# Non-negative Polynomials, Sums of Squares & The Moment Problem

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Except where otherwise indicated, this thesis is my original work.

Abhishek Bhardwaj
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To my parents

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# Abstract

This thesis studies *polynomial optimization*, that is, the problem of minimizing the value of a polynomial over a semi-algebraic set. Such polynomial optimization problems arise in a wide variety of contexts, both in mathematics, and more generally in science and engineering.

In the first part of this thesis, we study a polynomial optimization problem which arises when solving the *separability problem* in Quantum Information Theory. Our approach is via sums of squares decompositions for polynomials, which provide a natural relaxation for polynomial optimization. Our focus is on the development of practical computational methods to address these problems. We review classical sum of squares relaxations, and give a comparison of the computational complexities between some of the modern state-of-the-art relaxations. Using the insights gained from this analysis we develop a MATLAB package which is able to solve the separability problem in cases which were beyond the reach of previously existing software implementations.

In the second part of this thesis, we study *the tracial moment problem*, which can be thought of as a dual problem to non-commutative polynomial optimization. For the bivariate quartic tracial moment problem, the problem is well understood when the associated Hankel matrix (which has size $7 \times 7$) is positive definite, or positive semi-definite and of rank at most 4. Here we examine the Hankel matrix when it is of rank 5 or 6 and show that there are four canonical cases to study. In two out of the four rank 6 cases, we reformulate the existence of a representing measure, to a feasibility problem of three small linear matrix inequalities and a rank constraint. Our results significantly improve previous approaches to the bivariate quartic tracial moment problem.

Finally, we also study the tracial moment problem on elliptic curves, giving a reduction to the classical moment problem in two out of the three cases. Furthermore, for the classical moment problem on elliptic curves, we give sufficient conditions for a representing measure $\mu$ to exist.

# Contents

Chapter 1

# Introduction

Optimization is one of the most widely applicable branches of mathematics across science. It is ubiquitous in statistics [58], biology [68], cosmology [41], engineering [72, 89], and computer science [77] to name a few. In this thesis we will study the special subclass of *polynomial optimization* problems: given polynomials $p, g_1, \dots, g_k \in \mathbb{R}[x_1, \dots, x_n] \equiv \mathbb{R}[x]$, compute

$$\begin{aligned} p^{min} &= \min_{x \in \mathbb{R}^n} p(x), \\ s.t.\ g_1(x) &\geq 0, \dots, g_k(x) \geq 0. \end{aligned} \tag{1.1}$$

In other words, find the minimum (or more generally the infimum) of the polynomial $p$, over the semi-algebraic set $K = \{x \in \mathbb{R}^n : g_1(x) \geq 0, \dots, g_k(x) \geq 0\}$ which is the non-negativity set of the polynomials $g_1, \dots, g_k$. Many problems from different areas of mathematics can be formulated in this way; some notable examples are *the max-cut problem*, *testing matrix copositivity*, and *the stable set problem*. However, it is well known that problem (1.1) is NP-hard [40, 70, 75]. In the first part of this thesis (Chapters 2 and 3) we focus on approximating the solution to (1.1) via a sum of squares relaxations.

Sums of squares relaxations arise out of the following consideration, *'given a polynomial $p \in \mathbb{R}[x]$, if there are polynomials $h_1, \dots, h_k \in \mathbb{R}[x]$, such that the polynomial $p$ can be decomposed as $p = h_1^2 + \cdots + h_k^2$, then $p$ is non-negative on $\mathbb{R}^n$'*. Thus, a sum of squares decomposition provides a *certificate of non-negativity*. Furthermore, sum of squares decompositions make problem (1.1) easier, as such decompositions can be efficiently computed using the recent advances in semi-definite programming. As we can see, an essential component here is understanding when such a decomposition into a sum of squares is possible. This topic has a rich history, beginning with the work of Hilbert in the late 1800's [46]. For the univariate case, it has been known for a long time that if a univariate polynomial $p(x)$ is non-negative on $\mathbb{R}$, then it can be written as a sum of squares (two squares to be precise), a result often credited to Gauss. But in 1885, during his thesis defense, Minkowski conjectured that there are non-negative homogeneous polynomials which are not sums of squares. Fascinated by this, in 1888 Hilbert published [46] proving that this conjecture was in fact true. He further characterized the only cases where non-negativity is equivalent to the existence of a sum of squares decomposition.

This was the inspiration for Hilbert's $17^{th}$ problem, presented at the 1900 International Congress of Mathematicians in Paris, which questioned whether every non-negative polynomial could be decomposed as a sum of squares of *rational* functions. This question was answered in the affirmative by Artin in 1927 [3], and these results are usually regarded as the birthplace of Real Algebraic Geometry [13].

Since then, our understanding of sum of squares decompositions has grown considerably. In Chapter 2 we present these developments in more detail. The most groundbreaking being the Positivstellensatz, presented by Stengle [92] and now known to have been understood earlier by Krivine [55], which gives the most general conditions for decomposing non-negative polynomials into a sum of squares. We consider also the Positivstellensätze of Schmüdgen and Putinar, which under some additional natural assumptions, improve upon the result of Krivine. The representations due to the results of Schmüdgen or Putinar are undoubtedly simpler, and computationally advantageous in the context of optimization. We also show how to pose the existence of a sum of squares decomposition as a semi-definite program.

Hilbert's theorem proved the existence of non-negative polynomials which could not be written as sums of squares, however his proof was not constructive. The first known example, the Motzkin polynomial (Example 2.7), was discovered almost eight decades later [69]. In their recent work, Blekherman, Smith and Velasco [12] showed how to construct (random) non-negative polynomials, over varieties of non-minimal degrees, which are not sums of squares. The work of [51] further refines this process into an algorithm (Algorithm 1) to construct non-negative biquadratic polynomials which are not sums of squares and have a carefully chosen set of zeros. Biquadratic polynomials which are non-negative but not sums of squares are in direct correspondence with positive maps that are not completely positive from operator algebras (*pncp* maps for short). Our interest in this correspondence is motivated by *the separability problem* from Quantum Information Theory, which asks to determine if a given quantum state $\rho$ is *entangled*. A general approach to solving the separability problem relies on pncp maps, which can be constructed using Algorithm 1.

The underlying optimization problem in Algorithm 1 requires minimizing a non-negative polynomial. When we restrict to strictly positive polynomials, there are many methods to decompose a polynomial into a sum of squares which are guaranteed to work, and work well. On the contrary, when we consider non-negative polynomials, many of these methods (while useful) start to become limited and require additional information on intricate algebraic objects, which in most cases is difficult to obtain. Hence, the construction of pncp maps from Algorithm 1, requires a computationally suitable sum of squares relaxation for non-negative polynomials.

In Chapter 3 we examine several new relaxations to construct pncp maps. Our contributions towards this are as follows. Through our experiments we find the most stable, and the most efficient relaxation for Algorithm 1. In addition to this, we also illustrate how these randomly constructed pncp maps can help to detect entanglement in a quantum state represented by a density matrix $\rho \in \mathbb{R}^{n\times n}$. Our findings are nicely collected into a MATLAB package *PnCP*, designed for constructing random positive maps which are not completely positive. Moreover, PnCP can be used to check if a quantum state is entangled (see Algorithm 2 and Examples 3.15 and 3.16). While there are existing software packages for detecting quantum entanglement, they rely on a criterion (Criterion 3.13) which is no longer sufficient in higher dimensions; in contrast PnCP is applicable for arbitrary dimensions. As such we expect PnCP to significantly aid in the study of many problems in Quantum Information Theory.

In the second part of this thesis (Chapters 4 and 5) we study the dual theory of moments. The *moment problem* is a classical question in analysis, which asks when a linear functional on the space of univariate polynomials is represented by integration. Equivalently, for a sequence, $\beta$, of real (or complex) numbers, does there exist a *representing measure* $\mu$, such that the terms of $\beta$ are the moments of $\mu$?

Initiated by Stieltjes, the *power moment problem* in particular requires a real sequence $(\beta_k)_{k=0}^{\infty}$ to satisfy

$$\beta_i = \int_a^b x^i \, d\mu,$$

and is well studied. Let

$$\Delta_n = \begin{pmatrix} \beta_0 & \beta_1 & \dots & \beta_n \\ \beta_1 & \beta_2 & \dots & \beta_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_n & \beta_{n+1} & \dots & \beta_{2n} \end{pmatrix}, \text{ and } \Delta_n^{(1)} = \begin{pmatrix} \beta_1 & \beta_2 & \dots & \beta_{n+1} \\ \beta_2 & \beta_3 & \dots & \beta_{n+2} \\ \vdots & \vdots & \ddots & \vdots \\ \beta_{n+1} & \beta_{n+2} & \dots & \beta_{2n+1} \end{pmatrix}.$$

For the interval $[a, b] = [0, \infty)$, Stieltjes [93] gave necessary and sufficient conditions for a solution to the power moment problem using the Hankel matrices $\Delta_n$ and $\Delta_n^{(1)}$; there exists a representing measure $\mu$, such that $\beta_i = \int_0^\infty x^i \, d\mu$ if and only if $\det(\Delta_n) > 0$ and $\det(\Delta_n^{(1)}) > 0$ for every $n \geq 0$. Similar solutions for $[a, b] = (-\infty, \infty)$, and $[a, b] = [0, 1]$ are given by Hamburger [43] and Hausdorff [45] respectively, with each of these problems now named after the solver.

There are of course many generalizations, the first natural extension perhaps being to consider the problem on $\mathbb{R}^n$. To be precise, given a sequence $(\beta_\gamma)$ indexed by $\gamma = (\gamma_1, \dots, \gamma_n) \in \mathbb{N}^n$, we ask if there is a positive Borel measure $\mu$ on $\mathbb{R}^n$ such that

$$\beta_\gamma = \int_{\mathbb{R}^n} x^\gamma \, d\mu, \tag{1.2}$$

with the standard multi-index notation $x^\gamma = x_1^{\gamma_1} \cdots x_n^{\gamma_n}$. The general solution to this extension, the Riesz-Haviland Theorem [32, Theorem 1.1], provides a connection to non-negative polynomials through a duality relation: A sequence $(\beta_\gamma)_{\gamma \in \mathbb{N}^n}$, represents the moments of a positive Borel measure $\mu$ on $\mathbb{R}^n$ (i.e., $(\beta_\gamma)$ satisfies (1.2)), if and only if $\sum_\gamma p_\gamma \beta_\gamma \geq 0$ for every polynomial $p = \sum p_\gamma x^\gamma \in \mathbb{R}[x]$ which is non-negative on $\mathbb{R}^n$.

For the bivariate case ($\mathbb{R}^2$) in particular, there is a great deal of understanding and success for the *truncated moment problem*, which considers (1.2) with the truncation of $(\beta_\gamma)_{\gamma \in \mathbb{N}^2}$, i.e.,

$$\beta_{\gamma_1, \gamma_2} = \int_{\mathbb{R}^2} x_1^{\gamma_1} x_2^{\gamma_2} \, d\mu, \quad \gamma_1 + \gamma_2 \leq 2d, \tag{1.3}$$

and $d \in \mathbb{N}$. Stochel has shown in [95] that the truncated moment problem (1.3) is in fact more general than the full problem (1.2). In light of this, we only concern ourselves with the truncated moment problem.

Consider the following *(generalized) Hankel matrix*

$$\mathcal{M}_d(\beta) := \begin{array}{c} \\ \mathbb{1} \\ \mathbb{X} \\ \mathbb{Y} \\ \vdots \\ \mathbb{X}^d \\ \vdots \\ \mathbb{Y}^d \end{array} \begin{array}{c} \begin{array}{ccccccc} \mathbb{1} & \mathbb{X} & \mathbb{Y} & \dots & \mathbb{X}^d & \dots & \mathbb{Y}^d \end{array} \\ \begin{pmatrix} \beta_{0,0} & \beta_{1,0} & \beta_{0,1} & \dots & \beta_{d,0} & \dots & \beta_{0,d} \\ \beta_{1,0} & \beta_{2,0} & \beta_{1,1} & \dots & \beta_{d+1,0} & \dots & \beta_{1,d} \\ \beta_{0,1} & \beta_{1,1} & \beta_{0,2} & \dots & \beta_{d,1} & \dots & \beta_{0,d+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \beta_{d,0} & \beta_{d+1,0} & \beta_{d,1} & \dots & \beta_{2d,0} & \dots & \beta_{d,d} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \beta_{0,d} & \beta_{1,d} & \beta_{0,d+1} & \dots & \beta_{d,d} & \dots & \beta_{0,2d} \end{pmatrix} \end{array}.$$

Hankel matrices have been integral to the study of the moment problem. Curto and Fialkow paved the way forward through their seminal works [26, 27, 28, 29, 30, 31], in which they connected the solution of the truncated moment problem (1.3) to extensions of $\mathcal{M}_d(\beta)$. They developed a new functional calculus for the truncated moment problem, which studies polynomial equations defined on the columns and rows of $\mathcal{M}_d(\beta)$ (hence the suggestive column/row labels for $\mathcal{M}_d(\beta)$). This technique provided a complete characterization of the *quartic moment problem* ($\mathcal{M}_2(\beta)$, see Theorem 4.10), and is now an essential tool in studying not only the moment problem, but also some of its further generalizations.

Extending this problem further, Burgdorf and Klep introduced the *tracial moment problem* in [16], a non-commutative counterpart to (1.2). For a simple statement of the problem, consider the sequence $(\beta_{w(X,Y)})$ generated as

$$\beta_{w(X,Y)} = \int_{(\mathbb{SR}^{t\times t})^2} \operatorname{tr}(w(A,B))\, d\mu(A,B), \tag{1.4}$$

where $\mathbb{SR}^{t\times t}$ is the space of symmetric real matrices, $\mu$ a measure on this space, $w(X,Y)$ are monomials of the non-commutative variables $X$ and $Y$, and $\operatorname{tr}$ is the trace functional. The tracial moment problem is the converse : Given a sequence $(\beta_{w(X,Y)})$, is there a $t \in \mathbb{N}$ with a measure $\mu$ on $(\mathbb{SR}^{t\times t})^2$ such that $(\beta_{w(X,Y)})$ satisfies (1.4)?

Like the moment problem, the tracial moment problem is intertwined with optimization of non-commutative polynomials. Burgdorf and Klep have studied this connection well [15, 18], and in fact for the quartic tracial moment problem with sequences $(\beta_{w(X,Y)})$ that have their corresponding tracial Hankel matrix positive definite, they solved the problem entirely [16] (an alternative proof can be found in [19]). The tracial moment problem is further shown to be connected to many other important problems such as Connes' embedding conjecture in operator algebras [24, 52], or the now confirmed BMV conjecture [8, 14, 53, 91].

In the author's MSc thesis [9], we explored the quartic tracial moment problem when the associated Hankel matrix is singular and positive semi-definite, equivalently, when the representing measure $\mu$ must be contained in some quadratic variety. We used the extension approach of Curto and Fialkow to establish sufficient conditions for a solution to exist. During the PhD, collaboration with Aljaž Zalar led to refinements of these results, and moreover we established necessary conditions for the solution to exist, with our results published in [10].

In Chapter 4, we present some of these new results, developed during the PhD, on the quartic tracial moment problem, which provide a novel computational framework to search for solutions. We show that the quartic tracial moment problem reduces to the analysis of four canonical column relations in the Hankel matrix $\mathcal{M}_2$. We also illustrate that in many cases, the atoms of a potential representing measure have a nice form. This *atomic* approach enables us to completely characterize when a solution exists if the Hankel matrix $\mathcal{M}_2$ has rank 5. Finally, in the rank 6 case, we show that the quartic tracial moment problem can be reformulated into a feasibility problem of three small *linear matrix inequalities* and a rank constraint.

Chapter 5 generalizes this study to truncations of all orders $d$, where the representing measure lies on a cubic variety. This is the first presentation of the truncated tracial moment problem on cubic varieties. In particular, we study measures over Elliptic curves, which are the smooth cubics. Our first contribution is a reduction of the truncated tracial moment problem on elliptic curves, in two out of the three cases, to the classical (commutative) truncated moment problem on elliptic curves. The classical truncated moment problem has previously been studied on cubic varieties in special cases. For instance [33, 102, 103] study extremal cases of the sextic moment problem, with [102] giving special focus to harmonic cubic polynomials, and Fialkow [38] solves the classical truncated moment problem with representing measures supported on $y = x^3$. Elliptic varieties however remain largely unstudied, and to the best of our knowledge our presentation is the first analysis on elliptic varieties, even for the classical truncated moment problem. Our second contribution is an analysis of sufficient conditions for a representing measure to exist on elliptic curves in the classical setting. We also illustrate the distinctions with the quartic moment problem in Example 5.15.

Sums of squares relaxations and the dual theory of moments have become an increasingly popular approach to polynomial optimization problems. Indeed many state-of-the art optimization software such as SOStools, GloptiPoly3, RealCertify etc., are based on these ideas. The results of this thesis help to further our understanding of these concepts, highlight new directions for future research, and expand the horizon of applications to the realm of Quantum Information Theory.

Chapter 2

# Sums of Squares & Optimization

This chapter establishes a basic background for studying optimization through *sums of squares* (SOS) relaxations. The material presented is well understood and classical, with most texts on SOS theory having a similar presentation.

There is a vast amount of literature on the topic, but the survey of Laurent [59] is perhaps the best introduction, covering a broad range of topics. We follow the overall structure of [59] for sums of squares, and naturally adjust things for our purposes. We present proofs only when they are instructive, and otherwise refer the reader to appropriate literature.

We first settle on some notation which we use throughout the thesis. We denote by $\mathbb{N}$ (resp., $\mathbb{R}, \mathbb{C}$) the set of non-negative integers (resp., real numbers, complex numbers). We write $\mathbb{R}[x_1, \dots, x_n]$ for the ring of polynomials in $n$ variables and coefficients from $\mathbb{R}$, and often abbreviate to $\mathbb{R}[x]$, with $x = (x_1, \dots, x_n)$. When working with a small number of variables, for instance two, we normally write $\mathbb{R}[x, y]$ instead of $\mathbb{R}[x_1, x_2]$. We use bold face letters $\mathbf{x}, \mathbf{y}, \mathbf{z}, \dots$ for vectors. For $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$, $x^\alpha$ represents the monomial $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$, which has degree $|\alpha| = \alpha_1 + \cdots + \alpha_n$. A polynomial $p(x) \in \mathbb{R}[x]$ is of the form $p(x) = \sum_{\alpha \in \mathbb{N}^n} p_\alpha x^\alpha$, with only finitely many non-zero $p_\alpha$ (unless working with specific examples, we usually just write $p$ instead of $p(x)$). When $p_\alpha \neq 0$, we call $p_\alpha x^\alpha$ a *term* of $p$. The *degree* of a polynomial $p$ is defined as $\deg(p) := \max\{|\alpha| : p_\alpha \neq 0\}$. The set $\mathbb{R}[x]_d$ is the set of all polynomials with degree less than or equal to $d$.

We write $\mathbb{R}^{s \times t}$ for the set of real matrices of size $s \times t$, and $\mathbb{SR}^{s \times s}$ for the set of symmetric real matrices of size $s \times s$. We equip $\mathbb{R}^{s \times s}$ ($\mathbb{SR}^{s \times s}$) with the trace inner product

$$\langle A, B \rangle = \operatorname{tr}(A^T B),$$

for matrices $A, B \in \mathbb{R}^{s \times s}$.

We note that, in general, every polynomial $p \in \mathbb{R}[x]_{2d}$ can be written (in a non-unique way) as

$$p(x) = \mathbf{x}_d^T Q \mathbf{x}_d, \tag{2.1}$$

where $Q \in \mathbb{SR}^{s \times s}$ and $\mathbf{x}_d$ is the vector of all monomials with degree at most $d$. A matrix $Q \in \mathbb{SR}^{s \times s}$ is called *positive semi-definite* if for all *non-zero* vectors $\mathbf{x} \in \mathbb{R}^s$ we have

$$\mathbf{x}^T Q \mathbf{x} \geq 0. \tag{2.2}$$

We write $Q \succeq 0$. Similarly, $Q$ is called positive definite ($Q \succ 0$) if (2.2) is strict whenever

$\mathbf{x} \neq \mathbf{0}$. There are many equivalent formulations of positive semi-definiteness. Some important ones are the following: if $Q \in \mathbb{SR}^{s\times s}$ then the following are equivalent

(1) $Q \succeq 0$,

(2) there exists a $V \in \mathbb{R}^{s\times s}$ such that

$$Q = V^T V, \tag{2.3}$$

(3) $Q = \sum_{i=1}^k \mathbf{a}_i \mathbf{a}_i^T$ for some vectors $\mathbf{a}_i \in \mathbb{R}^s$,

(4) all eigenvalues of $Q$ are non-negative.

## 2.1 Polynomials and Non-negativity.

We say that $p \in \mathbb{R}[x]$ is *non-negative* if the evaluation $p(a) \geq 0$ for all $a \in \mathbb{R}^n$. In this case we write $p \geq 0$ (and similarly $p > 0$ when $p$ is *positive*). We say that $p$ has an SOS decomposition, or that $p$ is SOS, if there exist $q_1, \dots, q_k \in \mathbb{R}[x]$ such that

$$p = q_1^2 + \cdots + q_k^2.$$

We use the standard notation

$$\mathcal{P}_n = \{p \in \mathbb{R}[x_1, \dots, x_n] : p \geq 0\},$$
$$\Sigma_n = \{p \in \mathbb{R}[x_1, \dots, x_n] : p \text{ is SOS}\},$$

and

$$\mathcal{P}_{n,d} = \mathcal{P}_n \cap \mathbb{R}[x_1, \dots, x_n]_d,$$
$$\Sigma_{n,d} = \Sigma_n \cap \mathbb{R}[x_1, \dots, x_n]_d.$$

The following simple result is helpful when searching for SOS decompositions, as we will see in Example 2.7.

**Lemma 2.1** (Lemma 3.1, [59]). *If $p \in \Sigma_n$, then $\deg(p)$ is even. Moreover for any $q_i \in \mathbb{R}[x]$ such that $p = \sum_i q_i^2$, we have $\deg(q_i) \leq \deg(p)/2$.*

A polynomial $p$ is called *homogeneous* if all of its terms have the same degree. Let $p$ be a polynomial of degree $d$, i.e., $p = \sum_{|\alpha|\leq d} p_\alpha x^\alpha$, the homogenization of $p$ is the polynomial $\tilde{p} \in \mathbb{R}[x, x_{n+1}]$ defined as $\tilde{p} = \sum_{|\alpha|\leq d} p_\alpha x^\alpha x_{n+1}^{d-|\alpha|}$. As an example, consider the univariate quadratic

$$f(x) = x^2 + x + 1 \in \mathbb{R}[x].$$

The homogenization of $f$ is given by

$$\tilde{f}(x, y) = x^2 + xy + y^2 \in \mathbb{R}[x, y].$$

The following result shows that being non-negative or SOS is preserved under homogenization.

**Proposition 2.2.** *A polynomial $p \in \mathbb{R}[x]_{2d}$ is non-negative (resp. is SOS) if and only if the homogenization $\tilde{p} \in \mathbb{R}[x, x_{n+1}]_{2d}$ is non-negative (resp. is SOS).*

*Proof.* When $\tilde{p}$ is non-negative or SOS, the statement is clear (evaluate $x_{n+1} = 1$). Suppose that

$$p(x) = \sum_{|\alpha| \leq 2d} p_\alpha x^\alpha,$$

is non-negative on $\mathbb{R}^n$. Notice that we may write

$$\tilde{p}(x, x_{n+1}) = x_{n+1}^{2d} \sum_{|\alpha| \leq 2d} p_\alpha \left( \frac{x}{x_{n+1}} \right)^\alpha . \tag{2.4}$$

When $x_{n+1} \neq 0$, it is clear that $\tilde{p}$ is non-negative, as both $x_{n+1}^{2d}$ and $p$ are non-negative. On the other hand when $x_{n+1} = 0$, we instead write $p(x) = p_{2d} + \cdots + p_0$, where each $p_i$ is a term of degree $i$. Expanding (2.4) we find

$$\tilde{p} = x_{n+1}^{2d} \left( \frac{p_{2d}}{x_{n+1}^{2d}} + \cdots + \frac{p_0}{x_{n+1}^0} \right) = p_{2d} \geq 0,$$

where the last inequality holds because the highest degree term must be non-negative since $p$ is non-negative. The SOS property is proved similarly. □

It is clear to see that any SOS polynomial is non-negative on $\mathbb{R}^n$, the interesting question is when are these sets equal, i.e., $\Sigma_{n,d} = \mathcal{P}_{n,d}$? Two instances of this have been known for a long time.

**Theorem 2.3** (Gauss)**.** *Let $p \in \mathbb{R}[x]$ be a univariate polynomial. If $p(a) \geq 0$ for all $a \in \mathbb{R}$, then $p$ is SOS. In fact $p$ is a sum of* two *squares.*

**Theorem 2.4.** *Let $p \in \mathbb{R}[x]$ be a quadratic polynomial. If $p(a) \geq 0$ for all $a \in \mathbb{R}^n$, then $p$ is SOS.*

**Remark 2.5.** While there is a standard proof of Theorem 2.3 using the Fundamental Theorem of Algebra and the identity $(a^2 + b^2)(c^2 + d^2) = (ac + bd)^2 + (ad - bc)^2$, we recommend [67] for a far more interesting and general proof based on the Hahn-Banach Seperation theorem and Caratheodory's theorem on convex combinations.

Hilbert completely characterized when $\Sigma_{n,d} = \mathcal{P}_{n,d}$ [46], by proving that equality holds in exactly one other case.

**Theorem 2.6** (Hilbert)**.** $\Sigma_{n,d} = \mathcal{P}_{n,d}$ *if and only if $(n, d)$ is one of the following, $(1, d)$, $(n, 2)$ or $(2, 4)$.*

While this theorem proved the existence of non-negative polynomials which could not be written as sums of squares, the first concrete example, the *Motzkin polynomial*, was discovered much later in 1967 [69].

**Example 2.7** (Motzkin polynomial)**.** Let $M(x,y) = x^4y^2 + x^2y^4 - 3x^2y^2 + 1$. To see that $M(x,y) \geq 0$, set $a = xy^2$, $b = x^2y$ and $c = 1$, then the arithmetic geometric mean inequality gives

$$\frac{a^2+b^2+c^2}{3} \geq \sqrt[3]{a^2b^2c^2},$$

that is

$$x^4y^2 + x^2y^4 + 1 \geq 3x^2y^2.$$

Now suppose that $M$ is SOS. Using Lemma 2.1, we know that any decomposition $M = q_1^2 + \cdots + q_k^2$, requires $q_r$ to be of the form

$$q_r(x,y) = a_rx^3 + b_rx^2y + c_rxy^2 + d_ry^3 + e_rx^2 + f_rxy + g_ry^2 + h_rx + i_ry + j_r.$$

Comparing coefficients, we see that $\sum_r a_r^2 = 0$ and so $a_r = 0$. Similarly we find $e_r = g_r = 0$, and so (comparing coefficients for $x^2y^2$ terms) $\sum_r (f_r^2 + 2e_rg_r) = \sum_r f_r^2 = -3$, a contradiction. Hence $M(x,y) \notin \Sigma_{2,6}$.

Some other examples of polynomials which are non-negative but not SOS, such as the Robinson or Choi-Lam, can be found in [86].

## 2.2 SOS Programming

**Definition 2.8.** Given a finite set $G = \{g_1, \ldots, g_k\}$ of $\mathbb{R}[x]$, the *basic semi-algebraic set* associated to $G$ is defined as

$$K_G := \{x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_k(x) \geq 0\}.$$

Let us see now how the theory of sums of squares can be helpful in optimization. Recall our general optimization problem

$$p^{min} = \min_{x \in K_G} \; p(x). \tag{2.5}$$

We may rewrite this as

$$\begin{aligned} p^{min} &= \max_{\gamma \in \mathbb{R}} \; \gamma, \\ s.t. \text{ for all } x &\in K_G, \; p(x) - \gamma \geq 0, \end{aligned} \tag{2.6}$$

in other words, finding the minimum of $p$ on $K_G$ is equivalent to finding the largest scalar $\gamma$ such that the polynomial $(p - \gamma)$ is non-negative on $K_G$. This reformulation may seem unnecessary, however when $K_G = \mathbb{R}^n$, it allows to us to approximate $p^{min}$ by replacing the condition "$(p - \gamma) \geq 0$" with "$(p - \gamma)$ is SOS", i.e.,

$$\begin{aligned} p^{SOS} &= \max_{\gamma \in \mathbb{R}} \; \gamma, \\ s.t. \; p - \gamma &\text{ is SOS.} \end{aligned} \tag{2.7}$$

Problems with such SOS constraints, i.e., of the form (2.7), are called *SOS relaxations* or

*SOS programs*. Since $\Sigma_{n,d} \subseteq \mathcal{P}_{n,d}$, we must have $p^{SOS} \leq p^{min}$. Furthermore, by Hilbert's theorem (Theorem 2.6) there are polynomials where the inequality is strict; every polynomial $q \in \mathcal{P}_n \backslash \Sigma_n$ obviously satisfies $-\infty = q^{SOS} < 0 \leq q^*$.

At this point it is natural to wonder about one very important question, "is $p^{SOS}$ any easier to compute than $p^{min}$?"

### 2.2.1 Using Semi-definite Programs

While computing $p^{min}$ is known to be NP hard [70, 75], $p^{SOS}$ on the other hand can be computed efficiently thanks to recent advances in computational mathematics. Recall that every polynomial $p \in \mathbb{R}[x]_{2d}$ can be written as

$$p(x) = \mathbf{x}_d^T Q \mathbf{x}_d,$$

for some $Q \in \mathbb{SR}^{s\times s}$. For polynomials which are sums of squares, the following theorem gives information about $Q$.

**Theorem 2.9** (pg. 106, [23])**.** *A homogeneous polynomial $p \in \mathbb{R}[x]_{2d}$ is SOS if and only if we can write*

$$p(x) = \mathbf{x}_d^T Q \mathbf{x}_d,$$

*where $Q$ is a positive semi-definite matrix.*

*Proof.* Suppose $Q$ is positive semi-definite. Then we have the decomposition $Q = V^T V$ and

$$\begin{aligned} p(x) &= \mathbf{x}_d^T V^T V \mathbf{x}_d, \\ &= \|V\mathbf{x}_d\|^2, \end{aligned}$$

hence $p$ is SOS. Conversely, if $p$ is SOS, then we have that

$$p(x) = q_1(x)^2 + \cdots + q_k(x)^2.$$

For each $q_i$ there is some coefficient vector $\mathbf{a}_i$ such that we can write $q_i(x) = \mathbf{x}_d^T \mathbf{a}_i$ (note that we use the monomial vector $\mathbf{x}_d$ due to Lemma 2.1). Substituting this we see

$$\begin{aligned} p(x) &= \sum_{i=1}^k (\mathbf{x}_d^T \mathbf{a}_i)(\mathbf{x}_d^T \mathbf{a}_i), \\ &= \sum_{i=1}^k (\mathbf{x}_d^T \mathbf{a}_i)(\mathbf{x}_d^T \mathbf{a}_i)^T, \\ &= \sum_{i=1}^k \mathbf{x}_d^T (\mathbf{a}_i \mathbf{a}_i^T) \mathbf{x}_d, \\ &= \mathbf{x}_d^T \left( \sum_{i=1}^k \mathbf{a}_i \mathbf{a}_i^T \right) \mathbf{x}_d. \end{aligned}$$

Setting $Q = \left(\sum_{i=1}^{k} \mathbf{a}_i \mathbf{a}_i^T\right)$ proves the result. $\square$

Consequently, finding an SOS decomposition for a polynomial $p \in \mathbb{R}[x]_{2d}$ amounts to finding a positive semi-definite matrix $Q$ which satisfies the constraints

$$p(x) - \mathbf{x}_d^T Q \mathbf{x}_d = 0. \tag{2.8}$$

There are two important points to take note of here. Firstly, (2.8) gives a system of linear constraints with the entries of $Q$ as variables. Secondly, we *must* have $Q$ positive semi-definite. So finding such a $Q$ requires solving the linear program generated by (2.8) over the set of positive semi-definite matrices. This is precisely *semi-definite programming* [1, 97, 98, 100].

Semi-definite programs are a generalization of linear programs, and have the standard primal form

$$\begin{aligned} s^* = \sup_{X \in \mathbb{SR}^{s\times s}} &\langle C, X\rangle, \\ s.t.\ \langle A_j, X\rangle = b_j,\ &j = 1, \dots, k, \\ \text{and } X &\succeq 0, \end{aligned} \tag{2.9}$$

with the matrix variable $X$, problem data $C, A_1, \dots, A_k \in \mathbb{SR}^{s\times s}$, and $b = (b_1, \dots, b_k) \in \mathbb{R}^k$. When $C = \mathbf{0}_{s\times s}$, (2.9) is called a feasibility program. Finding an SOS decomposition for any $p \in \mathbb{R}[x]_{2d}$ can be written as the following semi-definite feasibility program,

$$\begin{aligned} &Q \succeq 0, \\ s.t.\ \langle A_\alpha, Q\rangle &= p_\alpha,\ |\alpha| \le 2d \end{aligned} \tag{2.10}$$

where

$$(A_\alpha)_{\beta,\gamma} = \begin{cases} 1, \text{if } \beta + \gamma = \alpha, \\ 0, \text{otherwise} \end{cases}.$$

Semi-definite programming has quickly become an invaluable tool for optimization. SOS programs in particular, are almost exclusively solved using semi-definite programming. The theory of semi-definite programming diverges too much from the core content of this thesis. We refer the reader to the books [1, 100] and the surveys [97, 98] for a more comprehensive discussion of semi-definite programming.

We simply state here that given some $\varepsilon > 0$, there are efficient methods and algorithms which can find $\varepsilon$-optimal solutions in polynomial time, given some mild regularity. In particular, the dependence of the complexity of these methods on $\varepsilon$, is polynomial in $\log(\frac{1}{\varepsilon})$ (cf. the references above, or Section 4.1 of [83] for a classical discussion of this). Therefore approximate solutions to $p^{SOS}$ are much easier to compute than approximate solutions to $p^{min}$.

### 2.2.2 Lasserre's Hierarchy

Until now we have only considered SOS programs for global optimization ($K_G = \mathbb{R}^n$). Let us consider SOS programs for optimization when we have constraints ($K_G \neq \mathbb{R}^n$).

As an alternative, instead of checking "$p - \gamma$ is SOS", we can first "divide out" the constraints by squares. With the constraint set $K_G = \{x \in \mathbb{R}^n : g_1(x) \ge 0, \dots, g_k(x) \ge 0\}$, we obtain the following SOS program for the problem (2.6)

$$\begin{aligned} p^{SOS} &= \max_{\gamma\in\mathbb{R}} \gamma, \\ s.t.\ \ p(x) - \gamma &= r + \sum_{i=1}^{k} q_i(x)g_i(x), \\ r, q_1, \ldots, q_k &\in \Sigma_n. \end{aligned} \tag{2.11}$$

Notice that (2.11) is not solvable with semi-definite programming because the constraints are now of arbitrary degree, so there is no bound for the dimension of the matrices required in an SDP program. This can be remedied by bounding the degrees of the unknown polynomials $r, q_1, \ldots, q_k$, giving us a sequence of approximations to $p^{min}$ with the following SDP,

$$\begin{aligned} p_d^{SOS} &= \max_{\gamma\in\mathbb{R}} \gamma, \\ s.t.\ \ p(x) - \gamma &= r + \sum_{i=1}^{k} q_i(x)g_i(x), \\ r, q_1, \ldots, q_k &\in \Sigma_n, \\ \deg(q_i g_i) &\le 2d. \end{aligned} \tag{2.12}$$

Lasserre [57] has shown that $p_d^{SOS} \to p^{min}$ as $d \to \infty$ under some natural conditions, and this hierarchy of approximations are often referred to as Lasserre's hierarchy.

#### 2.2.2.1 Duality

Let $\mathcal{B}(\mathbb{R}^n)$ be the space of probability measures on $\mathbb{R}^n$ (positive, normalized, Borel measures). Lasserre replaced the global optimization problem (2.5) ($K_G = \mathbb{R}^n$) with the following

$$p^{mom} = \min_{\mu\in\mathcal{B}(\mathbb{R}^n)} \int p(x)\, d\mu(x). \tag{2.13}$$

The equivalency of (2.5) and (2.13) of the problem can be seen as follows: $p(x) \ge p^{min}$ and hence $\int p d\mu \ge p^{min}$ since $\mu$ is normalized, and conversely if $x^{min}$ is a global minimizer, we may consider $\mu^{min} = \delta_{x^{min}}$, the Dirac measure at $x^{min}$ giving $p^{min} = \int p d\mu_{min} \ge p^{mom}$.

