedure for exploiting TS to each subsystem involving variables $\mathbf{x}(I_k), k \in [p]$ in the following way. Let

$$\mathscr{A} := \mathrm{supp}(f) \cup \bigcup_{j=1}^{m} \mathrm{supp}(g_j) \text{ and } \mathscr{A}_k := \{\alpha \in \mathscr{A} \mid \mathrm{supp}(\alpha) \subseteq I_k\} \tag{4.29}$$

for $k \in [p]$. Let $\mathbb{N}^{n_k}_{r-d_j}$ be the standard monomial basis for $j \in \{0\} \cup J_k, k \in [p]$. Let $G^{\mathrm{tsp}}_{r,k}$ be the tsp graph with nodes $\mathbb{N}^{n_k}_r$ associated to the support $\mathscr{A}_k$ defined as in Chapter 4.4, i.e., its node set is

$\mathbb{N}^{n_k}_r$ and $\{\beta,\gamma\}$ is an edge if $\beta+\gamma\in\mathscr{A}_k\cup 2\mathbb{N}^{n_k}_r$. Note that here we embed $\mathbb{N}^{n_k}_r$ into $\mathbb{N}^n_r$ via the map $\alpha=(\alpha_i)\in\mathbb{N}^{n_k}_r\mapsto\alpha'=(\alpha'_i)\in\mathbb{N}^n_r$ satisfying

$$\alpha'_i=\begin{cases}\alpha_i, & \text{if } i\in I_k,\\ 0, & \text{otherwise.}\end{cases}$$

Let us define $G^{(0)}_{r,k,0}:=G^{\text{tsp}}_{r,k}$ and $G^{(0)}_{r,k,j}, j\in J_k, k\in[p]$ are all empty graphs. Next for each $j\in\{0\}\cup J_k$ and each $k\in[p]$, we iteratively define an ascending chain of graphs $(G^{(s)}_{r,k,j}(V_{r,k,j},E^{(s)}_{r,k,j}))_{s\geq1}$ with $V_{r,k,j}:=\mathbb{N}^{n_k}_{r-d_j}$ via two successive operations:

(1) **support extension**. Define $F^{(s)}_{r,k,j}$ to be the graph with nodes $V_{r,k,j}$ and with edges

$$E(F^{(s)}_{r,k,j})=\left\{\{\beta,\gamma\}\mid\beta\neq\gamma\in V_{r,k,j},(\beta+\gamma+\text{supp}(g_j))\cap\mathscr{C}^{(s-1)}_r\neq\emptyset\right\},\tag{4.30}$$

where

$$\mathscr{C}^{(s-1)}_r:=\bigcup_{k=1}^{p}\left(\bigcup_{j\in\{0\}\cup J_k}\left(\text{supp}(g_j)+\text{supp}(G^{(s-1)}_{r,k,j})\right)\right).\tag{4.31}$$

(2) **chordal extension**. Let

$$G^{(s)}_{r,k,j}:=(F^{(s)}_{r,k,j})',\quad j\in\{0\}\cup J_k,k\in[p].\tag{4.32}$$

It is clear by construction that the sequences of graphs $(G^{(s)}_{r,k,j})_{s\geq1}$ stabilize for all $j\in\{0\}\cup J_k,k\in[p]$ after finitely many steps.

Example 4.22 *Let $f=1+x_1^2+x_2^2+x_3^2+x_1x_2+x_2x_3+x_3$ and consider the unconstrained POP: $\min\{f(\mathbf{x}):\mathbf{x}\in\mathbb{R}^n\}$. Take the relaxation order $r=r_{\min}=1$. The variables are decomposed into two cliques: $\{x_1,x_2\}$ and $\{x_2,x_3\}$. The tsp graphs with respect to these two cliques are illustrated in Figure 4.5. The left graph corresponds to the first clique: x_1 and x_2 are connected because of the term x_1x_2. The right graph corresponds to the second clique: 1 and x_3 are connected because of the term x_3; x_2 and x_3 are connected because of the term x_2x_3. It is not hard to see that the graph sequences $(G^{(s)}_{1,k})_{s\geq1}, k=1,2$ (the subscript j is omitted here since there is no constraint) stabilize at $s=2$ if the maximal chordal extension is used in (4.32).*

Figure 4.5: The tsp graphs of Example 4.22.

Let $t_{k,j}:=|\mathbb{N}^{n_k}_{r-d_j}|=\binom{n_k+r-d_j}{r-d_j}$ for all k,j. Then with $s\geq1$, the moment relaxation based on correlative-term sparsity for POP (3.1) is given by

$$\mathbf{P}^{r,s}_{\text{cs-ts}}:\quad\begin{cases}\inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f)\\ \text{s.t.} & \mathbf{B}_{G^{(s)}_{r,k,0}}\circ\mathbf{M}_r(\mathbf{y},I_k)\in\Pi_{G^{(s)}_{r,k,0}}(\mathbb{S}^+_{t_{k,0}}),\quad k\in[p]\\ & \mathbf{B}_{G^{(s)}_{r,k,j}}\circ\mathbf{M}_{r-d_j}(g_j\mathbf{y},I_k)\in\Pi_{G^{(s)}_{r,k,j}}(\mathbb{S}^+_{t_{k,j}}),\quad j\in J_k,k\in[p]\\ & L_{\mathbf{y}}(g_j)\geq0,\quad j\in J'\\ & y_{\mathbf{0}}=1\end{cases}\tag{4.33}$$

with optimum denoted by $f^{r,s}_{\text{cs-ts}}$.

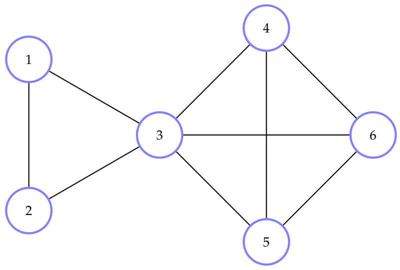

Figure 4.6: The csp graph of Example 4.23.

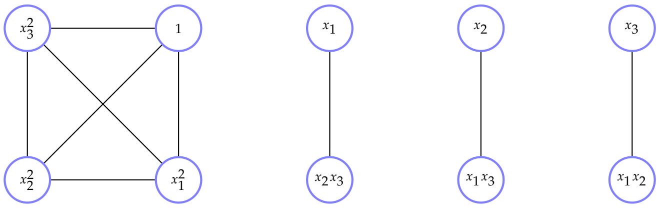

Figure 4.7: The tsp graph for the first clique of Example 4.23.

For all k, j, let us write $\mathbf{M}_{r-d_j}(g_j\mathbf{y}, I_k) = \sum_\alpha \mathbf{D}_\alpha^{k,j} y_\alpha$ for appropriate symmetry matrices $\{\mathbf{D}_\alpha^{k,j}\}$ and $g_j = \sum_\alpha g_{j,\alpha}\mathbf{x}^\alpha$. Then for each $s \geq 1$, the dual of $\mathbf{P}^{r,s}_{\text{cs-ts}}$ (4.33) reads as

$$(\mathbf{P}^{r,s}_{\text{cs-ts}})^* : \begin{cases} \sup\limits_{\mathbf{G}_{k,j},\lambda_j,b} & b \\ \text{s.t.} & \sum_{k=1}^p \sum_{j\in\{0\}\cup J_k} \langle \mathbf{G}_{k,j}, \mathbf{D}_\alpha^{k,j}\rangle + \sum_{j\in J'} \lambda_j g_{j,\alpha} \\ & \qquad\qquad + b\delta_{\mathbf{0}\alpha} = f_\alpha, \quad \forall \alpha \in \mathscr{C}_r^{(s)} \\ & \mathbf{G}_{k,j} \in \mathbf{S}_+^{t_{k,j}} \cap \mathbf{S}_{G^{(s)}_{r,k,j}}, \quad j \in \{0\}\cup J_k, k \in [p] \\ & \lambda_j \geq 0, \quad j \in J' \end{cases} \tag{4.34}$$

where $\mathscr{C}_r^{(s)}$ is defined in (4.31).

The primal-dual SDP relaxations (4.33)–(4.34) is called the CS-TSSOS hierarchy associated with $\mathbf{P}$ (3.1), which is indexed by two parameters: the relaxation order r and the sparse order s.

Example 4.23 *Let $f = 1 + \sum_{i=1}^6 x_i^4 + x_1x_2x_3 + x_3x_4x_5 + x_3x_4x_6 + x_3x_5x_6 + x_4x_5x_6$, and consider the unconstrained POP: $\min\{f(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^n\}$. Let us apply the CS-TSSOS hierarchy (using the maximal chordal extension in (4.32)) to this problem by taking $r = r_{\min} = 2, s = 1$. First, according to the csp graph (Figure 4.6), we decompose the variables into two cliques: $\{x_1, x_2, x_3\}$ and $\{x_3, x_4, x_5, x_6\}$. The tsp graphs for the first clique and the second clique are shown in Figure 4.7 and Figure 4.8, respectively. For the first clique one obtains four blocks of SDP matrices with respective sizes $4, 2, 2, 2$. For the second clique one obtains two blocks of SDP matrices with respective sizes $5, 10$. As a result, the original SDP matrix of size 28 has been reduced to six blocks of maximal size 10.*

Alternatively, if one applies the TSSOS hierarchy (using the maximal chordal extension in (4.23)) directly to this problem by taking $r = r_{\min} = 2, s = 1$ (i.e., without decomposing variables), then the tsp graph is shown in Figure 4.9 and one thereby obtains 11 PSD blocks with respective sizes $7, 2, 2, 2, 1, 1, 1, 1, 1, 1, 10$. Compared to the CS-TSSOS case, there are six additional blocks of size one and the two blocks with respective sizes $4, 5$ are replaced by a single block of size 7.

We summarize the basic properties of the CS-TSSOS hierarchy in the next theorem.

Theorem 4.24 *Let $f \in \mathbb{R}[\mathbf{x}]$ and $\mathbf{S}$ be defined as before. Then the following hold:*

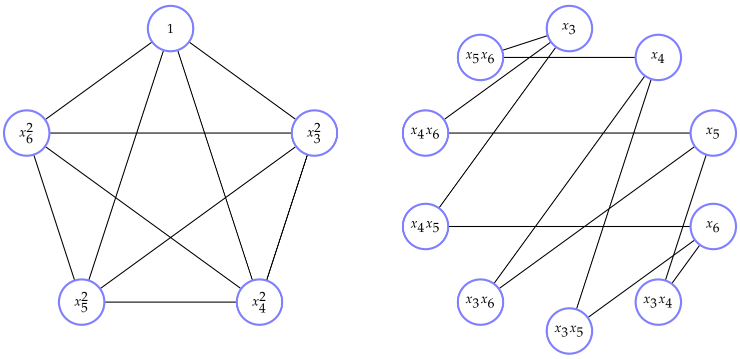

Figure 4.8: The tsp graph for the second clique of Example 4.23

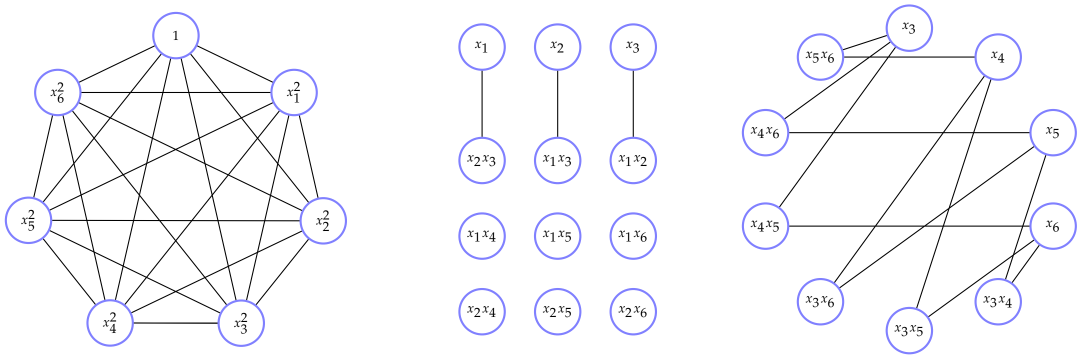

Figure 4.9: The tsp graph without decomposing variables of Example 4.23.

1. *If* $\mathbf{S}$ *has a nonempty interior, then there is no duality gap between* $\mathbf{P}^{r,s}_{\text{cs-ts}}$ *and* $(\mathbf{P}^{r,s}_{\text{cs-ts}})^*$ *for any* $r \geq r_{\min}$ *and* $s \geq 1$.
2. *For any* $r \geq r_{\min}$, *the sequence* $(f^{r,s}_{\text{cs-ts}})_{s\geq 1}$ *is monotonically non-decreasing and* $f^{r,s}_{\text{cs-ts}} \leq f^r_{\text{cs}}$ *for all* s *with* f^r_{cs} *being defined in Section 4.3.*
3. *For any* $s \geq 1$, *the sequence* $(f^{r,s}_{\text{cs-ts}})_{r\geq r_{\min}}$ *is monotonically non-decreasing.*

PROOF 1. By the duality theory of convex programming, this easily follows from Theorem 3.6 of [Las06b] and Theorem 1.5.

2. By construction, we have $G^{(s)}_{r,k,j} \subseteq G^{(s+1)}_{r,k,j}$ for all r, k, j and for all s. It follows that each maximal clique of $G^{(s)}_{r,k,j}$ is contained in some maximal clique of $G^{(s+1)}_{r,k,j}$. Hence by Theorem 1.5, $\mathbf{P}^{r,s}_{\text{cs-ts}}$ is a relaxation of $\mathbf{P}^{r,s+1}_{\text{cs-ts}}$ and is clearly also a relaxation of $\mathbf{P}^r_{\text{cs}}$. Therefore, $(f^{r,s}_{\text{cs-ts}})_{s\geq 1}$ is monotonically non-decreasing and $f^{r,s}_{\text{cs-ts}} \leq f^r_{\text{cs}}$ for all s.

3. The conclusion follows if we can show that the inclusion $G^{(s)}_{r,k,j} \subseteq G^{(s)}_{r+1,k,j}$ holds for all r, k, j, s, since by Theorem 1.5 this implies that $\mathbf{P}^{r,s}_{\text{cs-ts}}$ is a relaxation of $\mathbf{P}^{r+1,s}_{\text{cs-ts}}$. Let us prove $G^{(s)}_{r,k,j} \subseteq G^{(s)}_{r+1,k,j}$ by induction on s. For $s = 1$, we have $G^{(0)}_{r,k,0} = G^{\text{tsp}}_{r,k} \subseteq G^{\text{tsp}}_{r+1,k} = G^{(0)}_{r+1,k,0}$, which together with (4.30)-(4.31) implies that $F^{(1)}_{r,k,j} \subseteq F^{(1)}_{r+1,k,j}$ for $j \in \{0\} \cup J_k, k \in [p]$. It then follows that $G^{(1)}_{r,k,j} = (F^{(1)}_{r,k,j})' \subseteq (F^{(1)}_{r+1,k,j})' = G^{(1)}_{r+1,k,j}$. Now assume that $G^{(s)}_{r,k,j} \subseteq G^{(s)}_{r+1,k,j}$, $j \in \{0\} \cup J_k, k \in [p]$, hold for some $s \geq 1$. Then by (4.30)-(4.31) and by the induction hypothesis, we have $F^{(s+1)}_{r,k,j} \subseteq F^{(s+1)}_{r+1,k,j}$

for $j \in \{0\} \cup J_k, k \in [p]$. Thus $G^{(s+1)}_{r,k,j} = (F^{(s+1)}_{r,k,j})' \subseteq (F^{(s+1)}_{r+1,k,j})' = G^{(s+1)}_{r+1,k,j}$ which completes the induction. □

From Theorem 4.24, we deduce the following two-level hierarchy of lower bounds for the optimum $f_{\min}$ of **P** (3.1):

$$\begin{array}{ccccccc}
f^{r_{\min},1}_{\text{cs-ts}} & \leq & f^{r_{\min},2}_{\text{cs-ts}} & \leq & \cdots & \leq & f^{r_{\min}}_{\text{cs-ts}} \\
\wedge\vert & & \wedge\vert & & & & \wedge\vert \\
f^{r_{\min}+1,1}_{\text{cs-ts}} & \leq & f^{r_{\min}+1,2}_{\text{cs-ts}} & \leq & \cdots & \leq & f^{r_{\min}+1}_{\text{cs-ts}} \\
\wedge\vert & & \wedge\vert & & & & \wedge\vert \\
\vdots & & \vdots & & \vdots & & \vdots \\
\wedge\vert & & \wedge\vert & & & & \wedge\vert \\
f^{r,1}_{\text{cs-ts}} & \leq & f^{r,2}_{\text{cs-ts}} & \leq & \cdots & \leq & f^{r}_{\text{cs-ts}} \\
\wedge\vert & & \wedge\vert & & & & \wedge\vert \\
\vdots & & \vdots & & \vdots & & \vdots
\end{array} \tag{4.35}$$

As we have known for the TSSOS hierarchy, the block structure arising from the CS-TSSOS hierarchy is consistent with the sign symmetries of the POP. More precisely, we have the following theorem.

Theorem 4.25 *Let $\mathscr{A}$ be defined as in (4.29), $\mathscr{C}_r^{(s)}$ be defined as in (4.31), and assume that the sign symmetries of $\mathscr{A}$ are represented by the column vectors of the binary matrix $\mathbf{R}$. Then for any $r \geq r_{\min}$, $s \geq 1$ and any $\alpha \in \mathscr{C}_r^{(s)}$, it holds $\mathbf{R}^\intercal\alpha \equiv \mathbf{0}\,(\text{mod}\,2)$. As a consequence, if β, γ belong to the same block in the CS-TSSOS relaxations, then $\mathbf{R}^\intercal(\beta+\gamma) \equiv \mathbf{0}\,(\text{mod}\,2)$.*

We next show that if the chordal extension in (4.33) is chosen to be *maximal*, then for any relaxation order $r \geq r_{\min}$, the sequence of optima $(f^{r,s}_{\text{cs-ts}})_{s\geq 1}$ arising from the CS-TSSOS hierarchy converges to the optimum f^r_{cs} of the CSSOS relaxation.

It is clear by construction that the sequences of graphs $(G^{(s)}_{r,k,j})_{s\geq 1}$ stabilize for all $j \in \{0\} \cup J_k, k \in [p]$ after finitely many steps. We denote the resulting stabilized graphs by $G^{(\bullet)}_{r,k,j}, j \in \{0\} \cup J_k, k \in [p]$ and the corresponding SDP (4.33) by $\mathbf{P}^{r,\bullet}_{\text{cs-ts}}$.

Theorem 4.26 *If one uses the maximal chordal extension in (4.32), then for any $r \geq r_{\min}$, the sequence $(f^{r,s}_{\text{cs-ts}})_{s\geq 1}$ converges to f^r_{cs} in finitely many steps.*

PROOF Let $\mathbf{y} = (y_\alpha)$ be an arbitrary feasible solution of $\mathbf{P}^{r,\bullet}_{\text{cs-ts}}$ and $f^{r,\bullet}_{\text{cs-ts}}$ be the optimum of $\mathbf{P}^{r,\bullet}_{\text{cs-ts}}$. Note that $\{y_\alpha \mid \alpha \in \bigcup_{k=1}^p(\cup_{j\in\{0\}\cup J_k}(\text{supp}(g_j) + \text{supp}(G^{(\bullet)}_{r,k,j})))\}$ is the set of decision variables involved in $\mathbf{P}^{r,\bullet}_{\text{cs-ts}}$. Let $\mathscr{R}$ be the set of decision variables involved in $\mathbf{P}^r_{\text{cs}}$ (4.6). We then define a vector $\overline{\mathbf{y}} = (\overline{y}_\alpha)_{\alpha\in\mathscr{R}}$ as follows:

$$\overline{y}_\alpha = \begin{cases} y_\alpha, & \text{if } \alpha \in \bigcup_{k=1}^p(\cup_{j\in\{0\}\cup J_k}(\text{supp}(g_j) + \text{supp}(G^{(\bullet)}_{r,k,j}))), \\ 0, & \text{otherwise.} \end{cases}$$

By construction and since $G^{(\bullet)}_{r,k,j}$ stabilizes under support extension for all k, j, we have $\mathbf{M}_{r-d_j}(g_j\overline{\mathbf{y}}, I_k) = \mathbf{B}_{G^{(\bullet)}_{r,k,j}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y}, I_k)$. As the maximal chordal extension is chosen for (4.32), the matrix $\mathbf{B}_{G^{(\bullet)}_{r,k,j}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y}, I_k)$ is block diagonal up to permutation. It follows from $\mathbf{B}_{G^{(\bullet)}_{r,k,j}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y}, I_k) \in$

$\Pi_{G^{(\bullet)}_{r,k,j}}(\mathbf{S}^{t_{k,j}}_{+})$ that $\mathbf{M}_{r-d_j}(g_j\bar{\mathbf{y}}, I_k) \succeq 0$ for $j \in \{0\} \cup J_k, k \in [p]$. Therefore $\bar{\mathbf{y}}$ is a feasible solution of $\mathbf{P}^r_{\text{cs}}$ and so $L_{\mathbf{y}}(f) = L_{\bar{\mathbf{y}}}(f) \geq f^r_{\text{cs}}$. Hence $f^{r,\bullet}_{\text{cs-ts}} \geq f^r_{\text{cs}}$ since $\mathbf{y}$ is an arbitrary feasible solution of $\mathbf{P}^{r,\bullet}_{\text{cs-ts}}$. By Theorem 4.24, we already have $f^{r,\bullet}_{\text{cs-ts}} \leq f^r_{\text{cs}}$. Therefore, $f^{r,\bullet}_{\text{cs-ts}} = f^r_{\text{cs}}$. □

By Theorem 3.6 in [Las06b], the sequence $(f^r_{\text{cs}})_{r \geq r_{\min}}$ converges to the global optimum $f_{\min}$ of POP (3.1) (after adding some redundant quadratic constraints). Therefore, this together with Theorem 4.26 offers the global convergence of the CS-TSSOS hierarchy.

Proceeding along Theorem 4.24, we are able to provide a *sparse representation* theorem based on both CS and TS for a polynomial positive on a compact basic semialgebraic set.

Theorem 4.27 *Let $f \in \mathbb{R}[\mathbf{x}]$, $\mathbf{S} \subseteq \mathbb{R}^n$ and $\{I_k\}_{k=1}^p, \{J_k\}_{k=1}^p$ be defined in Assumption (4.1). Assume that the sign symmetries of $\mathscr{A} = \operatorname{supp}(f) \cup \bigcup_{j=1}^m \operatorname{supp}(g_j)$ are represented by the columns of the binary matrix $\mathbf{R}$. If f is positive on $\mathbf{S}$, then f admits a representation of form*

$$f = \sum_{k=1}^{p} \left(\sigma_{k,0} + \sum_{j \in J_k} \sigma_{k,j} g_j \right), \tag{4.36}$$

for some polynomials $\sigma_{k,j} \in \Sigma[\mathbf{x}(I_k)], j \in \{0\} \cup J_k, k \in [p]$, satisfying $\mathbf{R}^\intercal \alpha \equiv \mathbf{0} \pmod 2$ for any $\alpha \in \operatorname{supp}(\sigma_{k,j})$.

PROOF By Corollary 3.9 of [Las06b], there exist polynomials $\sigma'_{k,j} \in \Sigma[\mathbf{x}(I_k)], j \in \{0\} \cup J_k, k \in [p]$ such that

$$f = \sum_{k=1}^{p} \left(\sigma'_{k,0} + \sum_{j \in J_k} \sigma'_{k,j} g_j \right). \tag{4.37}$$

Let $r = \max\{\lceil \deg(\sigma'_{k,j} g_j)/2 \rceil : j \in \{0\} \cup J_k, k \in [p]\}$. Let $\mathbf{G}'_{k,j}$ be a PSD Gram matrix associated with $\sigma'_{k,j}$ and indexed by the monomial basis $\mathbb{N}^{n_k}_{r-d_j}$. Then for all k, j, we define $\mathbf{G}_{k,j} \in \mathbf{S}^{t_{k,j}}$ (indexed by $\mathbb{N}^{n_k}_{r-d_j}$) by

$$[\mathbf{G}_{k,j}]_{\beta\gamma} := \begin{cases} [Q'_{k,j}]_{\beta\gamma}, & \text{if } \mathbf{R}^\intercal(\beta+\gamma) \equiv \mathbf{0} \pmod 2, \\ 0, & \text{otherwise,} \end{cases}$$

and let $\sigma_{k,j} = (\mathbf{x}^{\mathbb{N}^{n_k}_{r-d_j}})^\intercal \mathbf{G}_{k,j} \mathbf{x}^{\mathbb{N}^{n_k}_{r-d_j}}$. One can easily verify that $\mathbf{G}_{k,j}$ is block diagonal up to permutation (see also [WML21b]) and each block is a principal submatrix of $\mathbf{G}'_{k,j}$. Then the positive semidefiniteness of $\mathbf{G}'_{k,j}$ implies that $\mathbf{G}_{k,j}$ is also positive semidefinite. Thus $\sigma_{k,j} \in \Sigma[\mathbf{x}(I_k)]$.

By construction, substituting $\sigma'_{k,j}$ with $\sigma_{k,j}$ in (4.37) boils down to removing the terms with exponents α that do not satisfy $\mathbf{R}^\intercal \alpha \equiv \mathbf{0} \pmod 2$ from the right hand side of (4.37). Since any $\alpha \in \operatorname{supp}(f)$ satisfies $\mathbf{R}^\intercal \alpha \equiv \mathbf{0} \pmod 2$, this does not change the match of coefficients on both sides of the equality. Thus we obtain

$$f = \sum_{k=1}^{p} \left(\sigma_{k,0} + \sum_{j \in J_k} \sigma_{k,j} g_j \right)$$

with the desired property. □

In the case of the dense moment-SOS hierarchy, there is a standard procedure described in [HL05a] to extract globally optimal solutions when the moment matrix satisfies the so-called flatness condition. This procedure was generalized to the correlative sparse setting in [Las06b, S 3.3] and [ND09]. In the term sparse setting, however, the corresponding procedure cannot be applied because the information on the moment matrix is incomplete. In order to extract a solution in this case, we may add an order-one (dense) moment matrix for each clique in (4.33):

$$\begin{cases}\inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f)\\ \text{s.t.} & \mathbf{M}_r(\mathbf{y}, I_k)\in\Pi_{G^{(s)}_{r,k,0}}(\mathbb{S}^+_{t_{k,0}}),\quad k\in[p]\\ & \mathbf{M}_1(\mathbf{y}, I_k)\succeq 0,\quad k\in[p]\\ & \mathbf{M}_{r-d_j}(g_j\mathbf{y}, I_k)\in\Pi_{G^{(s)}_{r,k,j}}(\mathbb{S}^+_{t_{k,j}}),\quad j\in J_k,\quad k\in[p]\\ & L_{\mathbf{y}}(g_j)\geq 0,\quad j\in J'\\ & y_{\mathbf{0}}=1\end{cases}\tag{4.38}$$

Let $\mathbf{y}^{\text{opt}}$ be an optimal solution of (4.38). Typically, $\mathbf{M}_1(\mathbf{y}^{\text{opt}}, I_k)$ (after identifying sufficiently small entries with zeros) is a block diagonal matrix (up to permutation). If for all k every block of $\mathbf{M}_1(\mathbf{y}^{\text{opt}}, I_k)$ is of rank one, then a globally optimal solution $\mathbf{x}^{\text{opt}}$ to $\mathbf{P}$ (3.1) which is unique up to sign symmetries can be extracted ([Las06b, Theorem 3.7]), and the global optimality is certified. Otherwise, the relaxation might be not exact or yield multiple global solutions.

Remark 4.28 *Note that* (4.38) *is a tighter relaxation of* $\mathbf{P}$ (3.1) *than* $\mathbf{P}^{r,s}_{\text{cs-ts}}$ (4.33)*, and so might provide a better lower bound for* $\mathbf{P}$*. In particular, if* $\mathbf{P}$ *is a QCQP, then* (4.38) *is always tighter than Shor's relaxation of* $\mathbf{P}$*.*

For POP (3.1), suppose that f is not a homogeneous polynomial or the constraint polynomials $\{g_j\}_{j\in[m]}$ are of different degrees. Then instead of using the uniform minimum relaxation order $r_{\min}$, it might be more beneficial, from the computational point of view, to assign different relaxation orders to different subsystems obtained from the csp for the initial relaxation step of the CS-TSSOS hierarchy. To this end, we redefine the csp graph $G^{\text{icsp}}(V, E)$ as follows: $V=[n]$ and $\{i,j\}\in E$ whenever there exists $\alpha\in\mathscr{A}$ such that $\{i,j\}\subseteq\text{supp}(\alpha)$. This is clearly a subgraph of G^{csp} defined in Chapter 4.1 and hence typically admits a smaller chordal extension. Let $(G^{\text{icsp}})'$ be a chordal extension of G^{icsp} and $\{I_k\}_{k\in[p]}$ be the list of maximal cliques of $(G^{\text{icsp}})'$ with $n_k:=|I_k|$. Now we partition the constraint polynomials $\{g_j\}_{j\in[m]}$ into groups $\{g_j\mid j\in J_k\}_{k\in[p]}$ and $\{g_j\mid j\in J'\}$ which satisfy

(1) $J_1,\ldots,J_p,J'\subseteq[m]$ are pairwise disjoint and $\bigcup_{k=1}^{p}J_k\cup J'=[m]$;

(2) for any $j\in J_k$, $\bigcup_{\alpha\in\text{supp}(g_j)}\text{supp}(\alpha)\subseteq I_k$, $k\in[p]$;

(3) for any $j\in J'$, $\bigcup_{\alpha\in\text{supp}(g_j)}\text{supp}(\alpha)\nsubseteq I_k$ for all $k\in[p]$.

Suppose f decomposes as $f=\sum_{k\in[p]}f_k$ such that $\bigcup_{\alpha\in\text{supp}(f_k)}\text{supp}(\alpha)\subseteq I_k$ for $k\in[p]$. We define the vector of minimum relaxation orders $\mathbf{o}=(o_k)_k\in\mathbb{N}^p$ with $o_k:=\max\{\{d_j: j\in J_k\}\cup\{\lceil\deg(f_k)/2\rceil\}\}$. Then with $s\geq 1$, we define the following minimal initial relaxation step of the CS-TSSOS hierarchy:

$$\begin{cases}\inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f)\\ \text{s.t.} & \mathbf{B}_{G^{(s)}_{o_k,k,0}}\circ\mathbf{M}_{o_k}(\mathbf{y}, I_k)\in\Pi_{G^{(s)}_{o_k,k,0}}(\mathbb{S}_+^{t_{k,0}}),\quad k\in[p]\\ & \mathbf{B}_{G^{(s)}_{o_k,k,j}}\circ\mathbf{M}_{o_k-d_j}(g_j\mathbf{y}, I_k)\in\Pi_{G^{(s)}_{o_k,k,j}}(\mathbb{S}_+^{t_{k,j}}),\quad j\in J_k, k\in[p]\\ & L_{\mathbf{y}}(g_j)\geq 0,\quad j\in J'\\ & y_{\mathbf{0}}=1\end{cases}\tag{4.39}$$

where $G^{(s)}_{o_k,k,j}, j\in J_k, k\in[p]$ are defined in the same spirit with Chapter 4.7 and $t_{k,j}:=\binom{n_k+o_k-d_j}{o_k-d_j}$ for all k,j.

Fore more details on term sparsity, please refer to [WML21b, WML21a, WMLM20].

4.8 Other structures

- Reduced monomial basis.
- Quotient ring. Please refer to [Par05].
- Symmetries. Please refer to [RTAL13].

Chapter 5

Extensions

5.1 Complex polynomial optimization

Let $\mathbf{i}$ be the imaginary unit, satisfying $\mathbf{i}^2 = -1$. Let $\mathbf{z} = (z_1, \ldots, z_n)$ be a tuple of complex variables and $\bar{\mathbf{z}} = (\bar{z}_1, \ldots, \bar{z}_n)$ its conjugate. We denote by $\mathbb{C}[\mathbf{z}] := \mathbb{C}[z_1, \ldots, z_n]$, $\mathbb{C}[\mathbf{z}, \bar{\mathbf{z}}] := \mathbb{C}[z_1, \ldots, z_n, \bar{z}_1, \ldots, \bar{z}_n]$ the complex polynomial ring in $\mathbf{z}$, the complex polynomial ring in $\mathbf{z}, \bar{\mathbf{z}}$, respectively. For $d \in \mathbb{N}$, let $\mathbb{C}_d[\mathbf{z}]$ denote the set of polynomials in $\mathbb{C}[\mathbf{z}]$ of degree no greater than d, and let $\mathbb{C}_d[\mathbf{z}, \bar{\mathbf{z}}]$ denote the set of polynomials in $\mathbb{C}[\mathbf{z}, \bar{\mathbf{z}}]$ of degree w.r.t $\mathbf{z}$ and $\bar{\mathbf{z}}$ no greater than d. A polynomial $f \in \mathbb{C}[\mathbf{z}, \bar{\mathbf{z}}]$ can be written as $f = \sum_{(\beta,\gamma)\in\mathscr{A}} f_{\beta,\gamma}\mathbf{z}^{\beta}\bar{\mathbf{z}}^{\gamma}$ with $\mathscr{A} \subseteq \mathbb{N}^n \times \mathbb{N}^n$ and $f_{\beta,\gamma} \in \mathbb{C}$. The support of f is defined by $\mathrm{supp}(f) = \{(\beta,\gamma) \in \mathscr{A} \mid f_{\beta,\gamma} \neq 0\}$. The conjugate of f is $\bar{f} = \sum_{(\beta,\gamma)\in\mathscr{A}} \bar{f}_{\beta,\gamma}\mathbf{z}^{\gamma}\bar{\mathbf{z}}^{\beta}$. A polynomial $\sigma = \sum_{(\beta,\gamma)} \sigma_{\beta,\gamma}\mathbf{z}^{\beta}\bar{\mathbf{z}}^{\gamma} \in \mathbb{C}_d[\mathbf{z}, \bar{\mathbf{z}}]$ is called a *Hermitian sum of squares* or an *HSOS* for short if there exist polynomials $f_i \in \mathbb{C}_d[\mathbf{z}], i \in [t]$ such that $\sigma = \sum_{i=1}^{t} f_i\bar{f}_i$. We use $\Sigma_d[\mathbf{z}, \bar{\mathbf{z}}]$ to denote the set of HSOS polynomials in $\mathbb{C}_d[\mathbf{z}, \bar{\mathbf{z}}]$.

For a positive integer r, the set of $r \times r$ Hermitian matrices is denoted by $\mathbf{H}^r$ and the set of $r \times r$ positive semidefinite (PSD) Hermitian matrices is denoted by $\mathbf{H}^r_+$. Let $A \circ B \in \mathbf{H}^r$ denote the Hadamard product of $A, B \in \mathbf{H}^r$, defined by $[A \circ B]_{ij} = A_{ij}B_{ij}$. The set $\{\mathbf{z}^{\beta} \mid \beta \in \mathbb{N}^n_d\}$ is called the standard (complex) *monomial basis* up to degree d. For the sake of convenience, we abuse notation slightly and use the exponent set $\mathbb{N}^n_d$ to denote the monomial basis.

In this section, we consider the following complex polynomial optimization problem (CPOP):

$$(\mathrm{Q}): \quad \begin{cases} \inf_{\mathbf{z}\in\mathbb{C}^n} & f(\mathbf{z}, \bar{\mathbf{z}}) := \sum_{\alpha,\beta} f_{\alpha,\beta}\mathbf{z}^{\alpha}\bar{\mathbf{z}}^{\beta} \\ \text{s.t.} & g_j(\mathbf{z}, \bar{\mathbf{z}}) := \sum_{\alpha,\beta} g_{j,\alpha,\beta}\mathbf{z}^{\alpha}\bar{\mathbf{z}}^{\beta} \geq 0, \quad j = 1, \ldots, m, \\ & h_i(\mathbf{z}, \bar{\mathbf{z}}) := \sum_{\alpha,\beta} h_{i,\alpha,\beta}\mathbf{z}^{\alpha}\bar{\mathbf{z}}^{\beta} = 0, \quad i = 1, \ldots, t, \end{cases} \tag{5.1}$$

where n, m, and t are positive integers, $\bar{\mathbf{z}} := (\bar{z}_1, \ldots, \bar{z}_n)$ stands for the conjugate of complex variables $\mathbf{z} := (z_1, \ldots, z_n)$. The functions $f, g_1, \ldots, g_m, h_1, \ldots, h_t$ are real-valued polynomials and their coefficients satisfy $f_{\alpha,\beta} = \bar{f}_{\beta,\alpha}$, $g_{j,\alpha,\beta} = \bar{g}_{j,\beta,\alpha}$, and $h_{i,\alpha,\beta} = \bar{h}_{i,\beta,\alpha}$. The feasible set is defined as $\{\mathbf{z} \in \mathbb{C}^n \mid g_j(\mathbf{z}, \bar{\mathbf{z}}) \geq 0, j = 1, \ldots, m, h_i(\mathbf{z}, \bar{\mathbf{z}}) = 0, i = 1, \ldots, t\}$. For the sake of brevity, we assume that there are only inequality constraints in (5.1) in the rest of this paper.