If we now consider the polynomial $p \in \mathbb{R}[x]_{2d}$, we see that

$$\int_{\mathbb{R}^n} p(x)\, d\mu(x) = \sum_{|\alpha|\le 2d} p_\alpha \int_{\mathbb{R}^n} x^\alpha\, d\mu(x) = \sum_{|\alpha|\le 2d} p_\alpha \beta_\alpha,$$

where $\beta_\alpha = \int x^\alpha\, d\mu(x)$ are the moments of $\mu$. We may thus replace the optimization problem (2.13) with

$$\begin{aligned} p^{mom} &= \min \sum_{|\alpha|\le 2d} p_\alpha \beta_\alpha, \\ s.t.\ \ \beta_\alpha &= \textstyle\int x^\alpha\, d\mu(x), \quad \mu \in \mathcal{B}(\mathbb{R}^n), \end{aligned} \tag{2.14}$$

which is known as the *moment relaxation*. Clearly this requires an understanding of when a sequence $(\beta_\alpha)_{\alpha\in\mathbb{N}}$ represents the moments of a measure $\mu \in \mathcal{B}(\mathbb{R}^n)$ (in other words, an understanding of *the moment problem*). We refer the reader to [57, 59] for a more detailed discussion of this duality, with computational considerations, formulations for the constrained setting and comparisons with the SOS relaxations.

## 2.3 SOS Representations

Hilbert's theorem (Theorem 2.6) classified all polynomials (in terms of the number of variables $n$, and degree $d$) where non-negativity was equivalent to being SOS. But as we have seen for constrained optimization problems, there are alternatives to the SOS condition that can be more useful. In this section we present some of the key relaxations which have had a significant impact in SOS programming. We also briefly discuss some more recent results.

### 2.3.1 The $17^{th}$ Problem

**Theorem 2.10** (Artin's Solution to Hilbert's $17^{th}$ Problem, [3]). *For any $p \in \mathbb{R}[x]$, if $p \geq 0$ on $\mathbb{R}^n$, then $p$ is a sum of squares of rational functions, i.e., there are polynomials $r, q_i \in \mathbb{R}[x]$, with $r \neq 0$, such that*

$$r^2 p = \sum_i q_i^2.$$

The solution to Hilbert's $17^{th}$ problem is one of the most general representation result for non-negative polynomials. In Chapter 3 we will see an application where the SOS program from Theorem 2.10 performs tremendously well.

For positive polynomials, Polya gave a concrete denominator, $r^2$, for Theorem 2.10 when restricted to the standard simplex $\Delta_n = \{x \in \mathbb{R}^n : x_i \geq 0 \text{ and } x_1 + \cdots + x_n = 1\}$.

**Theorem 2.11** (Polya, [79]). *Let $p \in \mathbb{R}[x]$ be homogeneous and positive on $\Delta_n$, then for sufficiently large $N$, the coefficients of*

$$(x_1 + \cdots + x_n)^{2N} p(x_1, ..., x_n),$$

*are positive.*

Since $x_i \geq 0$ in Theorem 2.11, we can use the change of variables $z_i = \sqrt{x_i}$ and obtain an SOS decomposition. Reznick and Powers [81] have in recent years extended Polya's theorem to non-negative polynomials, with specialized zeros.

**Definition 2.12.** Let $p \in \mathcal{P}_{n,d}$ be non-negative on $\Delta_n$. Then $p$ has a *simple zero* at the unit vector $e_j$ if the coefficient of $x_j^d$ is zero and the coefficient of $x_j^{d-1}x_i$ is non-zero for every $i \neq j$.

**Theorem 2.13** (Corollary 1, [81]). *Suppose $p \in \mathcal{P}_{n,d}$ is homogeneous and non-negative on $\Delta_n$ with the only zeros being simple zeros at the unit vectors $e_{j_1}, \ldots, e_{j_k}$. Then there is an $N \in \mathbb{N}$ such that*

$$(x_1 + \cdots + x_n)^N p$$

*has non-negative coefficients.*

Further refinements of this result are given in [22], where the zeros are allowed to be on faces of the simplex. Although restricted to positive homogeneous polynomials, computationally speaking, Theorem 2.11 is particularly useful because the certification can be written as a linear program.

Reznick generalizes the use of a similar denominator beyond the simplex for strictly positive polynomials.

**Theorem 2.14** (Theorem 3, [84])**.** *Suppose that a homogeneous polynomial $p \in \mathbb{R}[x]$ is strictly positive. Then there is an $\ell \in \mathbb{N}$ and $q_1, \ldots, q_k \in \mathbb{R}[x]$ such that*

$$(x_1^2 + \cdots + x_n^2)^\ell p = \sum_{i=1}^{k} q_i^2.$$

One might try and use this result for non-negative $p$ by considering $(p + \varepsilon(x_1^2 + \cdots + x_n^2))$ for some $\varepsilon > 0$, and then take limit as $\varepsilon \to 0$. However, in the same paper Reznick even gives a lower bound on $\ell$, which is inversely dependent on the infimum of $p$ (Theorem 2 [84]). Due to this $\ell \to \infty$, as $\varepsilon \to 0$. Therefore the denominator $(x_1^2 + \cdots + x_n^2)^\ell$ only works well when $p > 0$.

Moreover, Delzell has shown in his thesis [35], that there are non-negative polynomials $p \in \mathbb{R}[x_1, \ldots, x_n]$ with $n \geq 3$, such that in any decomposition

$$r^2 p = \sum_{i=1}^{k} q_i^2,$$

the zeros $z_j$ of $p$ are shared by $r$, i.e., $r(z_j) = p(z_j) = 0$. Such common zeros are known in as "bad points". The example (Example 3 [35])

$$f(x, y, z) = z^6 + x^6 y^2 - 3x^2 y^4 z^2 + y^{10}$$

is non-negative (arithmetic-geometric mean inequality), and in particular has the origin as a bad point, hence there is no $\ell \in \mathbb{N}$ such that $(x_1^2 + \cdots + x_n^2)^\ell f$ is SOS.

Reznick has also shown that in general no finite set of denominators is enough.

**Theorem 2.15** (Corollory 2, [85])**.** *Suppose that $\mathcal{P}_{n,d} \backslash \Sigma_{n,d} \neq \emptyset$. Then for any finite set $\{r_1, \ldots, r_k\}$, there is a polynomial $p \in \mathcal{P}_{n,d}$ such that*

$$r_i p \neq SOS,$$

*for all $i = 1, \ldots, k$.*

### 2.3.2 The Positivstellensätze

Recall the semi-algebraic set $K_G = \{x \in \mathbb{R}^n : g_1(x) \geq 0, \ldots, g_k(x) \geq 0\}$, which is the non-negativity set of $G = \{g_1, \ldots, g_k\}$. If a polynomial $p$ is non-negative on $K_G$, are there any SOS representations that $p$ is *guaranteed* to satisfy? To understand the answer, let us first define a *preordering*.

**Definition 2.16.** Given a finite set $G = \{g_1, \ldots, g_k\} \subseteq \mathbb{R}[x]$, the *preordering* associated to $G$ is defined as

$$T_G = \left\{ \sum_{\alpha \in \{0,1\}^k} \sigma_\alpha g_1^{\alpha_1} \cdots g_k^{\alpha_k} : \sigma_\alpha \in \Sigma_n \right\}.$$

The most general decomposition a non-negative polynomial will admit, is given by the Positivstellensatz (we present the statement from [65, 2.2.1]). This result was long credited to Stengle [92], but it is now known that core ideas of the result were presented by Krivine in [55] a decade earlier. The Positivstellensatz is a powerful result. We can even obtain a solution to Hilbert's $17^{th}$ problem by applying statement (2) with $K_G = \mathbb{R}^n$.

**Theorem 2.17** (The Positivstellensatz)**.** *Suppose $G$ is a finite subset of $\mathbb{R}[x]$, $K_G, T_G$ are the semi-algebraic set, and preordering associated to $G$, and $p \in \mathbb{R}[x]$. Then the following are true*

*(1) $p > 0$ on $K_G \Leftrightarrow$ there exists $r, q \in T_G$ such that $rp = 1 + q$.*

*(2) $p \geq 0$ on $K_G \Leftrightarrow$ there is an integer $m \geq 0$ and $r, q \in T_G$ such that $rp = p^{2m} + q$.*

*(3) $p = 0$ on $K_G \Leftrightarrow$ there is an integer $m \geq 0$ such that $-p^{2m} \in T_G$.*

*(4) $K_G = \emptyset \Leftrightarrow -1 \in T_G$.*

We present here the proof of the equivalency of (1)-(4) from [65]. This proof is very accessible, even to the unfamiliar reader, requiring nothing more than the basic definitions to understand. It is also instructive as it shows how each statement can be used. Note that the following proof does not establish the Positivstellensatz, only that the four statements are equivalent; the interested reader is referred to [65] to see that the four equivalent statements are indeed true.

*Proof.* **[(1)⇒(2)]** Suppose that $p \geq 0$ on $K_G$. We extend dimensions from $n$ to $n + 1$ with

$$(x, y) = (x_1, \ldots, x_n, y) \in \mathbb{R}^{n+1}, \ \mathbb{R}[x, y] = \mathbb{R}[x_1, \ldots, x_n, y].$$

We take

$$G' = \{g_1, \ldots, g_s, yp - 1, -yp + 1\},$$

so that

$$K_{G'} = \{(x, y) \in \mathbb{R}^{n+1} : yp(x) = 1, g_i \geq 0, i = 1, \ldots, s\}.$$

Thus on $K_{G'}$ we have $p(x, y) = p(x) > 0$, so by (1), there is a $r', q' \in T_{G'}$ such that

$$r'(x, y)p(x) = 1 + q'(x, y).$$

Replacing $y$ with $\frac{1}{p(x)}$ in this equation and clearing denominators by multiplying with $p(x)^{2m}$ and $m$ sufficiently large, we obtain

$$r(x)p(x) = p(x)^{2m} + q(x),$$

with

$$r(x) = p(x)^{2m} r'\left(x, \frac{1}{p(x)}\right), \; q(x) = p(x)^{2m} q'\left(x, \frac{1}{p(x)}\right).$$

It is enough now to show that $r, q \in T_G$ for sufficiently large $m$. By the definition of $T_{G'}$ we know that

$$r'(x,y) = \sum \sigma(x,y) g_1(x)^{e_1} \cdots g_s(x)^{e_s} (yp(x) - 1)^{e_{s+1}} (-yp(x) + 1)^{e_{s+2}},$$

with $\sigma(x,y) \in \Sigma_{n+1}$, say $\sigma(x,y) = \sum h_j(x,y)^2$. Replacing $y$ as before, the terms with $e_{s+1} = 1$ or $e_{s+2} = 1$ vanish. For all the other terms, it is clear that with $m$ large enough,

$$p(x)^{2m} \sigma\left(x, \frac{1}{p(x)}\right) \in \mathbb{R}[x].$$

We have the same for $q$, and so $r, q \in T_G$.

**[(2)⇒(3)]** Suppose $p = 0$ on $K_G$. Using (2) on $p$ and $-p$ yields

$$r_1 p = p^{2m_1} + q_1, \; -r_2 p = p^{2m_2} + q_2, \quad r_i, q_i \in T_G, \; i = 1, 2.$$

The product of these gives

$$-r_1 r_2 p^2 = p^{2(m_1+m_2)} + p^{2m_1} q_2 + p^{2m_2} q_1 + q_1 q_2,$$

meaning that

$$-p^{2m} = r,$$

with $m = m_1 + m_2$, and

$$r = r_1 r_2 p^2 + p^{2m_1} q_2 + p^{2m_2} q_1 + q_1 q_2,$$

which belongs to $T_G$ since preorderings are closed under addition, multiplication and contain all squares.

**[(3)⇒(4)]** Since $K_G = \emptyset$, we know that $1 = 0$ on $K_G$. Applying (3) with $p = 1$ shows that $-1 \in T_G$.

**[(4)⇒(1)]** Let $G' = G \cup \{-p\}$. Since $p > 0$ on $K_G$, $K_{G'} = \emptyset$, hence $-1 \in T_{G'}$ by (4). Moreover, since $G' = G \cup \{-p\}$, it follows $T_{G'} = T_G - pT_G$. Thus, $-1 = q - rp$, i.e., $rp = 1 + q$ with $r, q \in T_G$. □

Just like Theorem 2.10, the Positivestellensatz sees remarkable improvement when we work with *strictly positive* polynomials. When the set $K_G$ is compact, we have the following Positivstellensatz of Schmüdgen.

**Theorem 2.18** (Schmüdgen's Positivstellensatz [90]). *Suppose that $K_G$ is compact. If $p \in \mathbb{R}[x]$ is strictly positive on $K_G$, then $p \in T_G$.*

As noted in [65], there is a gap in Schmüdgen's original proof, but the result is still true (see [65]). The SOS program arising from Theorem 2.18 is computationally simpler than the program from the Positivstellensatz. However, Theorem 2.18 can not be extended to the realm of non-negative polynomials as shown by the following,

**Proposition 2.19.** *Let $n \geq 3$, and suppose $K_G$ has a non-empty interior. Then there exists a $q \in \mathbb{R}[x]$, such that $q \geq 0$ on $K_G$, but $q \notin T_G$.*

The above is a particular instance of a more general result by Scheiderer [87].

**Definition 2.20.** For $G = \{g_1, \ldots, g_k\}$, the *quadratic module* generated by $G$ is the set

$$M_G \equiv M(g_1, \ldots, g_k) = \left\{ r + \sum_{i=1}^{k} q_i g_i : r, q_i \in \Sigma_n \right\}.$$

Furthermore, $M_G$ is called *Archimedean* if there is an $N \in \mathbb{N}$ such that

$$N - \sum_{i=1}^{n} x_i^2 \in M_G.$$

Observe that the preordering $T_G$ is simply the quadratic module generated by all possible products of the $g_i$'s. Thus every preordering is a quadratic module, and hence quadratic modules are more fundamental objects than preorderings. Furthermore, quadratic modules are a natural object to study for SOS representations. Notice that the SOS program (2.11) is nothing more than a test of membership into $M_G$.

**Theorem 2.21** (Putinar's Positivstellensatz [82])**.** *Let $G$ be a finite subset of $\mathbb{R}[x]$, and suppose that $M_G$ is Archimedean. Given a polynomial $p \in \mathbb{R}[x]$, if $p > 0$ on $K_G$, then $p \in M_G$.*

Theorem 2.21 implies the asymptotic convergence of the relaxations (2.11) as shown by Lasserre in [57]. Degree bounds for such decompositions are discussed in [73]. Theorem 2.21 is also used in [71] to develop a new 'Jacobian' relaxation, which we utilize in Chapter 3.

While the Positivstellensätze of Schmüdgen and Putinar (Theorem 2.18, 2.21) provide improved, denominator-free SOS representations, they come at the cost of restricting to positive polynomials (among other things). Fortunately, there are some recent advances towards polynomials with zeros.

Schiederer extends Putinar's Positivstellensatz to non-negative polynomials with finitely many zeros, by considering local positivity and smoothness conditions on the zeros [88, Corollary 3.6]. Marshall further explores and refines this approach in [64], and considers degree bounds for applications to optimization in [66].

The basic idea is that for a polynomial $p \in \mathbb{R}[x]$ which is non-negative on $K_G$, in any neighborhood of a zero, the polynomial is positive. Hence smoothness at the zero implies the Hessian is positive definite. With these ideas in mind, Marshall shows that if there is a local system of parameters $\{t_1, \ldots, t_k, t_{k+1}, \ldots, t_j\}$, such that we can write $p = p_1 + p_2 + \cdots$, (where each $p_i$ is a term of degree $i$) with

$$p_1 = a_1 t_1 + \cdots + a_k t_k, \quad a_i > 0,$$

and $p_2(0, \ldots, 0, t_{k+1}, \ldots, t_j)$ is positive definite, then $p \in M_G$ [64, Theorem 2.3].

There are also other representation results, which diverge from the Positivstellensätze and instead rely on first and second order optimality conditions. We present these in Chapter 3 in the context of *completely positive maps*.

Chapter 3

# Detecting Quantum Entanglement

This chapter presents a modified version of the manuscript "Practical Construction of Positive Maps which are not Completely Positive" (https://arxiv.org/abs/2001.01181). We show how non-negative (and sum of squares) polynomials arise in Quantum Information Theory. We also give an account of modern sums of squares relaxations, and show how they can be used to detect entanglement in quantum states.

## 3.1 Constructing Positive & Completely Positive Maps

Given two matrix spaces $\mathcal{A}$ and $\mathcal{B}$, a linear map $\Phi : \mathcal{A} \to \mathcal{B}$ with the involution-preserving property $\Phi(A^*) = \Phi(A)^*$ for all $A \in \mathcal{A}$, is called *positive* if for all $A \succeq 0$, $\Phi(A) \succeq 0$. For a given $l \in \mathbb{N}$, such linear maps induce the *ampliation*

$$\Phi^{(l)} : \mathbb{R}^{l\times l} \otimes \mathcal{A} \to \mathbb{R}^{l\times l} \otimes \mathcal{B}; \qquad M \otimes A \to M \otimes \Phi(A),$$

where $\otimes$ is the standard Kronecker tensor product of matrices. If $\Phi^{(l)}$ is positive then we call $\Phi$ *l-positive*. If $\Phi^{(l)}$ is positive for all $l \in \mathbb{N}$, then $\Phi$ is called *completely positive*. Positive and completely positive maps arise naturally in matrix theory and operator algebras (e.g., positive linear functionals) [76, 101], frequently in quantum information theory [47, 74, 96], and have recently even been used in semi-definite programming [54].

We study these maps via their correspondence to non-negative and sum of squares polynomials. Restricting these involution-preserving maps to the space of symmetric matrices, each linear map $\Phi : \mathbb{SR}^{n\times n} \to \mathbb{SR}^{m\times m}$ gives rise to a biquadratic, bihomogeneous polynomial $p_\Phi \in \mathbb{R}[x_1, \dots, x_n, y_1, \dots, y_m]$, with

$$p_\Phi(x, y) = y^T \Phi(x^T x) y.$$

It is known (see, e.g., [51]) that $\Phi$ is positive if and only if $p_\Phi$ is non-negative on $\mathbb{R}^{n+m}$, and $\Phi$ is completely positive if and only if $p_\Phi$ is a sum of squares (SOS) on $\mathbb{R}^{n+m}$.

The connection between non-negative and SOS polynomials plays a central role in real algebraic geometry. There are many results concerning this interplay, see for instance the surveys [6, 59, 60, 80] or the book [65]. In particular, [12] explores the connection between varieties of minimal degrees and non-negative polynomials. Their main theorem (given below) shows that on varieties of minimal degrees, non-negative quadratic forms have an SOS decomposition with linear forms.

**Theorem 3.1** (Thereom 1.1, [12]). *Let $X \subseteq \mathbb{P}^n$ be a real irreducible non-degenerate projective sub-variety, with homogeneous coordinate ring R, such that the set $X(\mathbb{R})$ of real points is Zariski dense. Every non-negative real quadratic form on $X$ is a sum of squares of linear forms in $R$ if and only if $X$ is a variety of minimal degree.*

Moreover, when $X$ is not of minimal degree, [12] gave a construction for generic quadratic forms which are non-negative on $X$ but not SOS. In [51] the authors specialize this construction (Procedure 3.3 of [12]) to biquadratic, bihomogeneous polynomials over the Segre Variety, which is the image of the Segre embedding $\sigma : \mathbb{P}^{n-1} \times \mathbb{P}^{m-1} \to \mathbb{P}^{nm-1}$ (and is well known to not be of minimal degree for $n, m \geq 3$). This formalization of the method in [12], gives an algorithmic construction of positive maps which are not completely positive (pncp maps for short).

Letting $n, m \geq 3$, $t = n + m - 2$ and $N = n + m$, the algorithm of [12, 51] can be summarized as follows (see Section 3.2.1 for full details):

**Algorithm 1:** KMSZ Construction

1. Generate random points $x \in \mathbb{R}^n, y \in \mathbb{R}^m$
2. Use $x, y$ to create bilinear forms $\{h_0, \dots, h_t\}$ over $\mathbb{R}^N$
3. Generate $f \notin \langle h_0, \dots, h_t \rangle$ so that $f \neq SOS$ on $\mathbb{R}^N$
4. Choose $\delta$ small enough so that $F_\delta = \delta f + h_0^2 + \cdots + h_t^2 \geq 0$ on $\mathbb{R}^N$

Steps 1-3 are simple linear algebra computations, our contribution in this work is to find the most practical technique for Step 4, and to establish benchmarks for this type of construction.

This is an expository and experimental chapter in which we introduce the MATLAB package PnCP, currently the only implementation of Algorithm 1. We survey recent optimization techniques for verifying Step 4 and specify relaxations theoretically superior to those presented in [51]. We implement and test these methods in PnCP. Our package and test data are made available at https://github.com/Abhishek-B/PhD-Thesis-Supplementary-Material (as well as the official repository of PnCP, https://bitbucket.org/Abhishek-B/pncp/). We also consider rationalizations of the forms obtained with Algorithm 1 to construct exact certificates of non-negativity (PnCP is able to construct pncp maps with rational coefficients).

PnCP is developed as a consequence of the rising interest in quantum information and its purpose is to help identify *entangled* (quantum) states (see Section 3.5 for definitions); pncp maps preserve their positivity on *separable* states, however they may fail to preserve positivity on entangled states, which provides the following classification criterion.

**Criterion 3.2** (The general criteria, [4] section 8.4). A quantum state $\rho \in \mathbb{SR}^{s \times s}$ is entangled if there is a pncp map $\Phi$ such that the ampliation $(I \otimes \Phi)(\rho) \not\succeq 0$.

As an example, consider the Bell State, which has density matrix (see Section 3.5)

$$\rho = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \in \mathbb{R}^{2\times 2} \otimes \mathbb{R}^{2\times 2}.$$

and let $T$ be the standard transpose map (clearly positive, and known to be pncp). Then the partial ampliation $(I \otimes T) : \mathbb{R}^{2\times 2} \otimes \mathbb{R}^{2\times 2} \to \mathbb{R}^{2\times 2} \otimes \mathbb{R}^{2\times 2}$ applied to $\rho$ gives,

$$(I \otimes T)(\rho) = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

which has a negative eigenvalue of $-1/2$, and serves as evidence of entanglement in the Bell State. While the transpose map was sufficient in this simple example, in general finding a suitable map is difficult. With the help of PnCP one can generate many such maps to test for entanglement (see the examples in Section 3.5 for details).

The chapter is organized as follows. Section 3.2 reviews some notation and algebraic geometry background for the optimization involved in Step 4. In Section 3.3 we present some of the relaxations we surveyed and thought to be promising for using in Step 4. We also present our implementation of these methods using MATLAB and show their performance via computational efficiency (w.r.t. time) and success rate. Section 3.4 details issues in generating pncp maps with rational coefficients using Algorithm 1. We also show the difference in computational requirements for constructing maps with floating point coefficients and those with rational coefficients. Section 3.5 explains how we use PnCP to identify entanglement in quantum states. We demonstrate this usefulness through illustrative examples.

## 3.2 Background

In this section we present the necessary mathematical background and notation for understanding Algorithm 1, and then present the full Algorithm 1, for self-containment and convenience.

We use the following notation; for any integer $n > 0$, $[n] = \{1, \ldots, n\}$ and for a subset $I \subseteq [n]$, $|I|$ denotes its cardinality. For $k \in \mathbb{N}$, $[n]_k = \{I \subseteq [n] : |I| = k\}$.

A subset $I \subseteq \mathbb{R}[x]$ is called an *ideal* if $(\mathbb{R}[x] \cdot I) \subseteq I$. The set $\langle g_1, \ldots, g_k\rangle$ is the ideal generated by $\{g_1, \ldots, g_k\} \subseteq \mathbb{R}[x]$, which is the smallest ideal containing $\{g_1, \ldots, g_k\}$. According to the *Hilbert Basis Theorem* [25], every ideal has such a finite generating set. The *variety* of an ideal is the set of common complex zeros for the ideals' generators

$$V(I) = V(\langle g_1, \ldots, g_k\rangle) = \{x \in \mathbb{C}^n \ : \ g_j(x) = 0, \ \forall j = 1, ..., k\},$$

or more generally

$$V(I) = \{x \in \mathbb{C}^n \ : \ p(x) = 0, \ \forall p \in I\}.$$

The *real variety* of $I$ is simply the restriction of $V(I)$ to the reals. We denote this with $V^{\mathbb{R}}(I)$. If the variety $V(I)$ is a finite set, then $I$ is called *zero dimensional* (this is not the same as requiring $V^{\mathbb{R}}(I)$ to be finite). A variety $V(\langle g_1, \ldots, g_r\rangle) =: V \subseteq \mathbb{C}^n$ is called *smooth*, or *non-singular* if the associated $(r \times n)$ Jacobian matrix $\left(\frac{\partial g_i}{\partial x_j}(a)\right)_{i,j}$ has rank $n - \dim(V)$ at every point $a \in V$ (cf. [25, Chapter 9]). For every ideal $I \in \mathbb{R}[x]$, its *radical* is the ideal

$$\sqrt{I} = \{p \in \mathbb{R}[x] \ : \ p^r \in I \text{ for some } r \in \mathbb{N}\}.$$

For more details see [25]. Recall from Chapter 2, with any finite set $G = \{g_1, \dots, g_k\} \subseteq \mathbb{R}[x]$ we have the *semi-algebraic* set, and the *preorder* generated by $G$ resp.,

$$\begin{aligned} K_G &= \{x \in \mathbb{R}^n \;:\; g_j(x) \geq 0,\ \forall j = 1, ..., k\}, \\ T_G &= \left\{ \sum_{\gamma \in \{0,1\}^k} s_\gamma g_1^{\gamma_1} \cdots g_k^{\gamma_k} \;:\; s_\gamma \in \Sigma_n \right\}. \end{aligned} \tag{3.1}$$

### 3.2.1 Constructing Positive Maps

We will describe now Algorithm 1 in full detail, along with its relation to the Segre variety. As before letting

$$\begin{aligned} \sigma_{n,m} : \mathbb{P}^{n-1} \times \mathbb{P}^{m-1} &\to \mathbb{P}^{nm-1}, \\ ([x_1 : \dots : x_n], [y_1 : \dots : y_m]) &\mapsto [x_1 y_1 : x_1 y_2 : \dots : x_1 y_m : \dots : x_n y_m]. \end{aligned}$$

be the Segre embedding, then it is known that (the Segre variety) $\sigma_{n,m}(\mathbb{P}^{n-1} \times \mathbb{P}^{m-1})$ is the variety of the ideal $I_{n,m} \in \mathbb{C}[z_{11}, z_{12}, \dots, z_{1m}, \dots, z_{nm}]$ generated by all $2 \times 2$ minors of the matrix $(z_{ij})_{i,j}$ [44]. As in [51] we will write

$$V(I_{n,m}) = \{[z_{11} : \dots : z_{nm}] \in \mathbb{P}^{nm-1} \colon f(z) = 0 \text{ for every } f \in I_{n,m}\},$$

for the Segre variety, where

$$z = (z_{11}, z_{12}, \dots, z_{1m}, \dots, z_{nm}),$$

and $V_{\mathbb{R}}(I_{n,m})$ for the subset of its real points. Finally, as explained in [51], biquadratic forms in $\mathbb{R}[x, y]_{2,2}$ are in a bijective correspondence with quadratic forms in $\mathbb{R}[z]/I_{n,m}$. Let us write

$$\begin{aligned} \mathcal{P}(V_{\mathbb{R}}(I_{n,m})) &= \{f \in \mathbb{R}[z]/I_{n,m} \colon f(z) \geq 0 \quad \text{for all } z \in V_{\mathbb{R}}(I_{n,m})\}, \\ \Sigma(V_{\mathbb{R}}(I_{n,m})) &= \{f \in \mathbb{R}[z]/I_{n,m} \colon f = \sum_i f_i^2 \quad \text{for some } f_i \in \mathbb{R}[z]/I_{n,m}\}, \end{aligned}$$

then the construction is as follows.

**Algorithm 1.** Let $n > 2$, $m > 2$,

$$d = n+m-2 = \dim \sigma_{n,m}(\mathbb{P}^{n-1} \times \mathbb{P}^{m-1}) \ \text{ and } \ e = (n-1)(m-1) = \operatorname{codim} \sigma_{n,m}(\mathbb{P}^{n-1} \times \mathbb{P}^{m-1}).$$

To obtain a quadratic form in $\mathcal{P}(V_{\mathbb{R}}(I_{n,m})) \setminus \Sigma(V_{\mathbb{R}}(I_{n,m}))$ proceed as follows:

Step 1 Choose $e + 1$ random points $\mathbf{x}^{(i)} \in \mathbb{R}^n$ and $\mathbf{y}^{(i)} \in \mathbb{R}^m$ and calculate their Kronecker tensor products $\mathbf{z}^{(i)} = \mathbf{x}^{(i)} \otimes \mathbf{y}^{(i)} \in \mathbb{R}^{nm}$.

Step 2 Construction of linear forms $h_0, \dots, h_d$.

Step 2.1 Choose $d$ random vectors $\mathbf{v}_1, \ldots \mathbf{v}_d \in \mathbb{R}^{nm}$ from the kernel of the matrix

$$\begin{pmatrix} \mathbf{z}^{(1)} & \ldots & \mathbf{z}^{(e+1)} \end{pmatrix}^* .$$

The corresponding linear forms $h_1, \ldots, h_d$ are

$$h_j(z) = \mathbf{v}_j^* \cdot z \in \mathbb{R}[z] \quad \text{for } j = 1, \ldots, d.$$

If the number of points in the intersection

$$\ker(\begin{pmatrix} \mathbf{v}_1 & \ldots & \mathbf{v}_d \end{pmatrix}^*) \bigcap V(I_{n,m})$$

is not equal to $\deg(V(I_{n,m})) = \binom{n+m-2}{n-1}$ or if the points in the intersection are not in linearly general position, then repeat Step 1.

Step 2.2 Choose a random vector $\mathbf{v}_0$ from the kernel of the matrix

$$\begin{pmatrix} \mathbf{z}^{(1)} & \ldots & \mathbf{z}^{(e)} \end{pmatrix}^* .$$

(Note that we have omitted $\mathbf{z}^{(e+1)}$.) The corresponding linear form $h_0$ is

$$h_0(z) = \mathbf{v}_0^* \cdot z \in \mathbb{R}[z].$$

If $h_0$ intersects $h_1$, …, $h_d$ in more than $e$ points on $V(I_{n,m})$, then repeat Step 2.2.

Let $\mathfrak{a}$ be the ideal in $\mathbb{R}[\mathbf{z}]/I_{n,m}$ generated by $h_0, h_1, \ldots, h_d$.

Step 3 Construction of a quadratic form $f \in (\mathbb{R}[\mathbf{z}]/I_{n,m}) \setminus \mathfrak{a}^2$.

Step 3.1 Let $g_1(z), \ldots, g_{\binom{n}{2}\binom{m}{2}}(z)$ be the generators of the ideal $I_{n,m}$, i.e., the $2\times2$ minors $z_{ij}z_{kl} - z_{il}z_{kj}$ for $1 \leq i < k \leq n, 1 \leq j < l \leq m$. For each $i = 1, \ldots, e$ compute a basis $\{\mathbf{w}_1^{(i)}, \ldots, \mathbf{w}_{d+1}^{(i)}\} \subseteq \mathbb{R}^{nm}$ of the kernel of the matrix

$$\begin{pmatrix} \nabla g_1(z^{(i)})^* \\ \vdots \\ \nabla g_{\binom{n}{2}\binom{m}{2}}(z^{(i)})^* \end{pmatrix}.$$

(Note that this kernel is always $(d+1)$-dimensional, since the variety $V(I_{n,m})$ is $d$-dimensional (in $\mathbb{P}^{nm-1}$) and smooth.)

Step 3.2 Let $\mathbf{e}_i$ denote the $i$-th standard basis vector of the corresponding vector space, i.e., the vector with 1 on the $i$-th component and 0 elsewhere. Choose a random vector $\mathbf{v} \in \mathbb{R}^{n^2m^2}$ from the intersection of the kernels of the matrices

$$\begin{pmatrix} \mathbf{z}^{(i)} \otimes \mathbf{w}_1^{(i)} & \ldots & \mathbf{z}^{(i)} \otimes \mathbf{w}_{d+1}^{(i)} \end{pmatrix}^* \quad \text{for } i = 1, \ldots, e$$

with the kernels of the matrices

$$\big(\mathbf{e}_i \otimes \mathbf{e}_j - \mathbf{e}_j \otimes \mathbf{e}_i\big)^* \quad \text{for } 1 \le i < j \le nm.$$

(The latter condition ensures $\mathbf{v}$ is a symmetric tensor in $\mathbb{R}^{nm} \otimes \mathbb{R}^{nm}$. Note also that we have omitted the point $\mathbf{z}^{(e+1)}$.)

For $1 \le i, k \le n$ and $1 \le j, l \le m$ denote

$$E_{ijkl} = (\mathbf{e}_i \otimes \mathbf{e}_j) \otimes (\mathbf{e}_k \otimes \mathbf{e}_l) + (\mathbf{e}_k \otimes \mathbf{e}_l) \otimes (\mathbf{e}_i \otimes \mathbf{e}_j) \in \mathbb{R}^{n^2m^2}.$$

Let

$$\begin{aligned} A &= \{\mathbf{v}_i \otimes \mathbf{v}_j + \mathbf{v}_j \otimes \mathbf{v}_i \colon 0 \le i \le j \le d\}, \\ B &= \{E_{ijkl} - E_{ilkj}; 1 \le i < k \le n, 1 \le j < l \le m\}. \end{aligned}$$

If $\mathbf{v}$ is in

$$\operatorname{span}\big(A \cup B\big),$$

then repeat Step 3.2. Otherwise the corresponding quadratic form $f$

$$f(z) = \mathbf{v}^* \cdot (z \otimes z) \in \mathbb{R}[z]/I_{n,m},$$

does not belong to $\mathfrak{a}^2$.

Step 4 Construction of a quadratic form in $\mathbb{R}[z]/I_{n,m}$ that is positive but not a sum of squares. Calculate the greatest $\delta_0 > 0$ such that $\delta_0 f + \sum_{i=0}^{d} h_i^2$ is nonnegative on $V_{\mathbb{R}}(I_{n,m})$. Then for every $0 < \delta < \delta_0$ the quadratic form

$$(\delta f + \sum_{i=0}^{d} h_i^2)(z)$$

is nonnegative on $V_{\mathbb{R}}(I_{n,m})$ but is not a sum of squares.

As is explained in [51], with random data this algorithm works with probability 1 without implementing verifications (for Step 2.1, etc.). However, implementing this algorithm with truly generic data is difficult at best. Hence, in practice this algorithm will not work with probability 1, but with some other (likely smaller) probability.

## 3.3 Relaxations & Performance

We focus in this section on the general optimization problem of Step 4, and the underlying principles for finding a solution.

We first look at minimization techniques which we can use to ensure non-negativity, and then consider their relaxations which make them computationally feasible. We also describe how we implement these techniques in PnCP for practical success.

Recall the general minimization problem

$$\begin{aligned} &\min_{x\in\mathbb{R}^N} p(x) \\ &s.t.\;\; g_1(x)\geq 0,\cdots,g_k(x)\geq 0. \end{aligned} \tag{3.2}$$

Step 4 of Algorithm 1 involves solving a maximization problem similar to (3.2). To be more specific, in Algorithm 1 Step 4, we need to solve the following problem

$$\begin{aligned} &\max_{\delta>0} \delta \\ &s.t.\;\; F_\delta(x,y)\geq 0. \end{aligned} \tag{3.3}$$

The recommended SOS relaxation in [51] for (3.3) is the following

$$\begin{aligned} &\max_{\delta>0} \delta, \\ &s.t.\;\; \left(\sum (x_i y_j)^2\right)^\ell F_\delta(x,y)\in \Sigma_{n+m}, \\ &\ell\in\mathbb{N}. \end{aligned} \tag{3.4}$$

As we know (cf., Chapter 2 Section 2.2.1), relaxation problems such as the one above can be stated and solved as an appropriate optimization program (semi-definite, second order cone, quadratically constrained, etc.). In recent years, there have been many developments in optimization for computing minima, and the majority of solvers can handle the broad class of these problems.