5.1.1 The complex moment-HSOS hierarchy

Let $\mathbf{y} = (y_{\beta,\gamma})_{(\beta,\gamma)\in\mathbb{N}^n\times\mathbb{N}^n} \subseteq \mathbb{C}$ be a sequence indexed by $(\beta,\gamma) \in \mathbb{N}^n \times \mathbb{N}^n$ and satisfies $y_{\beta,\gamma} = \bar{y}_{\gamma,\beta}$. Let $L^{\mathrm{c}}_{\mathbf{y}} : \mathbb{C}[\mathbf{z}, \bar{\mathbf{z}}] \to \mathbb{R}$ be the linear functional

$$f = \sum_{(\beta,\gamma)} f_{\beta,\gamma}\mathbf{z}^{\beta}\bar{\mathbf{z}}^{\gamma} \mapsto L^{\mathrm{c}}_{\mathbf{y}}(f) = \sum_{(\beta,\gamma)} f_{\beta,\gamma}y_{\beta,\gamma}.$$

The *complex moment* matrix $\mathbf{M}^{\mathrm{c}}_r(\mathbf{y})$ ($r \in \mathbb{N}$) associated with $\mathbf{y}$ is the matrix with rows and columns indexed by $\mathbb{N}^n_r$ such that

$$\mathbf{M}^{\mathrm{c}}_d(\mathbf{y})_{\beta\gamma} := L^{\mathrm{c}}_{\mathbf{y}}(\mathbf{z}^{\beta}\bar{\mathbf{z}}^{\gamma}) = y_{\beta,\gamma}, \quad \forall \beta, \gamma \in \mathbb{N}^n_r.$$

Suppose that $g = \sum_{(\beta',\gamma')} g_{\beta',\gamma'}\mathbf{z}^{\beta'}\bar{\mathbf{z}}^{\gamma'} \in \mathbb{C}[\mathbf{z},\bar{\mathbf{z}}]$ is a Hermitian polynomial, i.e., $\bar{g} = g$. The *complex localizing* matrix $\mathbf{M}_r^{\mathrm{c}}(g\mathbf{y})$ associated with g and $\mathbf{y}$ is the matrix with rows and columns indexed by $\mathbb{N}_r^n$ such that

$$\mathbf{M}_r^{\mathrm{c}}(g\,\mathbf{y})_{\beta\gamma} := L_{\mathbf{y}}^{\mathrm{c}}(g\,\mathbf{z}^{\beta}\bar{\mathbf{z}}^{\gamma}) = \sum_{(\beta',\gamma')} g_{\beta',\gamma'}y_{\beta+\beta',\gamma+\gamma'}, \quad \forall \beta,\gamma \in \mathbb{N}_r^n.$$

Both the complex moment matrix and the complex localizing matrix are Hermitian matrices.

Note that a distinguished difference between the real moment matrix and the complex moment matrix is that the former has the Hankel property, whereas the latter does not have.

There are two ways to construct a "moment-SOS" hierarchy for CPOP (5.1). The first way is introducing real variables for both real and imaginary parts of each complex variable in (5.1), i.e., letting $z_i = x_i + x_{i+n}\mathbf{i}$ for $i \in [n]$. Then one can convert CPOP (5.1) to a POP involving only real variables at the price of doubling the number of variables. Therefore the usual real moment-SOS hierarchy applies to the resulting real POP.

On the other hand, as the second way, it might be advantageous to handle CPOP (5.1) directly with the complex moment-HSOS hierarchy introduced in [JM18]. Let $d_0 := \max\{|\beta|,|\gamma| : f_{\beta,\gamma} \neq 0\}$, $d_j := \max\{|\beta|,|\gamma| : g^j_{\beta,\gamma} \neq 0\}$, and let $r_{\min} := \max\{d_0, d_1, \ldots, d_m\}$. Then the complex moment hierarchy indexed by $r \geq r_{\min}$ (called the relaxation order) for CPOP (5.1) is given by

$$(\mathrm{Q}_r): \quad \begin{cases} \inf & L_{\mathbf{y}}^{\mathrm{c}}(f) \\ \text{s.t.} & \mathbf{M}_r^{\mathrm{c}}(\mathbf{y}) \succeq 0, \\ & \mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\mathbf{y}) \succeq 0, \quad j \in [m], \\ & y_{\mathbf{0},\mathbf{0}} = 1, \end{cases} \tag{5.2}$$

which is a semidefinite program (SDP) with optimum denoted by ρ_d. The dual of (Q_r) (5.2) can be formulized as the following HSOS relaxation:

$$(\mathrm{Q}_r)^*: \quad \begin{cases} \sup & \rho \\ \text{s.t.} & f - \rho = \sigma_0 + \sigma_1 g_1 + \ldots + \sigma_m g_m, \\ & \sigma_j \text{ is an HSOS}, \quad j = 0,\ldots,m, \\ & \sigma_0 \in \Sigma_r[\mathbf{z},\bar{\mathbf{z}}], \sigma_j \in \Sigma_{r-d_j}[\mathbf{z},\bar{\mathbf{z}}], \quad j \in [m]. \end{cases} \tag{5.3}$$

Remark 5.1 *In (5.2), the expression "$X \succeq 0$" means an Hermitian matrix X to be positive semidefinite. Since popular SDP solvers deal with only real SDPs, it is necessary to convert this condition to a condition involving only real matrices. The reader is referred to [Wan23].*

Remark 5.2 *The first order moment-(H)SOS relaxation for quadratically constrained quadratic programs (QCQP) is also known as Shor's relaxation. It was proved in [JM15] that the real Shor's relaxation and the complex Shor's relaxation for homogeneous QCQPs yield the same bound. However, generally the complex hierarchy is weaker (i.e., producing looser bounds) than the real hierarchy at the same relaxation order $r > 1$ as Hermitian sums of squares are a special case of real sums of squares; see [JM18].*

Remark 5.3 *By the complex Positivstellensatz theorem due to D'Angelo and Putinar [DP09], global convergence of the complex hierarchy is guaranteed when a sphere constraint is present.*

5.1.2 Correlative sparsity

The procedure to exploit correlative sparsity for the complex hierarchy consists of two steps: 1) partition the set of variables into subsets according to the correlations between variables emerging in the problem data, and 2) construct a sparse complex hierarchy with respect to the former partition of variables [JM18, WKKM06].

Let us discuss in more details. Consider the CPOP defined by (5.1). Fix a relaxation order $r \geq d_{min}$. Let $J' := \{j \in [m] \mid d_j = r\}$. For $\beta = (\beta_i)_i \in \mathbb{N}^n$, let $\mathrm{supp}(\beta) := \{i \in [n] \mid \beta_i \neq 0\}$. We define the *correlative sparsity pattern (csp) graph* associated with CPOP (5.1) to be the graph G^{csp} with nodes $V = [n]$ and edges E satisfying $\{i,j\} \in E$ if one of the following holds:

(i) there exists $(\beta,\gamma)\in \text{supp}(f)\cup\bigcup_{j\in J'}\text{supp}(g_j)$ such that $\{i,j\}\subseteq \text{supp}(\beta)\cup\text{supp}(\gamma)$;

(ii) there exists $k\in[m]\backslash J'$ such that $\{i,j\}\subseteq\bigcup_{(\beta,\gamma)\in\text{supp}(g_k)}(\text{supp}(\beta)\cup\text{supp}(\gamma))$.

Let $\overline{G}^{\text{csp}}$ be a chordal extension of G^{csp} and $\{I_l\}_{l\in[p]}$ be the list of maximal cliques of $\overline{G}^{\text{csp}}$ with $n_l:=|I_l|$. Let $\mathbb{C}[\mathbf{z}(I_l)]$ denote the ring of complex polynomials in the n_l variables $\mathbf{z}(I_l)=\{z_i\mid i\in I_l\}$. We then partition the constraint polynomials $g_j, j\in[m]\backslash J'$ into groups $\{g_j\mid j\in J_l\}, l\in[p]$ which satisfy:

(i) $J_1,\dots,J_p\subseteq[m]\backslash J'$ are pairwise disjoint and $\cup_{l=1}^p J_l=[m]\backslash J'$;

(ii) for any $j\in J_l$, $\bigcup_{(\beta,\gamma)\in\text{supp}(g_j)}(\text{supp}(\beta)\cup\text{supp}(\gamma))\subseteq I_l$, $l\in[p]$.

Example 5.4 *Consider the following CPOP*

$$\begin{cases}\inf_{\mathbf{z}\in\mathbb{C}^3} & z_1\bar{z}_2+\bar{z}_1z_2+|z_3|^2\\ s.t. & g_1=1-|z_1|^2-|z_2|^2\geq 0,\\ & g_2=1-|z_2|^2-|z_3|^2\geq 0,\\ & g_3=|z_1|^4+z_2\bar{z}_3+\bar{z}_2z_3\geq 0.\end{cases}$$

Taking $r=d_{min}=2$, we have two variable cliques $I_1=\{1,2\}, I_2=\{2,3\}$, and $J'=\{3\}, J_1=\{1\}, J_2=\{2\}$; taking $r=3$, we have one variable clique $I_1=\{1,2,3\}$, and $J'=\emptyset, J_1=\{1,2,3\}$.

Next, with $l\in[p]$ and $g\in\mathbb{C}[\mathbf{z}(I_l)]$, let $\mathbf{M}_d^c(\mathbf{y},I_l)$ (resp. $\mathbf{M}_d^c(g\mathbf{y},I_l)$) be the complex moment (resp. complex localizing) submatrix obtained from $\mathbf{M}_d^c(\mathbf{y})$ (resp. $\mathbf{M}_d^c(g\mathbf{y})$) by retaining only those rows and columns indexed by $\beta\in\mathbb{N}_d^n$ of $\mathbf{M}_d^c(\mathbf{y})$ (resp. $\mathbf{M}_d^c(g\mathbf{y})$) with $\text{supp}(\beta)\subseteq I_l$.

Then, the complex (moment) hierarchy based on correlative sparsity for CPOP (5.1) is defined as

$$(\mathrm{Q}_r^{\text{cs}}):\quad\begin{cases}\inf & L_{\mathbf{y}}^c(f)\\ \text{s.t.} & \mathbf{M}_d^c(\mathbf{y},I_l)\succeq 0,\quad l\in[p],\\ & \mathbf{M}_{r-d_j}^c(g_j\mathbf{y},I_l)\succeq 0,\quad j\in J_l, l\in[p],\\ & L_{\mathbf{y}}^c(g_j)\geq 0,\quad j\in J',\\ & y_{\mathbf{0},\mathbf{0}}=1.\end{cases}\tag{5.4}$$

We denote the optimum of $(\mathrm{Q}_r^{\text{cs}})$ by ρ_d^{cs}.

Proposition 5.5 *If CPOP (5.1) is a QCQP, then (Q_1^{cs}) and (Q_1) yield the same lower bound for (5.1), i.e., $\rho_1^{cs}=\rho_1$.*

PROOF By construction, the objective function and the affine constraints of (Q_1) involve only the decision variables $\{y_{\beta,\gamma}\}_{(\beta,\gamma)}$ with $\text{supp}(\beta)\cup\text{supp}(\gamma)\subseteq I_l$ for some $l\in[p]$. Therefore, we can replace $\mathbf{M}_1^c(\mathbf{y})\succeq 0$ by $B_G\circ\mathbf{M}_1^c(\mathbf{y})\in\Pi_G(\mathbf{H}_+^{n+1})$ without changing the optimum, where G is the graph obtained from $\overline{G}^{\text{csp}}$ by adding a node 0 (corresponding to $\mathbf{0}\in\mathbb{N}^n$) and adding edges $\{0,i\}, i\in[n]$. Note that G is again a chordal graph and so the equality of optima of (Q_1) and $(\mathrm{Q}_1^{\text{cs}})$ follows from Theorem 1.6.

5.1.3 Term sparsity

Let $\mathscr{A}=\text{supp}(f)\cup\bigcup_{j=1}^m\text{supp}(g_j)$. We define the *term sparsity pattern (tsp) graph* at relaxation order r associated with CPOP (5.1) or the set $\mathscr{A}$, to be the graph G_r^{tsp} with nodes $V=\mathbb{N}_r^n$ and edges

$$E:=\{\{\beta,\gamma\}\subseteq\mathbb{N}_d^n\mid(\beta,\gamma)\in\mathscr{A}\}.\tag{5.5}$$

Remark 5.6 *There is a difference on the definitions of tsp graphs between the complex and real cases. In the real case, we use $\mathscr{A}\cup 2\mathbb{N}_r^n$ rather than $\mathscr{A}$ in (5.5) due to the Hankel structure of real moment matrices.*

Example 5.7 *Consider the following CPOP*

$$\begin{cases} \inf_{\mathbf{z}\in\mathbb{C}^3} & z_1^2+\bar{z}_1^2+z_1\bar{z}_2+\bar{z}_1z_2+z_2\bar{z}_3+\bar{z}_2z_3+z_1z_2\bar{z}_3+\bar{z}_1\bar{z}_2z_3 \\ s.t. & g_1=1-|z_1|^2-|z_2|^2-|z_3|^2\ge 0. \end{cases}$$

Figure 5.1 illustrates the tsp graph G_2^{tsp} for this CPOP, where the nodes are labeled by $\mathbf{z}^\beta$ instead of β for better visualization.

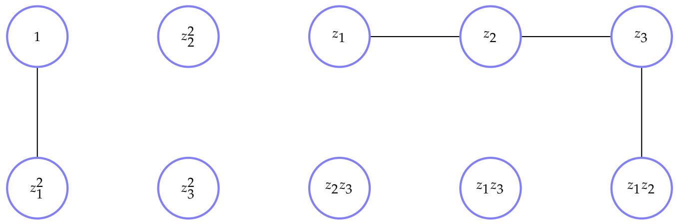

Figure 5.1: The tsp graph with $r=2$ for Example 5.7

For any graph G with $V\subseteq\mathbb{N}^n$ and $g=\sum_{(\beta',\gamma')}g_{\beta',\gamma'}\mathbf{z}^{\beta'}\bar{\mathbf{z}}^{\gamma'}\in\mathbb{C}[\mathbf{z},\bar{\mathbf{z}}]$, we define the *g-support* of G by

$$\mathrm{supp}_g(G):=\{(\beta+\beta',\gamma+\gamma')\mid\beta=\gamma\in V(G)\text{ or }\{\beta,\gamma\}\in E(G),(\beta',\gamma')\in\mathrm{supp}(g)\}.$$

Let us set $d_0:=0$ and $g_0:=1$. Now assume that $G_{r,0}^{(0)}=G_r^{\mathrm{tsp}}$ and $G_{r,j}^{(0)},j\in[m]$ are empty graphs. Then, we iteratively define an ascending chain of graphs $(G_{r,j}^{(k)}(V_{r,j},E_{r,j}^{(k)}))_{k\ge1}$ with $V_{r,j}=\mathbb{N}^n_{r-d_j}$ for each $j\in\{0\}\cup[m]$ by

$$G_{r,j}^{(k)}:=\overline{F_{r,j}^{(k)}}, \tag{5.6}$$

where $F_{r,j}^{(k)}$ is the graph with $V(F_{r,j}^{(k)})=\mathbb{N}^n_{r-d_j}$ and

$$E(F_{r,j}^{(k)})=\{\{\beta,\gamma\}\subseteq\mathbb{N}^n_{r-d_j}\mid((\beta,\gamma)+\mathrm{supp}(g_j))\cap(\bigcup_{i=0}^m\mathrm{supp}_{g_i}(G_{r,i}^{(k-1)}))\ne\emptyset\}. \tag{5.7}$$

Let $r_j:=\binom{n+r-d_j}{r-d_j}$ for $j\in\{0\}\cup[m]$. Then with $r\ge r_{\min}$ and $k\ge1$, the complex (moment) hierarchy based on term sparsity for CPOP (5.1) is defined as

$$(\mathrm{Q}_{r,k}^{\mathrm{ts}}):\quad\begin{cases}\inf & L_{\mathbf{y}}^{\mathrm{c}}(f)\\ \mathrm{s.t.} & B_{G_{r,0}^{(k)}}\circ\mathbf{M}_d^{\mathrm{c}}(\mathbf{y})\in\Pi_{G_{r,0}^{(k)}}(\mathbf{H}_+^{r_0}),\\ & B_{G_{r,j}^{(k)}}\circ\mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\mathbf{y})\in\Pi_{G_{r,j}^{(k)}}(\mathbf{H}_+^{r_j}),\quad j\in[m],\\ & y_{\mathbf{0},\mathbf{0}}=1,\end{cases} \tag{5.8}$$

with optimum denoted by $\rho_{r,k}^{\mathrm{ts}}$. The above hierarchy is called the (complex) *TSSOS* hierarchy, which is indexed by two parameters: the relaxation order r and the *sparse order* k.

Theorem 5.8 *Consider CPOP (5.1). The following hold:*

(i) Fixing a relaxation order $r\ge r_{\min}$, the sequence $(\rho_{r,k}^{ts})_{k\ge1}$ is monotonically nondecreasing and $\rho_{r,k}^{ts}\le\rho_r$ for all k (with ρ_r defined in Section 5.1.1).

(ii) Fixing a sparse order $k\ge1$, the sequence $(\rho_{r,k}^{ts})_{r\ge r_{\min}}$ is monotonically nondecreasing.

PROOF (i). For all j, k, by construction we have $G_{r,j}^{(k)} \subseteq G_{r,j}^{(k+1)}$, which implies that $B_{G_{r,j}^{(k)}} \circ \mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\mathbf{y}) \in \Pi_{G_{r,j}^{(k)}}(\mathbf{H}_+^{r_j})$ is less restrictive than $B_{G_{r,j}^{(k+1)}} \circ \mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\mathbf{y}) \in \Pi_{G_{r,j}^{(k+1)}}(\mathbf{H}_+^{r_j})$. Hence, $(\mathrm{Q}_{r,k}^{\mathrm{ts}})$ is a relaxation of $(\mathrm{Q}_{r,k+1}^{\mathrm{ts}})$ and is clearly also a relaxation of (Q_r). As a result, $(\rho_{r,k}^{\mathrm{ts}})_{k\geq 1}$ is monotonically nondecreasing and $\rho_{r,k}^{\mathrm{ts}} \leq \rho_r$ for all k.

(ii). The conclusion follows if we can show that the inclusion $G_{r,j}^{(k)} \subseteq G_{r+1,j}^{(k)}$ holds for all r, j since this implies that $(\mathrm{Q}_{r,k}^{\mathrm{ts}})$ is a relaxation of $(\mathrm{Q}_{r+1,k}^{\mathrm{ts}})$. Let us prove $G_{r,j}^{(k)} \subseteq G_{r+1,j}^{(k)}$ by induction on k. For $k = 1$, we have $E(G_r^{\mathrm{tsp}}) \subseteq E(G_{r+1}^{\mathrm{tsp}})$ by (5.5), which implies $G_{r,j}^{(1)} \subseteq G_{r+1,j}^{(1)}$ for all r, j. Now assume that $G_{r,j}^{(k)} \subseteq G_{r+1,j}^{(k)}$ holds for all r, j for a given $k \geq 1$. Then by (5.6), (5.7) and by the induction hypothesis, we deduce that $G_{r,j}^{(k+1)} \subseteq G_{r+1,j}^{(k+1)}$ holds for all r, j, which completes the induction.

When building $(\mathrm{Q}_{r,k}^{\mathrm{ts}})$, we have the freedom to choose a specific chordal extension for any involved graph $G_{r,j}^{(k)}$, which offers a trade-off between the quality of obtained bounds and the computational cost. We show that if the maximal chordal extension is chosen, then with r fixed, the resulting sequence of optima of the hierarchy (as k increases) converges in finitely many steps to the optimum of the corresponding dense relaxation.

Theorem 5.9 *Consider CPOP (5.1). If the maximal chordal extension is used in (5.6), then for $r \geq r_{\min}$, $(\rho_{r,k}^{ts})_{k\geq 1}$ converges to ρ_r in finitely many steps.*

PROOF Let r be fixed. It is clear that for all $j \in \{0\} \cup [m]$, the graph sequence $(G_{r,j}^{(k)})_{k\geq 1}$ stabilizes after finitely many steps and we denote the stabilized graph by $G_{r,j}^{(\circ)}$. Let $(\mathrm{Q}_{r,\circ}^{\mathrm{ts}})$ be the moment relaxation corresponding to the stabilized graphs and let $\mathbf{y}^* = (y_{\beta,\gamma}^*)$ be an arbitrary feasible solution. Notice that $\{y_{\beta,\gamma} \mid (\beta,\gamma) \in \bigcup_{i=0}^m \mathrm{supp}_{g_j}(G_{r,j}^{(\circ)})\}$ is the set of decision variables involved in $(\mathrm{Q}_{r,\circ}^{\mathrm{ts}})$ and $\{y_{\beta,\gamma} \mid (\beta,\gamma) \in \mathbb{N}_d^n \times \mathbb{N}_d^n\}$ is the set of decision variables involved in (Q_r). Define $\overline{\mathbf{y}}^* = (\overline{y}_{\beta,\gamma}^*)_{(\beta,\gamma)\in\mathbb{N}_d^n\times\mathbb{N}_d^n}$ as follows:

$$\overline{y}_{\beta,\gamma}^* = \begin{cases} y_{\beta,\gamma}^*, & \text{if } (\beta,\gamma) \in \bigcup_{i=0}^m \mathrm{supp}_{g_j}(G_{r,j}^{(\circ)}), \\ 0, & \text{otherwise.} \end{cases}$$

If the maximal chordal extension is used in (5.6), then we have that the matrices in $\Pi_{G_{r,j}^{(k)}}(\mathbf{H}_+^{r_j})$ are block-diagonal (up to permutation on rows and columns) for all j, k. As a consequence, $B_{G_{r,j}^{(k)}} \circ \mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\mathbf{y}) \in \Pi_{G_{r,j}^{(k)}}(\mathbf{H}_+^{r_j})$ implies $B_{G_{r,j}^{(k)}} \circ \mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\mathbf{y}) \succeq 0$. By construction, we have $\mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\overline{\mathbf{y}}^*) = B_{G_{r,j}^{(\circ)}} \circ \mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\mathbf{y}^*) \succeq 0$ for all $j \in \{0\} \cup [m]$. Therefore, $\overline{\mathbf{y}}^*$ is a feasible solution of (Q_r) and hence $L_{\mathbf{y}^*}^{\mathrm{c}}(f) = L_{\overline{\mathbf{y}}^*}^{\mathrm{c}}(f) \geq \rho_r$, which yields $\rho_{r,\circ}^{\mathrm{ts}} \geq \rho_r$ since $\mathbf{y}^*$ is an arbitrary feasible solution of $(\mathrm{Q}_{r,\circ}^{\mathrm{ts}})$. By (i) of Theorem 5.8, we already have $\rho_{r,\circ}^{\mathrm{ts}} \leq \rho_r$. So $\rho_{r,\circ}^{\mathrm{ts}} = \rho_r$ as desired.

Proposition 5.10 *If CPOP (5.1) is a QCQP, then $(Q_{1,1}^{ts})$ and (Q_1) yield the same lower bound for CPOP (5.1), i.e., $\rho_{1,1}^{ts} = \rho_1$.*

PROOF For a QCQP, (Q_1) reads as

$$(\mathrm{Q}_1): \quad \begin{cases} \inf & L_{\mathbf{y}}^{\mathrm{c}}(f) \\ \text{s.t.} & \mathbf{M}_1^{\mathrm{c}}(\mathbf{y}) \succeq 0, \\ & L_{\mathbf{y}}^{\mathrm{c}}(g_j) \geq 0, \quad j \in [m], \\ & y_{\mathbf{0},\mathbf{0}} = 1. \end{cases}$$

Note that the objective function and the affine constraints of (Q_1) involve only the decision variables $\{y_{\mathbf{0},\mathbf{0}}\} \cup \{y_{\beta,\gamma}\}_{(\beta,\gamma)\in\mathscr{A}}$ with $\mathscr{A} = \mathrm{supp}(f) \cup \bigcup_{j=1}^m \mathrm{supp}(g_j)$. Hence there is no discrepancy of optima in replacing (Q_1) with $(\mathrm{Q}_{1,1}^{\mathrm{ts}})$ by construction.

5.1.4 Correlative-term sparsity

We are now prepared to exploit correlative sparsity and term sparsity simultaneously in the complex hierarchy for CPOP (5.1).

Let $\{I_l\}_{l\in[p]}, \{n_l\}_{l\in[p]}, J', \{J_l\}_{l\in[p]}$ be defined as in Section 5.1.2. We apply the iterative procedure of exploiting term sparsity to each subsystem involving variables $\mathbf{z}(I_l)$ for $l \in [p]$ as follows. Let

$$\mathscr{A} := \mathrm{supp}(f) \cup \bigcup_{j=1}^{m} \mathrm{supp}(g_j) \tag{5.9}$$

and

$$\mathscr{A}_l := \{(\beta,\gamma) \in \mathscr{A} \mid \mathrm{supp}(\beta) \cup \mathrm{supp}(\gamma) \subseteq I_l\} \tag{5.10}$$

for $l \in [p]$. As before, $r_{\min} := \max\{\lceil \deg(f)/2 \rceil, d_1, \ldots, d_m\}$, $d_0 := 0$ and $g_0 := 1$. Fix a relaxation order $r \geq r_{\min}$. Let $G_{r,l}^{\mathrm{tsp}}$ be the tsp graph with nodes $\mathbb{N}_{r-d_j}^{n_l}$ associated with $\mathbf{A}_l$ defined as in Section 5.1.3. Note that here we embed $\mathbb{N}_{r-d_j}^{n_l}$ into $\mathbb{N}_{r-d_j}^{n}$ via the map $\alpha = (\alpha_i)_{i\in I_l} \in \mathbb{N}_{r-d_j}^{n_l} \mapsto \alpha' = (\alpha_i')_{i\in[n]} \in \mathbb{N}_{r-d_j}^{n}$ which satisfies

$$\alpha_i' = \begin{cases} \alpha_i, & \text{if } i \in I_l, \\ 0, & \text{otherwise.} \end{cases}$$

Assume that $G_{r,l,0}^{(0)} = G_{r,l}^{\mathrm{tsp}}$ and $G_{r,l,j}^{(0)}, j \in J_l, l \in [p]$ are empty graphs. Letting

$$\mathscr{C}_r^{(k-1)} := \bigcup_{l=1}^{p} \bigcup_{j\in\{0\}\cup J_l} \mathrm{supp}_{g_j}(G_{r,l,j}^{(k-1)}), \quad k \geq 1, \tag{5.11}$$

we iteratively define an ascending chain of graphs $(G_{r,l,j}^{(k)}(V_{r,l,j}, E_{r,l,j}^{(k)}))_{k\geq 1}$ with $V_{r,l,j} = \mathbb{N}_{r-d_j}^{n_l}$ for each $j \in \{0\} \cup J_l$ and each $l \in [p]$ by

$$G_{r,l,j}^{(k)} := \overline{F_{r,l,j}^{(k)}}, \tag{5.12}$$

where $F_{r,l,j}^{(k)}$ is the graph with $V(F_{r,l,j}^{(k)}) = \mathbb{N}_{r-d_j}^{n_l}$ and

$$E(F_{r,l,j}^{(k)}) = \{\{\beta,\gamma\} \subseteq \mathbb{N}_{r-d_j}^{n_l} \mid ((\beta,\gamma) + \mathrm{supp}(g_j)) \cap \mathscr{C}_r^{(k-1)} \neq \emptyset\}. \tag{5.13}$$

Let $r_{r,l,j} := \binom{n_l + r - d_j}{r - d_j}$ for all l, j. Then with $r \geq r_{\min}$ and $k \geq 1$, the complex (moment) hierarchy based on correlative-term sparsity for CPOP (5.1) is defined as

$$(\mathrm{Q}_{r,k}^{\mathrm{cs\text{-}ts}}): \quad \begin{cases} \inf & L_{\mathbf{y}}^{\mathrm{c}}(f) \\ \text{s.t.} & B_{G_{r,l,0}^{(k)}} \circ \mathbf{M}_d^{\mathrm{c}}(\mathbf{y}, I_l) \in \Pi_{G_{r,l,0}^{(k)}}(\mathbf{H}_+^{r_{r,l,0}}), \quad l \in [p], \\ & B_{G_{r,l,j}^{(k)}} \circ \mathbf{M}_{r-d_j}^{\mathrm{c}}(g_j\mathbf{y}, I_l) \in \Pi_{G_{r,l,j}^{(k)}}(\mathbf{H}_+^{r_{r,l,j}}), \quad j \in J_l, l \in [p], \\ & L_{\mathbf{y}}^{\mathrm{c}}(g_j) \geq 0, \quad j \in J', \\ & y_{\mathbf{0},\mathbf{0}} = 1, \end{cases} \tag{5.14}$$

with optimum denoted by $\rho_{r,k}^{\mathrm{cs\text{-}ts}}$. The above hierarchy is called the (complex) *CS-TSSOS* hierarchy indexed by the relaxation order r and the sparse order k.

By similar arguments as for Theorem 5.8, we can prove the following theorem.

Theorem 5.11 *Consider CPOP (5.1). The following hold:*

(i) Fixing a relaxation order $r \ge r_{\min}$, the sequence $(\rho^{cs\text{-}ts}_{r,k})_{k\ge1}$ is monotonically nondecreasing and $\rho^{cs\text{-}ts}_{r,k} \le \rho^{cs}_r$ for all k (with ρ^{cs}_r defined in Section 5.1.2).

(ii) Fixing a sparse order $k \ge 1$, the sequence $(\rho^{cs\text{-}ts}_{r,k})_{r\ge r_{\min}}$ is monotonically nondecreasing.

From Theorem 5.11, we have the following two-level hierarchy of lower bounds for the optimum of CPOP (5.1):

$$\begin{array}{ccccccc}
\rho^{\text{cs-ts}}_{r_{\min},1} & \le & \rho^{\text{cs-ts}}_{r_{\min},2} & \le & \cdots & \le & \rho^{\text{cs}}_{r_{\min}} \\
\wedge| & & \wedge| & & & & \wedge| \\
\rho^{\text{cs-ts}}_{r_{\min}+1,1} & \le & \rho^{\text{cs-ts}}_{r_{\min}+1,2} & \le & \cdots & \le & \rho^{\text{cs}}_{r_{\min}+1} \\
\wedge| & & \wedge| & & & & \wedge| \\
\vdots & & \vdots & & \vdots & & \vdots \\
\wedge| & & \wedge| & & & & \wedge| \\
\rho^{\text{cs-ts}}_{r,1} & \le & \rho^{\text{cs-ts}}_{r,2} & \le & \cdots & \le & \rho^{\text{cs}}_{r} \\
\wedge| & & \wedge| & & & & \wedge| \\
\vdots & & \vdots & & \vdots & & \vdots
\end{array} \tag{5.15}$$

By similar arguments as for Theorem 5.9, we can prove the convergence of the CS-TSSOS hierarchy at each relaxation order when the maximal chordal extension is chosen.

Theorem 5.12 *Consider CPOP (5.1). If the maximal chordal extension is used in (5.12), then for $r \ge r_{\min}$, $(\rho^{cs\text{-}ts}_{r,k})_{k\ge1}$ converges to ρ^{cs}_r in finitely many steps.*

Fore more details on exploiting structures in complex polynomial optimization, please refer to [WM22, WM23].

5.2 Noncommutative polynomial optimization

5.2.1 Noncommutative polynomials

We consider a finite alphabet $x_1, \ldots, x_n$ (called noncommutating variables) and generate all possible words (monomials) of finite length in these letters. The empty word is denoted by 1. The resulting set of words is $\langle \underline{x} \rangle$, with $\underline{x} = (x_1, \ldots, x_n)$. We denote by $\mathbb{R}\langle \underline{x} \rangle$ the ring of real polynomials in the noncommutating variables $\underline{x}$. An element in $\mathbb{R}\langle \underline{x} \rangle$ is called a *nc polynomial*. The *support* of an nc polynomial $f = \sum_{w\in\langle \underline{x} \rangle} a_w w$ is defined by $\mathrm{supp}(f) := \{w \in \langle \underline{x} \rangle \mid a_w \ne 0\}$ and the *degree* of f, denoted by $\deg(f)$, is the length of the longest word in $\mathrm{supp}(f)$. The set of nc polynomials of degree at most r is denoted by $\mathbb{R}\langle \underline{x} \rangle_r$. Let us denote by $\mathbf{W}_r$ the vector of all words of degree at most r with resepct to the lexicographic order. Note that $\mathbf{W}_r$ serves as a monomial basis of $\mathbb{R}\langle \underline{x} \rangle_r$ and the length of $\mathbf{W}_r$ is equal to $\sigma(n, r) := \sum_{i=0}^{r} n^i = \frac{n^{r+1}-1}{n-1}$. The ring $\mathbb{R}\langle \underline{x} \rangle$ is equipped with the involution $\star$ that fixes $\mathbb{R} \cup \{x_1, \ldots, x_n\}$ point-wise and reverses words, so that $\mathbb{R}\langle \underline{x} \rangle$ is the $\star$-algebra freely generated by n symmetric letters $x_1, \ldots, x_n$. For instance $(x_1x_2 + x_2^2 + 1)^\star = x_2x_1 + x_2^2 + 1$. The set of all *symmetric elements* is defined as $\mathrm{Sym}\,\mathbb{R}\langle \underline{x} \rangle := \{f \in \mathbb{R}\langle \underline{x} \rangle \mid f = f^\star\}$. A simple example of element of $\mathrm{Sym}\,\mathbb{R}\langle \underline{x} \rangle$ is $x_1x_2 + x_2x_1 + x_2^2 + 1$. An nc polynomial of the form $g^\star g$ is called an *hermitian square*. A given $f \in \mathrm{Sym}\,\mathbb{R}\langle \underline{x} \rangle$ is a SOHS if there exist nc polynomials $h_1, \ldots, h_t \in \mathbb{R}\langle \underline{x} \rangle$ such that $f = h_1^\star h_1 + \cdots + h_t^\star h_t$. Let $\Sigma\langle \underline{x} \rangle$ stand for the set of SOHS. We denote by $\Sigma\langle \underline{x} \rangle_r \subseteq \Sigma\langle \underline{x} \rangle$ the set of SOHS polynomials of degree at most $2r$. We now recall how to check whether a given $f \in \mathrm{Sym}\,\mathbb{R}\langle \underline{x} \rangle$ is an SOHS. The existing procedure, known as the *Gram matrix method*, relies on the following proposition.

Proposition 5.13 *Assume that $f \in \mathrm{Sym}\,\mathbb{R}\langle \underline{x} \rangle$ is of degree at most $2d$. Then $f \in \Sigma\langle \underline{x} \rangle$ if and only if there exists $\mathbf{G}_f \succeq 0$ satisfying*

$$f = \mathbf{W}_d^\star \mathbf{G}_f \mathbf{W}_d. \tag{5.16}$$

Conversely, given such $\mathbf{G}_f \succeq 0$ of rank t, one can construct $g_1, \ldots, g_t \in \mathbb{R}\langle \underline{x} \rangle$ of degree at most d such that $f = \sum_{i=1}^{t} g_i^\star g_i$.

Any symmetric matrix $\mathbf{G}_f$ (not necessarily positive semidefinite) satisfying (5.16) is called a *Gram matrix* of f.

Given a set of nc polynomials $\mathfrak{g} = \{g_1, \ldots, g_m\} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$, the nc semialgebraic set $\mathcal{D}_\mathfrak{g}$ associated to $\mathfrak{g}$ is defined as follows:

$$\mathcal{D}_\mathfrak{g} := \bigcup_{k \in \mathbb{N}^*} \{\underline{A} = (A_1, \ldots, A_n) \in (\mathbb{S}_k)^n \mid g_j(\underline{A}) \succeq 0, j \in [m]\}. \tag{5.17}$$

When considering only tuples of $k \times k$ symmetric matrices, we use the notation $\mathcal{D}_\mathfrak{g}^k := \mathcal{D}_\mathfrak{g} \cap (\mathbb{S}_k)^n$. The operator semialgebraic set $\mathcal{D}_\mathfrak{g}^\infty$ is the set of all bounded self-adjoint operators $\underline{A}$ on a Hilbert space $\mathcal{H}$ endowed with a scalar product $\langle \cdot \mid \cdot \rangle$, making $g(\underline{A})$ a positive semidefinite operator for all $g \in \mathfrak{g}$, i.e., $\langle g(\underline{A})v \mid v \rangle \geq 0$, for all $v \in \mathcal{H}$. We say that an nc polynomial f is positive (denoted by $f \succ 0$) on $\mathcal{D}_\mathfrak{g}^\infty$ if for all $\underline{A} \in \mathcal{D}_\mathfrak{g}^\infty$ the operator $f(\underline{A})$ is positive definite, i.e., $\langle f(\underline{A})v \mid v \rangle > 0$, for all nonzero $v \in \mathcal{H}$. The quadratic module $\mathcal{M}(\mathfrak{g})$, generated by $\mathfrak{g}$, is defined by

$$\mathcal{M}(\mathfrak{g}) := \left\{ \sum_{i=1}^{t} a_i^\star g_i a_i \mid t \in \mathbb{N}^*, a_i \in \mathbb{R}\langle \underline{x} \rangle, g_i \in \mathfrak{g} \cup \{1\} \right\}. \tag{5.18}$$

Given $r \in \mathbb{N}^*$, the truncated quadratic module $\mathcal{M}(\mathfrak{g})_r$ of order r, generated by $\mathfrak{g}$, is

$$\mathcal{M}(\mathfrak{g})_r := \left\{ \sum_{i=1}^{t} a_i^\star g_i a_i \mid t \in \mathbb{N}^*, a_i \in \mathbb{R}\langle \underline{x} \rangle, g_j \in \mathfrak{g} \cup \{1\}, \deg(a_i^\star g_i a_i) \leq 2r \right\}. \tag{5.19}$$

A quadratic module $\mathcal{M}$ is said to be *Archimedean* if for each $a \in \mathbb{R}\langle \underline{x} \rangle$, there exists $N > 0$ such that $N - a^\star a \in \mathcal{M}$. One can show that this is equivalent to the existence of an $N > 0$ such that $N - \sum_{i=1}^n x_i^2 \in \mathcal{M}$.