We now present alternate SOS relaxations to solving problem (3.2). We present the theory in this section with regards to an arbitrary function $p\in\mathbb{R}[x]$. We then give a description of how the results apply to our function of interest $F_\delta$ and problem (3.3).

To test the *success rate* of each relaxation, we do the following. We generate 50 random forms using Algorithm 1: Step 1 - Step 3 (with standard `rand` functions from MATLAB). Then we employ Step 4 with each relaxation, and note how many forms are identified as positive, but not completely positive.

### 3.3.1 Rational Functions

Let us begin by considering Artin's solution to Hilbert's $17^{th}$ problem [13], which we restate for convenience.

**Theorem 3.3** (Solution to Hilbert's $17^{th}$ Problem)**.** *For any $p\in\mathbb{R}[x]$, if $p\geq 0$ on $\mathbb{R}^n$, then $p$ is a sum of squares of rational functions, i.e., there are polynomials $g,q_i\in\mathbb{R}[x]$, with $g\neq 0$, such that*

$$g^2p=\sum_i q_i^2.$$

This result provides the most fundamental SOS relaxation. For Step 4, instead of minimizing $F_\delta$, we look for a decomposition into sums of rational squares, i.e.,

$$\begin{aligned} &\max_{\delta>0} \delta, \\ s.t.\ &\sigma(x,y)F_\delta(x,y) \in \Sigma_{n+m}, \\ &\sigma(x,y) \in \Sigma_{n+m}. \end{aligned} \tag{3.5}$$

If for some $\delta$, $F_\delta$ is non-negative, then by Theorem 3.3 the SOS decomposition in (3.5) always exists. Of course to solve the general problem (3.5) using semi-definite programming, we must first bound the degree of $\sigma(x,y) \neq 0$.

Note that (3.5) is a quadratically constrained optimization program (non-linear in the decision variables, $\delta$ and the coefficients of $\sigma$), which can be solved with solvers such as PENLAB [37], but our early tests indicated that this approach is not ideal. So we instead implement (3.5) with a "bisection" approach. This is already the suggested method in [51], which tries to solve (3.4), and increases $\ell$ if a solution is not found. While bisecting may seem like a simple idea, given some tolerance $\varepsilon$, bisection achieves an $\varepsilon$-optimal solution in $\log_2(\frac{1}{\varepsilon})$ calls to a feasibility oracle. And so it has comparable dependence on the tolerence $\varepsilon$ as interior-point methods for semi-definite programming.

For the Hilbert method (3.5), let $\mathcal{G}$ be the Gram matrix of $\sigma$. We fix $\delta = 2^0$, $d = 1$, and solve the following

$$\begin{aligned} \text{find } &\sigma(x,y) \in \Sigma_{n+m,d}, \\ s.t.\ &\operatorname{tr}(\mathcal{G}) = 1, \\ &\sigma(x,y)F_\delta(x,y) = \Sigma_{n+m}. \end{aligned}$$

If a solution is not found, we first bisect over $\delta$, and if still there is no solution we increase $d$ and repeat. We set the limits of $\delta$ to be $2^{-6}$ and $d$ to be 2.

The SOS decomposition and related optimization problems are generated using the symbolic computation package YALMIP [62, 63]. Our MATLAB code & data for the experiments, is available on https://github.com/Abhishek-B/PhD-Thesis-Supplementary-Material (as well as the official repository of PnCP, https://bitbucket.org/Abhishek-B/pncp/), so that the reader may verify the results of our experiments.

To solve the required semi-definite program we use the MOSEK solver [2] with our implementations. Verification of the SOS decomposition is done with the YALMIP command `sol.problem==0` (where `sol` is what we name our solution), as well as requiring the residual of the problem to be small ($\leq O(10^{-6})$).

All of the experiments were carried out on a standard Dell Optiplex 9020, with 12GB of memory, an Intel ®Core™ i5-4590 CPU @ 3.30GHz×4 processor, 500GB of storage and running Ubuntu 18.04 LTS.

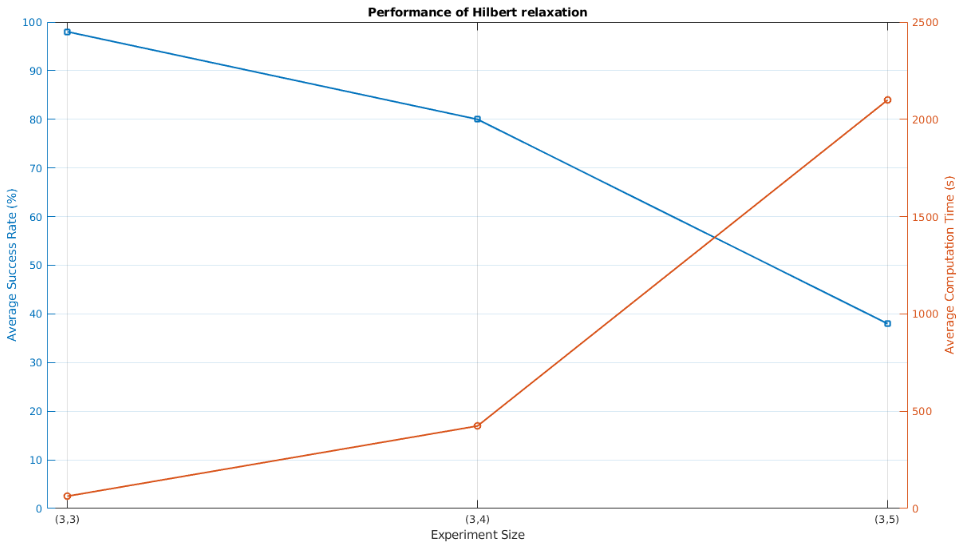


Figure 3.1: Performance of the Hilbert Relaxation (3.5) on problems of different sizes (3,$m$), tested on 50 randomly constructed biquadratic forms for each size.

The success rate of this relaxation for problems of small size is remarkable, as seen in Figure 3.1. Moreover, we observe from the average residual (which includes the failed examples as well) in Table 3.1, that if we were to allow the residual to be slightly larger (say $\leq O(10^{-5})$), we would see a higher success rate. This would also reduce computation times, increasing the appeal of this relaxation.

| Hilbert Relaxation | | | |
|---|---|---|---|
| $(n, m)$ | Success (%) | Time (s) | Residual |
| $(3, 3)$ | $98$ | $63.31$ | $7.19 \times 10^{-7}$ |
| $(3, 4)$ | $80$ | $423.99$ | $2.02 \times 10^{-6}$ |
| $(3, 5)$ | $38$ | $2098.93$ | $1.17 \times 10^{-5}$ |

Table 3.1: Average performance of relaxation (3.5)

**Remark 3.4.** After running a few experiments it becomes apparent that in the Hilbert method, we should initialize $d = 2$. While there are instances where $d = 1$ has a solution, it works with very small $\delta$ and hence requires a long runtime due to the number of bisections. We also add $\mathrm{tr}(\mathcal{G}) = 1$ in our constraints to avoid the trivial solution of $\sigma \equiv 0$.

The relaxation (3.4) is a simplified version of (3.5), which fixes the denominator

$$\sigma(x, y) = \left(\sum (x_i y_j)^2\right)^\ell .$$

We refer to this simplification as the *Coordinate Norm Relaxation* (CNR) and implement it similar to the Hilbert method. Since $\sigma$ is known, we maximize $\delta$ and "bisect" over $\ell \leq 2$. The verification of a solution is also similar, with the additional requirement $\delta > O(10^{-4})$ as otherwise $\delta$ becomes indistinguishable from numerical error.

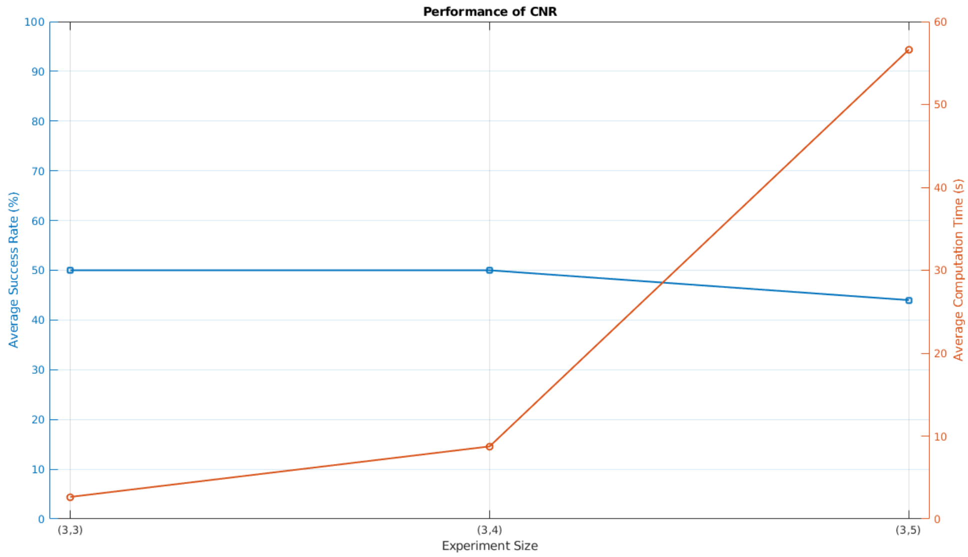


Figure 3.2: Performance of the Coordinate Norm Relaxation (3.4) on problems of different sizes (3,$m$), tested on 50 randomly constructed biquadratic forms for each size.

As we can see (Figure 3.2 or Table 3.2), this relaxation is incredibly fast (it is in fact the fastest relaxation). On problems of smaller size, it is not as successful compared to the Hilbert method, but we can see from the residuals, that if we relax our verification criteria, we might improve the success rate of the CNR quite dramatically.

| CNR | | | | |
|---|---|---|---|---|
| $(n, m)$ | Success (%) | Time (s) | Residual | Average $\delta$ |
| $(3, 3)$ | 50 | 2.65 | $4.89 \times 10^{-6}$ | 1.83 |
| $(3, 4)$ | 50 | 8.75 | $5.53 \times 10^{-6}$ | 0.13 |
| $(3, 5)$ | 44 | 56.61 | $1.34 \times 10^{-5}$ | 0.09 |

Table 3.2: Average performance of relaxation (3.4)

If we consider the variables $z_{ij} = x_i \otimes y_j$ over the Segre variety, then the CNR can be written as

$$\max_{\delta>0} \delta,$$
$$s.t. \ \left(\sum z_{ij}^2\right)^\ell F_\delta(z) \in \Sigma_{n+m},$$
$$\ell \in \mathbb{N}.$$

For polynomials with zeros, this denominator has been used in practice (see [61] for instance), but there is little theoretical justification for its use (see Theorem 2.14 and the discussion following it). Algorithm 1 works by fixing some zeros of $F_\delta$ in Step 1, hence the relaxation (3.4) while practically efficient, is not guaranteed to work, jeopardizing the entire construction.

### 3.3.2 Critical Points Ideal

A more modern relaxation comes from the gradient ideal $I_\nabla = \left\langle \frac{\partial p}{\partial x_1}, \dots, \frac{\partial p}{\partial x_n} \right\rangle$. The first order optimality test $\nabla p(x) = 0$ implies that minima exist in the gradient variety $V_\nabla^{\mathbb{R}}(I) = \{x \in \mathbb{R}^n : \nabla p(x) = 0\}$ (note that we may easily transform the equality constraint $\nabla p(x) = 0$, into the equivalent pair of inequality constraints $\nabla p(x) \geq 0, -\nabla p(x) \geq 0$). In [72] it is shown that one may consider searching for minimizers in the quotient ring $\mathbb{R}[x]/I_\nabla$ instead of $\mathbb{R}[x]$. Their main theorem is the following.

**Theorem 3.5** (Theorem 8, [72])**.** *Assume that the gradient ideal $I_\nabla$ is radical. If the real polynomial $p(x)$ is non-negative over $V_\nabla^{\mathbb{R}}(p)$, then there exist real polynomials $q_i(x)$ and $\phi_j(x)$ such that*

$$p(x) = \sum_{i=1}^{s} q_i(x) + \sum_{j=1}^{n} \phi_j(x) \frac{\partial p}{\partial x_j}(x)$$

*and each $q_i \in \Sigma_n$.*

Note that this is quite similar to (2.11), with the radicality of $I_\nabla$ providing a guarantee on the existence of the decomposition. Algorithms for extracting the minimum and minimizers of polynomials are also presented in [72] and tested on several notable examples. In cases where it is unknown if $I_\nabla$ is radical, one may use the following alternative result of [72].

**Theorem 3.6** (Theorem 9, [72])**.** *Suppose $p(x) \in \mathbb{R}[x]$ is strictly positive on its real gradient variety $V_\nabla^{\mathbb{R}}$. Then $p(x)$ is a SOS modulo its gradient ideal $I_\nabla$.*

Extending Theorem 3.5 and Theorem 3.6, [36] considers the ideal generated by the KKT system related to $f$ when minimizing over a semi-algebraic set. To this end let $\{g_1, \dots, g_k\} \subseteq \mathbb{R}[x]$ generate $K_G$ and $T_G$ (3.1). The KKT system associated to minimizing $p$ on $K_G$ is

$$\begin{gathered} \mathcal{P}_i = \frac{\partial p}{\partial x_i} - \sum_r \lambda_r \frac{\partial g_r}{\partial x_i} = 0, \\ g_r \geq 0, \\ \lambda_r g_r = 0, \end{gathered}$$

for $r = 1, \dots, k$ and $i = 1, \dots, n$. As in [36], we let

$$\begin{aligned} I_{\text{KKT}} &= \langle \mathcal{P}_1, \dots, \mathcal{P}_n, \lambda_1 g_1, \dots, \lambda_k g_k \rangle, \\ V_{\text{KKT}}^{\mathbb{R}} &= \{(x, \lambda) \in \mathbb{R}^n \times \mathbb{R}^k \ : \ q(x, \lambda) = 0, \ \forall q \in I_{\text{KKT}}\}, \\ \mathcal{H} &= \{(x, \lambda) \in \mathbb{R}^n \times \mathbb{R}^k \ : \ g_r(x) \geq 0, \ r = 1, \dots, k\}, \end{aligned}$$

and the KKT preorder generated by $G$ (now in the larger ring $\mathbb{R}[x, \lambda]$) is

$$T_{\text{KKT}} = T_G + I_{\text{KKT}}.$$

**Theorem 3.7** (Theorem 3.2, [36])**.** *Assume $I_{KKT}$ is radical. If $p(x)$ is non-negative on $V_{KKT}^{\mathbb{R}} \cap \mathcal{H}$, then $p(x)$ belongs to $T_{KKT}$.*

If the radicality of $I_{\text{KKT}}$ is not known, then similar to Theorem 3.5 positivity of $p(x)$ on the appropriate subset of $V^{\mathbb{R}}_{\text{KKT}}$, ensures membership in $T_{\text{KKT}}$.

**Theorem 3.8** (Theorem 3.5, [36])**.** *If $p(x) > 0$ on $V^{\mathbb{R}}_{KKT} \cap \mathcal{H}$, then $p(x)$ belongs to $T_{KKT}$.*

For our application we work on the sphere $\mathbb{S}^{N-1}$ (this can be replaced by any other suitable compact set) and the minimizers $(x^*, y^*)$ must now satisfy

$$s(x,y) = \sum_{i=1}^{n} x_i^2 + \sum_{j=1}^{m} y_j^2 - 1 = 0,$$
$$\nabla F_\delta(x,y) - \lambda \nabla s(x,y) = 0.$$

This allows us to use the following KKT relaxation, where we write $w$ for the variables $(x, y)$,

$$\begin{gathered} \max_{\delta>0} \delta \\ s.t.\ F_\delta(w) - \sum_{i=1}^{n} \phi_i(w) \left( \frac{\partial F_\delta}{\partial w_i}(w) - \lambda \frac{\partial s}{\partial w_i}(w) \right) - \lambda \eta(w) s(w) \in \Sigma_{n+m} \\ \phi_i, \eta \in \mathbb{R}[w] \end{gathered} \tag{3.6}$$

Notice that we do not search for membership of $F_\delta$ modulo $I_{\text{KKT}}$ into all of $T_G$, instead to simplify things we search only for elements of $T_G$ with $\gamma = (0, \ldots, 0)$. Since $F_\delta$ is known to have zeros, for this relaxation to be successful $I_{\text{KKT}}$ must be radical. While the random nature of $F_\delta$ implies a high probability of $I_{\text{KKT}}$ being radical, verifying this is computationally difficult, especially given the floating point construction of $F_\delta$.

This relaxation also has non-linear constraints, arising from the products of decision variables (coefficients of $\phi_i$ and $\delta$). Hence, we implement this with the same "bisection" approach and verification criteria as (3.5). We fix $\delta = 2^0, d = 1$, and solve

$$\begin{gathered} \text{find } \phi_i, \eta \in \mathbb{R}[w]_d, \\ s.t.\ F_\delta(w) - \phi(w)^T (\nabla F_\delta(w) - \lambda \nabla s(w)) - \lambda \eta(w) s(w) \in \Sigma_{n+m}. \end{gathered}$$

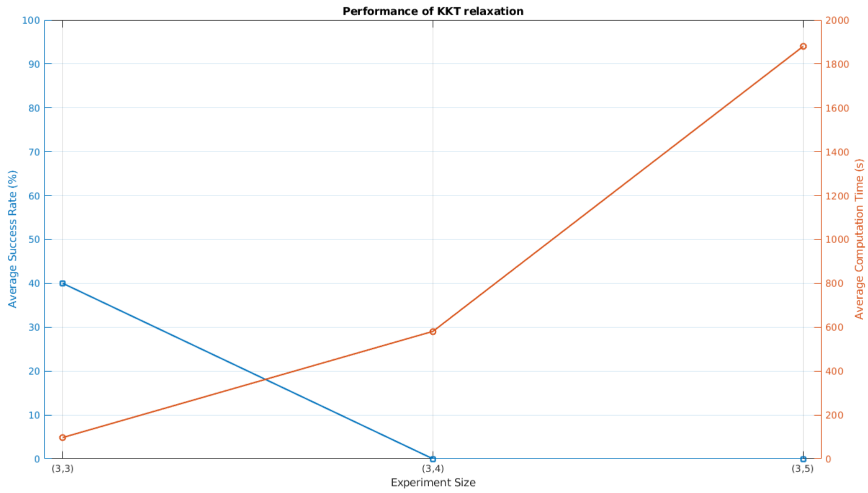


Figure 3.3: Performance of the KKT Relaxation (3.6) on problems of different sizes (3,$m$), tested on 50 randomly constructed biquadratic forms for each size.

To our surprise, this method fails completely on the (relatively) larger problems, and has quite poor performance even on the smaller ones of size $(3, 3)$. This suggests that the random construction alone is not enough to guarantee the radicalness of $I_{\text{KKT}}$. Unlike the previous two relaxations, the residuals here do not indicate any room for improvement. In our tests, increasing the relaxation degree $d$ offers some success, but this also greatly increases the computation time, making this relaxation impractical for the problem at hand.

| KKT Relaxation | | | |
|---|---|---|---|
| $(n, m)$ | Success (%) | Time (s) | Residual |
| $(3, 3)$ | 40 | 97.15 | 16.95 |
| $(3, 4)$ | 0 | 581.06 | 33.07 |
| $(3, 5)$ | 0 | 1879.94 | 56.57 |

Table 3.3: Average performance of relaxation (3.6)

### 3.3.3 Jacobian relaxation

We now present an exact relaxation which (in theory) always works for our problem of interest. This approach is similar to the KKT relaxation, only now to establish the dependence between derivatives of the constraints and the function, we consider determinants of an associated Jacobian matrix. Consider problems of the form (3.2) with a single constraint $g$. We define

$$B(x) = (\nabla p(x)\ \nabla g(x)),$$

to be the matrix with columns being the gradient vectors of $p$ and $g$. Let

$$\varphi_\ell(x) = \sum_{\substack{E \in [N]_2 \\ sum(E)=\ell}} \det B_E(x), \tag{3.7}$$

where $B_E$ is the submatrix of $B$ with rows listed in $E$, and $sum(E)$ is the sum of the elements in $E$. As shown in [71], (3.2) is equivalent to

$$\begin{aligned} &\min_{x\in\mathbb{R}^N} p(x) \\ &s.t.\ \ g(x) = 0, \\ &\varphi_\ell(x) = 0,\ \ \ell = 3,\dots,2N-1. \end{aligned} \tag{3.8}$$

We call this the *Jacobian* system related to (3.2). Letting $J = \langle g, \varphi_3, \dots, \varphi_{2N-1}\rangle$ and

$$J^{(d)} = \{q \in J : \deg(q) \leq 2d\},$$

we can write the SOS relaxation for (3.8) as

$$\begin{aligned} &\max_{\gamma>0} \gamma, \\ &s.t.\ \ p(x) - \gamma - q(x) \in \Sigma_n, \\ &q(x) \in J^{(d)}. \end{aligned} \tag{3.9}$$

Moreover, letting $p^*$ be the solution of (3.8), $p^{(d)}$ of the corresponding SOS relaxation (of order $d$) and $p^{min}$ the minimum of (3.2). Then the following holds.

**Theorem 3.9** (Theorem 2.3, [71]). *Assume that $V(g)$ is non-singular, then $p^* > -\infty$ and there is a $D \in \mathbb{N}$ such that $p^{(d)} = p^*$ for all $d \geq D$. Moreover, if $p^{min}$ is achievable, then $p^{(d)} = p^{min}$ for all $d \geq D$.*

For us, the minimum of $F_\delta$ is always achieved on $\mathbb{S}^{N-1}$, and it is clear that $V(s) = \mathbb{S}^{N-1}$ is non-singular. It follows that we can solve the Jocabian system (3.9) associated to $F_\delta$ exactly. This relaxation is given as

$$\begin{aligned} &\max_{\delta>0} \delta, \\ &s.t.\ \ F_\delta(x,y) - q(x,y) \in \Sigma_{n+m}, \\ &q(x,y) \in J^{(d)}. \end{aligned} \tag{3.10}$$

Due to non-linearity in the constraints of (3.10), we employ the bisection approach similar to the other methods and solve

$$\begin{aligned} &\text{find } q(x,y) \in J^{(d)}, \\ &s.t.\ \ F_\delta(x,y) - q(x,y) \in \Sigma_{n+m}, \end{aligned}$$

again with the limits of $\delta$ being $2^{-6}$ and $d$ being 2.

**Remark 3.10.** The functions $\varphi_\ell$ in (3.7) are quartic polynomials in our problem of interest. We could instead write this relaxation over the Segre variety in the variables $z_{ij} = x_i \otimes y_j$ which would lead to quadratic constraints $\varphi_\ell$. However, as detailed in [71] the generators of the Segre variety introduce an exponential number of constraints, and would in turn make (3.10) more difficult to solve numerically. This trade-off between the degree and the number of constraints is also present in the KKT relaxation.

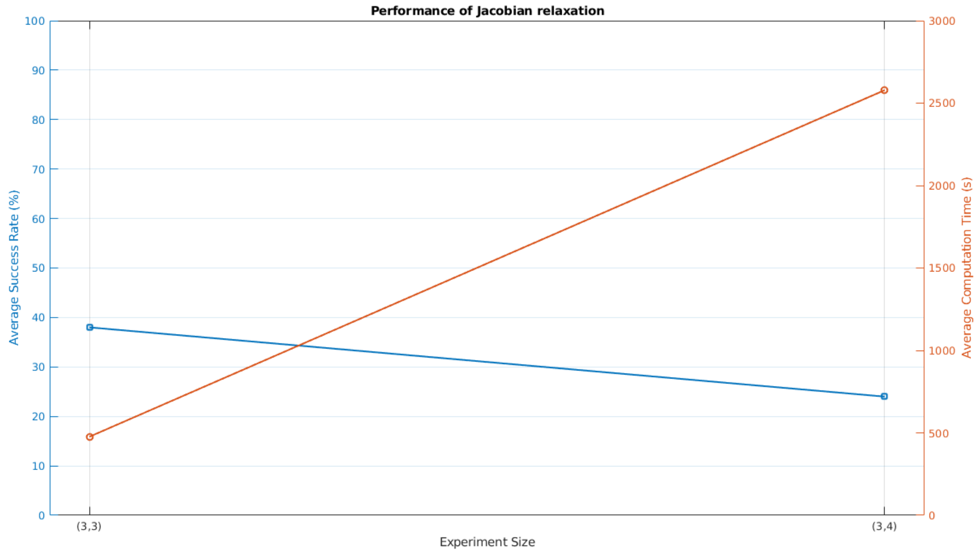


Figure 3.4: Performance of the Jacobian Relaxation (3.10), tested on 50 randomly constructed biquadratic forms. Problems of size (3,5) were too difficult for this relaxation.

Unsurprisingly, this is quite slow. The solve time on test cases of size $(3, 5)$ was close to one hour, and so we do not test the Jacobian relaxation on this set. We can also see (Figure/Table 3.4) that this relaxation exhibits low success rates and high residuals. Similar to KKT, the Jacobian relaxation is somewhat impractical in our context.

| Jacobian Relaxation | | | |
|---|---|---|---|
| $(n, m)$ | Success (%) | Time (s) | Residual |
| $(3, 3)$ | 38 | 476.63 | 18.64 |
| $(3, 4)$ | 24 | 2578.73 | 25.06 |

Table 3.4: Average performance of relaxation (3.10)

**Remark 3.11.** It should be noted again that these tests were conducted with limited freedom on the degrees of the relaxations. Based on our experience, we recommend using the Hilbert method with a high relaxation degree ($d = 3$) if memory is not a concern and the user wants more successful constructions. When memory becomes an issue, the CNR seems to be a better choice; although its success rate is lower, the speed of computation makes generating random examples more practical.

## 3.4 Rationalization

Constructing PnCP maps over floating point numbers provides quick numerical tests which can indicate positivity, but ideally we would like to have rational PnCP maps with exact certificates of positivity. Recall from Chapter 2, that the semi-definite programs arising from our SOS relaxations are feasibility problems of the form,

$$\begin{aligned} &\mathcal{G} \succeq 0 \\ s.t. \quad &\langle A_i, \mathcal{G} \rangle = b_i, \quad i = 1, \dots, m \end{aligned} \tag{3.11}$$

where $A_i$ and $b_i$ are obtained from the problem data (see [75] for a nice presentation of this). The following theorem, first proved in [78], provides a means to obtain rational solutions of (3.11) from numerical ones.

**Theorem 3.12** (Theorem 3.2, [20]). *Let $\mathcal{G}$ be a positive definite feasible point for (3.11) satisfying*

$$\mu := \min\left(eig(\mathcal{G})\right) > ||(\langle A_i, \mathcal{G}\rangle - b_i)_i|| =: \epsilon,$$

*then there is a (positive definite) rational feasible point $\hat{\mathcal{G}}$. This can be obtained in two step;*

*(1) Compute a rational approximation $\tilde{\mathcal{G}}$ with $\tau := ||\mathcal{G} - \tilde{\mathcal{G}}||$ satisfying $\tau^2 + \epsilon^2 \leq \mu^2$,*

*(2) Project $\tilde{\mathcal{G}}$ onto the affine subspace $\mathcal{L}$ defined by the equations $\langle A_i, \mathcal{G}\rangle = b_i$ to obtain $\hat{\mathcal{G}}$.*

For our problems, there are two key issues with using this rationalization. Firstly, our semi-definite programs will never satisfy the strict feasibility requirements of $\mathcal{G}$ being positive definite. This is because by construction, the form $F_\delta$ will always have non-trivial zeros chosen in Step 1 of Algorithm 1. To tackle this, there are many facial reduction methods available to allow this rationalization for positive semi-definite $\mathcal{G}$. To put it simply, these methods work by 'removing' the rational zeros, and allowing us to work with a smaller positive definite $\hat{\mathcal{G}}$. One such reduction is presented in [51], see also [56] for instance. However, we should note that in general even this strategy will not work in our setting. This is because, even though our initial choice of zeros for $F_\delta$ may be rational, it is still possible for $F_\delta$ to have some irrational zeros, which then can not be removed via facial reduction.

More importantly, the numbers $b_i$ are obtained from the coefficients of the polynomial being tested, in our case $F_\delta$. This means that the affine subspace $\mathcal{L}$ is being defined by floating point numbers, and any sort of rationalization of $\mathcal{G}$ will perturb this subspace.

In PnCP we combat this by restricting the randomization in the linear algebra steps of Algorithm 1; we restrict the choices of the initial points $x_i, y_j$, so that the generated linear/quadratic forms have rational entries with small (single digit) denominators. To be more specific, for the constructing the initial points $\mathbf{x}^{(i)}, \mathbf{y}^{(i)}$, instead of using `rand` in MATLAB to generate uniform random numbers, we use `randi` to generate pseudorandom integers, with the integers belonging to the interval $[-3, 3]$. This ensures that the points $\mathbf{z}^{(i)}$ has single digit entries, and as a result the required kernels of Step 2 and Step 3, have rational entries where the numerators and denominators normally have a small number of digits (two or three). For the linear forms $h_i$ and the quadratic form $f$, we choose the random vectors in Step 2 and Step 3 as a random linear combination of vectors that span the required kernels, with the linear combinations having coefficients $-1, 0$, or $1$.

As expected this reduces the base success rate of Algorithm 1, but it successfully constructs $F_\delta$ with rational coefficients. We also observe a significant increase in computation time to construct forms with rational coefficients; we test this by constructing 50 random forms with rational coefficients, and comparing the timing costs to constructing forms with floating point coefficients.

As we can see below, constructing rational forms is far more expensive than floating point forms. In fact, the average time taken to construct forms with floating point coefficients remains almost constant ($\sim$2 seconds). In constrast, the construction time for forms with rational coefficients can take close to 10 minutes.

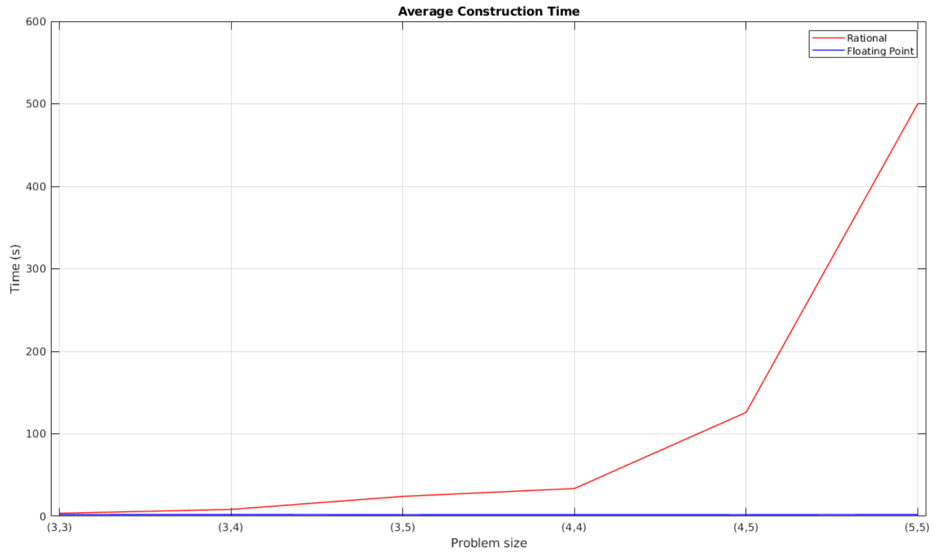


Figure 3.5

This rational construction can be used in PnCP with the command `Gen_PnCP` and setting the *'rationalize'* argument to 1. Currently, PnCP provides numerical verification of the constructed rational $F_\delta$, via the techniques of Section 3.3. This construction can be used in conjunction with the many rational SOS packages (such as RationalSOS, RealCertify, multivsos, etc.) to obtain exact certificates of non-negativity.

## 3.5 Detecting Quantum Entanglement

We will now show how we can use PnCP for detecting quantum entanglement. We start with a brief (and simplified) exposition into quantum states, the core object of interest for us, presenting some terminology and commonly known facts (for a more detailed introduction we refer the reader to [4, 50, 99], or any graduate text on Quantum Information Theory). We then state two entanglement criteria, and then give an example demonstrating how PnCP is used to implement the most general one.

A *quantum state* is a vector $\phi \in \mathbb{R}^n$, and with any quantum state there is an associated *(normalized) density matrix* $\phi\phi^T =: \rho \in \mathbb{SR}^{n\times n}$ (normalized to have unit trace). A density matrix

$$\rho = \sum_i p_i \phi_i \phi_i^T, \tag{3.12}$$

with $\{\phi_i\}$ an orthonormal system, $p_i \geq 0$ and $\sum_i p_i = 1$, represents a quantum system in one of several states $\phi_i$ with associated probabilities $p_i$. We use the following terminology; $\rho$ is a *pure state* if $\rho = \phi\phi^T$, otherwise if $\rho$ is of the form (3.12), then it is a *mixed state*. It should be noted that any (symmetric) positive semi-definite matrix $\rho$ with $\mathrm{tr}(\rho) = 1$ is a density matrix. It is known that pure states satisfy $\mathrm{tr}(\rho^2) = 1$ while for mixed states $\mathrm{tr}(\rho^2) < 1$.

Given a composite quantum system $\mathbb{SR}^{nm\times nm} = \mathbb{SR}^{n\times n} \otimes \mathbb{SR}^{m\times m}$ and a state $\rho^{nm} \in \mathbb{SR}^{nm\times nm}$, we call $\rho^{nm}$ *simply separable* if

$$\rho^{nm} = \rho^n \otimes \rho^m, \quad \text{with } \rho^i \in \mathbb{SR}^{i\times i}, \text{ and } \left\|\rho^i\right\| = 1,$$

*separable* if

$$\rho^{nm} = \sum_i p_i \rho_i^n \otimes \rho_i^m, \quad p_i \geq 0, \quad \sum_i p_i = 1,$$

and *entangled* if its not separable. A problem of interest in quantum information theory is the so called *separability problem*; *given a state (density matrix) $\rho$ in a composite system, determine if it is entangled.*

There are many different criteria and measures of entanglement throughout the literature. For pure states, things are relatively simple and separability can be determined by checking if the state is in the image of the Segre embedding. For mixed states however, the situation is more complicated.

In low dimensional composite systems, we have the Peres-Horodecki criterion, also known as the positive partial transpose (PPT) criterion; for $\rho^{nm} = \sum_i p_i \rho_i^n \otimes \rho_i^m$ define the partial ampliation map $(I \otimes \Phi)(\rho^{nm}) = \sum_i p_i \rho_i^n \otimes \Phi(\rho_i^m)$.

**Criterion 3.13** (PPT, [4] section 8.4)**.** For a quantum state $\rho \in \mathbb{SR}^{nm\times nm}$, if $(I \otimes T)(\rho)$ has a negative eigenvalue, i.e., $(I \otimes T)(\rho) \not\succeq 0$, then $\rho$ is entangled.

For systems of size $(n, m) = (2, 2)$ or $(2, 3)$, this criteria is both necessary and sufficient. In higher dimensional systems, we lose the sufficiency of this test, i.e., there are entangled states $\rho_{ent}$ with $(I \otimes T)(\rho_{ent}) \succeq 0$ (see [49] for the first such example). In this situation we instead have the more general entanglement criteria.

**Criterion 3.14** (The general criterion, [4] section 8.4)**.** A quantum state $\rho \in \mathbb{SR}^{nm\times nm}$ is entangled if there is a pncp map $\Phi$ such that the ampliation $(I \otimes \Phi)(\rho) \not\succeq 0$.