Theorem 5.14 (Helton-McCullough) *Let $\{f\} \cup \mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ and assume that $\mathcal{M}(\mathfrak{g})$ is Archimedean. If $f(\underline{A}) \succ 0$ for all $\underline{A} \in \mathcal{D}_\mathfrak{g}^\infty$, then $f \in \mathcal{M}(\mathfrak{g})$.*

Assuming $f = \sum_w a_w w \in \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ and $\mathfrak{g} = \{g_1, \ldots, g_m\} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$, we define the csp graph associated with f and $\mathfrak{g}$ to be the graph G^{csp} with nodes $V = [n]$ and with edges E satisfying $\{i, j\} \in E$ if one of following conditions holds:

(i) there exists $w \in \operatorname{supp}(f)$ s.t. $x_i, x_j \in \operatorname{var}(w)$;

(ii) there exists $k \in [m]$ s.t. $x_i, x_j \in \operatorname{var}(g_k)$,

where we use $\operatorname{var}(g)$ to denote the set of variables effectively involved in $g \in \mathbb{R}\langle \underline{x} \rangle$. Let $(G^{\text{csp}})'$ be a chordal extension of G^{csp} and $I_k, k \in [p]$ be the maximal cliques of $(G^{\text{csp}})'$ with cardinality being denoted by $n_k, k \in [p]$. We denote by $\langle \underline{x}(I_k) \rangle$ (resp. $\mathbb{R}\langle \underline{x}, I_k \rangle$) the set of words (resp. nc polynomials) in the n_k variables $\underline{x}(I_k) = \{x_i : i \in I_k\}$. We also define $\operatorname{Sym} \mathbb{R}\langle \underline{x}, I_k \rangle := \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle \cap \mathbb{R}\langle \underline{x}, I_k \rangle$. Let $\Sigma\langle \underline{x}, I_k \rangle$ stand for the set of SOHS in $\mathbb{R}\langle \underline{x}, I_k \rangle$ and we denote by $\Sigma\langle \underline{x}, I_k \rangle_r$ the restriction of $\Sigma\langle \underline{x}, I_k \rangle$ to nc polynomials of degree at most $2r$. In the sequel, we will rely on two specific assumptions. The first one is as follows.

Assumption 5.15 (Boundedness) *Let $\mathcal{D}_\mathfrak{g}$ be as in (5.17). There exists $N > 0$ such that $\sum_{i=1}^n x_i^2 \preceq N$, for all $\underline{x} \in \mathcal{D}_\mathfrak{g}^\infty$.*

Then, Assumption 5.15 implies that $\sum_{j \in I_k} x_j^2 \preceq N$, for all $k \in [p]$. Thus we define

$$g_{m+k} := N - \sum_{j \in I_k} x_j^2, \quad k \in [p], \tag{5.20}$$

and set $m' = m + p$ in order to describe the same set $\mathcal{D}_\mathfrak{g}$ again as

$$\mathcal{D}_\mathfrak{g} := \bigcup_{k \in \mathbb{N}^*} \{\underline{A} \in (\mathbb{S}_k)^n \mid g_j(\underline{A}) \succeq 0, j \in [m']\}, \tag{5.21}$$

as well as the operator semialgebraic set $\mathcal{D}_\mathfrak{g}^\infty$.

The second assumption, which is the strict nc analog of Assumption 4.1 (i)–(iii), is as follows.

Assumption 5.16 *Let $\mathcal{D}_{\mathfrak{g}}$ be as in (5.21) and let $f \in \operatorname{Sym}\mathbb{R}\langle \underline{x} \rangle$. The index set $J := \{1, \ldots, m'\}$ is partitioned into p disjoint sets $J_1, \ldots, J_p$ and the two collections $\{I_1, \ldots, I_p\}$ and $\{J_1, \ldots, J_p\}$ satisfy*

(i) The objective function f can be decomposed as $f = f_1 + \cdots + f_p$, with $f_k \in \operatorname{Sym}\mathbb{R}\langle \underline{x}, I_k \rangle$ for all $k \in [p]$;

(ii) For all $k \in [p]$ and $j \in J_k$, $g_j \in \operatorname{Sym}\mathbb{R}\langle \underline{x}, I_k \rangle$;

(iii) The RIP (1.7) holds for $I_1, \ldots, I_p$ (possibly after some reordering).

Given a sequence $\mathbf{y} = (y_w)_{w \in \mathbf{W}_{2r}} \in \mathbb{R}^{\sigma(n,2r)}$ (here we allow $r = \infty$), let us define the linear functional $L_{\mathbf{y}} : \mathbb{R}\langle \underline{x} \rangle_{2r} \to \mathbb{R}$ by $L_{\mathbf{y}}(f) := \sum_w a_w y_w$, for every polynomial $f = \sum_w a_w w$ of degree at most $2r$. The sequence $\mathbf{y}$ is said to be *unital* if $y_1 = 1$ and is said to be *symmetric* if $y_{w^\star} = y_w$ for all $w \in \mathbf{W}_{2r}$. Suppose $g \in \operatorname{Sym}\mathbb{R}\langle \underline{x} \rangle$ with $\deg(g) \leq 2r$. We further associate to $\mathbf{y}$ the following two matrices:

(1) the *(noncommutative) moment matrix* $\mathbf{M}_r(\mathbf{y})$ is the matrix indexed by words $u, v \in \mathbf{W}_r$, with $[\mathbf{M}_r(\mathbf{y})]_{u,v} = L_{\mathbf{y}}(u^\star v) = y_{u^\star v}$;

(2) the *localizing matrix* $\mathbf{M}_{r-\lceil \deg(g)/2 \rceil}(g\mathbf{y})$ is the matrix indexed by words $u, v \in \mathbf{W}_{r-\lceil \deg(g)/2 \rceil}$, with $[\mathbf{M}_{r-\lceil \deg(g)/2 \rceil}(g\mathbf{y})]_{u,v} = L_{\mathbf{y}}(u^\star g v)$.

We recall the following useful facts.

Lemma 5.17 *Let $g \in \operatorname{Sym}\mathbb{R}\langle \underline{x} \rangle$ with $\deg(g) \leq 2r$ and let L be the linear functional associated to a symmetric sequence $\mathbf{y} := (y_w)_{w \in \mathbf{W}_{2r}} \in \mathbb{R}^{\sigma(n,2r)}$. Then,*

(1) *$L_{\mathbf{y}}(h^\star h) \geq 0$ for all $h \in \mathbb{R}\langle \underline{x} \rangle_r$ if and only if the moment matrix $\mathbf{M}_r(\mathbf{y}) \succeq 0$;*

(2) *$L_{\mathbf{y}}(h^\star g h) \geq 0$ for all $h \in \mathbb{R}\langle \underline{x} \rangle_{r-\lceil \deg(g)/2 \rceil}$ if and only if the localizing matrix $\mathbf{M}_{r-\lceil \deg(g)/2 \rceil}(g\mathbf{y}) \succeq 0$.*

Definition 5.18 *Let $\mathbf{y} = (y_w)_{w \in \mathbf{W}_{2r+2\delta}} \in \mathbb{R}^{\sigma(n,2r+2\delta)}$ and $\tilde{\mathbf{y}} = (y_w)_{w \in \mathbf{W}_{2r}}$ be its truncation. We can write the moment matrix $\mathbf{M}_{r+\delta}(\mathbf{y})$ in block form:*

$$\mathbf{M}_{r+\delta}(\mathbf{y}) = \begin{bmatrix} \mathbf{M}_r(\tilde{\mathbf{y}}) & B \\ B^\intercal & C \end{bmatrix}.$$

*We say that $\mathbf{y}$ is δ-*flat *or that $\mathbf{y}$ is a* flat extension *of $\tilde{\mathbf{y}}$, if $\mathbf{M}_{r+\delta}(\mathbf{y})$ is flat over $\mathbf{M}_r(\tilde{L})$, i.e., if* $\operatorname{rank} \mathbf{M}_{r+\delta}(\mathbf{y}) = \operatorname{rank} \mathbf{M}_r(\tilde{\mathbf{y}})$.

For a subset $I \subseteq [n]$, let us define $\mathbf{M}_r(\mathbf{y}, I)$ to be the moment submatrix obtained from $\mathbf{M}_r(\mathbf{y})$ after retaining only those rows and columns indexed by $w \in \langle \underline{x}(I) \rangle_r$. For $g \in \mathbb{R}\langle \underline{x}, I \rangle$ with $\deg(g) \leq 2r$, we also define the localizing submatrix $\mathbf{M}_{r-\lceil \deg(g)/2 \rceil}(g\mathbf{y}, I)$ in a similar fashion.

5.2.2 Sparse representations

Here, we state our main theoretical result, which is a sparse version of the Helton-McCullough Positivstellensatz (Theorem 5.14). For this, we rely on amalgamation theory for $C^\star$-algebras.

Given a Hilbert space $\mathcal{H}$, we denote by $\mathcal{B}(\mathcal{H})$ the set of bounded operators on $\mathcal{H}$. A $C^\star$-algebra is a complex Banach algebra $\mathcal{A}$ (thus also a Banach space), endowed with a norm $\|\cdot\|$, and with an involution $\star$ satisfying $\|xx^\star\| = \|x\|^2$ for all $x \in \mathcal{A}$. Equivalently, it is a norm closed subalgebra with involution of $\mathcal{B}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$. Given a $C^\star$-algebra $\mathcal{A}$, a *state* φ is defined to be a positive linear functional of unit norm on $\mathcal{A}$, and we write often $(\mathcal{A}, \varphi)$ when $\mathcal{A}$ comes together with the state φ. Given two $C^\star$-algebras $(\mathcal{A}_1, \varphi_1)$ and $(\mathcal{A}_2, \varphi_2)$, a homomorphism $\iota : \mathcal{A}_1 \to \mathcal{A}_2$ is called *state-preserving* if $\varphi_2 \circ \iota = \varphi_1$. Given a $C^\star$-algebra $\mathcal{A}$, a *unitary representation* of $\mathcal{A}$ in $\mathcal{H}$ is a $*$-homomorphism $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ which is *strongly continuous*, i.e., the mapping $\mathcal{A} \to \mathcal{H}$, $g \mapsto \pi(g)\xi$ is continuous for every $\xi \in \mathcal{H}$.

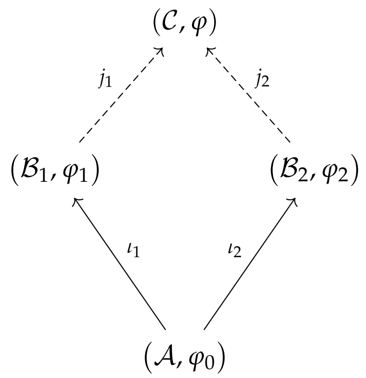

Figure 5.2: Illustration of Theorem 5.19 in the case $I = \{1, 2\}$.

Theorem 5.19 *Let $(\mathcal{A}, \varphi_0)$ and $\{(\mathcal{B}_k, \varphi_k) : k \in I\}$ be $C^\star$-algebras with states, and let ι_k be a state-preserving embedding of $\mathcal{A}$ into $\mathcal{B}_k$, for each $k \in I$. Then there exists a $C^\star$-algebra $\mathcal{C}$ amalgamating the $(\mathcal{B}_k, \varphi_k)$ over $(\mathcal{A}, \varphi_0)$. That is, there is a state φ on $\mathcal{C}$, and state-preserving homomorphisms $j_k : \mathcal{B}_k \to \mathcal{C}$, such that $j_k \circ \iota_k = j_i \circ \iota_i$, for all $k, i \in I$, and such that $\bigcup_{k \in I} j_k(\mathcal{B}_k)$ generates $\mathcal{C}$.*

Theorem 5.19 is illustrated in Figure 5.2 in the case $I = \{1, 2\}$. We also recall the GNS construction establishing a correspondence between $\star$-representations of a $C^\star$-algebra and positive linear functionals on it. In our context, the next result restricts to linear functionals on $\mathbb{R}\langle \underline{x} \rangle$ which are positive on an Archimedean quadratic module.

Theorem 5.20 *Let $\mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ be given such that its quadratic module $\mathcal{M}(\mathfrak{g})$ is Archimedean. Let $L : \mathbb{R}\langle \underline{x} \rangle \to \mathbb{R}$ be a nontrivial linear functional with $L(\mathcal{M}(\mathfrak{g})) \subseteq \mathbb{R}_{\geq 0}$. Then there exists a tuple $\underline{A} = (A_1, \ldots, A_n) \in \mathcal{D}_{\mathfrak{g}}^{\infty}$ and a vector $\mathbf{v}$ such that $L(f) = \langle f(\underline{A})\mathbf{v}, \mathbf{v} \rangle$, for all $f \in \mathbb{R}\langle \underline{x} \rangle$.*

Let $I_k, k \in [p]$ and $J_k, k \in [p]$ be given as in Chapter 4.1. For $k \in [p]$, let us define

$$\mathcal{M}(\mathfrak{g})^k := \left\{ a_0^\star a_0 + \sum_{i \in J_k} a_i^\star g_i a_i \mid a_i \in \mathbb{R}\langle \underline{x}, I_k \rangle, i \in J_k \cup \{0\} \right\}$$

and

$$\mathcal{M}(\mathfrak{g})^{\mathrm{cs}} := \mathcal{M}(\mathfrak{g})^1 + \cdots + \mathcal{M}(\mathfrak{g})^p. \tag{5.22}$$

Next, we state the main foundational result of this section.

Theorem 5.21 *Let $\{f\} \cup \mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ and let $\mathcal{D}_{\mathfrak{g}}$ be as in (5.21) with the additional quadratic constraints (5.20). Suppose Assumption 5.16 holds. If $f(\underline{A}) \succ 0$ for all $\underline{A} \in \mathcal{D}_{\mathfrak{g}}^{\infty}$, then $f \in \mathcal{M}(\mathfrak{g})^{\mathrm{cs}}$.*

We provide an example demonstrating that sparsity without an RIP-type condition is not sufficient to deduce sparsity in SOHS decompositions.

Example 5.22 *Consider the case of three variables $\underline{x} = (x_1, x_2, x_3)$ and the polynomial*

$$\begin{aligned} f &= (x_1 + x_2 + x_3)^2 \\ &= x_1^2 + x_2^2 + x_3^2 + x_1x_2 + x_2x_1 + x_1x_3 + x_3x_1 + x_2x_3 + x_3x_2 \in \Sigma\langle \underline{x} \rangle. \end{aligned}$$

Then $f = f_1 + f_2 + f_3$, with

$$f_1 = \frac{1}{2}x_1^2 + \frac{1}{2}x_2^2 + x_1x_2 + x_2x_1 \in \mathbb{R}\langle x_1, x_2\rangle,$$
$$f_2 = \frac{1}{2}x_2^2 + \frac{1}{2}x_3^2 + x_2x_3 + x_3x_2 \in \mathbb{R}\langle x_2, x_3\rangle,$$
$$f_3 = \frac{1}{2}x_1^2 + \frac{1}{2}x_3^2 + x_1x_3 + x_3x_1 \in \mathbb{R}\langle x_1, x_3\rangle.$$

However, the sets $I_1 = \{1,2\}$, $I_2 = \{2,3\}$ and $I_3 = \{1,3\}$ do not satisfy the RIP condition (1.7) and $f \notin \Sigma\langle \underline{x}\rangle^{\mathrm{cs}} := \Sigma\langle x_1, x_2\rangle + \Sigma\langle x_2, x_3\rangle + \Sigma\langle x_1, x_3\rangle$ since it has a unique Gram matrix by homogeneity.

Now consider $\mathfrak{g} = \{1 - x_1^2, 1 - x_2^2, 1 - x_3^2\}$. Then $\mathcal{D}_{\mathfrak{g}}$ is as in (5.21), $\mathcal{M}(\mathfrak{g})^{\mathrm{cs}}$ is as in (5.22) and $f|_{\mathcal{D}_{\mathfrak{g}}^{\infty}} \succeq 0$. However, we claim that $f - b \in \mathcal{M}(\mathfrak{g})^{\mathrm{cs}}$ if and only if $b \leq -3$. Clearly,

$$f + 3 = (x_1 + x_2)^2 + (x_1 + x_3)^2 + (x_2 + x_3)^2 + (1 - x_1^2) + (1 - x_2^2) + (1 - x_3^2) \in \mathcal{M}(\mathfrak{g})^{\mathrm{cs}}.$$

So one has $-3 \leq \sup\{b : f - b \in \mathcal{M}(\mathfrak{g})^{\mathrm{cs}}\}$, and the dual of this latter problem is given by

$$\begin{cases} \inf\limits_{\mathbf{y}_k} & \sum_{k=1}^3 L_{\mathbf{y}_k}(f_k) \\ \text{s.t.} & L_{\mathbf{y}_k}(1) = 1, \quad k = 1,2,3 \\ & L_{\mathbf{y}_k}(h^\star h) \succeq 0, \quad \forall h \in \mathbb{R}\langle \underline{x}, I_k\rangle, \quad k = 1,2,3 \\ & L_{\mathbf{y}_k}(h^\star(1 - x_i^2)h) \succeq 0, \quad \forall h \in \mathbb{R}\langle \underline{x}, I_k\rangle, i \in I_k, k = 1,2,3 \\ & L_{\mathbf{y}_j}|_{\mathbb{R}\langle \underline{X}(I_j \cap I_k)\rangle} = L_{\mathbf{y}_k}|_{\mathbb{R}\langle \underline{X}(I_j \cap I_k)\rangle}, \quad j,k = 1,2,3 \end{cases} \tag{5.23}$$

Hence, by weak duality, it suffices to show that there exist linear functionals $L_{\mathbf{y}_k} : \mathbb{R}\langle \underline{x}, I_k\rangle \to \mathbb{R}$ satisfying the constraints of problem (5.23) and such that $\sum_k L_{\mathbf{y}_k}(f_k) = -3$. Define

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad B = -A$$

and let

$$L_{\mathbf{y}_k}(g) = \mathrm{tr}(g(A, B)) \quad \text{for } g \in \mathbb{R}\langle \underline{x}, I_k\rangle.$$

Since $L_{\mathbf{y}_k}(f_k) = -1$, the three first constraints of problem (5.23) are easily verified and $\sum_k L_{\mathbf{y}_k}(f_k) = -3$. For the last one, given, say $h \in \mathbb{R}\langle \underline{x}, I_1\rangle \cap \mathbb{R}\langle \underline{x}, I_2\rangle = \mathbb{R}\langle x_2\rangle$, we have

$$L_{\mathbf{y}_1}(h) = \mathrm{tr}(h(B)),$$
$$L_{\mathbf{y}_2}(h) = \mathrm{tr}(h(A)),$$

since $L_{\mathbf{y}_1}$ (resp. $L_{\mathbf{y}_2}$) is defined on $\mathbb{R}\langle x_1, x_2\rangle$ (resp. $\mathbb{R}\langle x_2, x_3\rangle$) and h depends only on the second (resp. first) variable x_2 corresponding to B (resp. A).

But matrices A and B are orthogonally equivalent as $UAU^\intercal = B$ for

$$U = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

whence $h(B) = h(UAU^\intercal) = Uh(A)U^\intercal$ and $h(A)$ have the same trace.

5.2.3 Sparse GNS construction

Next, we provide the main theoretical tools to extract solutions of nc optimization problems with CS. To this end, we first present sparse nc versions of theorems by Curto and Fialkow. As recalled in Section 3.2 for the commutative case, Curto and Fialkow provided sufficient conditions for linear functionals on the set of degree $2r$ polynomials to be represented by integration with respect to a nonnegative measure. The main sufficient condition to guarantee such a representation is flatness (see Definition 5.18) of the corresponding moment matrix. We recall this result, which relies on a finite-dimensional GNS construction.

Theorem 5.23 *Let* $\mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ *and set* $\delta := \max\{\lceil \deg(g)/2 \rceil : g \in \mathfrak{g}\}$. *For* $r \in \mathbb{N}^*$, *let* $L_{\mathbf{y}} : \mathbb{R}\langle \underline{x} \rangle_{2r+2\delta} \to \mathbb{R}$ *be the linear functional associated to a unital sequence* $\mathbf{y} = (y_w)_{w \in \mathbf{W}_{2r+2\delta}} \in \mathbb{R}^{\sigma(n,2r+2\delta)}$ *satisfying* $L_{\mathbf{y}}(\mathcal{M}(\mathfrak{g})_{r+\delta}) \subseteq \mathbb{R}_{\geq 0}$. *If* $\mathbf{y}$ *is* δ*-flat, then there exists* $\hat{A} \in \mathcal{D}^r_{\mathfrak{g}}$ *for some* $t \leq \sigma(n,r)$ *and a unit vector* $\mathbf{v}$ *such that*

$$L_{\mathbf{y}}(g) = \langle g(\hat{A})\mathbf{v}, \mathbf{v} \rangle, \tag{5.24}$$

for all $g \in \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle_{2r}$.

We now give the sparse version of Theorem 5.23.

Theorem 5.24 *Suppose* $r \in \mathbb{N}^*$. *Let* $\mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle_{2r}$, *and assume* $\mathcal{D}_{\mathfrak{g}}$ *is as in* (5.21) *with the additional quadratic constraints* (5.20). *Suppose Assumption 5.16(i) holds. Set* $\delta := \max\{\lceil \deg(g)/2 \rceil : g \in \mathfrak{g}\}$. *Let* $L_{\mathbf{y}} : \mathbb{R}\langle \underline{x} \rangle_{2r+2\delta} \to \mathbb{R}$ *be the linear functional associated to a unital sequence* $\mathbf{y} = (y_w)_{w \in \mathbf{W}_{2r+2\delta}} \in \mathbb{R}^{\sigma(n,2r+2\delta)}$ *satisfying* $L_{\mathbf{y}}(\mathcal{M}(\mathfrak{g})_{r+\delta}) \subseteq \mathbb{R}_{\geq 0}$. *Assume that the following holds:*

(H1) $\mathbf{M}_{r+\delta}(\mathbf{y}, I_k)$ *and* $\mathbf{M}_{r+\delta}(\mathbf{y}, I_k \cap I_j)$ *are* δ*-flat, for all* $j, k \in [p]$.

Then, there exist finite-dimensional Hilbert spaces $\mathcal{H}(I_k)$ *with dimension* t_k, *for all* $k \in [p]$, *Hilbert spaces* $\mathcal{H}(I_j \cap I_k) \subseteq \mathcal{H}(I_j), \mathcal{H}(I_k)$ *for all pairs* (j,k) *with* $I_j \cap I_k \neq 0$, *and operators* $\hat{A}^k$, $\hat{A}^{jk}$, *acting on them, respectively. Further, there are unit vectors* $\mathbf{v}^j \in \mathcal{H}(I_j)$ *and* $\mathbf{v}^{jk} \in \mathcal{H}(I_j \cap I_k)$ *such that*

$$\begin{aligned} L_{\mathbf{y}}(f) &= \langle f(\hat{A}^j)\mathbf{v}^j, \mathbf{v}^j \rangle \quad \text{for all } f \in \mathbb{R}\langle \underline{x}, I_j \rangle_{2r}, \\ L_{\mathbf{y}}(g) &= \langle g(\hat{A}^{jk})\mathbf{v}^{jk}, \mathbf{v}^{jk} \rangle \quad \text{for all } g \in \mathbb{R}\langle \underline{X}(I_j \cap I_k) \rangle_{2r}. \end{aligned} \tag{5.25}$$

Assuming that for all pairs (j,k) *with* $I_j \cap I_k \neq \emptyset$, *one has*

(H2) the matrices $(\hat{A}^{jk}_i)_{i \in I_j \cap I_k}$ *have no common complex invariant subspaces,*

then there exist $\underline{A} \in \mathcal{D}^t_{\mathfrak{g}}$, *with* $t := t_1 \cdots t_p$, *and a unit vector* $\mathbf{v}$ *such that*

$$L_{\mathbf{y}}(f) = \langle f(\underline{A})\mathbf{v}, \mathbf{v} \rangle, \tag{5.26}$$

for all $f \in \sum_k \mathbb{R}\langle \underline{x}, I_k \rangle_{2r}$.

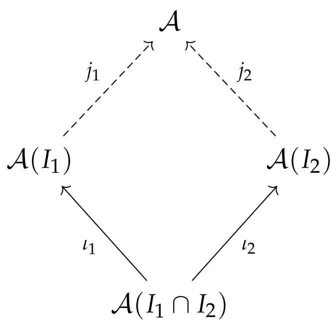

Figure 5.3: Amalgamation of finite-dimensional $C^\star$-algebras.

Example 5.25 (Non-amalgamation in finite-dimensional algebras) *Given* I_1 *and* I_2, *suppose* $\mathcal{A}(I_1 \cap I_2)$ *is generated by the* 2×2 *diagonal matrix*

$$A^{12} = \begin{bmatrix} 1 & \\ & 2 \end{bmatrix},$$

and assume $\mathcal{A}(I_1) = \mathcal{A}(I_2) = \mathbb{M}_3(\mathbb{R})$. (Observe that $\mathcal{A}(I_1 \cap I_2)$ is the algebra of all diagonal matrices.) For each $k \in \{1,2\}$, let us define $\iota_k(A) := A \oplus k$, for all $A \in \mathcal{A}(I_1 \cap I_2)$. We claim that there is no finite-dimensional $C^\star$-algebra $\mathcal{A}$ amalgamating the above Figure 5.3. Indeed, by the Skolem-Noether theorem, every homomorphism $\mathbb{M}_n(\mathbb{R}) \to \mathbb{M}_m(\mathbb{R})$ is of the form $x \mapsto P^{-1}(x \otimes \mathbf{I}_{m/n})P$ for some invertible P; in particular, n divides m. If a desired $\mathcal{A}$ existed, then the matrices $(A^{12} \oplus 1) \otimes \mathbf{I}_k$ and $(A^{12} \oplus 2) \otimes \mathbf{I}_k$ would be similar. But they are not as is easily seen from eigenvalue multiplicities.

As in the dense case, we can summarize the sparse GNS construction procedure described in the proof of Theorem 5.24 into an algorithm, called `SparseGNS` (see [KMP21, Algorithm 4.6]).

5.2.4 Eigenvalue optimization

We provide SDP relaxations allowing one to under-approximate the smallest eigenvalue that a given nc polynomial can attain on a tuple of symmetric matrices from a given semialgebraic set. We first recall the celebrated Helton-McCullough theorem stating the equivalence between SOHS and positive semidefinite nc polynomials.

Theorem 5.26 (Helton-McCullough) *Given $f \in \operatorname{Sym}\mathbb{R}\langle \underline{x} \rangle$, $f(\underline{A}) \succeq 0$, for all $\underline{A} \in (\mathbb{S}_k)^n$, $k \in \mathbb{N}^*$, if and only if $f \in \Sigma\langle \underline{x} \rangle$.*

In contrast with the constrained case where we obtain the analog of Putinar's Positivstellensatz in Theorem 5.21, there is no sparse analog of Theorem 5.26, as shown in the following example.

Lemma 5.27 *There exist polynomials which are sparse sums of hermitian squares but are not sums of sparse hermitian squares.*

PROOF Let $v = \begin{bmatrix} x_1 & x_1x_2 & x_2 & x_3 & x_3x_2 \end{bmatrix}$,

$$\mathbf{G}_f = \begin{bmatrix} 1 & -1 & -1 & 0 & \alpha \\ -1 & 2 & 0 & -\alpha & 0 \\ -1 & 0 & 3 & -1 & 9 \\ 0 & -\alpha & -1 & 6 & -27 \\ \alpha & 0 & 9 & -27 & 142 \end{bmatrix}, \qquad \alpha \in \mathbb{R}, \tag{5.27}$$

and consider

$$\begin{aligned} f &= v\mathbf{G}_f v^\star \\ &= x_1^2 - x_1x_2 - x_2x_1 + 3x_2^2 - 2x_1x_2x_1 + 2x_1x_2^2x_1 \\ &\quad - x_2x_3 - x_3x_2 + 6x_3^2 + 9x_2^2x_3 + 9x_3x_2^2 - 54x_3x_2x_3 + 142x_3x_2^2x_3. \end{aligned} \tag{5.28}$$

The polynomial f is clearly sparse with resepct to $I_1 = \{x_1, x_2\}$ and $I_2 = \{x_2, x_3\}$. Note that the matrix $\mathbf{G}_f$ is positive semidefinite if and only if $0.270615 \lesssim \alpha \lesssim 1.1075$, whence f is a sparse polynomial that is an SOHS.

We claim that $f \notin \Sigma\langle \underline{x}, I_1 \rangle + \Sigma\langle \underline{x}, I_2 \rangle$, i.e., f is not a sum of sparse hermitian squares. By the Newton chip method only monomials in v can appear in an SOHS decomposition of f. Further, every Gram matrix of f in the monomial basis v is of the form (5.27). However, the matrix $\mathbf{G}_f$ with $\alpha = 0$ is not positive semidefinite, and hence $f \notin \Sigma\langle \underline{x}, I_1 \rangle + \Sigma\langle \underline{x}, I_2 \rangle$.

Here, we focus on providing lower bounds for the constrained eigenvalue optimization of nc polynomials. Given $f \in \operatorname{Sym}\mathbb{R}\langle \underline{x} \rangle$ and $\mathfrak{g} = \{g_1, \ldots, g_m\} \subseteq \operatorname{Sym}\mathbb{R}\langle \underline{x} \rangle$ as in (5.17), let us define $\lambda_{\min}(f, \mathfrak{g})$ as follows:

$$\lambda_{\min}(f, \mathfrak{g}) := \inf\{\langle f(\underline{A})\mathbf{v}, \mathbf{v}\rangle : \underline{A} \in \mathcal{D}_{\mathfrak{g}}^{\infty}, \|\mathbf{v}\| = 1\}, \tag{5.29}$$

which is, as for the unconstrained case, equivalent to

$$\begin{aligned} \lambda_{\min}(f, \mathfrak{g}) = \quad & \sup_b \quad b \\ & \text{s.t.} \quad f(\underline{A}) - b\mathbf{I}_k \succeq 0, \quad \forall \underline{A} \in \mathcal{D}_{\mathfrak{g}}^{\infty}. \end{aligned} \tag{5.30}$$

As usual, let $d_j := \lceil \deg(g_j)/2 \rceil$ for each $j \in [m]$, and let

$$r_{\min} := \max\{\lceil \deg(f)/2 \rceil, d_1, \ldots, d_m\}.$$

One can approximate $\lambda_{\min}(f, \mathfrak{g})$ from below via the following hierarchy of SDP programs, indexed by $r \geq r_{\min}$:

$$\begin{aligned} \lambda^r(f, \mathfrak{g}) := \quad & \sup_b \quad b \\ & \text{s.t.} \quad f - b \in \mathcal{M}(\mathfrak{g})_r \end{aligned} \tag{5.31}$$

The dual of SDP (5.31) is

$$\begin{aligned} \eta^r(f, \mathfrak{g}) := \quad & \inf_{\mathbf{y}} \quad L_{\mathbf{y}}(f) \\ & \text{s.t.} \quad y_1 = 1, \quad \mathbf{M}_r(\mathbf{y}) \succeq 0 \\ & \qquad \mathbf{M}_{r-d_j}(g_j \mathbf{y}) \succeq 0, \quad j \in [m] \end{aligned} \tag{5.32}$$

Under additional assumptions, this hierarchy of primal-dual SDP (5.31)-(5.32) converges to the optimal value of the constrained eigenvalue problem.

Theorem 5.28 *Assume that $\mathcal{D}_\mathfrak{g}$ is as in (5.21) with the additional quadratic constraints (5.20) and that the quadratic module $\mathcal{M}(\mathfrak{g})$ is Archimedean. Then the following holds for $f \in \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$:*

$$\lim_{r \to \infty} \eta^r(f, \mathfrak{g}) = \lim_{r \to \infty} \lambda^r(f, \mathfrak{g}) = \lambda_{\min}(f, \mathfrak{g}). \tag{5.33}$$

The main ingredient of the proof is the nc analog of Putinar's Positivstellensatz, stated in Theorem 5.14.

Let $\mathcal{D}_\mathfrak{g}$ be as in (5.21) with the additional quadratic constraints (5.20). Let $\mathcal{M}(\mathfrak{g})^{\text{cs}}$ be as in (5.22) and let us define $\mathcal{M}(\mathfrak{g})^{\text{cs}}_r$ in the same way as the truncated quadratic module $\mathcal{M}(\mathfrak{g})_r$ in (5.19). Now, let us state the sparse variant of the primal-dual hierarchy (5.31)-(5.32) of lower bounds for $\lambda_{\min}(f, \mathfrak{g})$.

For $r \geq r_{\min}$, the sparse variant of SDP (5.32) is

$$\begin{aligned} \eta^r_{\text{cs}}(f, \mathfrak{g}) := \quad & \inf_{\mathbf{y}} \quad L_{\mathbf{y}}(f) \\ & \text{s.t.} \quad y_1 = 1, \quad \mathbf{M}_r(\mathbf{y}, I_k) \succeq 0, k \in [p] \\ & \qquad \mathbf{M}_{r-d_j}(g_j \mathbf{y}, I_k) \succeq 0, \quad j \in J_k, k \in [p] \end{aligned} \tag{5.34}$$

whose dual is the sparse variant of SDP (5.31):

$$\begin{aligned} \lambda^r_{\text{cs}}(f, \mathfrak{g}) := \quad & \sup_b \quad b \\ & \text{s.t.} \quad f - b \in \mathcal{M}(\mathfrak{g})^{\text{cs}}_r. \end{aligned} \tag{5.35}$$

An ε-neighborhood of 0 is the set $\mathcal{N}_\varepsilon$ defined for a given $\varepsilon > 0$ by

$$\mathcal{N}_\varepsilon := \bigcup_{k \in \mathbb{N}^*} \left\{ (A_1, \ldots, A_n) \in (\mathbb{S}_k)^n : \varepsilon^2 - \sum_{i=1}^n A_i^2 \succeq 0 \right\}.$$

Proposition 5.29 *Let $\{f\} \cup \mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$. Assume that $\mathcal{D}_\mathfrak{g}$ contains an ε-neighborhood of 0 and that $\mathcal{D}_\mathfrak{g}$ is as in (5.21) with the additional quadratic constraints (5.20). Then SDP (5.34) admits strictly feasible solutions. As a result, there is no duality gap between SDP (5.34) and its dual (5.35).*

Moreover, we have the following convergence result implied by Theorem 5.21.

Theorem 5.30 *Let $\{f\} \cup \mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$. Assume that $\mathcal{D}_\mathfrak{g}$ is as in (5.21) with the additional quadratic constraints (5.20). Let Assumption 5.16 hold. Then, one has*

$$\lim_{r \to \infty} \eta^r_{\text{cs}}(f, \mathfrak{g}) = \lim_{r \to \infty} \lambda^r_{\text{cs}}(f, \mathfrak{g}) = \lambda_{\min}(f, \mathfrak{g}). \tag{5.36}$$

There is no sparse variant of the "perfect" Positivstellensatz, for constrained eigenvalue optimization over convex nc semialgebraic sets [BKP16, Chapter 4.4], such as those associated either to the sparse nc ball $\mathbb{B}^{\text{cs}} := \{1 - \sum_{i \in I_1} x_i^2, \ldots, 1 - \sum_{i \in I_p} x_i^2\}$ or the nc polydisc $\mathbb{D} := \{1 - x_1^2, \ldots, 1 - x_n^2\}$. Namely, for an nc polynomial f of degree $2d+1$, computing only SDP (5.34) with optimal value $\lambda_{\text{cs}}^{d+1}(f, \mathfrak{g})$ when $\mathfrak{g} = \mathbb{B}^{\text{cs}}$ or $\mathfrak{g} = \mathbb{D}$ does not suffice to obtain the value of $\lambda_{\min}(f, \mathfrak{g})$. This is explained in Example 5.31 below.