The PPT entanglement criterion is a special case of Criterion 3.14, with $\Phi$ being the transpose map. With PnCP we can apply this test with many different random $\Phi$ in the following way;

**Algorithm 2:** Entanglement Detection

**Input:** $\rho$, $S$
**Output:** Status
$i = 0$; Status = "Unknown";
**while** $i < S$ **do**
  Generate random $\Phi$;
  Compute $I \otimes \Phi(\rho)$;
  **if** $I \otimes \Phi(\rho) \not\succeq 0$ **then**
    Status = "Entangled";
    break;
  **else**
    $i = i + 1$;
  **end**
**end**

**Example 3.15.** As an example consider the following state,

$$\begin{aligned}\Delta &= \begin{bmatrix} 1/3 & 0 & 0 & 0 & 1/3 & 0 & 0 & 0 & 1/3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 & 1/3 & 0 & 0 & 0 & 1/3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 & 1/3 & 0 & 0 & 0 & 1/3 \end{bmatrix} \\ &= \frac{1}{3}\sum_{i,j} E_{i,j} \otimes E_{i,j} \in \mathbb{R}^{3\times 3} \otimes \mathbb{R}^{3\times 3},\end{aligned}$$

where each $E_{i,j} \in \mathbb{R}^{3\times 3}$ is the unit matrix with $1$ in row $i$, column $j$ and zeros everywhere else. This state is modeled after the Bell states, and is entangled. We use PnCP to generate the following non-negative, non-SOS polynomial with the command `Ent_PnCP`,

$$\begin{aligned}F_1(x,y) = {} & 5x_1^2y_1^2 + 4x_1^2y_1y_3 + 12x_1x_2y_1^2 - 22x_1x_2y_1y_2 + 36x_1x_2y_1y_3 + 8x_1x_3y_1^2 \\ & +2x_1x_3y_1y_2 + 6x_1x_3y_1y_3 + 2x_1^2y_2^2 + 2x_1^2y_2y_3 + 60x_1x_2y_2^2 - 74x_1x_2y_2y_3 \\ & +4x_1x_3y_2^2 + 2x_1x_3y_2y_3 - 3x_1^2y_3^2 + 28x_1x_2y_3^2 - 2x_1x_3y_3^2 + 19x_2^2y_1^2 \\ & -66x_2^2y_1y_2 + 24x_2^2y_1y_3 - 4x_2x_3y_1^2 + 24x_2x_3y_1y_2 - 10x_2x_3y_1y_3 + 94x_2^2y_2^2 \\ & -36x_2^2y_2y_3 + 30x_2x_3y_2^2 + 2x_2x_3y_2y_3 + 5x_2^2y_3^2 - 2x_2x_3y_3^2 + 3x_3^2y_1^2 \\ & +2x_3^2y_1y_2 + 2x_3^2y_1y_3 + 2x_3^2y_2^2 + x_3^2y_3^2\end{aligned}$$

and the associated PnCP map $\Phi$,

$$\Phi(E_{1,1}) = \begin{bmatrix} 5 & 0 & 2 \\ 0 & 2 & 1 \\ 2 & 1 & -3 \end{bmatrix}, \quad \Phi(E_{1,3}+E_{3,1}) = \begin{bmatrix} 8 & 1 & 3 \\ 1 & 4 & 1 \\ 3 & 1 & -2 \end{bmatrix}$$

$$\Phi(E_{3,3}) = \begin{bmatrix} 3 & 1 & 1 \\ 1 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}, \quad \Phi(E_{1,2}+E_{2,1}) = \begin{bmatrix} 12 & -11 & 18 \\ -11 & 60 & -37 \\ 18 & -37 & 28 \end{bmatrix}$$

$$\Phi(E_{2,2}) = \begin{bmatrix} 19 & -33 & 12 \\ -33 & 94 & -18 \\ 12 & -18 & 5 \end{bmatrix}, \quad \Phi(E_{2,3}+E_{3,2}) = \begin{bmatrix} -4 & 12 & -5 \\ 12 & 30 & 1 \\ -5 & 1 & -2 \end{bmatrix}$$

Since we construct $\Phi$ on $\mathbb{SR}^{3\times 3}$, we make the canonical extension to $\mathbb{R}^{3\times 3}$ by setting $\Phi(E_{i,j}) = \frac{1}{2}\Phi(E_{i,j}+E_{j,i})$ for $i \neq j$. With this extension, we find that

$$(I \otimes \Phi)(\Delta) = \frac{1}{6}\begin{bmatrix} 10 & 0 & 4 & 12 & -11 & 18 & 8 & 1 & 3 \\ 0 & 4 & 2 & -11 & 60 & -37 & 1 & 4 & 1 \\ 4 & 2 & -6 & 18 & -37 & 28 & 3 & 1 & -2 \\ 12 & -11 & 18 & 38 & -66 & 24 & -4 & 12 & -5 \\ -11 & 60 & -37 & -66 & 188 & -36 & 12 & 30 & 1 \\ 18 & -37 & 28 & 24 & -36 & 10 & -5 & 1 & -2 \\ 8 & 1 & 3 & -4 & 12 & -5 & 6 & 2 & 2 \\ 1 & 4 & 1 & 12 & 30 & 1 & 2 & 4 & 0 \\ 3 & 1 & -2 & -5 & 1 & -2 & 2 & 0 & 2 \end{bmatrix},$$

with (numerical) eigenvalues $-8.45, -2.78, -0.83, -0.06, 0.23, 2.17, 3.28, 7.14, 41.96$.

**Example 3.16.** We consider now an example of a *bound entangled state*, which are known to be entangled whilst having a positive partial transpose (see [48] or [50, Section 6.11]). We take the example from [42], with

$$\sigma = \frac{1}{60}\begin{bmatrix} 5 & 5 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 5 & 5 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 5 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 5 \\ -1 & -1 & -1 & 5 & -1 & -1 & -1 & -1 & -1 & 5 & -1 & -1 \\ -1 & -1 & -1 & -1 & 5 & 5 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & 5 & 5 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & 5 & -1 & 5 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & 5 & -1 & -1 & 5 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & 5 & -1 & 5 & -1 & -1 & -1 \\ -1 & -1 & -1 & 5 & -1 & -1 & -1 & -1 & -1 & 5 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & 5 & -1 & -1 & 5 & -1 \\ -1 & -1 & 5 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & 5 \end{bmatrix}, \\ \in \mathbb{R}^{4\times 4} \otimes \mathbb{R}^{3\times 3}.$$

Note that $\mathrm{tr}(\sigma^2) = 0.2 < 1$, and so $\sigma$ is a mixed state (meaning we cannot simply check if it is in the image of the Segre embedding). PnCP generates the following

$$\Phi(E_{1,1}) = \begin{bmatrix} 7 & 17/2 & -5/2 \\ 17/2 & 13/2 & -7/2 \\ -5/2 & -7/2 & 2 \end{bmatrix}, \quad \Phi(E_{1,3}+E_{3,1}) = \begin{bmatrix} -6 & -3 & 3 \\ -3 & -2 & 3 \\ 3 & 3 & 0 \end{bmatrix},$$
$$\Phi(E_{3,3}) = \begin{bmatrix} 3 & -1 & 0 \\ -1 & 0 & -1 \\ 0 & -1 & 3 \end{bmatrix}, \quad \Phi(E_{1,2}+E_{2,1}) = \begin{bmatrix} -1/2 & 15/2 & -6 \\ 15/2 & 15 & -17/2 \\ -6 & -17/2 & 9/2 \end{bmatrix},$$
$$\Phi(E_{2,2}) = \begin{bmatrix} 3 & 0 & -1 \\ 0 & 17/2 & -4 \\ -1 & -4 & 3 \end{bmatrix}, \quad \Phi(E_{2,3}+E_{3,2}) = \begin{bmatrix} 2 & -3 & 0 \\ -3 & -2 & 3 \\ 0 & 3 & -2 \end{bmatrix}.$$

We find the ampliation $(I \otimes \Phi)(\sigma)$ to be

$$\frac{1}{120}\begin{bmatrix}
133 & 162 & -101 & -17 & -18 & 13 & -17 & -18 & 13 & 19 & -30 & 13 \\
162 & 308 & -182 & -18 & -52 & 22 & -18 & -52 & 22 & -30 & -52 & 10 \\
-101 & -182 & 129 & 13 & 22 & -21 & 13 & 22 & -21 & 13 & 10 & 15 \\
-17 & -18 & 13 & 163 & 36 & -29 & -17 & -18 & 13 & 67 & 84 & -17 \\
-18 & -52 & 22 & 36 & 104 & -44 & -18 & -52 & 22 & 84 & 26 & -20 \\
13 & 22 & -21 & -29 & -44 & 51 & 13 & 22 & -21 & -17 & -20 & 3 \\
-17 & -18 & 13 & -17 & -18 & 13 & 67 & 36 & 7 & 19 & -18 & 1 \\
-18 & -52 & 22 & -18 & -52 & 22 & 36 & 104 & -44 & -18 & 50 & -26 \\
13 & 22 & -21 & 13 & 22 & -21 & 7 & -44 & 75 & 1 & -26 & 15 \\
19 & -30 & 13 & 67 & 84 & -17 & 19 & -18 & 1 & 139 & 72 & -29 \\
-30 & -52 & 10 & 84 & 26 & -20 & -18 & 50 & -26 & 72 & 128 & -80 \\
13 & 10 & 15 & -17 & -20 & 3 & 1 & -26 & 15 & -29 & -80 & 75
\end{bmatrix},$$

with (numerical) eigenvalues of $-0.14, 0.00, 0.06, 0.10, 0.27, 0.37, 0.60, 0.79, 1.01, 1.81, 2.76, 4.69$. For this example, PnCP took $\sim$10 seconds to numerically check the entanglement status of the state, with majority of the time spent constructing the rational $\Phi$. If we desired only an indication of entanglement, we could repeat this with $\Phi$ having floating point entries, and the whole process would be significantly quicker.

**Remark 3.17.** With Example 3.16, PnCP only claims that the given state is entangled, it does not claim that $\sigma$ is bound entangled, i.e., it does not check whether $\sigma$ is *distillable* [7]. Distillation of quantum states is beyond the scope of this thesis.

There are many other entanglement criteria that rely on testing some condition with a PnCP map. As we can see from the examples, PnCP provides a means to implement these criteria by being able to generate random (*rational*) pncp maps.

## 3.6 Improvements for PnCP

In this chapter we presented PnCP; a MATLAB package for constructing positive maps which are not completely positive, with a focus on the practicality of this construction and its application to testing entanglement of quantum states.

PnCP is an open-source package available from https://bitbucket.org/Abhishek-B/pncp/. The package implements state of the art optimization techniques to numerically ensure positivity of the constructed maps. PnCP is even able to construct pncp maps with rational coefficients, which can be used in conjunction with existing software to obtain not only numerical, but exact certificates of positivity.

We use the KMSZ construction which additionally provides a priori knowledge of some of the zeros of the constructed polynomial. While there is work on optimizing polynomials with zeros [22, 81], there are restrictions on the zeros in these methods. Whether it is possible to adapt the zeros of the KMSZ construction to suit these methods, is something we wish to study in the future.

As the only package for this kind of construction, we intend to maintain and improve PnCP in various means; implementing better non-negativity tests as they become available, optimizing the existing code (perhaps even pursuing parallel computing where possible), and including more entanglement criteria to improve the classification of quantum states.

Our main focus moving forward will be to strengthen PnCP as a classification tool for quantum states; primarily by implementing a rational SOS decomposition method which will automatically provide exact certificates of positivity.

Chapter 4

# Truncated Tracial Moment Problem

The *truncated tracial moment problem* is a non-commutative analogue of the classical truncated moment problem. It is the study of positive linear functionals on the space of non-commutative polynomials that can be represented using traces of evaluations on tuples of real symmetric matrices. This chapter concerns the *bivariate quartic tracial moment problem*. As we have seen in Chapter 2 (Section 2.2.2.1), the classic moment problem is dual to polynomial optimization; likewise the truncated tracial moment problem is dual to trace optimization of non-commutative polynomials (see [18] for an introduction to this).

The author's MSc thesis [9] studied the bivariate quartic tracial moment problem when the associated Hankel matrix $\mathcal{M}_2$ is singular. Using the rank analysis approach of Curto and Fialkow, [9] gave a complete characterization of the bivariate quartic tracial moment problem when $\mathcal{M}_2$ is of rank at most 4. Furthermore, [9] gave sufficient conditions for when a representing measure exists.

While [9] studied sufficient conditions for the existence of a representing measure, it did not cover necessary conditions. During the PhD, we searched for these necessary conditions in collaboration with Aljaž Zalar, and our results are published in [10]. This chapter is based on our publication [10], and we will present here our novel, computationally oriented results; which provide a significant improvement (see below) to any existing algorithmic search for a representing measure.

For a more comprehensive discussion of bivariate quartic tracial moment problem, we refer the reader to [10], which includes the results of this chapter, as well as other (more technical) results, such as a complete characterization of the rank 5 case.

In Section 4.1 we present necessary definitions and preliminary results for the study of the truncated tracial moment problem. Section 4.2 gives the reduction of the bivariate quartic tracial moment problem with $\mathcal{M}_2$ of ranks 5 and 6 to four basic cases. This reduction helps to simplify future analysis of the tracial moment problem on quadratic varieties, by reducing it to the four canonical quadratics. Furthermore, our analysis is detailed and comprehensive, so it can easily be implemented to transform any given $\mathcal{M}_2$ of rank 5 or 6 into one with canonical relations.

Section 4.3 contains an analysis of the form of atoms in a potential representing measure; the results in this section were proved by Zalar in our article [10]. This atomic representation result was pivotal in analyzing the bivariate quartic tracial moment problem for ranks 5 and 6. In particular, a complete characterization of the rank 5 cases was obtainable thanks to this representation.

Section 4.4 gives the solution of the bivariate quartic tracial moment problem in two of the four rank 6 basic cases. The results include a consideration of the sizes of atoms in the minimal representing measure, and show that atoms of size 2 (i.e., $2 \times 2$ matrices) are sufficient. It is also shown how the problem can be rephrased as a feasibility problem of small linear matrix inequalities and a rank condition. This is reformulation is one of the main contributions of this thesis; ordinarily, the search for a representing measure is carried out via flat extensions, however this approach is teemed with numerical instabilities, and for larger size problems quickly becomes computationally intractable. In comparison, the computational complexity of the posed linear matrix inequalities remains the same, and these can be efficiently solved.

**Remark 4.1.** Note that all results in this chapter which have previously appeared in the author's MSc thesis will be cited as [9]. The results obtained during the PhD and subsequently published in the peer reviewed journal article [10], will be cited as such when required.

## 4.1 Preliminaries

### 4.1.1 Non-commutative bivariate polynomials

We denote by $\langle X, Y\rangle$ the *free monoid* generated by the non-commuting letters $X, Y$ and call its elements *words* in $X, Y$. Consider the free algebra $\mathbb{R}\langle X, Y\rangle$ of polynomials in $X, Y$ with coefficients in $\mathbb{R}$. Its elements are called *non-commutative (nc) polynomials*. Endow $\mathbb{R}\langle X, Y\rangle$ with the involution $p \mapsto p^*$ fixing $\mathbb{R} \cup \{X, Y\}$ pointwise. For a word $w \in \langle X, Y\rangle$, $w^*$ is its reverse, and $v \in \langle X, Y\rangle$ is *cyclically equivalent* to $w$, which we denote by $v \overset{\text{cyc}}{\sim} w$, if and only if $v$ is a cyclic permutation of $w$. The length of the longest word in a polynomial $f \in \mathbb{R}\langle X, Y\rangle$ is the *degree* of $f$ and is denoted by $\deg(f)$ or $|f|$. We write $\mathbb{R}\langle X, Y\rangle_k$ for all polynomials of degree at most $k$. For an nc polynomial $f$, its *commutative collapse* $\check{f}$ is obtained by replacing the nc variables $X, Y$, with commutative variables $x, y$.

### 4.1.2 Bivariate truncated tracial moment problem

Given a sequence of real numbers $\beta \equiv \beta^{(2n)} = (\beta_w)_{|w|\leq 2n}$, indexed by words $w$ of length at most $2n$ such that

$$\beta_v = \beta_w \quad \text{whenever } v \overset{\text{cyc}}{\sim} w \quad \text{and} \quad \beta_w = \beta_{w^*} \quad \text{for all } |w| \leq 2n, \tag{4.1}$$

we want to know if there exist $t \in \mathbb{N}$, and a probability measure (positive, normalized, Borel measure) $\mu$ on $(\mathbb{SR}^{t\times t})^2$ such that

$$\beta_w = \int_{(\mathbb{SR}^{t\times t})^2} \operatorname{Tr}(w(A, B)) \; d\mu(A, B).$$

By the tracial version [15, Theorem 3.8] of the Bayer-Teichmann theorem [5], this is equivalent to the following simpler problem.

Given $\beta$ as above, does there exist $N \in \mathbb{N}$, $t_i \in \mathbb{N}$, $\lambda_i \in (0, \infty)$ with $\sum_{i=1}^{N} \lambda_i = 1$ and pairs of matrices $(A_i, B_i) \in (\mathbb{SR}^{t_i \times t_i})^2$, such that

$$\beta_w = \sum_{i=1}^{N} \lambda_i \mathrm{Tr}(w(A_i, B_i)), \tag{4.2}$$

where $w$ runs over the indices of the sequence $\beta$ and Tr denotes the *normalized trace*, i.e.,

$$\mathrm{Tr}(A) = \frac{1}{t}\,\mathrm{tr}(A) \quad \text{for every } A \in \mathbb{R}^{t \times t}.$$

If such data exist, we say that $\beta$ admits a representing measure. The bivariate quartic tracial moment problem is the above with $n = 2$. The pair $(A_i, B_i) \in (\mathbb{SR}^{t_i \times t_i})^2$ *atoms of size* $t_i$ and the numbers $\lambda_i$ are *densities*. We say that $\mu$ is a representing measure of *type* $(m_1, m_2, \ldots, m_r)$ if it consists of exactly $m_i \in \mathbb{N} \cup \{0\}$ atoms of size $i$ and $m_r \neq 0$.

**Example 4.2.** As a very simple example, consider the following sequence

$$\begin{aligned}\theta^{(2)} &= (\theta_1, \theta_X, \theta_Y, \theta_{X^2}, \theta_{XY}, \theta_{YX}, \theta_{Y^2}) \\ &= (1, 1, \frac{1}{2}, 2, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}).\end{aligned}$$

For this sequence, one can write

$$\theta_w = \frac{1}{2}\mathrm{Tr}(w(A_1, B_1)) + \frac{1}{2}\mathrm{Tr}(w(A_2, B_2)),$$

where

$$(A_1, B_1) = (1, 0) \in (\mathbb{SR}^{1\times 1})^2, \quad (A_2, B_2) = \left( \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right) \in (\mathbb{SR}^{2\times 2})^2.$$

Then we know that $\theta^{(2)}$ has a representing measure $\mu_1$ which consists of two atoms, with equal densities ($\lambda_i = \frac{1}{2}$). Since the pair $(A_1, B_1)$ have size 1, and the pair $(A_2, B_2)$ have size 2, $\mu_1$ is of type $(1, 1)$. We could also take the alternative representing measure $\mu_2$, which consists of equal densities ($\lambda_i = \frac{1}{2}$ again), and the atoms

$$\left\{ \left( \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \right), \left( \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right) \right\} \in (\mathbb{SR}^{2\times 2})^2.$$

Because there are now no atoms of size 1, and two atoms of size 2, the representing measure $\mu_2$ is of type $(0, 2)$.

As seen in Example 4.2, given a representing measure, we can always present the atoms using matrices of a larger dimension. A representing measure of type $(m_1^{(1)}, m_2^{(1)}, \ldots, m_{r_1}^{(1)})$ is *minimal*, if there does not exist another representing measure of type $(m_1^{(2)}, m_2^{(2)}, \ldots, m_{r_2}^{(2)})$ such that

$$r_2 < r_1 \quad \text{or} \quad (r_2 = r_1, m_{r_2}^{(2)} < m_{r_1}^{(1)}) \quad \text{or} \quad (r_2 = r_1, m_{r_2}^{(2)} = m_{r_2}^{(1)}, m_{r_2-1}^{(2)} < m_{r_1-1}^{(1)})$$

$$\text{or} \quad \ldots \quad \text{or} \quad (r_2 = r_1, m_{r_2}^{(2)} = m_{r_2}^{(1)}, \ldots, m_2^{(2)} = m_2^{(1)}, m_1^{(2)} < m_1^{(1)}).$$

We say that $\beta$ admits a *non-commutative (nc) measure*, if it admits a minimal measure of type $(m_1, m_2, \ldots, m_r)$ with $r > 1$. If $\beta_1 = 1$, then we say $\beta$ is *normalized*. We may always assume that $\beta$ is normalized (otherwise we replace Tr with $\frac{1}{\beta_1}\mathrm{Tr}$). If $\beta_w = \beta_{\breve{w}}$ for all $w \in \langle X, Y \rangle$ with $|w| \leq 2n$, we call $\beta$ a *commutative (cm) sequence* and the moment problem reduces to the classical one solved by Curto and Fialkow. Otherwise we call $\beta$ a *non-commutative (nc) sequence*.

**Remark 4.3.** The following helps to simplify the problem at hand; Replacing a vector $(A_i, B_i)$ with any vector

$$(U_i A_i U_i^T, U_i B_i U_i^T) \in (\mathbb{S}\mathbb{R}^{t_i \times t_i})^2$$

where $U_i \in \mathbb{R}^{t_i \times t_i}$ is an orthogonal matrix, preserves (4.2).

We associate to the sequence $\beta$ the *(generalized) Hankel matrix* $\mathcal{M}_n = \mathcal{M}_n(\beta)$ *of order* $n$ with rows and columns indexed by words in $\mathbb{R}\langle X, Y \rangle_n$ in the graded reverse lexicographic order, in which we first sort elements by degree, and then in reverse lexicographic order (cf., [25, Chapter 2, Definition 6]). To illustrate,

$$1 < X < Y < X^2 < XY < YX < Y^2 < X^3 < X^2Y < XYX < XY^2 < \ldots$$

The entry in row $U$ and column $V$ is $\beta_{U^*V}$, i.e.,

$$\mathcal{M}_n(\beta) = \begin{array}{c c} & \begin{array}{ccccccc} \mathbb{1} & \mathbb{X} & \mathbb{Y} & \ldots & \mathbb{X}^n & \ldots & \mathbb{Y}^n \end{array} \\ \begin{array}{c} \mathbb{1} \\ \mathbb{X} \\ \mathbb{Y} \\ \vdots \\ \mathbb{X}^n \\ \vdots \\ \mathbb{Y}^n \end{array} & \begin{pmatrix} \beta_1 & \beta_X & \beta_Y & \ldots & \beta_{X^n} & \ldots & \beta_{Y^n} \\ \beta_X & \beta_{X^2} & \beta_{XY} & \ldots & \beta_{X^{n+1}} & \ldots & \beta_{XY^n} \\ \beta_Y & \beta_{XY} & \beta_{Y^2} & \ldots & \beta_{X^nY} & \ldots & \beta_{Y^{n+1}} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \beta_{X^n} & \beta_{X^{n+1}} & \beta_{X^nY} & \ldots & \beta_{X^{2n}} & \ldots & \beta_{X^nY^n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ \beta_{Y^n} & \beta_{XY^n} & \beta_{Y^{n+1}} & \ldots & \beta_{X^nY^n} & \ldots & \beta_{Y^{2n}} \end{pmatrix} \end{array}, \tag{4.3}$$

and in the special case of $n = 2$,

$$\mathcal{M}_2 = \begin{array}{c c} & \begin{array}{ccccccc} \mathbb{1} & \mathbb{X} & \mathbb{Y} & \mathbb{X}^2 & \mathbb{X}\mathbb{Y} & \mathbb{Y}\mathbb{X} & \mathbb{Y}^2 \end{array} \\ \begin{array}{c} \mathbb{1} \\ \mathbb{X} \\ \mathbb{Y} \\ \mathbb{X}^2 \\ \mathbb{Y}\mathbb{X} \\ \mathbb{X}\mathbb{Y} \\ \mathbb{Y}^2 \end{array} & \begin{pmatrix} \beta_1 & \beta_X & \beta_Y & \beta_{X^2} & \beta_{XY} & \beta_{XY} & \beta_{Y^2} \\ \beta_X & \beta_{X^2} & \beta_{XY} & \beta_{X^3} & \beta_{X^2Y} & \beta_{X^2Y} & \beta_{XY^2} \\ \beta_Y & \beta_{XY} & \beta_{Y^2} & \beta_{X^2Y} & \beta_{XY^2} & \beta_{XY^2} & \beta_{Y^3} \\ \beta_{X^2} & \beta_{X^3} & \beta_{X^2Y} & \beta_{X^4} & \beta_{X^3Y} & \beta_{X^3Y} & \beta_{X^2Y^2} \\ \beta_{XY} & \beta_{X^2Y} & \beta_{XY^2} & \beta_{X^3Y} & \beta_{X^2Y^2} & \beta_{XYXY} & \beta_{XY^3} \\ \beta_{XY} & \beta_{X^2Y} & \beta_{XY^2} & \beta_{X^3Y} & \beta_{XYXY} & \beta_{X^2Y^2} & \beta_{XY^3} \\ \beta_{Y^2} & \beta_{XY^2} & \beta_{Y^3} & \beta_{X^2Y^2} & \beta_{XY^3} & \beta_{XY^3} & \beta_{Y^4} \end{pmatrix} \end{array}, \tag{4.4}$$

where we have replaced the subscripts of the entries $\beta_{U^*V}$ with cyclically equivalent monomials, in accordance with the (degree-)lexicographic ordering. We will label the row/column vectors of $\mathcal{M}_n(\beta)$ with bold characters $\mathbb{X}, \mathbb{Y}$, etc. to distinguish from the nc variables $X, Y$, etc.

Observe that $\mathcal{M}_n$ is symmetric. Let $S_1, S_2 \subseteq \{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}^2, \mathbb{X}\mathbb{Y}, \mathbb{Y}\mathbb{X}, \dots, \mathbb{X}^n, \dots, \mathbb{Y}^n\}$. We will denote by $[\mathcal{M}_n]_{S_1,S_2}$ the submatrix of $\mathcal{M}_n$ consisting of the rows indexed by the elements of $S_1$ and the columns indexed by the elements of $S_2$. In case $S := S_1 = S_2$, we write $[\mathcal{M}_n]_S := [\mathcal{M}_n]_{S,S}$ for short, and if $S = \mathbb{R}\langle X, Y\rangle_k$ (with $k \le n$) we write $[\mathcal{M}_n]_k$. For any matrix $A$ with its rows and columns indexed by words in $\mathbb{R}\langle X, Y\rangle$, writing $w(\mathbb{X}, \mathbb{Y})$ we mean the column/row of $A$ indexed by the word $w$. Similarly for vectors. If $\beta$ admits a measure, then $\mathcal{M}_n$ is positive semi-definite; see Proposition 4.4. If $\mathcal{M}_n$ represents a cm sequence, we call it a *cm Hankel matrix*. Otherwise $\mathcal{M}_n$ is a *nc Hankel matrix*. By [17, Corollaries 3.19, 3.20], $\beta$ admits a measure if and only if there exists a Hankel matrix $\mathcal{M}_{n+k}$ extending $\mathcal{M}_n$, which admits a rank preserving extension $\mathcal{M}_{n+k+1}$. Furthermore, by [17, Corollary 3.2] in this case the atoms of size at most $\operatorname{rank}(\mathcal{M}_{n+k})$ are sufficient. When $n = 2$, if $\mathcal{M}_2$ is positive definite, then $\beta$ admits a measure since all trace-positive polynomials of degree 4 are cyclically equivalent to sums of hermitian squares [16]. This is the duality established by [17, Theorem 4.4]. Moreover, the measure consists of at most 15 atoms of size 2 [15, Remark 3.9].

### 4.1.3 Riesz functional and truncated Hankel matrix

For a polynomial $p \in \mathbb{R}\langle X, Y\rangle_{2n}$, let $\hat{p} = (a_w)_w$ be its coefficient vector with respect to the degree-lexicographic ordered basis

$$\{1, X, Y, X^2, XY, YX, Y^2, \dots, X^{2n}, \dots, Y^{2n}\}$$

of $\mathbb{R}\langle X, Y\rangle_{2n}$. Any sequence $\beta \equiv \beta^{(2n)} : \beta_1, \dots, \beta_{X^{2n}}, \dots, \beta_{Y^{2n}}$, which satisfies (4.1) defines the *Riesz functional* $L_{\beta^{(2n)}} : \mathbb{R}\langle X, Y\rangle_{2n} \to \mathbb{R}$ which is given by

$$L_{\beta^{(2n)}}(p) := \sum_{|w| \le 2n} a_w \beta_w, \quad \text{where } p = \sum_{|w| \le 2n} a_w w.$$

Notice that $\beta_w = L_{\beta^{(2n)}}(w)$ for every $|w| \le 2n$, and $\mathcal{M}_n$ is the unique matrix such that for $p, q \in \mathbb{R}\langle X, Y\rangle_n$ we have that

$$\langle \mathcal{M}_n \hat{p}, \hat{q}\rangle = L_{\beta^{(2n)}}(pq^*),$$

where $\langle \hat{p}, \hat{q}\rangle := \hat{p}^T \hat{q}$, and $q^*$ denotes the involution $*$ applied to $q$. In particular, the row $w_1(\mathbb{X}, \mathbb{Y})$ and column $w_2(\mathbb{X}, \mathbb{Y})$ entry of $\mathcal{M}_n$ is equal to

$$\left\langle \mathcal{M}_n \widehat{w_2(\mathbb{X}, \mathbb{Y})}, \widehat{w_1(\mathbb{X}, \mathbb{Y})} \right\rangle = L_{\beta^{(2n)}}(w_2 w_1^*).$$

If $\beta^{(2n)}$ admits a measure, i.e., (4.2) holds for every $\beta_w$, then for $p \in \mathbb{R}\langle X, Y\rangle$ of degree at most $n$ we have that

$$\langle \mathcal{M}_n \hat{p}, \hat{p}\rangle = L_{\beta^{(2n)}}(pp^*) = \sum_{i=1}^{m} \lambda_i Tr\left(p(A_i, B_i)\left(p(A_i, B_i)\right)^*\right) \geq 0,$$

where $\lambda_i, A_i, B_i$ are as in (4.2). This proves the following proposition, which is also well understood in the commutative setting.

**Proposition 4.4.** *If $\beta^{(2n)}$ admits a measure, then $\mathcal{M}_n$ is positive semi-definite.*

### 4.1.4 Support and Recursive Generation

We write $\mathbf{0}_{m\times n}$ for the $m \times n$ matrix with zero entries. Usually we will omit the subindex $m \times n$, when the size is clear from context.

Let $\mathcal{C}_{\mathcal{M}_n}$ denote the column space of $\mathcal{M}_n$, i.e.,

$$\mathcal{C}_{\mathcal{M}_n} = \operatorname{span}\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \ldots, \mathbb{X}^n \ldots, \mathbb{Y}^n\}.$$

For a polynomial $p \in \mathbb{R}\langle X, Y\rangle_n$ of the form $p = \sum a_w w(X, Y)$, we define

$$p(\mathbb{X}, \mathbb{Y}) = \sum_w a_w w(\mathbb{X}, \mathbb{Y}).$$

Note that $p(\mathbb{X}, \mathbb{Y}) \in \mathcal{C}_{\mathcal{M}_n}$. We express linear dependencies among the columns of $\mathcal{M}_n$ as

$$p_1(\mathbb{X}, \mathbb{Y}) = \mathbf{0}, \ldots, p_m(\mathbb{X}, \mathbb{Y}) = \mathbf{0},$$

for some $p_1, \ldots, p_m \in \mathbb{R}\langle X, Y\rangle_n$, with $m \in \mathbb{N}$. We define the *free zero set* $\mathcal{Z}(p)$ of $p \in \mathbb{R}\langle X, Y\rangle$ by

$$\mathcal{Z}(p) := \left\{(A, B) \in (\mathbb{SR}^{t\times t})^2 : t \in \mathbb{N},\ p(A, B) = \mathbf{0}_{t\times t}\right\},$$

and the variety $\mathcal{V}(\mathcal{M}_n)$ as

$$\mathcal{V}(\beta^{(2n)}) \equiv \mathcal{V}(\mathcal{M}_n) := \bigcap_{\substack{p\in\mathbb{R}\langle X,Y\rangle_n \\ p(\mathbb{X},\mathbb{Y})=\mathbf{0}}} \mathcal{Z}(p). \tag{4.5}$$

Theorem 4.5 (1) (resp. (3)) is a real tracial analogue of [26, Proposition 3.1] (resp. [27, Theorem 1.6]) and was first established in [9, Lemma 4.1.1] (resp. [9, Theorem 4.1.3]).

**Theorem 4.5** (Theorem 2.2, [10])**.** *Suppose $\beta^{(2n)}$ admits a representing measure consisting of finitely many atoms $(A_i, B_i) \in (\mathbb{SR}^{t_i\times t_i})^2$, $t_i \in \mathbb{N}$, with the corresponding densities $\lambda_i \in (0, 1)$. Let $p \in \mathbb{R}\langle X, Y\rangle_n$ be a polynomial. Then the following are true:*

1. *We have*

$$\bigcup_i (X_i, Y_i) \subseteq \mathcal{Z}(p) \quad \Leftrightarrow \quad p(\mathbb{X}, \mathbb{Y}) = \mathbf{0} \ \text{ in } \mathcal{M}_n.$$

2. *Suppose the sequence* $\beta^{(2n+2)} = (\beta_w)_{|w|\leq n+1}$ *is the extension of* $\beta$ *generated by*

$$\beta_w = \sum_i \lambda_i Tr(w(A_i, B_i)).$$

*Let* $\mathcal{M}_{n+1}$ *be the corresponding Hankel matrix. Then:*

$$p(\mathbb{X}, \mathbb{Y}) = \mathbf{0} \ \text{ in } \mathcal{M}_n \quad \Rightarrow \quad p(\mathbb{X}, \mathbb{Y}) = \mathbf{0} \ \text{ in } \mathcal{M}_{n+1}.$$

3. *(Recursive generation) For* $q \in \mathbb{R}\langle X, Y\rangle_n$ *such that* $(pq) \in \mathbb{R}\langle X, Y\rangle_n$*, we have*

$$p(\mathbb{X}, \mathbb{Y}) = \mathbf{0} \ \text{ in } \mathcal{M}_n \quad \Rightarrow \quad (pq)(\mathbb{X}, \mathbb{Y}) = (qp)(\mathbb{X}, \mathbb{Y}) = \mathbf{0} \ \text{ in } \mathcal{M}_n.$$

Column relations forced upon $\mathcal{M}_n$ with an application of Theorem 4.5 (3) will be important in solving bivariate quartic tracial moment problem and we will refer to them as the *RG relations*. If $\mathcal{M}_n$ satisfies RG relations, we say $\mathcal{M}_n$ is *recursively generated*. The first consequence of the RG relations is the following important observation about an nc Hankel matrix $\mathcal{M}_n$.

**Corollary 4.6** (Lemma 4.1.5, [9])**.** *Suppose* $n \geq 2$ *and let* $\beta^{(2n)}$ *be a sequence such that* $\beta_{X^2Y^2} \neq \beta_{XYXY}$*. Then the columns* $\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{XY}$ *of* $\mathcal{M}_n$ *are linearly independent.*

**Corollary 4.7** (Corollary 4.2.1, [9])**.** *Suppose* $n \geq 2$ *and let* $\beta^{(2n)}$ *be a sequence such that* $\beta_{X^2Y^2} \neq \beta_{XYXY}$*. If* $\mathcal{M}_n$ *is of rank at most 3, then* $\beta$ *does not admit a measure.*

### 4.1.5 Flat extensions

For a matrix $A \in \mathbb{SR}^{s\times s}$, an *extension* $\widetilde{A} \in \mathbb{SR}^{(s+u)\times(s+u)}$ of the form

$$\widetilde{A} = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}$$

for some $B \in \mathbb{R}^{s\times u}$ and $C \in \mathbb{R}^{u\times u}$, is called *flat* if $\operatorname{rank}(A) = \operatorname{rank}(\widetilde{A})$. This is equivalent to saying that there is a matrix $W \in \mathbb{R}^{s\times u}$ such that $B = AW$ and $C = W^T AW$. The connection between flat extensions and the bivariate truncated tracial moment problem is the following.

**Theorem 4.8** (Theorem 3.19, [17])**.** *Let* $\beta \equiv \beta^{(2n)}$ *be a sequence satisfying (4.1). If* $\mathcal{M}_n(\beta)$ *is positive semi-definite and is a flat extension of* $\mathcal{M}_{n-1}(\beta)$*, then* $\beta$ *admits a representing measure.*

### 4.1.6 Affine linear transformations

An important result for converting a given moment problem into a simpler, equivalent moment problem is the application of affine linear transformations to a sequence $\beta$. For $a, b, c, d, e, f \in \mathbb{R}$ with $bf - ce \neq 0$, let us define

$$\phi(X, Y) = (\phi_1(X, Y), \phi_2(X, Y)) := (aI_s + bX + cY, dI_s + eX + fY), \ (X, Y) \in (\mathbb{SR}^{s\times s})^2,$$

where $I_s$ is the identity matrix in $\mathbb{SR}^{s\times s}$. Let $\widetilde{\beta}^{(2n)}$ be the sequence obtained by the rule

$$\widetilde{\beta}_w = L_{\beta^{(2n)}}(w \circ \phi) \quad \text{for every } |w| \leq n.$$

Notice that $L_{\widetilde{\beta}^{(2n)}}(p) = L_{\beta^{(2n)}}(p \circ \phi) \quad$ for every $p \in \mathbb{R}\langle X, Y\rangle_n$.