Example 5.31 *Let us consider a randomly generated cubic polynomial $f = f_1 + f_2$ with*

$$\begin{aligned}
f_1 =& 4 - x_1 + 3x_2 - 3x_3 - 3x_1^2 - 7x_1x_2 + 6x_1x_3 - x_2x_1 - 5x_3x_1 + 5x_3x_2 \\
& - 5x_1^3 - 3x_1^2x_3 + 4x_1x_2x_1 - 6x_1x_2x_3 + 7x_1x_3x_1 + 2x_1x_3x_2 - x_1x_3^2 \\
& - x_2x_1^2 + 3x_2x_1x_2 - x_2x_1x_3 - 2x_2^3 - 5x_2^2x_3 - 4x_2x_3^2 - 5x_3x_1^2 \\
& + 7x_3x_1x_2 + 6x_3x_2x_1 - 4x_3x_2x_2 - x_3^2x_1 - 2x_3^2x_2 + 7x_3^3, \\
f_2 =& -1 + 6x_2 + 5x_3 + 3x_4 - 5x_2^2 + 2x_2x_3 + 4x_2x_4 - 4x_3x_2 + x_3^2 - x_3x_4 \\
& + x_4x_2 - x_4x_3 + 2x_4^2 - 7x_2^3 + 4x_2x_3^2 + 5x_2x_3x_4 - 7x_2x_4x_3 - 7x_2x_4^2 \\
& + x_3x_2^2 + 6x_3x_2x_3 - 6x_3x_2x_4 - 3x_3^2x_2 - 7x_3^2x_4 + 6x_3x_4x_2 \\
& - 3x_3x_4x_3 - 7x_3x_4^2 + 3x_4x_2^2 - 7x_4x_2x_3 - x_4x_2x_4 - 5x_4x_3^2 \\
& + 7x_4x_3x_4 + 6x_4^2x_2 - 4x_4^3,
\end{aligned}$$

and the nc polyball $\mathfrak{g} = \mathbb{B}^{\text{cs}} = \{1 - x_1^2 - x_2^2 - x_3^2, 1 - x_2^2 - x_3^2 - x_4^2\}$ corresponding to $I_1 = \{1,2,3\}$ and $I_2 = \{2,3,4\}$. Then, one has $\lambda_{\text{cs}}^2(f,\mathfrak{g}) \simeq -27.536 < \lambda_{\text{cs}}^3(f,\mathfrak{g}) \simeq -27.467 \simeq \lambda_{\min}^2(f,\mathfrak{g}) = \lambda_{\min}(f,\mathfrak{g})$.

Corollary 5.32 *Let $\{f\} \cup \mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$, and assume that $\mathcal{D}_{\mathfrak{g}}$ is as in (5.21) with the additional quadratic constraints (5.20). Suppose Assumptions 5.16(i)-(ii) hold. Let $\mathbf{y}$ be an optimal solution of SDP (5.34) with optimal value $\eta_{\text{cs}}^r(f,\mathfrak{g})$ for $r \geq r_{\min} + \delta$, such that $\mathbf{y}$ satisfies the assumptions of Theorem 5.24. Then, there exist $t \in \mathbb{N}^*$, $\underline{A} \in \mathcal{D}_{\mathfrak{g}}^t$ and a unit vector $\mathbf{v}$ such that*

$$\lambda_{\min}(f,\mathfrak{g}) = \langle f(\underline{A})\mathbf{v}, \mathbf{v} \rangle = \eta_{\text{cs}}^r(f,\mathfrak{g}).$$

Example 5.33 *Consider the sparse polynomial $f = f_1 + f_2$ from Example 5.31. The moment matrix $\mathbf{M}_3(\mathbf{y})$ obtained by solving (5.34) with $r = 3$ satisfies the flatness (H1) and irreducibility (H2) conditions of Theorem 5.24. We can thus apply the `SparseGNS` algorithm yielding*

$$A_1 = \begin{bmatrix} 0.0059 & 0.0481 & 0.1638 & 0.4570 \\ 0.0481 & -0.2583 & 0.5629 & -0.2624 \\ 0.1638 & 0.5629 & 0.3265 & -0.3734 \\ 0.4570 & -0.2624 & -0.3734 & -0.2337 \end{bmatrix}$$

$$A_2 = \begin{bmatrix} -0.3502 & 0.0080 & 0.1411 & 0.0865 \\ 0.0080 & -0.4053 & 0.2404 & -0.1649 \\ 0.1411 & 0.2404 & -0.0959 & 0.3652 \\ 0.0865 & -0.1649 & 0.3652 & 0.4117 \end{bmatrix}$$

$$A_3 = \begin{bmatrix} -0.7669 & -0.0074 & -0.1313 & -0.0805 \\ -0.0074 & -0.4715 & -0.2238 & 0.1535 \\ -0.1313 & -0.2238 & 0.0848 & -0.3400 \\ -0.0805 & 0.1535 & -0.3400 & -0.2126 \end{bmatrix}$$

$$A_4 = \begin{bmatrix} 0.3302 & -0.1839 & 0.1811 & -0.0404 \\ -0.1839 & -0.1069 & 0.5114 & -0.0570 \\ 0.1811 & 0.5114 & 0.1311 & -0.3664 \\ -0.0404 & -0.0570 & -0.3664 & 0.4440 \end{bmatrix}$$

where

$$f(\underline{A}) = \begin{bmatrix} -10.3144 & 3.9233 & -5.0836 & -7.7828 \\ 3.9233 & 1.8363 & 4.5078 & -7.5905 \\ -5.0836 & 4.5078 & -19.5827 & 13.9157 \\ -7.7828 & -7.5905 & 13.9157 & 8.3381 \end{bmatrix}$$

has minimal eigenvalue -27.4665 *with unit eigenvector*

$$\mathbf{v} = \begin{bmatrix}0.1546 & -0.2507 & 0.8840 & -0.3631\end{bmatrix}^{\intercal}.$$

In this case all the ranks involved are equal to four. So A_2 *and* A_3 *are computed from* $\mathbf{M}_3(\mathbf{y}, I_1 \cap I_2)$*, after an appropriate basis change* A_1 *(and the same* A_2, A_3*) is obtained from* $\mathbf{M}_3(\mathbf{y}, I_1)$*, and finally* A_4 *is computed from* $\mathbf{M}_3(\mathbf{y}, I_2)$*.*

For more details on exploiting correlative sparsity in noncommutative polynomial optimization, please refer to [KMP21].

5.2.5 Eigenvalue optimization with term sparsity

Recall that the eigenvalue optimization problem is defined by

$$\lambda_{\min}(f, \mathfrak{g}) := \inf\{\langle f(\underline{A})\mathbf{v}, \mathbf{v}\rangle : \underline{A} \in \mathcal{D}_{\mathfrak{g}}^{\infty}, \|\mathbf{v}\| = 1\}, \tag{5.37}$$

for $f \in \operatorname{Sym}\mathbb{R}\langle \underline{x}\rangle$ and $\mathfrak{g} = \{g_1, \ldots, g_m\} \subseteq \operatorname{Sym}\mathbb{R}\langle \underline{x}\rangle$. Let

$$\mathscr{A} = \operatorname{supp}(f) \cup \bigcup_{j=1}^{m} \operatorname{supp}(g_j). \tag{5.38}$$

Fixing a relaxation order $r \geq r_{\min}$, we define a graph G_r^{tsp} with nodes $\mathbf{W}_r$[1] and edges

$$E(G_r^{\text{tsp}}) = \{\{u, v\} \mid (u, v) \in \mathbf{W}_r \times \mathbf{W}_r,\ u \neq v,\ u^{\star}v \in \mathscr{A} \cup \mathbf{W}_r^2\}, \tag{5.39}$$

where $\mathbf{W}_r^2 := \{u^{\star}u \mid u \in \mathbf{W}_r\}$. We call G_r^{tsp} the tsp graph associated with the support $\mathscr{A}$.

For a graph $G(V, E)$ with $V \subseteq \langle \underline{x}\rangle$ and $g \in \mathbb{R}\langle \underline{x}\rangle$, let us define

$$\operatorname{supp}_g(G) := \{u^{\star}wv \mid u = v \in V \text{ or } \{u, v\} \in E, w \in \operatorname{supp}(g)\}. \tag{5.40}$$

Let $G_{r,0}^{(0)} = G_r^{\text{tsp}}$ and $G_{r,j}^{(0)}$ be the empty graph with nodes $V_{r,j} := \mathbf{W}_{r-d_j}$ for $j \in [m]$. Then for each $j \in \{0\} \cup [m]$, we iteratively define a sequence of graphs $(G_{r,j}^{(s)}(V_{r,j}, E_{r,j}^{(s)}))_{s \geq 1}$ via two successive operations:

(1) **support extension**. Let $F_{r,j}^{(s)}$ be the graph with nodes $V_{r,j}$ and

$$\begin{aligned} E(F_{r,j}^{(s)}) = &\{\{u, v\} \mid (u, v) \in V_{r,j} \times V_{r,j},\ u \neq v, \\ &u^{\star} \operatorname{supp}(g_j) v \cap \bigcup_{j=0}^{m} \operatorname{supp}_{g_j}(G_{r,j}^{(s-1)}) \neq \emptyset\}, \end{aligned} \tag{5.41}$$

where $u^{\star} \operatorname{supp}(g_j) v := \{u^{\star}wv \mid w \in \operatorname{supp}(g_j)\}$.

(2) **chordal extension**. Let

$$G_{r,j}^{(s)} := (F_{r,j}^{(s)})'. \tag{5.42}$$

By construction, one has $G_{r,j}^{(s)} \subseteq G_{r,j}^{(s+1)}$ for all j, s. Therefore, for every j, the sequence of graphs $(G_{r,j}^{(s)})_{s \geq 1}$ stabilizes after a finite number of steps.

Let $t_j = |\mathbf{W}_{r-d_j}|$ for $j \in \{0\} \cup [m]$. Then by replacing the csp constraint $\mathbf{M}_{r-d_j}(g_j\mathbf{y}) \succeq 0$ with the weaker constraint $\mathbf{B}_{G_{r,j}^{(s)}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y}) \in \Pi_{G_{r,j}^{(s)}}(\mathbb{S}_{t_j}^{+})$ for $j \in \{0\} \cup [m]$ in (5.32), we obtain the following series of sparse moment relaxations for (5.37) indexed by $s \geq 1$:

$$\begin{aligned} \lambda_{\text{ts}}^{r,s}(f, \mathfrak{g}) := \inf_{\mathbf{y}} \quad & L_{\mathbf{y}}(f) \\ \text{s.t.} \quad & \mathbf{B}_{G_{r,0}^{(s)}} \circ \mathbf{M}_r(\mathbf{y}) \in \Pi_{G_{r,0}^{(s)}}(\mathbb{S}_{t_0}^{+}) \\ & \mathbf{B}_{G_{r,j}^{(s)}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y}) \in \Pi_{G_{r,j}^{(s)}}(\mathbb{S}_{t_j}^{+}), \quad j \in [m] \\ & y_1 = 1 \end{aligned} \tag{5.43}$$

[1] If $\mathfrak{g} = \emptyset$, then we may replace the monomial basis $\mathbf{W}_r$ with the one returned by the Newton chip method; see [BKP16, §2.3].

We call s the *sparse order*. For each $s \geq 1$, the dual of (5.43) reads as

$$\begin{cases} \sup\limits_{\mathbf{G}_j, b} & b \\ \text{s.t.} & \sum_{j=0}^{m} \langle \mathbf{G}_j, \mathbf{D}_w^j \rangle + b\delta_{1w} = f_w, \quad \forall w \in \bigcup_{j=0}^{m} \text{supp}_{g_j}(G_{r,j}^{(s)}) \\ & \mathbf{G}_j \in \mathbb{S}_{t_j}^+ \cap \mathbb{S}_{G_{r,j}^{(s)}}, \quad j \in \{0\} \cup [m] \end{cases} \tag{5.44}$$

where $\{\mathbf{D}_w^j\}_{j,w}$ are appropriate matrices satisfying $\mathbf{M}_{r-d_j}(g_j \mathbf{y}) = \sum_w \mathbf{D}_w^j y_w$. We then call the TS-adapted moment-SOHS relaxations (5.43)–(5.44) the *NCTSSOS hierarchy* associated with (5.37).

Theorem 5.34 *Let $\{f\} \cup \mathfrak{g} \subseteq \text{Sym}\,\mathbb{R}\langle \underline{x} \rangle$. Then the following hold:*

(1) Suppose that $\mathcal{D}_{\mathfrak{g}}$ contains an nc ε-neighborhood of 0. Then for all r, s, there is no duality gap between (5.43) and its dual (5.44).

(2) Fixing a relaxation order $r \geq r_{\min}$, the sequence $(\lambda_{ts}^{r,s}(f, \mathfrak{g}))_{s\geq 1}$ is monotonically non-decreasing and $\lambda_{ts}^{r,s}(f, \mathfrak{g}) \leq \lambda^r(f, \mathfrak{g})$ for all s (with $\lambda^r(f, \mathfrak{g})$ being defined in (5.32)).

(3) Fixing a sparse order $s \geq 1$, the sequence $(\lambda_{ts}^{r,s}(f, \mathfrak{g}))_{r \geq r_{\min}}$ is monotonically non-decreasing.

(4) If the maximal chordal extension is chosen in (5.42), then $(\lambda_{ts}^{r,s}(f, \mathfrak{g}))_{s\geq 1}$ converges to $\lambda^r(f, \mathfrak{g})$ in finitely many steps.

Following from Theorem 5.34, we have the following two-level hierarchy of lower bounds for the optimum $\lambda_{\min}(f, \mathfrak{g})$ of (5.37):

$$\begin{array}{ccccccc} \lambda_{\text{ts}}^{r_{\min},1}(f, \mathfrak{g}) & \leq & \lambda_{\text{ts}}^{r_{\min},2}(f, \mathfrak{g}) & \leq & \cdots & \leq & \lambda^{r_{\min}}(f, \mathfrak{g}) \\ \wedge| & & \wedge| & & & & \wedge| \\ \lambda_{\text{ts}}^{r_{\min}+1,1}(f, \mathfrak{g}) & \leq & \lambda_{\text{ts}}^{r_{\min}+1,2}(f, \mathfrak{g}) & \leq & \cdots & \leq & \lambda^{r_{\min}+1}(f, \mathfrak{g}) \\ \wedge| & & \wedge| & & & & \wedge| \\ \vdots & & \vdots & & \vdots & & \vdots \\ \wedge| & & \wedge| & & & & \wedge| \\ \lambda_{\text{ts}}^{r,1}(f, \mathfrak{g}) & \leq & \lambda_{\text{ts}}^{r,2}(f, \mathfrak{g}) & \leq & \cdots & \leq & \lambda^{r}(f, \mathfrak{g}) \\ \wedge| & & \wedge| & & & & \wedge| \\ \vdots & & \vdots & & \vdots & & \vdots \end{array} \tag{5.45}$$

Example 5.35 *Consider $f = 2 - x^2 + xy^2x - y^2 + xyxy + yxyx + x^3y + yx^3 + xy^3 + y^3x$ and $\mathfrak{g} = \{1 - x^2, 1 - y^2\}$. The graph sequence $(G_{2,0}^{(s)})_{s\geq 1}$ for f and $\mathfrak{g}$ is given in Figure 5.4. In fact the graph sequence $(G_{2,j}^{(s)})_{s\geq 1}$ stabilizes at $s = 2$ for $j = 0, 1, 2$ (with approximately smallest chordal extensions). Using* `TSSOS`*, we obtain that $\lambda_{ts}^{2,1}(f, \mathfrak{g}) \approx -2.55482$, $\lambda_{ts}^{2,2}(f, \mathfrak{g}) = \lambda^2(f, \mathfrak{g}) \approx -2.05111$.*

5.2.6 Combining correlative and term sparsity

Combining CS with TS for eigenvalue optimization proceeds in a similar manner as for the commutative case in Chapter 4.7.

Let $f = \sum_w f_w w \in \text{Sym}\,\mathbb{R}\langle \underline{x} \rangle$ and $\mathfrak{g} = \{g_1, \ldots, g_m\} \subseteq \text{Sym}\,\mathbb{R}\langle \underline{x} \rangle$. Suppose that G^{csp} is the csp graph associated with f and $\mathfrak{g}$, and $(G^{\text{csp}})'$ is a chordal extension of G^{csp}. Let $\{I_k\}_{k\in[p]}$ be the maximal cliques of $(G^{\text{csp}})'$ with cardinality being denoted by $n_k, k \in [p]$. Then the set of variables $\underline{x}$ is decomposed into $\underline{x}(I_1), \underline{x}(I_2), \ldots, \underline{x}(I_p)$. Let $J_1, \ldots, J_p$ be defined as before.

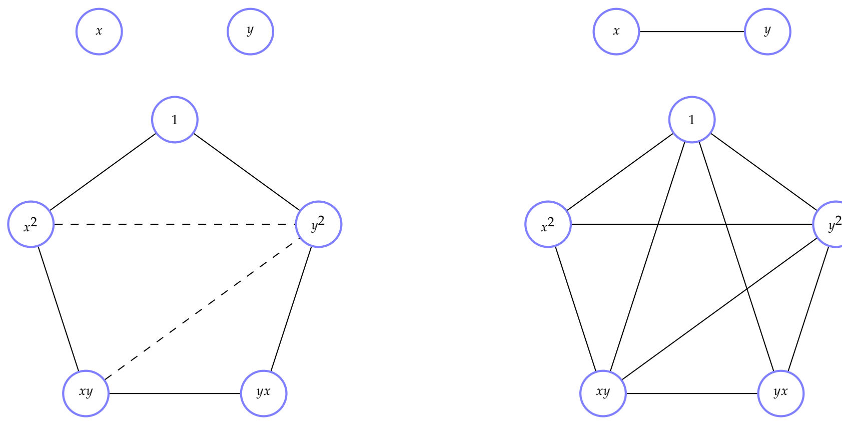

Figure 5.4: The graph sequence $(G_{2,0}^{(s)})_{s\geq 1}$ in Example 5.35: left for $s=1$; right for $s=2$. The dashed edges are added after a chordal extension.