The following is the tracial analogue of [30, Proposition 1.9], which will allow us to make affine linear changes of variables.

**Proposition 4.9** (Proposition 3.1.5, [9]). *Suppose $\beta^{(2n)}$ and $\widetilde{\beta}^{(2n)}$ are as above and $\mathcal{M}_n$ and $\widetilde{\mathcal{M}}_n$ the corresponding Hankel matrices. Let $J_\phi : \mathbb{R}\langle X, Y\rangle_{2n} \to \mathbb{R}\langle X, Y\rangle_{2n}$ be the linear map given by*

$$J_\phi \widehat{p} := \widehat{p \circ \phi}.$$

*Then the following hold:*

1. $\widetilde{\mathcal{M}}_n = (J_\phi)^T \mathcal{M}_n J_\phi$.
2. *$J_\phi$ is invertible.*
3. $\widetilde{\mathcal{M}}_n \succeq 0 \Leftrightarrow \mathcal{M}_n \succeq 0$.
4. $\operatorname{rank}(\widetilde{\mathcal{M}}_n) = \operatorname{rank}(\mathcal{M}_n)$.
5. *The formula $\mu = \tilde{\mu} \circ \phi$ establishes a one-to-one correspondence between the sets of representing measures of $\beta$ and $\tilde{\beta}$, and $\phi$ maps $\operatorname{supp}(\mu)$ bijectively onto $\operatorname{supp}(\tilde{\mu})$.*
6. *$\mathcal{M}_n$ admits a flat extension if and only if $\widetilde{\mathcal{M}}_n$ admits a flat extension.*
7. *For $p \in \mathbb{R}\langle X, Y\rangle_n$, we have $p(\widetilde{X}, \widetilde{Y}) = (J_\phi)^T (p \circ \phi)(X, Y)$.*

### 4.1.7 Classical bivariate quartic real moment problem

The classical bivariate quartic moment problem has been solved by Curto and Fialkow in a series of papers, e.g., [26, 27, 28, 29, 30, 31, 32, 39]. The main technique used was the analysis of the existence of a flat extension of the Hankel matrix $\mathcal{M}_2$. Curto and Fialkow's solution to the singular bivariate quartic real moment problem is given in Theorem 4.10 below. Given a polynomial $p \in \mathbb{R}[x, y]_2$ we write $\mathcal{Z}_{cm}(p) = \{(x, y) \in \mathbb{R}^2 : p(x, y) = 0\}$ for the variety generated by $p$.

**Theorem 4.10.** *Suppose $\beta \equiv \beta^{(4)}$ is a commutative sequence with the associated Hankel matrix $\mathcal{M}_2$. Let*

$$\mathcal{V} := \bigcap_{\substack{g \in \mathbb{R}[x,y]_2 \\ g(\mathbb{X},\mathbb{Y})=\mathbf{0}}} \mathcal{Z}_{cm}(g)$$

*be the variety associated to $\mathcal{M}_2$ and $p \in \mathbb{R}[x, y]$ a polynomial with $\deg(p) = 2$. Then $\beta$ has a representing measure supported in $\mathcal{Z}_{cm}(p)$ if and only if $\mathcal{M}_2$ is positive semi-definite, recursively generated, satisfies $\operatorname{rank}(\mathcal{M}_2) \leq \operatorname{card}(\mathcal{V})$ and has a column dependency relation $p(\mathbb{X}, \mathbb{Y}) = 0$.*

*Moreover, assume that $\mathcal{M}_2$ is positive semi-definite, recursively generated and satisfies the column dependency relation $p(\mathbb{X}, \mathbb{Y})$. The following statements are true:*

1. *If* $\operatorname{rank}(\mathcal{M}_2) \leq 3$*, then* $\mathcal{M}_2$ *always admits a flat extension to a Hankel matrix* $\mathcal{M}_3$ *and hence* $\beta$ *admits a 3-atomic minimal measure.*

2. *If* $\operatorname{rank}(\mathcal{M}_2) = 4$*, then* $\beta$ *does not necessarily come from a cm measure.*

3. *If* $\operatorname{rank}(\mathcal{M}_2) = 5$*, then* $\beta$ *always admits a cm measure, but* $\mathcal{M}_2$ *does not necessarily admit a flat extension to a Hankel matrix* $\mathcal{M}_3$*. There exists an affine linear transformation such that* $\mathcal{V}$ *is one of* $x^2 + y^2 = 1$*,* $y = x^2$*,* $xy = 1$*,* $x^2 = 1$ *or* $xy = 0$*. In the first four cases* $\mathcal{M}_2$ *always admits a flat extension to a Hankel matrix* $\mathcal{M}_3$ *and hence* $\beta$ *admits a 5-atomic measure. However, in the last case there always exists a measure with 6 representing atoms, but not necessarily 5.*

4. *If* $\operatorname{rank}(\mathcal{M}_2) = 6$*, then* $\mathcal{M}_2$ *always admits a flat extension to a Hankel matrix* $\mathcal{M}_3$ *and hence* $\beta$ *admits a 6-atomic measure.*

## 4.2 Ranks 5 and 6 - Canonical forms

When the Hankel matrix for the bivariate quartic tracial moment problem has rank 5 or 6, it suffices to study some basic cases satisfying "nice" column relations. We proved this in Proposition 4.1 of [10].

**Proposition 4.11.** *Suppose an nc sequence* $\beta \equiv \beta^{(4)}$ *has a Hankel matrix* $\mathcal{M}_2$ *of rank 5 or 6. Let* $L_\beta$ *be the Riesz functional belonging to* $\beta$*. If* $\beta$ *admits an nc measure, then there exists an affine linear transformation* $\phi$ *such that a sequence* $\widehat{\beta}$*, given by* $\widehat{\beta}_w = L_\beta(w \circ \phi)$ *for every* $|w(X,Y)| \leq 4$*, has a Hankel matrix* $\widehat{\mathcal{M}_2}$ *such that:*

1. *If* $\mathcal{M}_2$ *is of rank 5, then* $\widehat{\mathcal{M}_2}$ *satisfies* $\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}$ *and one of the following relations:*

   *Basic case 1* $\mathbb{X}^2 + \mathbb{Y}^2 = \mathbb{1}$,

   *Basic case 2* $\mathbb{Y}^2 = \mathbb{1}$,

   *Basic case 3* $\mathbb{Y}^2 - \mathbb{X}^2 = \mathbb{1}$,

   *Basic case 4* $\mathbb{Y}^2 = \mathbb{X}^2$.

2. *If* $\mathcal{M}_2$ *is of rank 6, then* $\widehat{\mathcal{M}_2}$ *satisfies one of the following relations:*

   *Basic relation 1* $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$,

   *Basic relation 2* $\mathbb{Y}^2 = \mathbb{1} + \mathbb{X}^2$,

   *Basic relation 3* $\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}$,

   *Basic relation 4* $\mathbb{Y}^2 = \mathbb{1}$.

To prove Proposition 4.11 we need some lemmas. We proved the following in Lemma 4.2 of [10].

**Lemma 4.12.** *Suppose an nc sequence* $\beta \equiv \beta^{(4)}$ *has a Hankel matrix* $\mathcal{M}_2$ *of rank 5 or 6 satisfying the relation*

$$\mathbb{Y}^2 = a_1\mathbb{1} + a_2\mathbb{X} + a_3\mathbb{Y} + a_4\mathbb{X}^2 + a_5\mathbb{X}\mathbb{Y} + a_6\mathbb{Y}\mathbb{X}, \tag{4.6}$$

*where $a_i \in \mathbb{R}$ for each $i$. Let $L_\beta$ be the Riesz funtional belonging to $\beta$. If $\beta$ admits an nc measure, then there exists an affine linear transformation $\phi$ of the form*

$$\phi(X,Y) = (\alpha_1 X + \alpha_2 I, \alpha_3 Y + \alpha_4 I), \tag{4.7}$$

*where $\alpha_i \in \mathbb{R}$ for each $i$, $\alpha_1 \neq 0$, $\alpha_4 \neq 0$, such that the sequence $\widehat{\beta}$ given by $\widehat{\beta}_w = L_\beta(w \circ \phi)$ for every $|w(X,Y)| \leq 4$, has a Hankel matrix $\widehat{\mathcal{M}_2}$ satisfying one of the following relations:*

*Relation 1* $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$,

*Relation 2* $\mathbb{Y}^2 = \mathbb{1}$,

*Relation 3* $\mathbb{Y}^2 = \mathbb{1} + \mathbb{X}^2$,

*Relation 4* $\mathbb{Y}^2 = \mathbb{X}^2$.

*Moreover, relation 4 is equivalent to*

*Relation 4′* $\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}$.

*Proof.* By comparing the rows $\mathbb{X}\mathbb{Y}$, $\mathbb{Y}\mathbb{X}$ on both sides of (4.6) we conclude that $a_5 = a_6$. We rewrite the relation (4.6) as

$$(\mathbb{Y} - a_5\mathbb{X})^2 = a_1\mathbb{1} + a_2\mathbb{X} + a_3\mathbb{Y} + (a_4 + a_5^2)\mathbb{X}^2.$$

Applying an affine linear transformation $\phi_1(X,Y) = (X, Y - a_5 X)$ to $\beta$ we get $\widetilde{\beta}$ with the Hankel matrix $\widetilde{\mathcal{M}_2}$ satisfying the relation

$$\mathbb{Y}^2 = a_1\mathbb{1} + (a_2 + a_3 a_5)\mathbb{X} + a_3\mathbb{Y} + a_4\mathbb{X}^2. \tag{4.8}$$

We separate three possibilities according to the sign of $a_4 \in \mathbb{R}$.

**Case 1:** $a_4 < 0$. The relation (4.8) can be rewritten as

$$\Big(\mathbb{Y} - \frac{a_3}{2}\Big)^2 = -\Big(\sqrt{|a_4|}\mathbb{X} - \frac{a_2 + a_3 a_5}{2\sqrt{|a_4|}}\Big)^2 + \Big(a_1 + \frac{a_3^2}{4} + \frac{(a_2 + a_3 a_5)^2}{4a_4}\Big)\mathbb{1}.$$

Applying an affine linear transformation $\phi_2(X,Y) = (\sqrt{|a_4|}X - \frac{a_2+a_3a_5}{2\sqrt{|a_4|}}, Y - \frac{a_3}{2})$ to $\widetilde{\beta}$ we get $\overline{\beta}$ with $\overline{\mathcal{M}_2}$ satisfying the relation

$$\mathbb{Y}^2 = -\mathbb{X}^2 + \Big(a_1 + \frac{a_3^2}{4} + \frac{(a_2 + a_3 a_5)^2}{4a_4}\Big)\mathbb{1}. \tag{4.9}$$

If $C_1 := a_1 + \frac{a_3^2}{4} + \frac{(a_2+a_3a_5)^2}{4a_4} \leq 0$, then by comparing the row $\mathbb{Y}^2$ on both sides of (4.9) we get

$$0 \leq \beta_{Y^4} + \beta_{X^2Y^2} = C_1 \cdot \beta_{Y^2} \leq 0,$$

where we used that $\beta_{Y^4} \geq 0$, $\beta_{X^2Y^2} \geq 0$, $\beta_{Y^2} \geq 0$. But then $\beta_{Y^4} = \beta_{X^2Y^2} = \beta_{Y^2} = 0$, which contradicts the rank of $\widetilde{\mathcal{M}_2}$ being 5 or 6. Therefore $C_1 > 0$. Applying an affine linear transformation $\phi_3(X,Y) = (\frac{X}{\sqrt{C_1}}, \frac{Y}{\sqrt{C_1}})$ to $\overline{\beta}$ we get $\widehat{\beta}$ with $\widehat{\mathcal{M}_2}$ satisfying

$$\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2,$$

which is the relation 1.

**Case 2:** $a_4 = 0$. Multiplying (4.8) with $\mathbb{Y}$ we get

$$\mathbb{Y}^3 = a_1\mathbb{Y} + (a_2 + a_3a_5)\mathbb{X}\mathbb{Y} + a_3\mathbb{Y}^2. \tag{4.10}$$

By comparing the rows $\mathbb{X}\mathbb{Y}$, $\mathbb{Y}\mathbb{X}$ on both sides of (4.10) we conclude that $a_2 + a_3a_5 = 0$. We can rewrite (4.8) as

$$\Big(\mathbb{Y} - \frac{a_3}{2}\Big)^2 = \Big(a_1 + \frac{a_3^2}{4}\Big)\mathbb{1}.$$

Applying an affine linear transformation $\phi_4(X,Y) = (X, Y - \frac{a_3}{2})$ to $\widetilde{\beta}$ we get $\overline{\beta}$ with $\overline{\mathcal{M}_2}$ satisfying

$$\mathbb{Y}^2 = \Big(a_1 + \frac{a_3^2}{4}\Big)\mathbb{1}. \tag{4.11}$$

If $C_2 := a_1 + \frac{a_3^2}{4} \leq 0$, then by comparing the row $\mathbb{Y}^2$ on both sides of (4.11) we get

$$0 \leq \beta_{Y^4} = (a_2 + \frac{c_2^2}{4})\beta_{Y^2} \leq 0,$$

where we used that $\beta_{Y^4} \geq 0$, $\beta_{Y^2} \geq 0$. But then $\beta_{Y^4} = \beta_{Y^2} = 0$ and hence also $\beta_{X^2Y^2} = 0$, which contradicts the rank of $\widehat{\mathcal{M}_2}$ being 5 or 6. Therefore $C_2 > 0$. Applying an affine linear transformation $\phi_5(X,Y) = (X, \frac{Y}{\sqrt{C_2}})$ to $\overline{\beta}$ we get $\widehat{\beta}$ with $\widehat{\mathcal{M}_2}$ satisfying

$$\mathbb{Y}^2 = \mathbb{1},$$

which is the relation 2.

**Case 3:** $a_4 > 0$. The relation (4.8) can be rewritten as

$$\Big(\mathbb{Y} - \frac{a_3}{2}\Big)^2 = \Big(\sqrt{a_4}\mathbb{X} + \frac{a_2 + a_3a_5}{2\sqrt{a_4}}\Big)^2 + \Big(a_1 + \frac{a_3^2}{4} - \frac{(a_2 + a_3a_5)^2}{4a_4}\Big)\mathbb{1}.$$

Applying an affine linear transformation $\phi_6(X,Y) = (\sqrt{a_4}X + \frac{a_2+a_3a_5}{2\sqrt{a_4}}, Y - \frac{a_3}{2})$ to $\widetilde{\beta}$ we get $\overline{\beta}$ with $\overline{\mathcal{M}_2}$ satisfying

$$\mathbb{Y}^2 = \mathbb{X}^2 + \Big(a_1 + \frac{a_3^2}{4} - \frac{(a_2 + a_3a_5)^2}{4a_4}\Big)\mathbb{1}. \tag{4.12}$$

We separate three possibilities according to the sign of $C_3 := a_1 + \frac{a_3^2}{4} - \frac{(a_2+a_3a_5)^2}{4a_4}$.

**Case 3.1:** $C_3 > 0$. Applying an affine linear transformation $\phi_7(X,Y) = (\frac{X}{\sqrt{C_3}}, \frac{Y}{\sqrt{C_3}})$ to $\overline{\beta}$ we get $\widehat{\beta}$ with $\widehat{\mathcal{M}_2}$ satisfying

$$\mathbb{Y}^2 = \mathbb{1} + \mathbb{X}^2,$$

which is the relation 3.

**Case 3.2:** $C_3 = 0$. The relation (4.12) is

$$\mathbb{Y}^2 = \mathbb{X}^2,$$

which is the relation 4. Applying an affine linear transformation $\phi_8(X,Y) = (X-Y, X+Y)$ to $\widetilde{\beta}$ we get $\overline{\beta}$ with $\overline{\mathcal{M}_2}$ satisfying

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0},$$

which is the relation $4'$.

**Case 3.3:** $C_3 < 0$. Applying an affine linear transformation $\phi_9(X,Y) = (Y,X)$ to $\overline{\beta}$ we come into Case 3.1. □

**Lemma 4.13** (Lemma 4.4.1, [9]). *Suppose an nc sequence $\beta \equiv \beta^{(4)}$ has a Hankel matrix $\mathcal{M}_2$ of rank 5 with linearly independent columns $\mathbb{1}$, $\mathbb{X}$, $\mathbb{Y}$, $\mathbb{X}\mathbb{Y}$. Then one of the following cases occurs:*

*Case 1: The set $\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}\mathbb{Y}, \mathbb{Y}\mathbb{X}\}$ is the basis for $\mathcal{C}_{\mathcal{M}_2}$ and the columns $\mathbb{X}^2, \mathbb{Y}^2$ belong to the $\mathrm{span}\{\mathbb{1}, \mathbb{X}, \mathbb{Y}\}$.*

*Case 2: The set $\left\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}^2, \mathbb{X}\mathbb{Y}\right\}$ is the basis for $\mathcal{C}_{\mathcal{M}_2}$.*

*Case 3: The set $\left\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{Y}^2, \mathbb{Y}\mathbb{X}\right\}$ is the basis for $\mathcal{C}_{\mathcal{M}_2}$.*

**Lemma 4.14** (Lemma 4.5.1, [9]). *Suppose an nc sequence $\beta \equiv \beta^{(4)}$ has a Hankel matrix $\mathcal{M}_2$ of rank 6 with linearly independent columns $\mathbb{1}$, $\mathbb{X}$, $\mathbb{Y}$, $\mathbb{X}\mathbb{Y}$. There exists an affine linear transformation $\phi$ such that a sequence $\widehat{\beta}$, given by $\widehat{\beta}_w = L_\beta(w \circ \phi)$ for every $|w(X,Y)| \leq 4$, has a Hankel matrix $\widehat{\mathcal{M}_2}$ such that:*

*Case 1: The set $\left\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}^2, \mathbb{X}\mathbb{Y}, \mathbb{Y}\mathbb{X}\right\}$ is the basis for $\mathcal{C}_{\widehat{\mathcal{M}_2}}$.*

*Case 2: The set $\left\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}^2, \mathbb{X}\mathbb{Y}, \mathbb{Y}^2\right\}$ is the basis for $\mathcal{C}_{\widehat{\mathcal{M}_2}}$.*

**Lemma 4.15** (Section 4.5, [9]). *Suppose an nc sequence $\beta \equiv \beta^{(4)}$ has a Hankel matrix $\mathcal{M}_2$ satisfying one of the relations*

$$\mathbb{Y}^2 + \mathbb{X}^2 = \mathbb{1} \quad \text{or} \quad \mathbb{Y}^2 - \mathbb{X}^2 = \mathbb{1} \quad \text{or} \quad \mathbb{Y}^2 = \mathbb{X}^2.$$

*If $\beta$ admits an nc measure $\mu$, then the extension $\mathcal{M}_3 := \begin{pmatrix} \mathcal{M}_2 & B_3 \\ B_3^t & C_3 \end{pmatrix}$ generated by $\mu$ satisfies the relations*

$$\mathbb{X}^2\mathbb{Y} = \mathbb{Y}\mathbb{X}^2 \quad \text{and} \quad \mathbb{X}\mathbb{Y}^2 = \mathbb{Y}^2\mathbb{X}.$$

*In particular, the rows $\mathbb{X}\mathbb{Y}$, $\mathbb{Y}\mathbb{X}$ are the same in the columns $\mathbb{X}^2\mathbb{Y}$, $\mathbb{Y}\mathbb{X}^2$ and the columns $\mathbb{X}\mathbb{Y}^2$, $\mathbb{Y}^2\mathbb{X}$.*

Finally we give the proof of Proposition 4.11 (1).

*Proof of Proposition 4.11 (1).* By Proposition 4.6 the columns $\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}\mathbb{Y}$ of $\mathcal{M}_2$ are linearly independent. By Lemma 4.13 there are three cases to consider.

**Case 1: The set $\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}\mathbb{Y}, \mathbb{Y}\mathbb{X}\}$ is the basis for $\mathcal{C}_{\mathcal{M}_2}$ and the columns $\mathbb{X}^2, \mathbb{Y}^2$ belong to the $\operatorname{span}\{\mathbb{1}, \mathbb{X}, \mathbb{Y}\}$.**

By assumption there are constants $a_j, b_j, c_j \in \mathbb{R}$ for $j = 1, 2$ such that

$$\mathbb{X}^2 = a_1\mathbb{1} + b_1\mathbb{X} + c_1\mathbb{Y} \quad \text{and} \quad \mathbb{Y}^2 = a_2\mathbb{1} + b_2\mathbb{X} + c_2\mathbb{Y}.$$

By multiplying the first relation with $\mathbb{X}$ and the second with $\mathbb{Y}$ it follows that if $\beta$ admits an nc measure, then $c_1 = b_2 = 0$. Let

$$\phi_1(X, Y) = \Big(X - \frac{b_1}{2}, Y - \frac{c_3}{2}\Big), \quad \phi_2(X, Y) = \Big(\frac{X}{\sqrt{a_1 + \frac{b_1^2}{4}}}, \frac{Y}{\sqrt{a_3 + \frac{c_3^2}{4}}}\Big).$$

Applying an affine linear transformation $\phi_2 \circ \phi_1$ to $\beta$ we get $\widetilde{\beta}$ with $\widetilde{\mathcal{M}_2}$ satisfying

$$\mathbb{X}^2 = \mathbb{Y}^2 = \mathbb{1}.$$

Equivalently, the relations are

$$\mathbb{Y}^2 - \mathbb{X}^2 = \mathbf{0}, \quad \mathbb{Y}^2 = \mathbb{1}.$$

Finally applying an affine linear transformation $\phi_3(X, Y) = (\frac{X+Y}{2}, \frac{Y-X}{2})$ to $\widetilde{\beta}$ we get $\widehat{\beta}$ with $\widehat{\mathcal{M}_2}$ satisfying

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}, \quad \mathbb{X}^2 + \mathbb{Y}^2 = \mathbb{1}.$$

Hence we are in a basic case 1 of Proposition 4.11.

**Case 2: The set $\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}^2, \mathbb{X}\mathbb{Y}\}$ is the basis for $\mathcal{C}_{\mathcal{M}_2}$.**

By assumption there are constants $a_j, b_j, c_j, d_j, e_j \in \mathbb{R}$ for $j = 1, 2$ such that

$$\mathbb{Y}\mathbb{X} = a_1\mathbb{1} + b_1\mathbb{X} + c_1\mathbb{Y} + d_1\mathbb{X}^2 + e_1\mathbb{X}\mathbb{Y}, \quad \mathbb{Y}^2 = a_2\mathbb{1} + b_2\mathbb{X} + c_2\mathbb{Y} + d_2\mathbb{X}^2 + e_2\mathbb{X}\mathbb{Y}.$$

By comparing the rows $\mathbb{X}\mathbb{Y}, \mathbb{Y}\mathbb{X}$ of the both sides of equations we conclude that $e_1 = -1$ and $e_2 = 0$, so that the relation are

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_1\mathbb{1} + b_1\mathbb{X} + c_1\mathbb{Y} + d_1\mathbb{X}^2 \quad \text{and} \quad \mathbb{Y}^2 = a_2\mathbb{1} + b_2\mathbb{X} + c_2\mathbb{Y} + d_2\mathbb{X}^2. \tag{4.13}$$

By Lemma 4.12 there exists an affine linear transformation $\phi_4$ of the form (4.7) such that after applying $\phi_4$ to $\beta$ the second relation in (4.13) of the corresponding matrix $\overline{\mathcal{M}_2}$ becomes one of the following:

$$\mathbb{Y}^2 = \mathbb{1} \quad \text{or} \quad \mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2 \quad \text{or} \quad \mathbb{Y}^2 = \mathbb{X}^2 \quad \text{or} \quad \mathbb{Y}^2 = \mathbb{1} + \mathbb{X}^2, \tag{4.14}$$

while the first relation in (4.13) becomes

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_3\mathbb{1} + b_3\mathbb{X} + c_3\mathbb{Y} + d_3\mathbb{X}^2, \tag{4.15}$$

where $a_3, b_3, c_3, d_3 \in \mathbb{R}$. We separate four possibilities according to the relation in (4.14).

**Case 2.1:** $\mathbb{Y}^2 = \mathbb{1}$ **in (4.14).** The relation (4.15) can be rewritten in the form

$$\mathbb{Y}\big(\mathbb{X} - \frac{c_3}{2}\big) + \big(\mathbb{X} - \frac{c_3}{2}\big)\mathbb{Y} = a_3\mathbb{1} + b_3\mathbb{X} + d_3\mathbb{X}^2.$$

Applying an affine linear transformation $\phi_5(X, Y) = (X - \frac{c_3}{2}, Y)$ to $\overline{\beta}$ we get $\breve{\beta}$ with $\breve{\mathcal{M}}_2$ satisfying

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_4\mathbb{1} + b_4\mathbb{X} + d_4\mathbb{X}^2 \quad \text{and} \quad \mathbb{Y}^2 = \mathbb{1}, \tag{4.16}$$

where $a_4, b_4, d_4 \in \mathbb{R}$. Multiplying the first relation in (4.16) with $\mathbb{X}$ on left (resp. right) we get

$$\mathbb{X}^2\mathbb{Y} + \mathbb{X}\mathbb{Y}\mathbb{X} = a_4\mathbb{X} + b_4\mathbb{X}^2 + d_4\mathbb{X}^3 = \mathbb{X}\mathbb{Y}\mathbb{X} + \mathbb{Y}\mathbb{X}^2.$$

Hence, $\mathbb{X}^2\mathbb{Y} = \mathbb{Y}\mathbb{X}^2$. Multiplying the first relation in (4.16) with $\mathbb{Y}$ on right and using the second relation in (4.16), we get

$$\mathbb{X} + \mathbb{Y}\mathbb{X}\mathbb{Y} = a_4\mathbb{Y} + b_4\mathbb{X}\mathbb{Y} + d_4\mathbb{X}^2\mathbb{Y}. \tag{4.17}$$

Comparing the rows $\mathbb{X}\mathbb{Y}$, $\mathbb{Y}\mathbb{X}$ on both sides of (4.17) gives $b_4 = 0$. We now separate two possibilities depending on $d_4$.

**Case 2.1.1:** $d_4 = 0$ **in (4.16).** The relations (4.16) are

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_4\mathbb{1}, \quad \mathbb{Y}^2 = \mathbb{1}.$$

Using the second relation we can rewrite the first relation in the form

$$\big(\mathbb{X} - \frac{a_4}{2}\mathbb{Y}\big)\mathbb{Y} + \mathbb{Y}\big(\mathbb{X} - \frac{a_4}{2}\mathbb{Y}\big) = \mathbf{0}.$$

Applying an affine linear transformation $\phi_6(\mathbb{X}, \mathbb{Y}) = (x - \frac{a_4}{2}y, y)$ to $\breve{\beta}$ we get $\widehat{\beta}$ with $\widehat{\mathcal{M}_2}$ satisfying

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}, \quad \mathbb{Y}^2 = \mathbb{1}.$$

Hence we are in the basic case 2 of Proposition 4.11 (1).

**Case 2.1.2: $d_4 \neq 0$ in (4.16).** The relations (4.16) are

$$\mathbb{X}^2 - \frac{1}{d_4}(\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X}) = -\frac{a_4}{d_4}\mathbb{1} \quad \text{and} \quad \mathbb{Y}^2 = \mathbb{1}.$$

Summing together the first relation and the second relation multiplied by $\frac{1}{d_4^2}$ we get

$$\frac{1}{d_4^2}\mathbb{Y}^2 - \frac{1}{d_4}(\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X}) + \mathbb{X}^2 = \big(\frac{1}{d_4^2} - \frac{a_4}{d_4}\big)\mathbb{1}. \tag{4.18}$$

Now we rewrite (4.18) in the form

$$\big(\frac{1}{d_4}\mathbb{Y} - \mathbb{X}\big)^2 = \big(\frac{1}{d_4^2} - \frac{a_4}{d_4}\big)\mathbb{1}.$$

Applying an affine linear transformation $\phi_7(X,Y) = \big(\frac{1}{d_4}y - X, Y\big)$ to $\breve{\beta}$ we get $\acute{\beta}$ with $\acute{\mathcal{M}}_2$ satisfying

$$\mathbb{X}^2 = \big(\frac{1}{d_4^2} - \frac{a_4}{d_4}\big)\mathbb{1} \quad \text{and} \quad \mathbb{Y}^2 = \mathbb{1}.$$

Hence we are in Case 1.

**Case 2.2: $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$ in (4.14).** Multiplying the relation (4.15) from the left by $\mathbb{X}$ (resp. $\mathbb{Y}$) and comparing the rows $\mathbb{X}\mathbb{Y}$, $\mathbb{Y}\mathbb{X}$ on both sides using Lemma 4.15 we conclude that $c_3 = 0$ (resp. $b_3 = 0$). Thus the relation of $\overline{\mathcal{M}_2}$ are

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_3\mathbb{1} + d_3\mathbb{X}^2 \quad \text{and} \quad \mathbb{Y}^2 + \mathbb{X}^2 = \mathbb{1}.$$

Summing together the first relation and the second relation multiplied by $\alpha$ we get

$$\alpha\mathbb{Y}^2 + (\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X}) + (\alpha - d_3)\mathbb{X}^2 = (\alpha + a_3)\mathbb{1}. \tag{4.19}$$

Choosing

$$\alpha = \frac{1}{2}\sqrt{4 + d_3^2} + \frac{d_3}{2},$$

we see that

$$\alpha > 0, \quad \alpha - d_3 > 0 \quad \text{and} \quad \sqrt{(\alpha - d_3)\alpha} = 1,$$

and thus (4.19) can be rewritten in the form

$$(\sqrt{\alpha - d_3}\mathbb{X} + \sqrt{\alpha}\mathbb{Y})^2 = (\alpha + a_3)\mathbb{1}.$$

Applying an affine linear transformation $\phi_8(X,Y) = (X, \sqrt{\alpha - d_3}X + \sqrt{\alpha}Y)$ to $\overline{\beta}$ we get $\widehat{\beta}$ with $\widehat{\mathcal{M}_2}$ satisfying

$$\mathbb{Y}^2 = (\alpha + a_3)\mathbb{1} \quad \text{and} \quad \mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_4\mathbb{1} + d_4\mathbb{X}^2, \tag{4.20}$$

where $a_4, d_4 \in \mathbb{R}$. Since $\widehat{\mathcal{M}_2}$ is positive semi-definite of rank 5, $\alpha + a_3 > 0$ and after normalization the relations (4.20) become

$$\mathbb{Y}^2 = \mathbb{1} \quad \text{and} \quad \mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_5\mathbb{1} + d_5\mathbb{X}^2,$$

where $a_5, d_5 \in \mathbb{R}$. Hence we are in Case 2.1.

**Case 2.3: $\mathbb{Y}^2 = \mathbb{X}^2$ in (4.14).** As in the first paragraph of Case 2.2 we conclude that the relations of $\overline{\mathcal{M}_2}$ are

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_3\mathbb{1} + d_3\mathbb{X}^2 \quad \text{and} \quad \mathbb{Y}^2 = \mathbb{X}^2.$$

Applying an affine linear transformation $\phi_9(X,Y) = (X+Y, Y-X)$ to $\overline{\beta}$ we get $\widetilde{\beta}$ with $\widetilde{\mathcal{M}_2}$ satisfying

$$(2-d_3)\mathbb{X}^2 - (2+d_3)\mathbb{Y}^2 = 4a_3\mathbb{1} \quad \text{and} \quad \mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}, \quad .$$

If $d_3 = 2$, then after normalization we come into Case 2.1. If $d_3 = -2$, then we come into Case 2.1 after we apply a transformation $(X,Y) \mapsto (Y,X)$ to change the roles of $\mathbb{X}$ and $\mathbb{Y}$ and normalize. Otherwise we apply an affine linear transformation

$$\phi_{10}(X,Y) = (\sqrt{|2-d_3|}X, \sqrt{|2+d_3|}Y)$$

to $\widetilde{\beta}$ and get $\breve{\beta}$ with $\breve{\mathcal{M}}_2$ satisfying

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}$$

and one of the following:

$$\mathbb{X}^2 + \mathbb{Y}^2 = 4a_3\mathbb{1} \quad \text{or} \quad \mathbb{X}^2 - \mathbb{Y}^2 = 4a_3\mathbb{1} \quad \text{or} \quad -\mathbb{X}^2 - \mathbb{Y}^2 = 4a_3\mathbb{1}. \tag{4.21}$$

The first and the last cases are equivalent, since the third relation can be rewritten as $\mathbb{X}^2+\mathbb{Y}^2 = -4a_3\mathbb{1}$. Thus we separate two possibilities in (4.21).

**Case 2.3.1: $\mathbb{X}^2 + \mathbb{Y}^2 = 4a_3\mathbb{1}$ in (4.21).** It is easy to see that $a_3 > 0$ (by $\breve{\mathcal{M}}_2$ being positive semi-definite of rank 5, since otherwise $\beta_{Y^2} = \beta_{X^2Y^2} = \beta_{Y^4} = 0$). Thus after the normalization we are in the basic case 1 of Proposition 4.11.

**Case 2.3.2: $\mathbb{X}^2 - \mathbb{Y}^2 = 4a_3\mathbb{1}$ in (4.21).** We may assume that $a_3 \leq 0$ (otherwise we change the roles of $\mathbb{X}$ and $\mathbb{Y}$). If $a_3 < 0$, then after normalization we come into the basic case 3. Otherwise $a_3 = 0$ and we are in the basic case 4.

**Case 2.4: $\mathbb{Y}^2 = \mathbb{1} + \mathbb{X}^2$ in (4.14).** As in the first paragraph of Case 2.2 we conclude that the relations of $\overline{\mathcal{M}_2}$ are

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a_3\mathbb{1} + d_3\mathbb{X}^2 \quad \text{and} \quad \mathbb{Y}^2 = \mathbb{1} + \mathbb{X}^2,$$

and after applying an affine linear transformation $\phi_9(X,Y) = (X+Y, Y-X)$ to $\overline{\beta}$ to get $\breve{\beta}$ with $\breve{\mathcal{M}}_2$ satisfying

$$(2-d_3)\mathbb{X}^2 - (2+d_3)\mathbb{Y}^2 = (4a_3 - 2d_3)\mathbb{1} \quad \text{and} \quad \mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = 2 \cdot \mathbb{1}.$$

If $d_3 = 2$, then after normalization we come into Case 2.1. If $d_3 = -2$ then we come into Case 2.1 after we apply a transformation $(X,Y) \mapsto (Y,X)$ to change the roles of $\mathbb{X}$ and $\mathbb{Y}$ and normalize. Otherwise we apply an affine linear transformation

$$\phi_{11}(X,Y) = (\sqrt{|2-d_3|}X, \sqrt{|2+d_3|}Y)$$

to $\breve{\beta}$ and get $\acute{\beta}$ with $\acute{\mathcal{M}}_2$ satisfying

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = 2\sqrt{|(4-d_3^2|}\mathbb{1}$$

and one of the following

$$\mathbb{X}^2 + \mathbb{Y}^2 = \tilde{a}\mathbb{1} \quad \text{or} \quad \mathbb{X}^2 - \mathbb{Y}^2 = \tilde{a}\mathbb{1} \quad \text{or} \quad -\mathbb{X}^2 - \mathbb{Y}^2 = \tilde{a}\mathbb{1}, \tag{4.22}$$

where $\tilde{a} = 4a_3 - 2d_3$. The first and the last cases are equivalent, since the third relation can be rewritten as $\mathbb{X}^2 + \mathbb{Y}^2 = -\tilde{a}\mathbb{1}$. Thus we separate two possibilities in (4.22).

**Case 2.4.1:** $\mathbb{X}^2 + \mathbb{Y}^2 = \tilde{a}\mathbb{1}$**.** It is easy to see that $\tilde{a} > 0$ (by $\acute{\mathcal{M}}_2$ being positive semi-definite of rank 5, since otherwise $\beta_{Y^2} = \beta_{X^2Y^2} = \beta_{Y^4} = 0$). Hence after normalization we come into Case 2.2.

**Case 2.4.2:** $\mathbb{Y}^2 - \mathbb{X}^2 = \tilde{a}\mathbb{1}$**.** We may assume that $\tilde{a} \geq 0$ (otherwise we change the roles of $\mathbb{X}$ and $\mathbb{Y}$). If $\tilde{a} = 0$, we are in Case 2.3. Otherwise we apply a transformation

$$\phi_{12}(X,Y) = \Big(X, X - \frac{2\sqrt{|(4-d_3^2|}}{\tilde{a}}Y\Big)$$

to $\acute{\beta}$ and get $\widehat{\beta}$ with $\widehat{\mathcal{M}_2}$ satisfying

$$\mathbb{Y}^2 + \Big(1 - \frac{4(4-d_3^2)^2}{\tilde{a}^2}\Big)\mathbb{X}^2 = \mathbf{0} \quad \text{and} \quad \mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = -\tilde{a}\mathbb{1} + \tilde{a}\mathbb{X}^2.$$

It is easy to see that $1 - \frac{4(4-d_3^2)^2}{\tilde{a}^2} < 0$ (by $\widehat{\mathcal{M}_2}$ being positive semi-definite of rank 5, since otherwise $\beta_{Y^4} = \beta_{X^2Y^2} = \beta_{Y^2} = \beta_{X^2} = 0$) and after a further normalization of $\mathbb{X}$ the relations of the corresponding matrix $\widehat{\mathcal{M}_2}$ become

$$\mathbb{Y}^2 - \mathbb{X}^2 = \mathbf{0} \quad \text{and} \quad \mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = -\hat{a}\mathbb{1} - \hat{a}\mathbb{X}^2, \quad \text{for some } \hat{a} \in \mathbb{R}.$$

Hence we come into Case 2.3.

**Case 3: The set** $\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{Y}^2, \mathbb{Y}\mathbb{X}\}$ **is the basis for** $\mathcal{C}_{\mathcal{M}_2}$**.**

Applying an affine linear transformation $(X,Y) \mapsto (Y,X)$ we come into Case 2. □

Now we prove Proposition 4.11 (2).

*Proof of Proposition 4.11 (2).* By Lemma 4.14 we have to consider 2 different cases.

**Case 1: The set $\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}^2, \mathbb{X}\mathbb{Y}, \mathbb{Y}\mathbb{X}\}$ is the basis for $\mathcal{C}_{\mathcal{M}_2}$.**

By assumption there are constants $a_i$, $i = 1, \ldots, 6$, such that

$$\mathbb{Y}^2 = a_1\mathbb{1} + a_2\mathbb{X} + a_3\mathbb{Y} + a_4\mathbb{X}^2 + a_5\mathbb{X}\mathbb{Y} + a_6\mathbb{Y}\mathbb{X}.$$

By Lemma 4.12 the statement of Proposition 4.11 follows.

**Case 2: The set $\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}^2, \mathbb{X}\mathbb{Y}, \mathbb{Y}^2\}$ is the basis for $\mathcal{C}_{\mathcal{M}_2}$.**

By assumption there are constants $a_i$, $i = 1, \ldots, 6$, such that

$$\mathbb{Y}\mathbb{X} = a_1\mathbb{1} + a_2\mathbb{X} + a_3\mathbb{Y} + a_4\mathbb{X}^2 + a_5\mathbb{X}\mathbb{Y} + a_6\mathbb{Y}^2. \tag{4.23}$$

By comparing the rows $\mathbb{X}\mathbb{Y}$, $\mathbb{Y}\mathbb{X}$ of the both sides of equation we conclude that $a_5 = -1$. We separate two cases.

**Case 2.1:** $a_4 \neq 0$ **or** $a_6 \neq 0$**.** By symmetry we may assume that $a_6 \neq 0$. We rewrite the relation (4.23) as

$$\mathbb{Y}^2 = -\frac{a_1}{a_6}\mathbb{1} - \frac{a_2}{a_6}\mathbb{X} - \frac{a_3}{a_6}\mathbb{Y} - \frac{a_4}{a_6}\mathbb{X}^2 - \frac{a_5}{a_6}\mathbb{X}\mathbb{Y} + \frac{1}{a_6}\mathbb{Y}\mathbb{X}.$$

By Lemma 4.12 the statement of Proposition 4.11 follows.

**Case 2.2:** $a_4 = a_6 = 0$. We rewrite the relation (4.23) as

$$(\mathbb{X} + \mathbb{Y})\mathbb{Y} + \mathbb{Y}(\mathbb{X} + \mathbb{Y}) - 2\mathbb{Y}^2 = a_1\mathbb{1} + a_2(\mathbb{X} + \mathbb{Y}) + (a_3 - a_2)\mathbb{Y}.$$

Applying an affine linear transformation $\phi_1(X, Y) = (X + Y, Y)$ to $\beta$ we get $\widetilde{\beta}$ with $\widetilde{\mathcal{M}_2}$ satisfying

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} - 2\mathbb{Y}^2 = a_1\mathbb{1} + a_2\mathbb{X} + (a_3 - a_2)\mathbb{Y}.$$

By Lemma 4.12 the statement of Proposition 4.11 (2) follows. □

## 4.3 Atoms in the minimal measure of ranks 5 and 6

Every nc sequence $\beta \equiv \beta^{(4)}$ which admits an nc measure with $\mathcal{M}_2$ in one of the basic cases of rank 5 or one of the first three basic cases of rank 6 given by Proposition 4.11, admits a minimal measure with all the atoms of special form. This form is crucial in the analysis of each basic case.

The next result and its proof are due to Zalar, and are proved in Proposition 5.1 of our article [10].

**Proposition 4.16.** *Suppose an nc sequence $\beta \equiv \beta^{(4)}$ has a Hankel matrix $\mathcal{M}_2$ satisfying one* *of the column relations*

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0} \quad or \quad \mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2 \quad or \quad \mathbb{Y}^2 = \mathbb{1} + \mathbb{X}^2. \tag{4.24}$$

*If $\beta$ admits an nc measure, then the atoms are of the following two forms:*

1. $(x_i, y_i) \in \mathbb{R}^2$.

2. $(X_i, Y_i) \in (\mathbb{SR}^{2t_i \times 2t_i})^2$ *for some* $t_i \in \mathbb{N}$ *such that*

$$X_i = \begin{pmatrix} \gamma_i I_{t_i} & B_i \\ B_i^T & -\gamma_i I_{t_i} \end{pmatrix} \quad and \quad Y_i = \begin{pmatrix} \mu_i I_{t_i} & \mathbf{0} \\ \mathbf{0} & -\mu_i I_{t_i} \end{pmatrix}$$

*where $\gamma_i \geq 0$, $\mu_i > 0$ and $B_i$ are $t_i \times t_i$ matrices.*

*Proof.* Suppose $\mu$ is any nc measure representing $\beta$. By Theorem 4.5 every atom $(X_i, Y_i)$ in $\mu$ satisfies the relation (4.24).

**Claim 1:** We may assume that $X_iY_i + Y_iX_i$ and $Y_i$ are diagonal matrices.

Observe that $X_iY_i + Y_iX_i$ is symmetric and commutes with $Y_i$. Therefore after a orthogonal transformation we may assume that $X_iY_i + Y_iX_i$ and $Y_i$ are diagonal matrices.

**Claim 2:** We may assume that the atoms $(X_i, Y_i)$ of size greater than 1 are of the forms

$$X_i = \begin{pmatrix} D_{i1} & B_i \\ B_i^T & D_{i2} \end{pmatrix} \quad \text{and} \quad Y_i = \begin{pmatrix} \mu_i I_{n_{i1}} & \mathbf{0} \\ \mathbf{0} & -\mu_i I_{n_{i2}} \end{pmatrix}, \tag{4.25}$$

where $\mu_i > 0$, $n_{i1}, n_{i2} \in \mathbb{N}$, $D_{i1} \in \mathbb{R}^{n_{i1} \times n_{i1}}$ and $D_{i2} \in \mathbb{R}^{n_{i2} \times n_{i2}}$ are diagonal matrices and $B_i \in \mathbb{R}^{n_{i1} \times n_{i2}}$.

By an appropriate permutation we may assume that $Y_i$ is of the form

$$Y_i = \bigoplus_{j=1}^{\ell_i} \begin{pmatrix} \mu_j^{(i)} I_{n_{ij}} & \mathbf{0} \\ \mathbf{0} & -\mu_j^{(i)} I_{m_{ij}} \end{pmatrix} \bigoplus \mathbf{0}_{m \times m},$$

where $\ell_i, n_{ij}, m_{ij}, m \in \mathbb{N} \cup \{0\}$, $\mu_j^{(i)} > 0$ and $\mu_{j_1}^{(i)} \neq \mu_{j_2}^{(i)}$ for $j_1 \neq j_2$. Let

$$X_i = (X_{pr}^{(i)})_{pr}$$

be the corresponding block decomposition of $X_i$. Since $X_iY_i + Y_iX_i$ is diagonal, it follows that

1. for $1 \le p, r \le \ell_i$ and $p \ne r$ we have that

$$\begin{aligned}
[X_iY_i + Y_iX_i]_{2p-1,2r-1} &= (\mu_p^{(i)} + \mu_r^{(i)})X_{2p-1,2r-1}^{(i)} = \mathbf{0} \quad \Rightarrow \quad X_{2p-1,2r-1}^{(i)} = \mathbf{0},\\
[X_iY_i + Y_iX_i]_{2p-1,2r} &= (\mu_p^{(i)} - \mu_r^{(i)})X_{2p-1,2r}^{(i)} = \mathbf{0} \quad \Rightarrow \quad X_{2p-1,2r}^{(i)} = \mathbf{0},\\
[X_iY_i + Y_iX_i]_{2p,2r} &= -(\mu_p^{(i)} + \mu_r^{(i)})X_{2p,2r}^{(i)} = \mathbf{0} \quad \Rightarrow \quad X_{2p,2r}^{(i)} = \mathbf{0}.
\end{aligned}$$

2. for $1 \le p \le \ell_i$ we have that

$$\begin{aligned}
[X_iY_i + Y_iX_i]_{2p-1,2\ell_i+1} &= \mu_p^{(i)}X_{2p-1,2\ell_i+1}^{(i)} = \mathbf{0} \quad \Rightarrow \quad X_{2p-1,2\ell_i+1}^{(i)} = \mathbf{0},\\
[X_iY_i + Y_iX_i]_{2p,2\ell_i+1} &= -\mu_p^{(i)}X_{2p,2\ell_i+1}^{(i)} = \mathbf{0} \quad \Rightarrow \quad X_{2p,2\ell_i+1}^{(i)} = \mathbf{0},\\
[X_iY_i + Y_iX_i]_{2\ell_i+1,2p-1} &= \mu_p^{(i)}X_{2\ell_i+1,2p-1}^{(i)} = \mathbf{0} \quad \Rightarrow \quad X_{2\ell_i+1,2p-1}^{(i)} = \mathbf{0},\\
[X_iY_i + Y_iX_i]_{2\ell_i+1,2p} &= -\mu_p^{(i)}X_{2\ell_i+1,2p}^{(i)} = \mathbf{0} \quad \Rightarrow \quad X_{2\ell_i+1,2p}^{(i)} = \mathbf{0}.
\end{aligned}$$

3. for $1 \le p = r \le \ell_i$ we have that

$$\begin{aligned}
[X_iY_i + Y_iX_i]_{2p-1,2p-1} &= 2\mu_p^{(i)}X_{2p-1,2p-1}^{(i)} \text{ is diagonal} \quad \Rightarrow \quad X_{2p-1,2p-1}^{(i)} \text{ is diagonal},\\
[X_iY_i + Y_iX_i]_{2p,2p} &= -2\mu_p^{(i)}X_{2p,2p}^{(i)} \text{ is diagonal} \quad \Rightarrow \quad X_{2p,2p}^{(i)} \text{ is diagonal}.
\end{aligned}$$

So $X_i$ is of the form

$$X_i = \bigoplus_{j=1}^{\ell_i} \begin{pmatrix} X_{11}^{(ij)} & X_{12}^{(ij)} \\ (X_{12}^{(ij)})^T & X_{22}^{(ij)} \end{pmatrix} \bigoplus X_{\ell_i+1}^{(i)}.$$

Thus we can replace the atom $(X_i, Y_i)$ with the atoms of the form

$$\widetilde{X}_{ij} = \begin{pmatrix} X_{11}^{(ij)} & X_{12}^{(ij)} \\ (X_{12}^{(ij)})^T & X_{22}^{(kij)} \end{pmatrix} \quad \text{and} \quad \widetilde{Y}_{ij} = \begin{pmatrix} \mu_j^{(i)} I_{n_{ij}} & \mathbf{0} \\ \mathbf{0} & -\mu_j^{(i)} I_{m_{ij}} \end{pmatrix}, \tag{4.26}$$

or

$$\widetilde{X}_{ij} = X_{\ell_i+1}^{(i)} \quad \text{and} \quad \widetilde{Y}_{ij} = \mathbf{0}. \tag{4.27}$$

By orthogonal transformation the atom (4.27) can be replaced by the atom

$$\widehat{X}_{ij} = D_{\ell_i+1}^{(i)} \quad \text{and} \quad \widetilde{Y}_{ij} = \mathbf{0},$$

where $D_{\ell_i+1}^{(i)}$ is a diagonal matrix and further on by atoms of size 1 of the form $(x, 0)$, where $x$ runs over the diagonal of $D_{\ell_i+1}^{(i)}$. Hence we may assume that the atoms of size greater than 1 in the representing measure for $\beta$ are of the form (4.26). Furthermore, by appropriate orthogonal transformation we may assume that they are of the form (4.25). This proves the claim.

**Claim 3:** We may assume that the atoms $(X_i, Y_i)$ of size greater than 1 are of the forms

$$X_i = \begin{pmatrix} \gamma_i I_{t_i} & B_i \\ B_i^T & -\gamma_i I_{t_i} \end{pmatrix} \quad \text{and} \quad Y_i = \begin{pmatrix} \mu_i I_{t_i} & \mathbf{0} \\ \mathbf{0} & -\mu_i I_{t_i} \end{pmatrix},$$

where $\gamma_i \geq 0$, $\mu_i > 0$ and $B_i$ are $t_i \times t_i$ matrices for some $t_i \in \mathbb{N}$.

First we prove Claim 3 in case we have $\mathbb{XY} + \mathbb{YX} = \mathbf{0}$ in (4.24). Let us prove that we may assume invertibility of $X_i$. After applying an orthogonal transformation to $(X_i, Y_i)$ we have $X_i = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \widehat{X}_i \end{pmatrix}$ where $\widehat{X}$ is invertible and $Y_i = \begin{pmatrix} Y_{i1} & Y_{i2} \\ Y_{i2}^t & Y_{i3} \end{pmatrix}$. From $X_iY_i + Y_iX_i = \mathbf{0}$ it follows that $Y_{i2}\widehat{X}_i = \mathbf{0}$. Since $\widehat{X}_i$ is invertible, $Y_{i2} = \mathbf{0}$. Hence we can replace the atom $(X_i, Y_i)$ with the atoms $(\mathbf{0}, Y_{i1})$ and $(\widehat{X}_i, Y_{i3})$. Since the atom $(\mathbf{0}, Y_{i1})$ can be further replaced with the atoms of size 1, we may assume the $X_i$ is invertible.

Observe that in (3) from the proof of Claim 2 we have

$$\begin{aligned} \mathbf{0} = [X_iY_i + Y_iX_i]_{2p-1,2p-1} = 2\mu_p^{(i)} X_{2p-1,2p-1}^{(i)} \quad &\Rightarrow \quad X_{2p-1,2p-1}^{(i)} = \mathbf{0}, \\ \mathbf{0} = [X_iY_i + Y_iX_i]_{2p,2p} = -2\mu_p^{(i)} X_{2p,2p}^{(i)} \quad &\Rightarrow \quad X_{2p,2p}^{(i)} = \mathbf{0}. \end{aligned}$$

Therefore $X_i$ in (4.25) is of the form $X_i = \begin{pmatrix} \mathbf{0} & B_i \\ B_i^T & \mathbf{0} \end{pmatrix}$ with $B_i \in \mathbb{R}^{n_{i1} \times n_{i2}}$ and $n_{i1} = n_{i2}$ by the invertibility of $X_i$. This proves Claim 3 in case we have $\mathbb{XY} + \mathbb{YX} = \mathbf{0}$ in (4.24).

It remains to prove Claim 3 in case we have $\mathbb{Y}^2 = \mathbb{1} \pm \mathbb{X}^2$ in (4.24). By Claim 2 and after an appropriate permutation we may assume that $X_i$, $Y_i$ are of the form (4.25) with

$$D_{i1} = \bigoplus_{j=1}^{p_i} \lambda_j^{(i)} I_{s_{ij}} \quad \text{and} \quad D_{i2} = \bigoplus_{j=1}^{r_i} \gamma_j^{(i)} I_{v_{ij}},$$

where $p_i, s_{ij}, r_i, v_{ij} \in \mathbb{N}$ and

$$\lambda_1^{(i)} > \lambda_2^{(i)} > \ldots > \lambda_{p_i}^{(i)} \quad \text{and} \quad \gamma_1^{(i)} > \gamma_2^{(i)} > \ldots > \gamma_{r_i}^{(i)}.$$

Let

$$B_i = (B_{pr}^{(i)})_{pr}$$

be the corresponding block decomposition of $B_i$, where

$$B_{pr}^{(i)} \in \mathbb{R}^{s_{ip} \times v_{ri}}$$

for $p = 1, \ldots, p_i$, $r = 1, \ldots, r_i$. Calculating $X_i^2$ we get that

$$X_i^2 = \begin{pmatrix} D_{i1}^2 + B_iB_i^T & D_{i1}B_i + B_i^TD_{i2} \\ B_i^TD_{i1} + D_{i2}B_i & B_i^TB_i + D_{i2}^2 \end{pmatrix}.$$

Since $X_i^2$ is a diagonal matrix, we conclude that

$$D_{i1}B_i + B_i^TD_{i2} = \mathbf{0}.$$

Thus

$$[D_{i1}B_i + B_i^TD_{i2}]_{pr} = (\lambda_p^{(i)} + \gamma_r^{(i)})B_{pr}^{(i)} = \mathbf{0},$$

for $1 \le p \le p_i$, $1 \le r \le r_i$. We conclude that

$$\lambda_p^{(i)} = -\gamma_r^{(i)} \quad \text{or} \quad B_{pr}^{(i)} = \mathbf{0}.$$

So in every row and every column in the block decomposition of $B_i$ at most one block $B_{pr}^{(i)}$ is possibly non-zero, i.e., $B_{pr}^{(i)}$ may be non-zero if and only if $\lambda_p^{(i)} = -\gamma_r^{(i)}$ So after a suitable permutation $X_i$ has the following block decomposition

$$X_i = \bigoplus_{\substack{1\le p\le p_i\\ 1\le r\le r_i\\ \lambda_p^{(i)}+\gamma_r^{(i)}=0}} \begin{pmatrix} \lambda_p^{(i)} I_{s_{ip}} & B_{pr}^{(i)} \\ (B_{pr}^{(i)})^T & \gamma_r^{(i)} I_{v_{ir}} \end{pmatrix} \bigoplus \bigoplus_{\substack{1\le p\le p_k\\ \lambda_p^{(i)}\neq-\gamma_r^{(i)}\ \forall r}} \left(\lambda_p^{(i)} I_{s_{ip}}\right)$$
$$\bigoplus \bigoplus_{\substack{1\le r\le r_k\\ \lambda_p^{(i)}\neq-\gamma_r^{(i)}\ \forall p}} \left(\gamma_r^{(i)} I_{v_{ir}}\right).$$

The corresponding block decomposition of $Y_i$ is of the form

$$Y_i = \bigoplus_{\substack{1\le p\le p_i\\ 1\le r\le r_i\\ \lambda_p^{(i)}+\gamma_r^{(i)}=0}} \begin{pmatrix} \mu_i I_{s_{ip}} & 0 \\ 0 & -\mu_i I_{v_{ir}} \end{pmatrix} \bigoplus \bigoplus_{\substack{1\le p\le p_k\\ \lambda_p^{(i)}\neq-\gamma_r^{(i)}\ \forall r}} \left(\mu_i I_{s_{ip}}\right)$$
$$\bigoplus \bigoplus_{\substack{1\le r\le r_k\\ \lambda_p^{(i)}\neq-\gamma_r^{(i)}\ \forall p}} \left(-\mu_i I_{v_{ir}}\right).$$

Thus we can replace the atom $(X_i, Y_i)$ with the atoms of the form

$$\widetilde{X}_{ij} = \begin{pmatrix} \lambda_p^{(i)} I_{s_{ip}} & B_{pr}^{(i)} \\ (B_{pr}^{(i)})^T & -\lambda_p^{(i)} I_{v_{ir}} \end{pmatrix} \quad \text{and} \quad \widetilde{Y}_{ij} = \begin{pmatrix} \mu_i I_{s_{ip}} & 0 \\ 0 & -\mu_i I_{v_{ir}} \end{pmatrix} \tag{4.28}$$

or

$$\widetilde{X}_{ij} = \lambda_p^{(i)} \quad \text{and} \quad \widetilde{Y}_{ij} = \mu_i$$

or

$$\widetilde{X}_{ij} = \gamma_r^{(i)} \quad \text{and} \quad \widetilde{Y}_{ij} = -\mu_i.$$

Hence we may assume that the atoms $(X_i, Y_i)$ of size greater than 1 in the representing measure for $\mathcal{M}_2$ are of the form (4.28). Now

$$X_i^2 = \begin{pmatrix} (\lambda_p^{(i)})^2 I_{s_{ip}} + B_{pr}^{(i)}(B_{pr}^{(i)})^T & \mathbf{0} \\ \mathbf{0} & (B_{pr}^{(i)})^T B_{pr}^{(i)} + (\lambda_p^{(i)})^2 I_{v_{ir}} \end{pmatrix}$$

Since

$$X_i^2 = \mathbb{1} \pm Y_i^2 = \begin{pmatrix} (1 \pm \mu_i^2) I_{s_{ip}} & \mathbf{0} \\ \mathbf{0} & (1 \pm \mu_i^2) I_{v_{ir}} \end{pmatrix},$$

it follows that

$$B_{pr}^{(i)}(B_{pr}^{(i)})^T = (1 \pm \mu_i^2 - (\lambda_p^{(i)})^2)I_{s_{ip}} \tag{4.29}$$
$$(B_{pr}^{(i)})^T B_{pr}^{(i)} = (1 \pm \mu_i^2 - (\lambda_p^{(i)})^2)I_{v_{ir}}. \tag{4.30}$$

We separate two cases according to the value of $1 \pm \mu_i^2 - (\lambda_p^{(i)})$.

**Case 1:** $1 \pm \mu_i^2 - (\lambda_p^{(i)}) = 0$**.**

It follows that $B_{pr}^{(i)} = \mathbf{0}$. Then $X_i$ is diagonal and commutes with $Y_i$. Therefore the atom $(X_i, Y_i)$ can be replaced by the atoms $(\lambda_p^{(i)}, \mu_i)$ and $(-\lambda_p^{(i)}, -\mu_i)$.

**Case 2:** $1 \pm \mu_i^2 - (\lambda_p^{(i)}) \neq 0$**.**

From (4.29) and (4.30) it follows that

$$s_{ip} = \operatorname{rank}(B_{pr}^{(i)}(B_{pr}^{(i)})^T) \leq \min(\operatorname{rank}(B_{pr}^{(i)}), \operatorname{rank}((B_{pr}^{(i)})^T)) \leq \min(s_{ip}, v_{ir}) \tag{4.31}$$
$$v_{ir} = \operatorname{rank}((B_{pr}^{(i)})^T B_{pr}^{(i)}) \leq \min(\operatorname{rank}((B_{pr}^{(i)})^T), \operatorname{rank}(B_{pr}^{(i)})) \leq \min(v_{ir}, s_{ip}). \tag{4.32}$$

It follows from (4.31) and (4.32) that $s_{ip} = v_{ir}$ in (4.28) which proves Claim 3 and concludes the proof of Proposition 4.16. □

## 4.4 $\mathcal{M}_2$ in the basic cases 1 and 2 of rank 6

In this section we solve the bivariate quartic tracial moment problem for $\mathcal{M}_2$ in the basic cases 1 and 2 of rank 6 given by Proposition 4.11. In Subsections 4.4.1 and 4.4.2 each case is presented separately, characterizing when $\mathcal{M}_2$ admits an nc measure, see Theorems 4.21 and 4.24. Corollaries 4.22 and 4.25 translate the existence of an nc measure into the feasibility problem of three linear matrix inequalities and a rank condition from Theorem 4.10.

The following proposition states that if $\beta$ has a Hankel matrix $\mathcal{M}_2$ of rank 6 in the basic cases 1, 2 or 3 given by Proposition 4.11 (2) and $\beta$ admits an nc measure, then it has a representing measure with the atoms of size at most 2.

The following three propositions are due to Zalar and were proved in Proposition 7.1, 7.2 and 7.3 of our article [10].

**Proposition 4.17.** *Let us fix a basic case relation 1, 2 or 3 given by Proposition 4.11 (2) and denote it by $R$. If an nc sequence $\beta$ with a Hankel matrix $\mathcal{M}_2(\beta)$ of rank 6 satisfying $R$ admits an nc measure, then it admits an nc measure with atoms of size at most 2.*

The following two propositions say more about the minimal measure.

**Proposition 4.18.** *Let us fix a basic case relation 1, 2 or 3 given by Proposition 4.11 (2) and denote it by $R$. If a sequence $\beta$ with a Hankel matrix $\mathcal{M}_2$ satisfying $R$ admits an nc measure of type $(k, 1)$, then*

1. $2 \leq k \leq 5$ *if* $R$ *is equal to* $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$ *or* $\mathbb{Y}^2 = \mathbb{1} + \mathbb{X}^2$.

2. $2 \leq k \leq 6$ *if* $R$ *is equal to* $\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}$.

**Proposition 4.19.** *Let us fix a basic case relation 1 or 2 given by Proposition 4.11 (2) and denote it by $R$. If every sequence $\beta$ with $\beta_X = \beta_Y = \beta_{X^3} = \beta_{X^2Y} = \beta_Y^3 = 0$ and a Hankel matrix $\mathcal{M}_2(\beta)$ of rank 6 with column relation $R$, admits an nc measure with exactly one atom of size 2 and some atoms of size 1, then every sequence $\widetilde{\beta}$ which admits an nc measure and has a Hankel matrix $\widetilde{\mathcal{M}}_2$ of rank 6 with the column relation $R$, admits an nc measure with exactly one atom of size 2 and some atoms of size 1.*

### 4.4.1 Relation $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$.

In this subsection we present results for an nc sequence $\beta$ with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying the relation $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$. Theorem 4.21 characterizes when $\beta$ admits an nc measure. Corollary 4.22 shows that the existence of an nc measure is equivalent to the feasibility problem of three linear matrix inequalities (LMIs) and a rank condition from Theorem 4.10.

The form of $\mathcal{M}_2$ is given by the following, and was proven in Proposition 7.4 of our article [10].

**Proposition 4.20.** *Let $\beta \equiv \beta^{(4)}$ be an nc sequence with a Hankel matrix $\mathcal{M}_2$ satisfying the relation*

$$\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2. \tag{4.33}$$

*Then $\mathcal{M}_2$ is of the form*

$$\begin{pmatrix}
\beta_1 & \beta_X & \beta_Y & \beta_{X^2} & \beta_{XY} & \beta_{XY} & \beta_1 - \beta_{X^2} \\
\beta_X & \beta_{X^2} & \beta_{XY} & \beta_{X^3} & \beta_{X^2Y} & \beta_{X^2Y} & \beta_X - \beta_{X^3} \\
\beta_Y & \beta_{XY} & \beta_1 - \beta_{X^2} & \beta_{X^2Y} & \beta_X - \beta_{X^3} & \beta_X - \beta_{X^3} & \beta_Y - \beta_{X^2Y} \\
\beta_{X^2} & \beta_{X^3} & \beta_{X^2Y} & \beta_{X^4} & \beta_{X^3Y} & \beta_{X^3Y} & \beta_{X^2} - \beta_{X^4} \\
\beta_{XY} & \beta_{X^2Y} & \beta_X - \beta_{X^3} & \beta_{X^3Y} & \beta_{X^2} - \beta_{X^4} & \beta_{XYXY} & \beta_{XY} - \beta_{X^3Y} \\
\beta_{XY} & \beta_{X^2Y} & \beta_X - \beta_{X^3} & \beta_{X^3Y} & \beta_{XYXY} & \beta_{X^2} - \beta_{X^4} & \beta_{XY} - \beta_{X^3Y} \\
\beta_1 - \beta_{X^2} & \beta_X - \beta_{X^3} & \beta_Y - \beta_{X^2Y} & \beta_{X^2} - \beta_{X^4} & \beta_{XY} - \beta_{X^3Y} & \beta_{XY} - \beta_{X^3Y} & \beta_1 - 2\beta_{X^2} + \beta_{X^4}
\end{pmatrix}. \tag{4.34}$$

*Proof.* The relation (4.33) gives us the following system in $\mathcal{M}_2$

$$\begin{aligned}
\beta_{Y^2} &= \beta_1 - \beta_{X^2}, & \beta_{X^2Y^2} &= \beta_{X^2} - \beta_{X^4}, \\
\beta_{XY^2} &= \beta_X - \beta_{X^3}, & \beta_{XY^3} &= \beta_{XY} - \beta_{X^3Y}, \\
\beta_{Y^3} &= \beta_Y - \beta_{X^2Y}, & \beta_{Y^4} &= \beta_{Y^2} - \beta_{X^2Y^2}.
\end{aligned} \tag{4.35}$$

Plugging in the expressions for $\beta_{Y^2}$ and $\beta_{X^2Y^2}$ in the expression for $\beta_{Y^4}$ gives the form (4.34) of $\mathcal{M}_2$. □

The following theorem characterizes normalized nc sequences $\beta$ with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying the relation $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$, which admit an nc measure, and is proven in Theorem 7.5 of our article [10].

**Theorem 4.21.** *Suppose $\beta \equiv \beta^{(4)}$ is a normalized nc sequence with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying the relation $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$. Then $\beta$ admits an nc measure if and only if $\mathcal{M}_2$ is positive semi-definite and one of the following is true:*

*(1)* $\beta_X = \beta_Y = \beta_{X^3} = \beta_{X^2Y} = 0$. *Moreover, there exists an nc measure of type (4,1).*

*(2) There exist*

$$a_1 \in (0,1), \quad a_2 \in \left(-2\sqrt{a_1(1-a_1)}, 2\sqrt{a_1(1-a_1)}\right)$$

*such that*

$$M := \mathcal{M}_2 - \xi \mathcal{M}_2^{(X,Y)}$$

*is a positive semi-definite cm Hankel matrix satisfying* $\operatorname{rank}(M) \leq \operatorname{card}(\mathcal{V}_M)$, *where* $\mathcal{V}_M$ *is the variety associated to $M$ (as in Theorem 4.10),*

$$X = \begin{pmatrix} \sqrt{a_1} & 0 \\ 0 & -\sqrt{a_1} \end{pmatrix}, \quad Y = \sqrt{(1-a_1)} \begin{pmatrix} \frac{a}{2} & \frac{1}{2}\sqrt{4-a^2} \\ \frac{1}{2}\sqrt{4-a^2} & -\frac{a}{2} \end{pmatrix}, \tag{4.36}$$

$$a = \frac{a_2}{\sqrt{a_1(1-a_1)}},$$

*and $\xi > 0$ is the smallest positive number such that the rank of $\mathcal{M}_2 - \xi \mathcal{M}_2^{(X,Y)}$ is smaller than the rank of $\mathcal{M}_2$.*

*Proof.* We first consider the reverse implication. Suppose $\mathcal{M}_2$ is positive definite. If (2) holds it is easy to see from the solutions of the commutative moment problems, that $\beta$ admits a representing measure. Now suppose $\mathcal{M}_2$ is positive definite and (1) holds, we will show that $\beta$ admits a measure. Then by Proposition (4.20), $\mathcal{M}_2$ is of the form

$$\begin{pmatrix}
1 & 0 & 0 & \beta_{X^2} & \beta_{XY} & \beta_{XY} & 1-\beta_{X^2} \\
0 & \beta_{X^2} & \beta_{XY} & 0 & 0 & 0 & 0 \\
0 & \beta_{XY} & 1-\beta_{X^2} & 0 & 0 & 0 & 0 \\
\beta_{X^2} & 0 & 0 & \beta_{X^4} & \beta_{X^3Y} & \beta_{X^3Y} & \beta_{X^2}-\beta_{X^4} \\
\beta_{XY} & 0 & 0 & \beta_{X^3Y} & \beta_{X^2}-\beta_{X^4} & \beta_{XYXY} & \beta_{XY}-\beta_{X^3Y} \\
\beta_{XY} & 0 & 0 & \beta_{X^3Y} & \beta_{XYXY} & \beta_{X^2}-\beta_{X^4} & \beta_{XY}-\beta_{X^3Y} \\
1-\beta_{X^2} & 0 & 0 & \beta_{X^2}-\beta_{X^4} & \beta_{XY}-\beta_{X^3Y} & \beta_{XY}-\beta_{X^3Y} & 1-2\beta_{X^2}+\beta_{X^4}
\end{pmatrix}.$$

We define the matrix function

$$B(\alpha) := \mathcal{M}_2 - \alpha\big(\mathcal{M}_2^{(1,0)} + \mathcal{M}_2^{(-1,0)}\big),$$

where $\mathcal{M}_2^{(x,y)}$ are the moment matrices generated by the atom $(x,y)$.

We have that

$$B(\alpha) = \begin{pmatrix}
1-2\alpha & 0 & 0 & \beta_{X^2}-2\alpha & \beta_{XY} & \beta_{XY} & D \\
0 & \beta_{X^2}-\alpha & \beta_{XY} & 0 & 0 & 0 & 0 \\
0 & \beta_{XY} & D & 0 & 0 & 0 & 0 \\
\beta_{X^2}-2\alpha & 0 & 0 & \beta_{X^4}-2\alpha & \beta_{X^3Y} & \beta_{X^3Y} & C \\
\beta_{XY} & 0 & 0 & \beta_{X^3Y} & C & E & \beta_{XY}-\beta_{X^3Y} \\
\beta_{XY} & 0 & 0 & \beta_{X^3Y} & E & C & \beta_{XY}-\beta_{X^3Y} \\
D & 0 & 0 & C & \beta_{XY}-\beta_{X^3Y} & \beta_{XY}-\beta_{X^3Y} & D-C
\end{pmatrix},$$

where

$$C = \beta_{X^2} - \beta_{X^4}, \quad D = 1 - \beta_{X^2}, \quad E = \beta_{XYXY}.$$

We have that

$$\det\left([B(\alpha)]_{\{\mathbb{1},\mathbb{X},\mathbb{Y},\mathbb{X}^2,\mathbb{XY},\mathbb{YX}\}}\right) = JK(-F + 2\alpha G), \tag{4.37}$$

where

$$\begin{aligned}
J &= -(\beta_{XYXY} - \beta_{X^2} + \beta_{X^4}) \\
K &= (-\beta_{XY}^2 + \beta_{X^2} - \beta_{X^2}^2 + 2\alpha(-1 + \beta_X^2)) \\
F &= \beta_{XYXY}(\beta_{X^2}^2 - \beta_{X^4}) + \beta_{X^2}(\beta_{X^2}^2 - 4\beta_{XY}\beta_{X^3Y} - \beta_{X^4}(1 + \beta_{X^2})) \\
&\quad + 2\beta_{X^3Y}^2 + \beta_{X^4}(\beta_{X^4} + 2\beta_{XY}^2), \\
G &= 2\beta_{XY}(\beta_{XY} - 2\beta_{X^3Y}) + \beta_{XYXY}(2\beta_{X^2} - 1 - \beta_{X^4}) + \beta_{X^2}(2\beta_{X^2} - 1 - 3\beta_{X^4}) \\
&\quad + 2\beta_{X^3Y}^2 + \beta_{X^4}(1 + \beta_{X^4}).
\end{aligned}$$

Let $\alpha_0 > 0$ be the smallest positive number such that the rank of $B(\alpha_0)$ is smaller than 6. By (4.37) we get

$$\alpha_0 = \min\left(\frac{\beta_{XY}^2 - \beta_{X^2} + \beta_{X^2}^2}{2(-1 + \beta_{X^2})}, \frac{F}{2G}\right).$$

**Claim 1:** $\alpha_0 = \frac{F}{2G} < \alpha_1$.

Since

$$\begin{aligned}
\det\left([B(\alpha)]_{\{\mathbb{1},\mathbb{X}^2\}}\right) &= \beta_{X^4} - \beta_{X^2}^2 + 2\alpha(-1 + 2\beta_{X^2} - \beta_{X^4}), \\
\det\left([B(\alpha)]_{\{\mathbb{1},\mathbb{XY}\}}\right) &= C - \beta_{XY}^2 - 2\alpha \cdot C, \\
\det\left([B(\alpha)]_{\{\mathbb{1},\mathbb{XY},\mathbb{YX}\}}\right) &= (E - C)(-E - C + 2\beta_{X^2Y} + 2\alpha \cdot (E + C)),
\end{aligned}$$

the system

$$\det\left([B(\alpha_2)]_{\{\mathbb{1},\mathbb{X}^2\}}\right) = 0, \quad \det\left([B(\alpha_3)]_{\{\mathbb{1},\mathbb{XY}\}}\right) = 0, \quad \det\left([B(\alpha_4)]_{\{\mathbb{1},\mathbb{XY},\mathbb{YX}\}}\right) = 0$$

has a solution

$$\alpha_2 = \frac{\beta_{X^2}^2 - \beta_{X^4}}{2(-1 + 2\beta_{X^2} - \beta_{X^4})}, \quad \alpha_3 = \frac{-\beta_{XY}^2 + \beta_{X^2} - \beta_{X^4}}{2(\beta_{X^2} - \beta_{X^4})}, \quad \alpha_4 = \frac{-2\beta_{XY}^2 + \beta_{XYXY} + \beta_{X^2} - \beta_{X^4}}{2(\beta_{XYXY} + \beta_{X^2} - \beta_{X^4})}.$$

If $\alpha_1 \le \frac{F}{2G}$, then since $B(\alpha_1) \succeq 0$, it follows that $\alpha_1 \le \min(\alpha_2, \alpha_3, \alpha_4)$. Using *Mathematica*, the system

$$\alpha_1 \le \min(\alpha_2, \alpha_3, \alpha_4), \quad \det\left(\mathcal{M}_2|_{\{\mathbb{Y}\}}\right) > 0, \quad \det\left(\mathcal{M}_2|_{\{\mathbb{XY}\}}\right) > 0, \tag{4.38}$$

$$\det\left(\mathcal{M}_2|_{\{\mathbb{X},\mathbb{Y}\}}\right) > 0, \quad \det\left(\mathcal{M}_2|_{\{1,X^2\}}\right) > 0, \quad \det\left(\mathcal{M}_2|_{\{1,\mathbb{XY},\mathbb{YX}\}}\right) > 0, \tag{4.39}$$

does not have solutions (see https://github.com/Abhishek-B/TTMP for the Mathematica file, note that the Mathematica file pertains to Theorem 7.5 from [10]). Hence $\alpha_0 = \frac{F}{2G} < \alpha_1$.