Now we consider the tsp for each subsystem involving the variables $\underline{x}(I_k)$, $k\in[p]$ respectively as follows. Let

$$\mathscr{A} := \mathrm{supp}(f) \cup \bigcup_{j=1}^{m} \mathrm{supp}(g_j) \text{ and } \mathscr{A}_k := \{w \in \mathscr{A} \mid \mathrm{var}(w) \subseteq \underline{x}(I_k)\}, \tag{5.46}$$

for $k\in[p]$. As before, let $g_0=1$, $d_j=\lceil \deg(g_j)/2\rceil$, $j\in\{0\}\cup[m]$ and $r_{\min}=\max\{\lceil\deg(f)/2\rceil, d_1,\ldots,d_m\}$. Fix a relaxation order $r\geq r_{\min}$. Let $\mathbf{W}_{r-d_j,k}$ be the standard monomial basis of degree $\leq r-d_j$ with respect to the variables $\underline{x}(I_k)$ and $G_{r,k}^{\mathrm{tsp}}$ be the tsp graph with nodes $\mathbf{W}_{r,k}$ associated with $\mathscr{A}_k$ defined as in Chapter 5.2.5. Let $G_{r,k,0}^{(0)}=G_{r,k}^{\mathrm{tsp}}$ and $G_{r,k,j}^{(0)}$ be the empty graph with nodes $V_{r,k,j}:=\mathbf{W}_{r-d_j,k}$ for $j\in J_k, k\in[p]$. Letting

$$\mathscr{C}_r^{(s)} := \bigcup_{k=1}^{p} \bigcup_{j\in\{0\}\cup J_k} \mathrm{supp}_{g_j}(G_{r,k,j}^{(s)}), \tag{5.47}$$

we iteratively define a sequence of graphs $(G_{r,k,j}^{(s)}(V_{r,k,j},E_{r,k,j}^{(s)}))_{s\geq 1}$ for each $j\in\{0\}\cup J_k, k\in[p]$ by

$$G_{r,k,j}^{(s)} := (F_{r,k,j}^{(s)})', \tag{5.48}$$

where $F_{r,k,j}^{(s)}$ is the graph with nodes $V_{r,k,j}$ and edges

$$E(F_{r,k,j}^{(s)}) = \{\{u,v\} \mid u\neq v\in V_{r,k,j}, u^\star\,\mathrm{supp}(g_j)v \cap \mathscr{C}_r^{(s-1)} \neq \emptyset\}. \tag{5.49}$$

Let $t_{k,j}=|\mathbf{W}_{r-d_j,k}|$ for all k,j. Then for each $s\geq 1$ (called the *sparse order*), the moment relaxation based on correlative-term sparsity for (5.37) is given by

$$\begin{array}{rll} \lambda_{\text{cs-ts}}^{r,s}(f,\mathfrak{g}) := & \inf\limits_{\mathbf{y}} & L_{\mathbf{y}}(f) \\ & \text{s.t.} & \mathbf{B}_{G_{r,k,0}^{(s)}} \circ \mathbf{M}_r(\mathbf{y},I_k) \in \Pi_{G_{r,k,0}^{(s)}}(\mathbb{S}_{r_{k,0}}^{+}), \quad k\in[p] \\ & & \mathbf{B}_{G_{r,k,j}^{(s)}} \circ \mathbf{M}_{r-d_j}(g_j\mathbf{y},I_k) \in \Pi_{G_{r,k,j}^{(s)}}(\mathbb{S}_{r_{k,j}}^{+}), \quad j\in J_k, k\in[p] \\ & & y_1 = 1 \end{array} \tag{5.50}$$

For all k,j, let us write $\mathbf{M}_{r-d_j}(g_j\mathbf{y},I_k)=\sum_w \mathbf{D}_w^{k,j} y_w$ for appropriate matrices $\{\mathbf{D}_w^{k,j}\}_{k,j,w}$. Then for each $s\geq 1$, the dual of (5.50) reads as

$$\begin{cases} \sup\limits_{\mathbf{G}_{k,j},b} & b \\ \text{s.t.} & \sum_{k=1}^{p}\sum_{j\in\{0\}\cup J_k}\langle \mathbf{G}_{k,j}, \mathbf{D}_w^{k,j}\rangle + b\delta_{1w} = f_w, \quad \forall w\in\mathscr{C}_r^{(s)} \\ & \mathbf{G}_{k,j}\in\mathbb{S}_{t_{k,j}}^{+}\cap\mathbb{S}_{G_{r,k,j}^{(s)}}, \quad j\in\{0\}\cup J_k, k\in[p] \end{cases} \tag{5.51}$$

where $\mathscr{C}_r^{(s)}$ is defined in (5.47).

The properties of the relaxations (5.50)–(5.51) are summarized in the following theorem.

Theorem 5.36 *Assume that $\{f\} \cup \mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$. Then the following hold:*

(1) *Fixing a relaxation order $r \geq r_{\min}$, the sequence $(\lambda^{r,s}_{cs\text{-}ts}(f, \mathfrak{g}))_{s\geq 1}$ is monotonically non-decreasing and $\lambda^{r,s}_{cs\text{-}ts}(f, \mathfrak{g}) \leq \lambda^{r}_{cs}(f, \mathfrak{g})$ for all $s \geq 1$ (with $\lambda^{r}_{cs}(f, \mathfrak{g})$ being defined in Chapter 5.34).*

(2) *Fixing a sparse order $s \geq 1$, the sequence $(\lambda^{r,s}_{cs\text{-}ts}(f, \mathfrak{g}))_{r\geq r_{\min}}$ is monotonically non-decreasing.*

(3) *If the maximal chordal extension is chosen in (5.48), then $(\lambda^{r,s}_{cs\text{-}ts}(f, \mathfrak{g}))_{s\geq 1}$ converges to $\lambda^{r}_{cs}(f, \mathfrak{g})$ in finitely many steps.*

5.2.7 Trace optimization

We start this section by introducing useful notations about commutators and trace zero polynomials. Given $g, h \in \mathbb{R}\langle \underline{x} \rangle$, the nc polynomial $[g, h] := gh - hg$ is called a *commutator*. Two nc polynomials $g, h \in \mathbb{R}\langle \underline{x} \rangle$ are called *cyclically equivalent* ($g \overset{\text{cyc}}{\sim} h$) if $g - h$ is a sum of commutators. Given $\mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ with corresponding quadratic module $\mathcal{M}(\mathfrak{g})$ and truncated variant $\mathcal{M}(\mathfrak{g})_d$, one defines $\Theta(\mathfrak{g})_d := \{g \in \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle_{2d} : g \overset{\text{cyc}}{\sim} h \text{ for some } h \in \mathcal{M}(\mathfrak{g})_d\}$ and $\Theta(\mathfrak{g}) := \bigcup_{d\in\mathbb{N}} \Theta(\mathfrak{g})_d$. In this case, $\Theta(\mathfrak{g})$ stands for the *cyclic quadratic module* generated by $\mathfrak{g}$ and $\Theta(\mathfrak{g})_d$ stands for the *truncated cyclic quadratic module* generated by $\mathfrak{g}$.

For $\mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ and $\mathcal{D}_{\mathfrak{g}}$ as in (5.21) with the additional quadratic constraints (5.20), let us define $\Theta(\mathfrak{g})^k_d := \{g \in \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle_{2d} : g \overset{\text{cyc}}{\sim} h \text{ for some } h \in \mathcal{M}(\mathfrak{g})^k_d\}$, $\Theta(\mathfrak{g})^k := \bigcup_{d\in\mathbb{N}} \Theta(\mathfrak{g})^k_d$, for all $k \in [p]$ and the sum

$$\Theta(\mathfrak{g})^{\text{cs}}_d := \Theta(\mathfrak{g})^1_d + \cdots + \Theta(\mathfrak{g})^p_d, \tag{5.52}$$

as well as $\Theta(\mathfrak{g})^{\text{cs}} := \bigcup_{d\in\mathbb{N}} \Theta(\mathfrak{g})^{\text{cs}}_d$. If $\mathfrak{g}$ is empty, we drop the $\mathfrak{g}$ in the above notations. The normalized trace of a matrix $A \in \mathbb{S}_t$ is given by $\operatorname{tr} A = \frac{1}{t} \operatorname{trace} A$. An nc polynomial $g \in \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ is called a *trace zero* nc polynomial if $\operatorname{tr}(g(\underline{A})) = 0$, for all $\underline{A} \in \mathbb{S}^n$. This is equivalent to $g \overset{\text{cyc}}{\sim} 0$ (see e.g. [KS08, Proposition 2.3]). For a given nc polynomial g, the cyclic degree of g, denoted by $\operatorname{cdeg}(g)$, is the smallest degree of a polynomial cyclically equivalent to g. The next theorem allows one to obtain a sparse tracial representation of a tracial linear functional, under the same flatness and irreducibility conditions stated in Theorem 5.24. This is a sparse variant of [BKP16, Theorem 1.71].

Theorem 5.37 *Let $\mathfrak{g} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle_{2d}$, and assume that the semialgebraic set $\mathcal{D}_{\mathfrak{g}}$ is as in (5.21) with the additional quadratic constraints (5.20). Let Assumption 5.16(i) hold. Set $\delta := \max\{\lceil \deg(g)/2 \rceil : g \in \mathfrak{g} \cup \{1\}\}$. Let $L : \mathbb{R}\langle \underline{x} \rangle_{2d+2\delta} \to \mathbb{R}$ be a unital tracial linear functional satisfying $L(\Theta(\mathfrak{g})^{\text{cs}}_d) \subseteq \mathbb{R}^{\geq 0}$. Assume that the flatness (H1) and irreducibility (H2) conditions of Theorem 5.24 hold. Then there are finitely many n-tuples $\underline{A}^{(j)}$ of symmetric matrices in $\mathcal{D}^r_{\mathfrak{g}}$ for some $r \in \mathbb{N}$, and positive scalars λ_j with $\sum_j \lambda_j = 1$, such that for all $f \in \mathbb{R}\langle \underline{x}, I_1 \rangle_{2d} + \cdots + \mathbb{R}\langle \underline{x}, I_p \rangle_{2d}$, one has:*

$$L(f) = \sum_j \lambda_j \operatorname{tr} f(\underline{A}^{(j)}). \tag{5.53}$$

In this subsection, we provide the sparse tracial version of Lasserre's hierarchy to minimize the trace of a noncommutative polynomial on a semialgebraic set. Given $f \in \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ and $\mathfrak{g} = \{g_1, \ldots, g_m\} \subset \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ as in (5.17), let us define $\operatorname{tr}_{\min}(f, \mathbf{S})$ as follows:

$$\operatorname{tr}_{\min}(f, \mathfrak{g}) := \inf\{\operatorname{tr} f(\underline{A}) : \underline{A} \in \mathcal{D}_{\mathfrak{g}}\}. \tag{5.54}$$

Since an infinite-dimensional Hilbert space does not admit a trace, we obtain lower bounds on the minimal trace by considering a particular subset of $\mathcal{D}_{\mathfrak{g}}^{\infty}$. This subset is obtained by restricting from the algebra of all bounded operators $\mathcal{B}(\mathcal{H})$ on a Hilbert space $\mathcal{H}$ to finite von Neumann algebras of type I and type II. We introduce $\operatorname{tr}_{\min}(f,\mathfrak{g})^{\mathrm{II}_1}$ as the trace-minimum of f on $\mathcal{D}_{\mathfrak{g}}^{\mathrm{II}_1}$. This latter set is defined as follows (see [BKP16, Definition 1.59]):

Definition 5.38 *Let $\mathcal{F}$ be a type-II_1-von Neumann algebra [Tak03, Chapter 5]. Let us define $\mathcal{D}_{\mathfrak{g}}^{\mathcal{F}}$ as the set of all tuples $\underline{A} = (A_1,\ldots,A_n) \in \mathcal{F}^n$ making $g(\underline{A})$ a positive semidefinite operator for every $g \in \mathfrak{g}$. The von Neumann semialgebraic set $\mathcal{D}_{\mathfrak{g}}^{\mathrm{II}_1}$ generated by $\mathfrak{g}$ is defined as*

$$\mathcal{D}_{\mathfrak{g}}^{\mathrm{II}_1} := \bigcup_{\mathcal{F}} \mathcal{D}_{\mathfrak{g}}^{\mathcal{F}},$$

where the union is over all type-II_1-von Neumann algebras with separable predual.

By [BKP16, Proposition 1.62], if $f \in \Theta(\mathfrak{g})$, then $\operatorname{tr} f(\underline{A}) \geq 0$, for all $A \in \mathcal{D}_{\mathfrak{g}}$ and $A \in \mathcal{D}_{\mathfrak{g}}^{\mathrm{II}_1}$. Since $\mathcal{D}_{\mathfrak{g}}$ can be modeled by $\mathcal{D}_{\mathfrak{g}}^{\mathrm{II}_1}$, one has $\operatorname{tr}_{\min}(f,\mathfrak{g})^{\mathrm{II}_1} \leq \operatorname{tr}_{\min}(f,\mathfrak{g})$. With $r_{\min}$ being defined as before, one can approximate $\operatorname{tr}_{\min}(f,\mathfrak{g})^{\mathrm{II}_1}$ from below via the following hierarchy of SDP programs, indexed by $r \geq r_{\min}$:

$$\operatorname{tr}^r(f,\mathfrak{g}) = \sup\{b : f - b \in \Theta(\mathfrak{g})_r\}, \tag{5.55}$$

whose dual is

$$\begin{aligned} L_{\Theta}^r(f,\mathfrak{g}) := \inf_{\mathbf{y}} \quad & \langle \mathbf{M}_r(\mathbf{y}), \mathbf{G}_f \rangle \\ \text{s.t.} \quad & (\mathbf{M}_r(\mathbf{y}))_{u,v} = (\mathbf{M}_r(\mathbf{y}))_{w,z}, \quad \text{for all } u^\star v \overset{\text{cyc}}{\sim} w^\star z, \\ & y_1 = 1, \\ & \mathbf{M}_r(\mathbf{y}) \succeq 0, \quad \mathbf{M}_{r-d_j}(g_j \mathbf{y}) \succeq 0, \quad j \in [m], \\ & L : \mathbb{R}\langle \underline{x} \rangle_{2d} \to \mathbb{R} \text{ linear.} \end{aligned} \tag{5.56}$$

If the quadratic module $\mathcal{M}(\mathfrak{g})$ is Archimedean, the resulting hierarchy of SDP programs provides a sequence of lower bounds $\operatorname{tr}^r(f,\mathfrak{g})$ monotonically converging to $\operatorname{tr}_{\min}(f,\mathfrak{g})^{\mathrm{II}_1}$, see e.g. [BKP16, Corollary 3.5].

Next, we present a sparse variant hierarchy of SDP programs providing a sequence of lower bounds $\operatorname{tr}_{\mathrm{cs}}^r(f,\mathfrak{g})$ monotonically converging to $\operatorname{tr}_{\min}(f,\mathfrak{g})^{\mathrm{II}_1}$. Let $\mathfrak{g} \cup \{f\} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ and let $\mathcal{D}_{\mathfrak{g}}$ be as in (5.21) with the additional quadratic constraints (5.20). Let us define the sparse variant of SDP (5.56), indexed by $r \geq r_{\min}$:

$$\begin{aligned} L_{\Theta,\mathrm{cs}}^r(f,\mathfrak{g}) = \inf_{\mathbf{y}} \quad & \sum_{k=1}^{p} \langle \mathbf{M}_r(\mathbf{y}, I_k), \mathbf{G}_{f_k} \rangle \\ \text{s.t.} \quad & (\mathbf{M}_r(\mathbf{y}, I_k))_{u,v} = (\mathbf{M}_r(\mathbf{y}, I_k))_{w,z}, \quad \text{for all } u^\star v \overset{\text{cyc}}{\sim} w^\star z, \\ & y_1 = 1, \\ & \mathbf{M}_r(\mathbf{y}, I_k) \succeq 0, \quad k \in [p], \\ & \mathbf{M}_{r-d_j}(g_j L, I_k) \succeq 0, \quad j \in J_k, \quad k \in [p], \\ & L : \mathbb{R}\langle \underline{x}, I_1 \rangle_{2d} + \cdots + \mathbb{R}\langle \underline{x}, I_p \rangle_{2d} \to \mathbb{R} \text{ linear.} \end{aligned} \tag{5.57}$$

whose dual is the sparse variant of SDP (5.55):

$$\operatorname{tr}_{\mathrm{cs}}^r(f,\mathfrak{g}) = \sup\{b : f - b \in \Theta(\mathfrak{g})_d^{\mathrm{cs}}\}, \tag{5.58}$$

With the same conditions as the ones assumed in Proposition 5.29 for constrained eigenvalue optimization, SDP (5.57) admits strictly feasible solutions, so there is no duality gap between SDP (5.57) and SDP (5.58). The proof is the same since the constructed linear functional in Proposition 5.29 is tracial. In order to prove convergence of the hierarchy of bounds given by the SDP (5.57)-(5.58), we need the following proposition, which is the sparse variant of [BKP16, Proposition 1.63].

Proposition 5.39 *Let* $\mathfrak{g} \cup \{f\} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ *and let* $\mathcal{D}_{\mathfrak{g}}$ *be as in* (5.21) *with the additional quadratic constraints* (5.20)*. Let Assumption 5.16 hold. Then the following are equivalent:*

(i) $\operatorname{tr} f(\underline{A}) \geq 0$ *for all* $\underline{A} \in \mathcal{D}_{\mathfrak{g}}^{\mathrm{II}_1}$*;*

(ii) for all $\varepsilon > 0$*, there exists* $g \in \mathcal{M}(\mathfrak{g})^{\mathrm{cs}}$ *with* $f + \varepsilon \overset{cyc}{\sim} g$*.*

Proposition 5.39 implies the following convergence property.

Corollary 5.40 *Let* $\mathfrak{g} \cup \{f\} \subseteq \operatorname{Sym} \mathbb{R}\langle \underline{x} \rangle$ *and let* $\mathcal{D}_{\mathfrak{g}}$ *be as in* (5.21) *with the additional quadratic constraints* (5.20)*. Let Assumption 5.16 hold. Then*

$$\lim_{r \to \infty} \operatorname{tr}_{\mathrm{cs}}^{r}(f, \mathfrak{g}) = \lim_{r \to \infty} L_{\Theta,\mathrm{cs}}^{r}(f, \mathfrak{g}) = \operatorname{tr}_{\min}(f, \mathfrak{g})^{\mathrm{II}_1}.$$

For more details on noncommutative polynomial optimization, please refer to [BKP16]. For more details on exploiting term sparsity in noncommutative polynomial optimization, please refer to [WM21].

5.3 Other extensions

• Polynomial matrix inequality: please refer to [GW23].

Chapter 6

Applications

6.1 Software

SDP:

- MOSEK: https://www.mosek.com/

POP:

- TSSOS: https://github.com/wangjie212/TSSOS

6.2 Optimal power flow

Please refer to [WML22].

6.3 Polyphase wave design

Please refer to [WM23].

6.4 Quantum maximal violation of Bell inequalities

Please refer to [KMVW23].

6.5 Ground state energy of local Hamiltonian

Please refer to [WSF+23].

6.6 Other applications

Please refer to [Las09, Las15, MW23].

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