Using *Mathematica* to calculate the kernel of $B(\frac{F}{2G})$ we conclude that $B(\frac{F}{2G})$ satisfies the relations

$$\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = a\mathbb{1} + d\mathbb{X}^2, \quad \mathbb{Y}^2 + \mathbb{X}^2 = \mathbb{1}$$

for some $a, d \in \mathbb{R}$. We also have

$$\beta_X^{(B)} = \beta_Y^{(B)} = \beta_{X^3}^{(B)} = \beta_{X^2Y}^{(B)} = \beta_{XY^2}^{(B)} = \beta_{Y^3}^{(B)} = 0,$$

where $\beta_{w(X,Y)}^{(B)}$ are the moments of $B(\frac{F}{2G})$. This is a special case in the proof of Proposition 4.11, i.e., Case 2.2. Following the proof we see that after using only transformations of type

$$(x, y) \mapsto (\alpha_1 x + \beta_1 y, \alpha_2 x + \beta_2 y)$$

for some $\alpha_1, \alpha_2, \beta_1, \beta_2 \in \mathbb{R}$, we come into the basic case 1 or 2 of rank 5 with $\widetilde{\beta}_X = \widetilde{\beta}_Y = \widetilde{\beta}_{X^3} = 0$. But every such sequence admits a measure of type (2,1) by Theorems 6.5 and 6.8 of [10]. Hence $\beta$ admits a measure of type $(4, 1)$.

Now we show the forward implication. Suppose that $\beta$ admits an nc measure, we will show that (2) holds. By Proposition 4.19 and Theorem 4.21 (1),

$$\mathcal{M}_2 = \sum_i \lambda_i \mathcal{M}^{(x_i,y_i)}(2) + \xi \mathcal{M}^{(X,Y)}(2), \tag{4.40}$$

where $(x_i, y_i) \in \mathbb{R}^2$, $(X, Y) \in (\mathbb{SR}^{2\times 2})^2$, $\lambda_i > 0$, $\xi > 0$ and $\sum_i \lambda_i + \xi = 1$. Therefore

$$\mathcal{M}_2 - \xi \mathcal{M}_2^{(X,Y)}$$

is a cm Hankel matrix satisfying the relations

$$\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2 \quad \text{and} \quad \mathbb{X}\mathbb{Y} = \mathbb{Y}\mathbb{X}.$$

By Theorem 4.10, $M$ admits a measure if and only if $M$ is psd and satisfies $\operatorname{rank} M \leq \operatorname{card} \mathcal{V}_M$. To conclude the proof it only remains to prove that $X, Y$ are of the form (4.36). $\mathcal{M}_2^{(X,Y)}$ is an nc Hankel matrix rank 4. Therefore the columns $\{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}\mathbb{Y}\}$ are linearly independent and hence

$$\mathbb{X}^2 = a_1\mathbb{1} + b_1\mathbb{X} + c_1\mathbb{Y} + d_1\mathbb{X}\mathbb{Y}, \quad \text{and} \quad \mathbb{Y}^2 = a_3\mathbb{1} + b_3\mathbb{X} + c_3\mathbb{Y} + d_3\mathbb{X}\mathbb{Y},$$

where $a_j, b_j, c_j, d_j \in \mathbb{R}$ for $j = 1, 3$. By Theorem 3.1 (1) of [10], $d_1 = d_3 = 0$. By Theorem 3.1 (3) of [10], $c_1 = b_3 = 0$. Since $\mathbb{X}^2 + \mathbb{Y}^2 = \mathbb{1}$ it follows that $b_1 = c_3 = 0$ and $a_3 = 1 - a_1$. By Theorem 3.1 (4), $X$ and $Y$ are of the form (4.36). □

As a consequence we can translate the bivariate quartic tracial moment problem for $\beta$ with $\mathcal{M}_2$ of rank 6 satisfying $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$ into the feasibility problem of some small linear matrix inequalities and a rank condition from Theorem 4.10. We proved this result in Corollary 7.6 of our article [10].

**Corollary 4.22.** *Suppose $\beta \equiv \beta^{(4)}$ is a normalized nc sequence with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying the relation $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$. Let $L(a,b,c,d,e)$ be the following linear matrix polynomial*

$$\begin{pmatrix} a & \beta_X & \beta_Y & b & c & c & a-b \\ \beta_X & b & c & \beta_{X^3} & \beta_{X^2Y} & \beta_{X^2Y} & \beta_X - \beta_{X^3} \\ \beta_Y & c & a-b & \beta_{X^2Y} & \beta_X - \beta_{X^3} & \beta_X - \beta_{X^3} & \beta_Y - \beta_{X^2Y} \\ b & \beta_{X^3} & \beta_{X^2Y} & d & e & e & b-d \\ c & \beta_{X^2Y} & \beta_X - \beta_{X^3} & e & b-d & b-d & c-e \\ c & \beta_{X^2Y} & \beta_X - \beta_{X^3} & e & b-d & b-d & c-e \\ a-b & \beta_X - \beta_{X^3} & \beta_Y - \beta_{X^2Y} & b-d & c-e & c-e & a-2b+d \end{pmatrix},$$

*where $a,b,c,d,e \in \mathbb{R}$. Then $\beta$ admits an nc measure if and only if there exist $a,b,c,d,e \in \mathbb{R}$ such that*

1. *$L(a,b,c,d,e) \succeq 0$,*
2. *$\mathcal{M}_2 - L(a,b,c,d,e) \succeq 0$,*
3. *$(\mathcal{M}_2 - L(a,b,c,d,e))_{\{\mathbb{1},\mathbb{X},\mathbb{Y},\mathbb{XY}\}} \succ 0$,*
4. *$\operatorname{rank}(L(a,b,c,d,e)) \leq \operatorname{card}(\mathcal{V}_L)$, where $\mathcal{V}_L$ is the variety associated to the Hankel matrix $L(a,b,c,d,e)$ (see Theorem 4.10).*

*Proof.* By Theorem 4.21, $\beta$ admits an nc measure if and only if

$$\mathcal{M}_2 = \sum_{i=1}^{k} \lambda_i \mathcal{M}_2^{(x_i,y_i)} + \xi \mathcal{M}_2^{(X,Y)}, \tag{4.41}$$

where $(x_i,y_i) \in \mathbb{R}^2$, $(X,Y) \in (\mathbb{SR}^{2\times 2})^2$, $\lambda_i > 0$, $\xi > 0$ and $\sum_i \lambda_i + \xi = 1$. By Corollary 3.2 of [10],

$$\beta_X^{(X,Y)} = \beta_Y^{(X,Y)} = \beta_{X^3}^{(X,Y)} = \beta_{X^2Y}^{(X,Y)} = \beta_{XY^2}^{(X,Y)} = \beta_{Y^3}^{(X,Y)} = 0, \tag{4.42}$$

where $\beta_{w(X,Y)}^{(X,Y)}$ are the moments of $\mathcal{M}_2^{(X,Y)}$. Using (4.41) and (4.42), we conclude that $\sum_i \lambda_i \mathcal{M}_2^{(x_i,y_i)}$ and $\xi \mathcal{M}_2^{(X,Y)}$ are of the forms

$$\begin{pmatrix} a & \beta_X & \beta_Y & b & c & c & a-b \\ \beta_X & b & c & \beta_{X^3} & \beta_{X^2Y} & \beta_{X^2Y} & \beta_X - \beta_{X^3} \\ \beta_Y & c & a-b & \beta_{X^2Y} & \beta_X - \beta_{X^3} & \beta_X - \beta_{X^3} & \beta_Y - \beta_{X^2Y} \\ b & \beta_{X^3} & \beta_{X^2Y} & d & e & e & b-d \\ c & \beta_{X^2Y} & \beta_X - \beta_{X^3} & e & b-d & b-d & c-e \\ c & \beta_{X^2Y} & \beta_X - \beta_{X^3} & e & b-d & b-d & c-e \\ a-b & \beta_X - \beta_{X^3} & \beta_Y - \beta_{X^2Y} & b-d & c-e & c-e & a-2b+d \end{pmatrix}, \tag{4.43}$$

$$\begin{pmatrix} 1-a & 0 & 0 & \beta_{X^2}-b & A_1(c) & A_1(c) & A_2(a,b) \\ 0 & \beta_{X^2}-b & A_1(c) & 0 & 0 & 0 & 0 \\ 0 & A_1(c) & A_2(a,b) & 0 & 0 & 0 & 0 \\ \beta_{X^2}-b & 0 & 0 & \beta_{X^4}-d & A_3(e) & A_3(e) & A_4(b,d) \\ A_1(c) & 0 & 0 & A_3(e) & A_4(b,d) & \beta_{XYXY}-(b-d) & A_5(c,e) \\ A_1(c) & 0 & 0 & A_3(e) & \beta_{XYXY}-(b-d) & A_4(b,d) & A_5(c,e) \\ A_2(a,b) & 0 & 0 & A_4(b,d) & A_5(c,e) & A_5(c,e) & A_6(a,b,d) \end{pmatrix}, \tag{4.44}$$

where

$$
\begin{aligned}
A_1(c) &= \beta_{XY} - c, \quad A_2(a,b) = 1 - \beta_{X^2} - (a-b),\\
A_3(e) &= \beta_{X^3Y} - e, \quad A_4(b,d) = \beta_{X^2} - \beta_{X^4} - (b-d),\\
A_5(c,e) &= \beta_{XY} - \beta_{X^3Y} - (c-e), \quad A_6(a,b,d) = 1 - 2\beta_{X^2} + \beta_{X^4} - (a-2b+d),
\end{aligned}
$$

for some $a,b,c,d,e \in \mathbb{R}$. Notice that the matrix (4.43) equals to $L(a,b,c,d,e)$ and the matrix (4.44) to $\mathcal{M}_2 - L(a,b,c,d,e)$. Since $L(a,b,c,d,e)$ is a cm Hankel matrix, it admits an nc measure by Theorem 4.10 if and only if (1) and (4) of Theorem 4.22 are true. Since $\mathcal{M}_2 - L(a,b,c,d,e)$ is an nc Hankel matrix satisfying $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$ and $\widetilde{\beta}_X = \widetilde{\beta}_Y = \widetilde{\beta}_{X^3} = \widetilde{\beta}_{X^2Y} = \widetilde{\beta}_{XY^2} = \widetilde{\beta}_{Y^3} = 0$, it admits an nc measure by the results of rank 4 and 5 cases and Theorem 4.21 (1) if and only if (2) and (3) of Theorem 4.22 are true. □

### 4.4.2 Relation $\mathbb{XY} + \mathbb{YX} = \mathbf{0}$.

In this subsection we present the results for an nc sequence $\beta \equiv \beta^{(4)}$ with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying the relation $\mathbb{XY} + \mathbb{YX} = \mathbf{0}$. Theorem 4.24 characterizes when $\beta$ admits an nc measure. Corollary 4.25 we show that the existence of an nc measure is equivalent to the feasibility problem of three linear matrix inequalities and a rank condition from Theorem 4.10. We omit the proofs as they are similar to the $\mathbb{Y}^2 = \mathbb{1} - \mathbb{X}^2$ case, and can be readily found in our article [10].

The form of $\mathcal{M}_2$ is given by the following, and is proven in Proposition 7.7 of our article [10].

**Proposition 4.23.** *Let $\beta \equiv \beta^{(4)}$ be an nc sequence with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying the relation*

$$\mathbb{XY} + \mathbb{YX} = \mathbf{0} \tag{4.45}$$

*Then $\mathcal{M}_2$ is of the form*

$$
\begin{pmatrix}
\beta_1 & \beta_X & \beta_Y & \beta_{X^2} & 0 & 0 & \beta_{Y^2}\\
\beta_X & \beta_{X^2} & 0 & \beta_{X^3} & 0 & 0 & 0\\
\beta_Y & 0 & \beta_{Y^2} & 0 & 0 & 0 & \beta_{Y^3}\\
\beta_{X^2} & \beta_{X^3} & 0 & \beta_{X^4} & 0 & 0 & \beta_{X^2Y^2}\\
0 & 0 & 0 & 0 & \beta_{X^2Y^2} & -\beta_{X^2Y^2} & 0\\
0 & 0 & 0 & 0 & -\beta_{X^2Y^2} & \beta_{X^2Y^2} & 0\\
\beta_{Y^2} & 0 & \beta_{Y^3} & \beta_{X^2Y^2} & 0 & 0 & \beta_{Y^4}
\end{pmatrix}. \tag{4.46}
$$

*Proof.* The relation (4.45) gives us the following system in $\mathcal{M}_2$

$$
\begin{aligned}
2\beta_{XY} &= 0, & \qquad 2\beta_{X^3Y} &= 0,\\
2\beta_{X^2Y} &= 0, & \qquad \beta_{X^2Y^2} + \beta_{XYXY} &= \beta_{XY},\\
2\beta_{XY^2} &= 0, & \qquad 2\beta_{XY^3} &= 0.
\end{aligned} \tag{4.47}
$$

Thus the solution of the system (4.47) is given by the statement of the proposition. □

The following theorem characterizes normalized sequences $\beta$ with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying $\mathbb{XY} + \mathbb{YX} = \mathbf{0}$, which admit an nc measure, and is proven in Theorem 7.8 of our article [10].

**Theorem 4.24.** *Suppose $\beta \equiv \beta^{(4)}$ is a normalized nc sequence with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying the relation $\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}$. Then $\beta$ admits an nc measure if and only if $\mathcal{M}_2$ is positive semi-definite and one of the following is true:*

1. $\beta_X = \beta_Y = \beta_{X^3} = \beta_{Y^3} = 0$. *There exists an nc measure of type (2,1) or (3,1).*
2. *There exist*
$$a_1 > 0, \quad a_3 > 0,$$
*such that*
$$M := \mathcal{M}_2 - \xi \mathcal{M}_2^{(X,Y)}$$
*is a positive semi-definite cm Hankel matrix satisfying* $\operatorname{rank}(M) \le \operatorname{card}(\mathcal{V}_M)$, *where* $\mathcal{V}_M$ *is the variety associated to* $M$ *(as in Theorem 4.10),*
$$X = \begin{pmatrix} \sqrt{a_1} & 0 \\ 0 & -\sqrt{a_1} \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & \sqrt{a_3} \\ \sqrt{a_3} & 0 \end{pmatrix} \tag{4.48}$$
*and* $\xi > 0$ *is the smallest positive number such that rank of* $\mathcal{M}_2 - \xi \mathcal{M}_2^{(X,Y)}$ *is smaller than the rank of* $\mathcal{M}_2$.

As a consequence we can translate the bivariate quartic tracial moment problem for $\beta$ with $\mathcal{M}_2$ of rank 6 satisying $\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}$ into the feasibility problem of some small linear matrix inequalities and a rank condition from Theorem 4.10. We proved this result in Corollary 7.9 of our article [10].

**Corollary 4.25.** *Suppose $\beta \equiv \beta^{(4)}$ is a normalized nc sequence with a Hankel matrix $\mathcal{M}_2$ of rank 6 satisfying the relation $\mathbb{X}\mathbb{Y} + \mathbb{Y}\mathbb{X} = \mathbf{0}$. Let us define a linear matrix polynomial*

$$L(a,b,c,d,e) = \begin{pmatrix} a & \beta_X & \beta_Y & b & 0 & 0 & c \\ \beta_X & b & 0 & \beta_{X^3} & 0 & 0 & 0 \\ \beta_Y & 0 & c & 0 & 0 & 0 & \beta_{Y^3} \\ b & \beta_{X^3} & 0 & d & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c & 0 & \beta_{Y^3} & 0 & 0 & 0 & e \end{pmatrix},$$

*where $a, b, c, d, e \in \mathbb{R}$. Then $\beta$ admits an nc measure if and only there exist*

$$a \in (0,1), \quad b \in (0, \beta_{X^2}), \quad c \in (0, \beta_{Y^2}), \quad d \in (0, \beta_{X^4}), \quad e \in (0, \beta_{Y^4}), \tag{4.49}$$

*such that*

1. $L(a,b,c,d,e) \succeq 0$,
2. $\mathcal{M}_2 - L(a,b,c,d,e) \succeq 0$,
3. $\operatorname{rank}(L(a,b,c,d,e)) \le \operatorname{card}(\mathcal{V}_L)$, *where $\mathcal{V}_L$ is the variety associated to the Hankel matrix $L(a,b,c,d,e)$ (see Theorem 4.10).*

Chapter 5

# The Moment Problem on Elliptic Curves

The characterization of the quartic moment problem (both classical and tracial) has been to a great extent successful for two reasons. Firstly, the problem maintains a manageable size, and so can be tackled via computational approaches. Secondly, because the representing measure is supported in a quadratic variety, and thanks to Hilbert's theorem (Theorem 2.6), positive linear functionals on quadratic varieties are well understood. In contrast, the solution to the moment problem on varieties of higher degree curves, for the most part, remains elusive.

For the classic moment problem, [33, 102, 103] investigate measures supported on special cubic varieties, while [38] completely characterizes the solutions with measures supported on the variety $y = x^3$. In this chapter we take the first steps to understanding the tracial moment problem when the representative measure is supported on cubic varieties.

We focus on the smooth cubics, namely the *elliptic* curves, which to the best of our knowledge have not been studied in association with the tracial moment problem (and not even in the classical moment problem). We refer to this class of problems (tracial and classical) as *the elliptic moment problem*.

This chapter is currently being prepared for joint publication with Zalar. Except where specifically indicated the results here are the author's work.

## 5.1 Tracial Sequences

We start by making precise what we mean by the elliptic moment problem. Suppose we have a truncated tracial sequence $\beta^{(2n)}$, and associated Hankel matrix $\mathcal{M}_n$. Suppose that $\mathcal{M}_n$ is positive semi-definite, recursively generated, and in $\mathcal{C}_{\mathcal{M}_n}$ we have the relation

$$\mathbb{Y}^2 = \mathbb{X}^3 + a\mathbb{X} + b\mathbb{1}, \tag{5.1}$$

or those following from (5.1) via recursive generation, i.e., $\mathcal{V}(\mathcal{M}_n) = \{(X, Y) \in \mathbb{R}^{s\times s} : Y^2 = X^3 + aX + bI_s\}$. We call such a Hankel matrix *elliptic-pure*.

**Remark 5.1.** Our analysis and results from this chapter also extend to the *Neile curve*, $y^2 = x^3$ (non-smooth, with a cusp at the origin), and so we will abuse terminology and include this special curve in our discussion of elliptic moment problem.

Let us begin by analyzing the form of nc atoms if a measure exists.

**Proposition 5.2.** *If $\mathcal{M}_n$ is as described above and has a representing measure $\mu$, then the atoms $(X_i, Y_i)$ of size greater than 1 have the form*

$$X_i = \begin{pmatrix} D_{i1} & B_i \\ B_i^T & D_{i2} \end{pmatrix}, \quad \text{and} \quad Y_i = \begin{pmatrix} \mu_i I_{n_{i1}} & 0 \\ 0 & -\mu_i I_{n_{i2}} \end{pmatrix},$$

*where $\mu_i > 0, n_{i1}, n_{i2} \in \mathbb{N}, B_i \in \mathbb{R}^{n_{i1}\times n_{i2}}$ and $D_{i1} \in \mathbb{R}^{n_{i1}\times n_{i1}}, D_{i2} \in \mathbb{R}^{n_{i2}\times n_{i2}}$ are diagonal matrices.*

*Proof.* We start by showing that $(X_iY_i + Y_iX_i)$ and $Y_i$ commute.

$$\begin{aligned}(X_iY_i + Y_iX_i)Y_i - Y_i(X_iY_i + Y_iX_i) &= X_iY_i^2 - Y_i^2X_i, \\ &= X_i(X_i^3 + aX_i + bI_s) - (X_i^3 + aX_i + bI_s)X_i, \\ &= 0.\end{aligned}$$

And now following the proofs of Claims 1 & 2 in the proof of Proposition 4.16 provides the form of the atoms. □

With the given representation of the non-commutative atoms, Hankel matrices $\mathcal{M}_n$ satisfying $\mathbb{Y}^2 = \mathbb{X}^3 + a\mathbb{X} + b\mathbb{1}$ can in some instances be simplified considerably. The next result was first communicated to me by Zalar for Horn's problem [21] on the Neile curve.

**Lemma 5.3.** *Suppose $\mathcal{M}_n$ satisfies $\mathbb{Y}^2 = \mathbb{X}^3 + a\mathbb{X} + b\mathbb{1}$ and has a representing measure $\mu$ consisting of atoms $\{(X_1, Y_1), \dots, (X_t, Y_t)\}$ (which have the form in Proposition 5.2). If we have*

$$4a^3 + 27(b - \mu_i^2)^2 \geq 0, \quad \text{for} \quad i = 1, \dots, t$$

*then $\mathcal{M}_n$ is a commutative Hankel matrix, and has a commutative representing measure.*

*Proof.* We begin as before by looking at an atom $(X_i, Y_i)$ in the measure of $\mathcal{M}_n$. By Proposition 5.2 we know that

$$Y_i^2 = \mu_i^2 \begin{pmatrix} I_{n_{i1}} & 0 \\ 0 & I_{n_{i2}} \end{pmatrix}.$$

Since $\operatorname{supp}(\mu) \subseteq \mathcal{V}(\mathcal{M}_n)$ (Theorem 4.5), this implies now that

$$X_i^3 + aX_i + bI_s = \mu_i^2 I_s \;\Leftrightarrow\; X_i^3 + aX_i + (b - \mu_i^2)I_s = 0. \tag{5.2}$$

Let $X_i = V_i^* D_i V_i$ be a diagonalization of $X_i$. The preceding equation implies

$$V_i^*(D_i^3 + aD_i + (b - \mu_i^2)I_s)V = 0,$$

and so it follows that the diagonal matrix $\Phi = D_i^3 + aD_i + (b - \mu_i^2)I_s = 0$. Since each diagonal element of $\Phi$ is a depressed cubic with the same linear and constant coefficient, namely $a$ and $(b - \mu_i^2)$, and we have that $4a^3 + 27(b - \mu_i^2)^2 \geq 0$, we have a unique (perhaps repeated) real solution. And hence, $D_i = \phi_i I_s$, which now shows that $X_iY_i = Y_iX_i$.

This is true of all the atoms, and hence the result follows. □

Lemma 5.3 offers a very nice reduction of the tracial elliptic moment problem. We can go even further with this simplification by consider the different possibilities for $a$.

**Corollary 5.4.** *Let $\mathcal{M}_n$ be a positive semi-definite, recursively generated Hankel matrix which satisfies $\mathbb{Y}^2 = \mathbb{X}^3 + a\mathbb{X} + b\mathbb{1}$. If $\mathcal{M}_n$ has a representing measure $\mu$ and $a \geq 0$, then $\mathcal{M}_n$ is a commutative Hankel matrix, and has a commutative represeating measure $\mu_{\boldsymbol{cm}}$.*

*Proof.* Letting $\{(X_1, Y_1), \ldots, (X_t, Y_t)\}$ be the atoms of the measure. Since we assume $a \geq 0$ it is clear that

$$4a^3 + 27(b - \mu_i^2)^2 \geq 0,$$

as $(b - \mu_i^2)^2 \geq 0$ is also non-negative (since it is a square). Hence the result follows from Lemma 5.3. □

**Proposition 5.5.** *Let $\mathcal{M}_n$ satisfy $\mathbb{Y}^2 = \mathbb{X}^3 + a\mathbb{X} + b\mathbb{1}$, and $a \neq 0$, then we can transform into one of the following;*

*(i)* $a > 0 : \widehat{\mathbb{Y}}^2 = \widehat{\mathbb{X}}^3 + \widehat{\mathbb{X}} + \tau\mathbb{1}$,

*(ii)* $a < 0 : \widehat{\mathbb{Y}}^2 = \widehat{\mathbb{X}}^3 - \widehat{\mathbb{X}} + \tau\mathbb{1}$.

*Proof.* $(i)$: When $a > 0$, we can apply a linear transformation (Proposition 4.9) to achieve

$$\mathbb{X} = (a^{\frac{1}{2}})\widehat{\mathbb{X}}, \quad \text{and} \quad \mathbb{Y} = (a^{\frac{3}{4}})\widehat{\mathbb{Y}}.$$

Under this scaling we have

$$(a^{\frac{3}{2}})\widehat{\mathbb{Y}}^2 = (a^{\frac{3}{2}})\widehat{\mathbb{X}}^3 + (a^{\frac{3}{2}})\widehat{\mathbb{X}} + b\mathbb{1},$$

and the result follows with $\tau = b/a^{\frac{3}{2}}$.

$(ii)$: Since $a < 0$, we know $a = -\sqrt{|a|^2}$. Together with the transformation

$$\mathbb{X} = (|a|^{\frac{1}{2}})\widehat{\mathbb{X}}, \quad \text{and} \quad \mathbb{Y} = (|a|^{\frac{3}{4}})\widehat{\mathbb{Y}},$$

the result is proved as in $(i)$. □

It is clear now that when $\mathbb{Y}^2 = \mathbb{X}^3 + \mathbb{X} + \tau\mathbb{1}$ is satisfied in $\mathcal{M}_n$, we always have a commutative Hankel matrix, and hence the entire class of problems is reduced to the commutative case.

We will return to this in Section 5.3. For now we will explore moment matrices $\mathcal{M}_n$ satisfying $\mathbb{Y}^2 = \mathbb{X}^3 - \mathbb{X} + \tau\mathbb{1}$, and demonstrate some properties through illustrative examples. These examples were generated by Zalar in our study of Horn's problem [21], which is closely related to the moment problem.

## 5.2 $\mathcal{M}_n$ generated by single atom $(X, Y)$

In this section we will provide an example of a Hankel matrix $\mathcal{M}_3$, generated by $(X, Y) \in (\mathbb{SR}^{3\times 3})^2$, satisfying the relations

$$\mathbb{Y}^2 = \mathbb{1} \quad \text{and} \quad \frac{48}{9}\mathbb{X}^3 - \frac{39}{9}\mathbb{X} = \mathbb{1}, \tag{5.3}$$

which must have an atoms of size 3 (or higher) in any representing measure. The relation $\mathbb{Y}^2 = \mathbb{1}$ is always present when we have only one atom (cf., Propositions 5.2 and 4.9).

**Example 5.6.** Let $(X, Y) \in (\mathbb{SR}^{3\times 3})^2$ be

$$X = \begin{pmatrix} \frac{1}{4} & \frac{1}{6} & \frac{2}{3} \\ \frac{1}{6} & -\frac{1}{3} & \frac{1}{2} \\ \frac{2}{3} & \frac{1}{2} & \frac{1}{12} \end{pmatrix}, \quad Y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{5.4}$$

**Claim 1.** *The Hankel matrix $\mathcal{M}_3^{(X,Y)}$ generated by $(X, Y)$ satisfies the relations (5.3), and any representing measure $\mu$ for $\mathcal{M}_3^{(X,Y)}$ must have an atom of size 3 (or higher).*

*Proof.* It is easy to check that the atom (5.4) generates the following $\mathcal{M}_3^{(X,Y)}$

$$\mathcal{M}_3^{(X,Y)} = \begin{pmatrix} \mathcal{M}_2^{(X,Y)} & B_3 \\ B_3^T & C_3 \end{pmatrix},$$

where

$$\mathcal{M}_2^{(X,Y)} = \begin{array}{c} \\ \mathbb{1} \\ \mathbb{X} \\ \mathbb{Y} \\ \mathbb{X}^2 \\ \mathbb{XY} \\ \mathbb{YX} \\ \mathbb{Y}^2 \end{array} \begin{array}{c} \begin{array}{ccccccc} \mathbb{1} & \mathbb{X} & \mathbb{Y} & \mathbb{X}^2 & \mathbb{XY} & \mathbb{YX} & \mathbb{Y}^2 \end{array} \\ \begin{pmatrix} 1 & 0 & \frac{1}{3} & \frac{13}{24} & -\frac{1}{18} & -\frac{1}{18} & 1 \\ 0 & \frac{13}{24} & -\frac{1}{18} & \frac{3}{16} & \frac{2}{27} & \frac{2}{27} & 0 \\ \frac{1}{3} & -\frac{1}{18} & 1 & \frac{2}{27} & 0 & 0 & \frac{1}{3} \\ \frac{13}{24} & \frac{3}{16} & \frac{2}{27} & \frac{169}{384} & \frac{5}{288} & \frac{5}{288} & \frac{13}{24} \\ -\frac{1}{18} & \frac{2}{27} & 0 & \frac{5}{288} & \frac{13}{24} & -\frac{83}{216} & -\frac{1}{18} \\ -\frac{1}{18} & \frac{2}{27} & 0 & \frac{5}{288} & -\frac{83}{216} & \frac{13}{24} & -\frac{1}{18} \\ 1 & 0 & \frac{1}{3} & \frac{13}{24} & -\frac{1}{18} & -\frac{1}{18} & 1 \end{pmatrix} \end{array},$$

$$B_3 = \begin{array}{c} \\ \mathbb{1} \\ \mathbb{X} \\ \mathbb{Y} \\ \mathbb{X}^2 \\ \mathbb{X}\mathbb{Y} \\ \mathbb{Y}\mathbb{X} \\ \mathbb{Y}^2 \end{array} \begin{array}{c} \begin{array}{cccccccc} \mathbb{X}^3 & \mathbb{X}^2\mathbb{Y} & \mathbb{X}\mathbb{Y}\mathbb{X} & \mathbb{X}\mathbb{Y}^2 & \mathbb{Y}\mathbb{X}^2 & \mathbb{Y}\mathbb{X}\mathbb{Y} & \mathbb{Y}^2\mathbb{X} & \mathbb{Y}^3 \end{array} \\ \begin{pmatrix} \frac{3}{16} & \frac{2}{27} & \frac{2}{27} & 0 & \frac{2}{27} & 0 & 0 & \frac{1}{3} \\ \frac{169}{384} & \frac{5}{288} & \frac{5}{288} & \frac{13}{24} & \frac{5}{288} & -\frac{83}{216} & \frac{13}{24} & -\frac{1}{18} \\ \frac{5}{288} & \frac{13}{24} & -\frac{83}{216} & -\frac{1}{18} & \frac{13}{24} & -\frac{1}{18} & -\frac{1}{18} & 1 \\ \frac{65}{256} & \frac{43}{864} & \frac{43}{864} & \frac{3}{16} & \frac{43}{864} & -\frac{97}{1296} & \frac{3}{16} & \frac{2}{27} \\ \frac{43}{864} & \frac{3}{16} & -\frac{97}{1296} & \frac{2}{27} & -\frac{97}{1296} & \frac{2}{27} & \frac{2}{27} & 0 \\ \frac{43}{864} & -\frac{97}{1296} & -\frac{97}{1296} & \frac{2}{27} & \frac{3}{16} & \frac{2}{27} & \frac{2}{27} & 0 \\ \frac{3}{16} & \frac{2}{27} & \frac{2}{27} & 0 & \frac{2}{27} & 0 & 0 & \frac{1}{3} \end{pmatrix} \end{array},$$

$$C_3 = \begin{array}{c} \\ \mathbb{X}^3 \\ \mathbb{X}^2\mathbb{Y} \\ \mathbb{X}\mathbb{Y}\mathbb{X} \\ \mathbb{X}\mathbb{Y}^2 \\ \mathbb{Y}\mathbb{X}^2 \\ \mathbb{Y}\mathbb{X}\mathbb{Y} \\ \mathbb{Y}^2\mathbb{X} \\ \mathbb{Y}^3 \end{array} \begin{array}{c} \begin{array}{cccccccc} \mathbb{X}^3 & \mathbb{X}^2\mathbb{Y} & \mathbb{X}\mathbb{Y}\mathbb{X} & \mathbb{X}\mathbb{Y}^2 & \mathbb{Y}\mathbb{X}^2 & \mathbb{Y}\mathbb{X}\mathbb{Y} & \mathbb{Y}^2\mathbb{X} & \mathbb{Y}^3 \end{array} \\ \begin{pmatrix} \frac{2413}{6144} & \frac{43}{1536} & \frac{43}{1536} & \frac{169}{384} & \frac{43}{1536} & -\frac{1079}{3456} & \frac{169}{384} & \frac{5}{288} \\ \frac{43}{1536} & \frac{169}{384} & -\frac{1079}{3456} & \frac{5}{288} & \frac{9809}{31104} & \frac{5}{288} & \frac{5}{288} & \frac{13}{24} \\ \frac{43}{1536} & -\frac{1079}{3456} & \frac{9809}{31104} & \frac{5}{288} & -\frac{1079}{3456} & -\frac{235}{2592} & \frac{5}{288} & -\frac{83}{216} \\ \frac{169}{384} & \frac{5}{288} & \frac{5}{288} & \frac{13}{24} & \frac{5}{288} & -\frac{83}{216} & \frac{13}{24} & -\frac{1}{18} \\ \frac{43}{1536} & \frac{9809}{31104} & -\frac{1079}{3456} & \frac{5}{288} & \frac{169}{384} & \frac{5}{288} & \frac{5}{288} & \frac{13}{24} \\ -\frac{1079}{3456} & \frac{5}{288} & -\frac{235}{2592} & -\frac{83}{216} & \frac{5}{288} & \frac{13}{24} & -\frac{83}{216} & -\frac{1}{18} \\ \frac{169}{384} & \frac{5}{288} & \frac{5}{288} & \frac{13}{24} & \frac{5}{288} & -\frac{83}{216} & \frac{13}{24} & -\frac{1}{18} \\ \frac{5}{288} & \frac{13}{24} & -\frac{83}{216} & -\frac{1}{18} & \frac{13}{24} & -\frac{1}{18} & -\frac{1}{18} & 1 \end{pmatrix} \end{array},$$

A computational check with *Mathematica* reveals the kernel of $\mathcal{M}_3^{(X,Y)}$ to be of dimension 7 with columns dependencies

$$\begin{aligned} \mathbf{0} &= \mathbb{Y}^2 - \mathbb{1}, \\ \mathbf{0} &= \mathbb{X}^3 - \frac{13}{16}\mathbb{X} - \frac{3}{16}\mathbb{1}, \\ \mathbf{0} &= \mathbb{X}\mathbb{Y}^2 - \mathbb{X}, \\ \mathbf{0} &= \mathbb{Y}\mathbb{X}^2 + \mathbb{X}^2\mathbb{Y} + \mathbb{X}\mathbb{Y}\mathbb{X} - \mathbb{X}^2 - \frac{13}{16}\mathbb{Y} + \frac{1}{6}\mathbb{X} + \frac{85}{144}\mathbb{1}, \\ \mathbf{0} &= \mathbb{Y}\mathbb{X}\mathbb{Y} - \mathbb{Y}\mathbb{X} - \mathbb{X}\mathbb{Y} + \frac{1}{6}\mathbb{Y} + \mathbb{X} - \frac{1}{6}\mathbb{1}, \\ \mathbf{0} &= \mathbb{Y}^2\mathbb{X} - \mathbb{X}, \\ \mathbf{0} &= \mathbb{Y}^3 - \mathbb{Y}. \end{aligned} \tag{5.5}$$

The only possible commutative atoms in the measure for $\mathcal{M}_3^{(X,Y)}$ are those which satisfy all these relations. However, there are no such atoms. This can be easily seen by noticing that the only candidates are

$$P_1 = (1,1),\ P_2 = (-\frac{1}{4},1),\ P_3 = (-\frac{3}{4},1),\ P_4 = (1,-1),\ P_5 = (-\frac{1}{4},-1),\ P_6 = (-\frac{3}{4},-1),$$

which are the points in the intersection of the relations (5.3). Substituting these points in the function

$$f(x,y) = 3x^2y - \frac{13}{16}y - x^2 + \frac{1}{6}x + \frac{85}{144},$$

(the commutative collapse of (5.5)) we get

$$\frac{35}{18},\ -\frac{5}{36},\ \frac{7}{9},\ -\frac{175}{72},\ \frac{10}{9},\ -\frac{35}{36},$$

respectively. Hence none of the points $P_i$, $i = 1,\dots,6$, satisfy the relation (5.5), and so there are no commutative atoms in the measure for $\mathcal{M}_3^{(X,Y)}$. Now notice that for any atom $(X',Y') \in (\mathbb{SR}^{2\times 2})^2$ in the measure, $Y'$ must be of the form

$$Y' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

So if there are only atoms of size at most 2 in the measure for $\mathcal{M}_3^{(X,Y)}$, then $\beta_Y = 0$. In the example above $\beta_Y = \frac{1}{4}$. Hence there must be atoms of size 3 (or higher) present in the measure. □

We believe that the technique we have used to generate Example 5.6 is much more general. Let us consider a larger Hankel matrix $\mathcal{M}_4$ generated with $(X,Y) \in (\mathbb{SR}^{3\times 3})^2$, satisfying the relations

$$\mathbb{Y}^2 = \mathbb{1} \quad \text{and} \quad \frac{1}{64}(\mathbb{X} + 2\cdot\mathbb{1})(\mathbb{X}+\mathbb{1})(\mathbb{X}-\mathbb{1})(\mathbb{X}-2\cdot\mathbb{1}) = \mathbf{0}, \tag{5.6}$$

for which any representing measure must contain an atom of size 4 (or higher).

**Example 5.7.** Let $(X,Y) \in (\mathbb{SR}^{4\times 4})^2$ be

$$X = \begin{pmatrix} 0 & -\frac{3}{2} & 0 & -\frac{1}{2} \\ -\frac{3}{2} & 0 & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & 0 & -\frac{3}{2} \\ -\frac{1}{2} & 0 & -\frac{3}{2} & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{5.7}$$

**Claim 2.** *Then the Hankel matrix $\mathcal{M}_4^{(X,Y)}$ generated by $(X,Y)$ satisfies the relations (5.6), and any representing measure for $\mathcal{M}_4^{(X,Y)}$ must contain an atoms of size 4 (or higher).*

*Proof.* It is easy to check that the atom (5.7) satisfies the relations (5.6). A computation of the kernel of $\mathcal{M}_4^{(X,Y)}$ reveals it to be of dimension 18 and among those dependencies we have the following relation

$$5\mathbb{X} - 5\mathbb{X}\mathbb{Y} - 5\mathbb{Y}\mathbb{X} - 2\mathbb{X}^3 + \mathbb{X}^3\mathbb{Y} + \mathbb{X}^2\mathbb{Y}\mathbb{X} + \mathbb{X}\mathbb{Y}\mathbb{X}^2 + \mathbb{Y}\mathbb{X}^3 = \mathbf{0}. \tag{5.8}$$

As before, the only possible commutative atoms in the measure for $\mathcal{M}_4^{(X,Y)}$ are those that satisfy all of the dependencies in the kernel. The only possibilities for such atoms are

$$P_1 = (-2,1),\ P_2 = (-1,1),\ P_3 = (1,1),\ P_4 = (2,1),$$
$$P_5 = (-2,-1),\ P_6 = (-1,-1),\ P_7 = (1,-1),\ P_8 = (2,-1),$$

which are the points in the intersection of (5.6). The commutative collapse of (5.8)

$$f(x,y) = 4x^3y - 10xy - 2x^2 + 5x,$$

evaluated at these points gives

$$-6, 3, -3, 6, 18, -9, 9, -18,$$

respectively. Hence none of the points $P_i$, $i = 1, \dots, 8$, satisfies the relation (5.8). So there are no commutative atoms in the measure for $\mathcal{M}_4^{(X,Y)}$. For any atom $(X', Y') \in (\mathbb{SR}^{3\times 3})^2$ in the measure, $Y'$ must be of the form

$$Y' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

So if there are only atoms of size at most 3 in the measure for $\mathcal{M}_3^{(X,Y)}$, then $\beta_Y \leq \frac{1}{3}$. In the example above $\beta_Y = \frac{1}{2}$. Hence there must be atoms of size 4 (or higher) present in the measure. □

## 5.3 Commutative Sequences

In this section we analyze the commutative truncated moment problem with variety $y^2 = x^3 + ax + b$. Our results here provide (numerical) sufficient conditions which can be used to test for the existence of a measure. It should be noted that these are not necessary conditions, as demonstrated by Example 5.15.

We will use below the extension principle of Curto and Fialkow, and so we state it here for convenience.

**Theorem 5.8** (Proposition 3.9, [26]). *Let $A \in \mathbb{R}^{s\times s}$. If there exists a $t$ with $0 \leq t \leq (s-1)$, and a vector $\mathbf{x} \in \mathbb{R}^t$ such that $[A]_t\mathbf{x} = 0$, then for $\mathbf{y} = \begin{pmatrix}\mathbf{x} & \mathbf{0}_{(s-t)}\end{pmatrix}^T$ we have*

$$A\mathbf{y} = \mathbf{0}.$$

Let $\mathcal{M}_n$ be elliptic-pure, i.e., positive semi-definite, recursively generated, and satisfying $\mathbb{Y}^2 = \mathbb{X}^3 + a\mathbb{X} + b\mathbb{1}$ with all others following from recursive generation,

$$\mathbb{X}^i\mathbb{Y}^{j+2} = (\mathbb{X}^{i+3} + a\mathbb{X}^{i+1} + b\mathbb{X}^i)\mathbb{Y}^j \quad (i, j \geq 0, i+j+3 \leq n). \tag{5.9}$$

We have in this case $\mathcal{V}(\mathcal{M}_n) = \{(x,y) : y^2 = x^3 + ax + b\}$. In the commutative setting we are fortunate enough to write a basis $\mathcal{B}$ for $\mathcal{C}_{\mathcal{M}_n}$ as

$$\mathcal{B} = \{\mathbb{1}, \mathbb{X}, \mathbb{Y}, \mathbb{X}^2, \mathbb{X}\mathbb{Y}, \mathbb{Y}^2, \mathbb{X}^2\mathbb{Y}, \mathbb{X}\mathbb{Y}^2, \mathbb{Y}^3, \dots, \mathbb{X}^2\mathbb{Y}^{n-2}, \mathbb{X}\mathbb{Y}^{n-1}, \mathbb{Y}^n\}, \tag{5.10}$$

and so $\operatorname{rank}(\mathcal{M}_n) = 3n$. We know that if a representing measure exists, then there is a positive, recursively generated, Hankel matrix extension

$$\mathcal{M}_{n+1} = \begin{pmatrix} \mathcal{M}_n & B_{n+1} \\ B_{n+1}^T & C_{n+1} \end{pmatrix}. \tag{5.11}$$

Moreover, we know that if we can construct such an extension, which is flat then a representing measure does indeed exist. We follow the approach of [38] and examine conditions for a flat extension to exists. Our discussion will follow the same structure as [38], split into different subsections.

In Subsection 5.3.1, we will show the following result, which shows that a compatible block $B_{n+1}$ always exists for elliptic-pure problems.

**Proposition 5.9.** *If $\mathcal{M}_n$ is elliptic-pure, then there is a Hankel block $B_{n+1} \equiv B_{n+1}[\theta, \phi, \psi]$ which is compatible with a recursively generated Hankel extension $\mathcal{M}_{n+1}$. Moreover, we have* $\operatorname{Ran}(B_{n+1}) \subseteq \operatorname{Ran}(\mathcal{M}_n)$.

Once this is established, in Subsection 5.3.2 we will then examine the hypothetical block $C_{n+1}$, to see what conditions it must satisfy for $\mathcal{M}_{n+1}$ to be flat. From this examination we will obtain the following

**Theorem 5.10.** *Let $n \geq 3$. Suppose that $\mathcal{M}_n$ is positive and Elliptic-pure. Then there is a quartic polynomials $\mathcal{Q}(\theta)$, such that a flat extension $\mathcal{M}_{n+1}$ of $\mathcal{M}_n$ exists if $\mathcal{Q}(\theta)$ has a real root.*

### 5.3.1 Constructing $B_{n+1}$

Our first step is to construct $B_{n+1}$ which satisfies $B_{n+1} = \mathcal{M}_n W$ for some matrix $W$, i.e., the range inclusion $\operatorname{Ran}(B_{n+1}) \subseteq \operatorname{Ran}(\mathcal{M}_n)$. Positivity of $\mathcal{M}_{n+1}$ and Theorem 5.8 imply that the relations in $\mathcal{C}_{\mathcal{M}_n}$ hold also in $\mathcal{C}_{\mathcal{M}_{n+1}}$, and so we have the following relations in $\mathcal{M}_{n+1}$

$$\mathbb{X}^i\mathbb{Y}^{j+2} = (\mathbb{X}^{i+3} + a\mathbb{X}^{i+1} + b\mathbb{X}^i)\mathbb{Y}^j \quad (i, j \geq 0, i + j + 3 \leq n). \tag{5.12}$$

Using recursive generation we now have the following column relations in $B_{n+1}$

$$\begin{aligned} \mathbb{X}^{n+1} &= \mathbb{X}^{n-2}(\mathbb{Y}^2 - a\mathbb{X} - b\mathbb{1}) \\ \mathbb{X}^n\mathbb{Y} &= \mathbb{X}^{n-3}(\mathbb{Y}^3 - a\mathbb{X}\mathbb{Y} - b\mathbb{Y}) \\ &\vdots \\ \mathbb{X}^3\mathbb{Y}^{n-2} &= \mathbb{Y}^n - a\mathbb{X}\mathbb{Y}^{n-2} - b\mathbb{Y}^{n-2}. \end{aligned} \tag{5.13}$$

Due to recursive generation, these columns inherit the required Hankel structure from the corresponding columns in $\mathcal{M}_n$. To define $\mathbb{X}^2\mathbb{Y}^{n-1}, \mathbb{X}\mathbb{Y}^n$, and $\mathbb{Y}^{n+1}$ we use 'old moments' as follows;

$$\left\langle B_{n+1}\widetilde{x^iy^{n+1-j}}, \widetilde{x^ky^l} \right\rangle = \beta_{i+k,n+1-i+l}, \tag{5.14}$$

where $i = 0, 1, 2$, and $l, k \geq 0$, with $l + k \leq n - 1$. Now every column in $B_{n+1}$ has the Hankel structure in all rows up to degree $n-1$. For a column $w(\mathbb{X}, \mathbb{Y})$ of $B_{n+1}$, let $[w(\mathbb{X}, \mathbb{Y})]_S$

(respectively $[w(\mathbb{X},\mathbb{Y})]_k$) be the restriction to rows from the set $S$ (respectively rows of degree at most $k$). First we must ensure that the moment structure from $[\mathbb{X}^3\mathbb{Y}^{n-2}]_{n-1}$ carries into $[\mathbb{X}^2\mathbb{Y}^{n-1}]_{n-1}$.

**Lemma 5.11.** *With the notation and definitions as above, for* $i \geq 1, j \geq 0, i+j \leq n-1$

$$\left\langle B_{n+1}\widetilde{x^3y^{n-2}}, \widetilde{x^{i-1}y^{j+1}}\right\rangle = \left\langle B_{n+1}\widetilde{x^2y^{n-1}}, \widetilde{x^iy^j}\right\rangle.$$

*Proof.* We have,

$$\begin{aligned}
\left\langle B_{n+1}\widetilde{x^3y^{n-2}}, \widetilde{x^{i-1}y^{j+1}}\right\rangle &= \left\langle \mathcal{M}_n(\widetilde{y^n} - a\widetilde{xy^{n-2}} - b\widetilde{y^{n-2}}), \widetilde{x^{i-1}y^{j+1}}\right\rangle \\
&= \left\langle \mathcal{M}_n\widetilde{y^n}, \widetilde{x^{i-1}y^{j+1}}\right\rangle - a\left\langle \mathcal{M}_n\widetilde{xy^{n-2}}, \widetilde{x^{i-1}y^{j+1}}\right\rangle \\
&\quad -b\left\langle \mathcal{M}_n\widetilde{y^{n-2}}, \widetilde{x^{i-1}y^{j+1}}\right\rangle \\
&= \beta_{i-1,n+j+1} - a\beta_{i,n+j-1} - b\beta_{i-1,n+j-1}
\end{aligned}$$

and

$$\left\langle B_{n+1}\widetilde{x^2y^{n-1}}, \widetilde{x^iy^j}\right\rangle = \beta_{i+2,n+j-1}.$$

So it is enough to show $\beta_{i+2,n+j-1} = \beta_{i-1,n+j+1} - a\beta_{i,n+j-1} - b\beta_{i-1,n+j-1}$ where $i,j \geq 0, i+j \leq n-1$. Since $i+j+1 \leq n$, in $\mathcal{M}_n$ we have

$$\begin{aligned}
\beta_{i+2,n+j-1} &= \left\langle \mathcal{M}_n\widetilde{x^3y^{n-3}}, \widetilde{x^{i-1}y^{j+2}}\right\rangle \\
&= \left\langle \mathcal{M}_n(\widetilde{y^{n-1}} - a\widetilde{xy^{n-3}} - b\widetilde{y^{n-3}}), \widetilde{x^{i-1}y^{j+2}}\right\rangle \\
&= \left\langle \mathcal{M}_n\widetilde{y^{n-1}}, \widetilde{x^{i-1}y^{j+2}}\right\rangle \\
&\quad -a\left\langle \mathcal{M}_n\widetilde{xy^{n-3}}, \widetilde{x^{i-1}y^{j+2}}\right\rangle \\
&\quad -b\left\langle \mathcal{M}_n\widetilde{y^{n-3}}, \widetilde{x^{i-1}y^{j+2}}\right\rangle \\
&= \beta_{i-1,n+j+1} - a\beta_{i,n+j-1} - b\beta_{i-1,n+j-1}.
\end{aligned}$$

□

We now define the (potential) moments in $\mathbb{X}^2\mathbb{Y}^{n-1}, \mathbb{X}\mathbb{Y}^n, \mathbb{Y}^{n+1}$ in the rows of degree $n$ (the other columns have these defined through recursive generation). To keep the Hankel structure, we propagate the moments from $\mathbb{X}^3\mathbb{Y}^{n-2}$ along the cross diagonals; for $k = 0,1,2, i,j \geq$

$0, i+j=n$ and $0 \le j \le n-3+k$ we have

$$
\begin{aligned}
\left\langle B_{n+1}\widetilde{x^k y^{n+1-k}}, \widetilde{x^i y^j}\right\rangle &= \left\langle B_{n+1}\widetilde{x^3 y^{n-2}}, \widetilde{x^{i+k-3}y^{j-k+3}}\right\rangle \\
&= \left\langle B_{n+1}\widetilde{y^n}, \widetilde{x^{i+k-3}y^{j-k+3}}\right\rangle \\
&\quad -a\left\langle B_{n+1}\widetilde{xy^{n-2}}, \widetilde{x^{i+k-3}y^{j-k+3}}\right\rangle \\
&\quad -b\left\langle B_{n+1}\widetilde{y^{n-2}}, \widetilde{x^{i+k-3}y^{j-k+3}}\right\rangle \\
&= \beta_{i+k-3,n+j-k+3} \\
&\quad -a\beta_{i+k-2,n+j-k+1} - b\beta_{i+k-3,n+j-k+1}.
\end{aligned}
\tag{5.15}
$$

To complete the definition of $B_{n+1}$, we parameterize it via the following

$$
\begin{aligned}
\left\langle B_{n+1}\widetilde{x^2 y^{n-1}}, \widetilde{y^n}\right\rangle &= \left\langle B_{n+1}\widetilde{xy^n}, \widetilde{xy^{n-1}}\right\rangle \\
&= \left\langle B_{n+1}\widetilde{y^{n+1}}, \widetilde{x^2 y^{n-2}}\right\rangle \\
&= \theta, \\
\left\langle B_{n+1}\widetilde{xy^n}, \widetilde{y^n}\right\rangle &= \left\langle B_{n+1}\widetilde{y^{n+1}}, \widetilde{xy^{n-1}}\right\rangle \\
&= \phi, \\
\left\langle B_{n+1}\widetilde{y^{n+1}}, \widetilde{y^{n+1}}\right\rangle &= \psi.
\end{aligned}
\tag{5.16}
$$

So the component of $B_{n+1}$ with rows of degree $n$, now has the structure

$$
B_{n+1} = \begin{array}{c} \\ \mathbb{X}^n \\ \mathbb{X}^{n-1}\mathbb{Y} \\ \vdots \\ \mathbb{X}^2\mathbb{Y}^{n-2} \\ \mathbb{X}\mathbb{Y}^{n-1} \\ \mathbb{Y}^n \end{array}
\begin{array}{c}
\begin{array}{cccccc} \mathbb{X}^{n+1} & \mathbb{X}^n\mathbb{Y} & \dots & \mathbb{X}^2\mathbb{Y}^{n-1} & \mathbb{X}\mathbb{Y}^n & \mathbb{Y}^{n+1} \end{array} \\
\begin{pmatrix}
\beta_{2n+1,0} & \beta_{2n,1} & \cdots & \cdots & \cdots & \beta_{n,n+1} \\
\beta_{2n,1} & \iddots & \iddots & \iddots & \iddots & \beta_{n-1,n+2} \\
\vdots & \iddots & \iddots & \iddots & \iddots & \vdots \\
\vdots & \iddots & \iddots & \iddots & \iddots & \theta \\
\vdots & \beta_{n+1,n} & \iddots & \iddots & \theta & \phi \\
\beta_{n+1,n} & \iddots & \iddots & \theta & \phi & \psi
\end{pmatrix}
\end{array},
$$

where $\beta_{i,2n+1-i} = \beta_{i-3,2n+3-i} - a\beta_{i-2,2n+1-i} - b\beta_{i-3,2n+1-i}$ for $3 \le i \le 2n+1$.

Having created $B_{n+1} \equiv B_{n+1}[\theta, \phi, \psi]$, let us now examine the condition $\operatorname{Ran}(B_{n+1}) \subseteq \operatorname{Ran}(\mathcal{M}_n)$. Clearly $\mathbb{X}^{n+1}, \dots, \mathbb{X}^3\mathbb{Y}^{n-2} \subseteq \mathcal{C}_{\mathcal{M}_n}$, so consider the three remaining columns. Given a basis $\mathcal{B}$ for $\mathcal{C}_{\mathcal{M}_n}$, let $\mathcal{J} = [\mathcal{M}_n]_{\mathcal{B}}$, which implies that $\mathcal{J}$ is positive definite. For $k, l \ge 0$ we let $\widehat{\mathbb{X}^k\mathbb{Y}^l}$ be the compression of $\mathbb{X}^k\mathbb{Y}^l \in [\mathcal{M}_n, B_{n+1}]$ to the rows indexed by elements in $\mathcal{B}$. Note that columns of $\mathcal{J}$ are of the form $\widehat{\mathbb{X}^p\mathbb{Y}^q}$ with $p, q \ge 0, p+q \le n, p \le 2$.

Since $\mathcal{J}$ is invertible, for $0 \leq i \leq 2, j = n+1-i$ we may write

$$\mathcal{J}c^{(ij)} = \widehat{\mathbb{X}^i\mathbb{Y}^j}, \qquad \text{or,}$$

$$\widehat{\mathbb{X}^i\mathbb{Y}^j} = \sum_{\substack{p,q\geq 0\\ p+q\leq n\\ p\leq 2}} c_{pq}^{(ij)}\widehat{\mathbb{X}^p\mathbb{Y}^q} \qquad (c_{pq}^{(ij)} \in \mathbb{R}). \tag{5.17}$$

**Lemma 5.12.** *With the notation and definition as above, we have*

$$\mathbb{X}^i\mathbb{Y}^j = \sum_{\substack{p,q\geq 0\\ p+q\leq n\\ p\leq 2}} c_{pq}^{(ij)}\mathbb{X}^p\mathbb{Y}^q$$

*in* $[\mathcal{M}_n, B_{n+1}]$ *for* $0 \leq i \leq 2, j = n+1-j$.

*Proof.* To prove the claim it is enough to show

$$\left\langle B_{n+1}\widetilde{x^iy^j}, \widetilde{x^ky^l}\right\rangle = \sum_{\substack{p,q\geq 0\\ p+q\leq n\\ p\leq 2}} c_{pq}^{(ij)}\left\langle \mathcal{M}_n\widetilde{x^py^q}, \widetilde{x^ky^l}\right\rangle \tag{5.18}$$

for $k,l \geq 0, k+l \leq n, k \geq 3$, which is to say that the rows of the column on the left and the rows of the sum of columns on the right are equal in $B_{n+1}$. In $\mathcal{M}_n$ this is given by (5.17), and so (5.18) is true when $k,l \geq 0, k+l \leq n, k \leq 2$.

To prove (5.18) we attempt induction on $\rho = k+l \geq 3$ (with $k \geq 3$).

**Base Case:** $\rho = 3 \Rightarrow k = 3, l = 0$.

In $\mathcal{C}_{\mathcal{M}_n}$, $\mathbb{Y}^2 = \mathbb{X}^3 + a\mathbb{X} + b\mathbb{1}$, so row $\mathbb{X}^3$ equals the row combination $\mathbb{Y}^2 - a\mathbb{X} - b\mathbb{1}$, and by the definition of $\mathbb{X}^{n+1}, \ldots, \mathbb{X}^3\mathbb{Y}^{n-2}$, these columns have row $\mathbb{X}^3$ equal to the same combination in $B_{n+1}$. We will show that these rows are also equal in the columns $\mathbb{X}^2\mathbb{Y}^{n-1}, \mathbb{X}\mathbb{Y}^n, \mathbb{Y}^{n+1}$. Let $i = 0,1,2, j = n+1-i$ and consider the equation

$$\left\langle B_{n+1}\widetilde{x^iy^j}, \widetilde{x^3}\right\rangle = \left\langle B_{n+1}\widetilde{x^iy^j}, (\widetilde{y^2} - a\widetilde{x} - b\widetilde{1})\right\rangle.$$

**Case 1** $(n = 3)$:

From (5.15) we have

$$\begin{aligned}
\left\langle B_4\widetilde{x^iy^j}, \widetilde{x^3}\right\rangle &= \left\langle B_4\widetilde{x^iy^{4-i}}, \widetilde{x^3}\right\rangle \\
&= \left\langle B_4\widetilde{x^3y}, \widetilde{x^iy^{3-i}}\right\rangle \\
&= \left\langle \mathcal{M}_3(\widetilde{y^3} - a\widetilde{xy} - b\widetilde{y}), \widetilde{x^iy^{3-i}}\right\rangle \\
&= \beta_{i,6-i} - a\beta_{i+1,4-i} - b\beta_{i,4-i} \\
&= \left\langle B_4\widetilde{x^iy^{4-i}}, (\widetilde{y^2} - a\widetilde{x} - b\widetilde{1})\right\rangle
\end{aligned}$$

where the last step is using (5.14).

**Case 2** ($n > 3$):

$$\text{(using (5.14))} \qquad \left\langle B_{n+1}\widetilde{x^i y^j}, \widetilde{x^3}\right\rangle = \beta_{i+3,n+1-i}$$
$$= \left\langle \mathcal{M}_n \widetilde{x^3 y}, \widetilde{x^i y^{n-i}}\right\rangle$$
$$= \left\langle \mathcal{M}_n (\widetilde{y^3} - a\widetilde{xy} - b\widetilde{y}), \widetilde{x^i y^{n-i}}\right\rangle$$
$$= \beta_{i,n+3-i} - a\beta_{i+1,n+1-i} - b\beta_{i,n+1-i}$$
$$= \left\langle B_{n+1}\widetilde{x^i y^j}, (\widetilde{y^2} - a\widetilde{x} - b\widetilde{1})\right\rangle$$

So we see now that when $\rho = 3$ the row $\mathbb{X}^3$ is equal to the row combination $\mathbb{Y}^2 - a\mathbb{X} - b\mathbb{1}$ in $[\mathcal{M}_n, B_{n+1}]$. As (5.18) holds for $\mathbb{Y}^2 - a\mathbb{X} - b\mathbb{1}$ and $\mathbb{Y}^2, \mathbb{X}, \mathbb{1} \in \mathcal{B}$, it also holds for $\mathbb{X}^3$, and so (5.18) is true for $\rho = 3$.

**Inductive Step:** Suppose now that (5.18) is true for $3 \le \rho < k + l$. First we consider

$$\left\langle B_{n+1}\widetilde{x^i y^{n+1-i}}, \widetilde{x^k y^l}\right\rangle = \beta_{i+k-3,n+l-i+3} - a\beta_{i+k-2,n+l+1-i} - b\beta_{i+k-3,n+l+1-i} \tag{5.19}$$

for $k, l \ge 0, k + l \le n, k \ge 3, 0 \le i \le 2$.

**Case 1:** $(k + l < n)$

$$\text{(from (5.14))} \quad \left\langle B_{n+1}\widetilde{x^i y^{n+1-i}}, \widetilde{x^k y^l}\right\rangle = \beta_{i+k,n+l+1-i}$$
$$(k + l \le n - 1) \qquad = \left\langle \mathcal{M}_n \widetilde{x^k y^{l+1}}, \widetilde{x^i y^{n-i}}\right\rangle$$
$$\text{(RG in } \mathcal{M}_n) \qquad = \left\langle \mathcal{M}_n \widetilde{x^{k-3} y^{l+3}}, \widetilde{x^i y^{n-i}}\right\rangle$$
$$-a\left\langle \mathcal{M}_n \widetilde{x^{k-2} y^{l+2}}, \widetilde{x^i y^{n-i}}\right\rangle$$
$$-b\left\langle \mathcal{M}_n \widetilde{x^{k-3} y^{l+1}}), \widetilde{x^i y^{n-i}}\right\rangle$$
$$= \beta_{i+k-3,n+l-i+3} - a\beta_{i+k-2,n+l+1-i} - b\beta_{i+k-3,n+l+1-i}$$

**Case 2:** $(k + l = n)$

$$\text{(from (5.15))} \quad \left\langle B_{n+1}\widetilde{x^i y^{n+1-i}}, \widetilde{x^k y^l}\right\rangle = \left\langle B_{n+1}\widetilde{x^3 y^{n-2}}, \widetilde{x^{k+i-3} y^{l-i+3}}\right\rangle$$
$$(k + l = n) \qquad = \left\langle \mathcal{M}_n \widetilde{x^3 y^{n-2}}, \widetilde{x^{k+i-3} y^{l-i+3}}\right\rangle$$
$$= \left\langle \mathcal{M}_n \widetilde{y^n}, \widetilde{x^{k+i-3} y^{l-i+3}}\right\rangle$$
$$-a\left\langle \mathcal{M}_n \widetilde{xy^{n-2}}, \widetilde{x^{k+i-3} y^{l-i+3}}\right\rangle$$
$$\text{(RG in } \mathcal{M}_n) \qquad -b\left\langle \mathcal{M}_n \widetilde{y^{n-2}}, \widetilde{x^{k+i-3} y^{l-i+3}}\right\rangle$$
$$= \beta_{i+k-3,n+l-i+3} - a\beta_{i+k-2,n+l+1-i} - b\beta_{i+k-3,n+l+1-i}$$

And so (5.19) is proved. Coming back to (5.18) we have

$$\begin{aligned}
\text{(self adjointness)} \quad \sum_{\substack{p,q\geq 0\\ p+q\leq n\\ p\leq 2}} c_{pq}^{(ij)} \left\langle \mathcal{M}_n \widetilde{x^p y^q}, \widetilde{x^k y^l} \right\rangle &= \sum_{\substack{p,q\geq 0\\ p+q\leq n\\ p\leq 2}} c_{pq}^{(ij)} \left\langle \mathcal{M}_n \widetilde{x^k y^l}, \widetilde{x^p y^q} \right\rangle \\
&= \sum_{\substack{p,q\geq 0\\ p+q\leq n\\ p\leq 2}} c_{pq}^{(ij)} \Big( \left\langle \mathcal{M}_n \widetilde{x^{k-3} y^{l+2}}, \widetilde{x^p y^q} \right\rangle \\
&\quad - a \left\langle \mathcal{M}_n \widetilde{x^{k-2} y^l}, \widetilde{x^p y^q} \right\rangle \\
&\quad - b \left\langle \mathcal{M}_n \widetilde{x^{k-3} y^l}, \widetilde{x^p y^q} \right\rangle \Big) \\
&= \chi.
\end{aligned}$$

Using self adjointness again we see

$$\begin{aligned}
\chi = \sum_{\substack{p,q\geq 0\\ p+q\leq n\\ p\leq 2}} c_{pq}^{(ij)} &\Big( \left\langle \mathcal{M}_n \widetilde{x^p y^q}, \widetilde{x^{k-3} y^{l+2}} \right\rangle \\
&- a \left\langle \mathcal{M}_n \widetilde{x^p y^q}, \widetilde{x^{k-2} y^l} \right\rangle \\
&- b \left\langle \mathcal{M}_n \widetilde{x^p y^q}, \widetilde{x^{k-3} y^l} \right\rangle \Big) \\
= &\Big( \left\langle B_{n+1} \widetilde{x^i y^{n+1-i}}, \widetilde{x^{k-3} y^{l+2}}, \right\rangle \\
&- a \left\langle B_{n+1} \widetilde{x^i y^{n+1-i}}, \widetilde{x^{k-2} y^l} \right\rangle \\
&- b \left\langle B_{n+1} \widetilde{x^i y^{n+1-i}}, \widetilde{x^{k-3} y^l} \right\rangle \Big) \\
= &\ \beta_{k+i-3,n+l-i+3} \\
&- a\beta_{k+i-2,n+l+1-i} \\
\text{(from (5.14))} \quad &- b\beta_{k+i-3,n+l+1-i} \\
\text{(from (5.19))} \quad = &\left\langle B_{n+1} \widetilde{x^i y^{n+1-i}}, \widetilde{x^k y^l} \right\rangle
\end{aligned}$$

where the change from $\mathcal{M}_n$ to $B_{n+1}$ is from (5.18) if $(k-3) \leq 2$, or by induction since $\rho = (k-3) + (l+2) = k + l - 1 < k + l$. This shows that (5.18) is always true, and so Lemma 5.12 is proved. □

We have now shown the following result.

**Proposition 5.13.** *If $\mathcal{M}_n$ is elliptic-pure, then there is a Hankel block $B_{n+1} \equiv B_{n+1}[\theta, \phi, \psi]$ which is compatible with a recursively generated Hankel extension $\mathcal{M}_{n+1}$. Moreover, we have* $\operatorname{Ran}(B_{n+1}) \subseteq \operatorname{Ran}(\mathcal{M}_n)$.

### 5.3.2 Examining $C_{n+1}$

We concentrate now on the remaining block $C_{n+1}$. The analysis below will shed insights into when flat extensions of $\mathcal{M}_n$ exist, and lead to a constructive proof of Theorem 5.14.

Since $\operatorname{Ran}(B_{n+1}) \subseteq \operatorname{Ran}(\mathcal{M}_n)$, we know that there exists a $W$ such that $B_{n+1} = \mathcal{M}_n W$, and that $\mathcal{M}_{n+1}$ is positive semi-definite if and only if

$$C_{n+1} \geq \widehat{C} \equiv B_{n+1}^T W (= W^T \mathcal{M}_n W),$$

furthermore $\mathcal{M}_{n+1}$ is a flat extension of $\mathcal{M}_n$ if and only if $C_{n+1} = \widehat{C}$.

Recall that we have the following column relations in $\mathcal{M}_{n+1}$

$$\begin{aligned} \mathbb{X}^{n+1} &= \mathbb{X}^{n-2}(\mathbb{Y}^2 - a\mathbb{X} - b\mathbb{1}), \\ \mathbb{X}^n\mathbb{Y} &= \mathbb{X}^{n-3}(\mathbb{Y}^3 - a\mathbb{X}\mathbb{Y} - b\mathbb{Y}), \\ &\vdots \\ \mathbb{X}^3\mathbb{Y}^{n-2} &= \mathbb{Y}^n - a\mathbb{X}\mathbb{Y}^{n-2} - b\mathbb{Y}^{n-2}. \end{aligned} \tag{5.20}$$

In particular, these relations must hold in $[B_{n+1}^T, C_{n+1}]$. The construction of $B_{n+1}$ shows that they also hold in $[B_{n+1}^T, \widehat{C}]$, which implies that $C_{n+1}$ and $\widehat{C}$ are the same in the columns $\mathbb{X}^{n+1}, \ldots, \mathbb{X}^3\mathbb{Y}^{n-2}$.

Positivity and symmetry of $\widehat{C}$ imply that $\widehat{C}$ has a Hankel structure if and only if the following hold

$$\widehat{C}_{n,n} = \widehat{C}_{n+1,n-1}, \tag{5.21}$$

$$\widehat{C}_{n+1,n} = \widehat{C}_{n+2,n-1}, \tag{5.22}$$

$$\widehat{C}_{n+1,n+1} = \widehat{C}_{n+2,n}, \tag{5.23}$$

where the first two equations are matching moments in the columns $\mathbb{X}^3\mathbb{Y}^{n-2}$ with $\mathbb{X}^2\mathbb{Y}^{n-1}$, and the last one is checking different locations of the moment $\beta_{2,2n}$. The element in row $n$, column $n$ of $C_{n+1}$ is

$$\langle C_{n+1}\widetilde{x^2y^{n-1}}, \widetilde{x^2y^{n-1}}\rangle,$$

and $C_{n+1} \geq \widehat{C}$ implies

$$\langle C_{n+1}\widetilde{x^2y^{n-1}}, \widetilde{x^2y^{n-1}}\rangle \geq \widehat{C}_{n,n} \tag{5.24}$$

We build and analyse $\widehat{C}$ to examine (5.21)-(5.23). Let $\mathcal{J} = [\mathcal{M}_n]_{\mathcal{B}}$, where $\mathcal{B}$ is a basis for $\mathcal{M}_n$. Write

$$\mathcal{J} = \begin{bmatrix} M & x \\ x^T & \Delta \end{bmatrix}$$

where $M$ is the submatrix of $\mathcal{M}_n$, with rows and columns indexed by $\mathcal{B}$ except $\mathbb{Y}^n$,

$$\mathbb{Y}^n = \begin{bmatrix} x \\ \Delta \end{bmatrix}$$

and thus $\Delta = \beta_{0,2n}$. Since both $\mathcal{J}$ and $M$ are positive definite, we have $\Delta > x^T M^{-1} x$. Let

$$\mathcal{J}^{-1} = \begin{bmatrix} P & v \\ v^T & \varepsilon \end{bmatrix}$$

with

$$P = M^{-1}(1 + \varepsilon x x^T M^{-1}), \quad v = -\varepsilon M^{-1} x, \quad \varepsilon = (\Delta - x^T M^{-1} x)^{-1}$$

Let $\widehat{W} = \mathcal{J}^{-1}[B_{n+1}]_{\mathcal{B}}$. So we have $[\mathcal{M}_n]_{\mathcal{B}}\widehat{W} = [B_{n+1}]_{\mathcal{B}}$, and we use this to define $W$. For each $\mathbb{X}^i\mathbb{Y}^j$, if $\mathbb{X}^i\mathbb{Y}^j \in \mathcal{B}$ then we let row $\mathbb{X}^i\mathbb{Y}^j$ in $W$ be the corresponding row of $\widehat{W}$. If $\mathbb{X}^i\mathbb{Y}^j \notin \mathcal{B}$, then we set row $\mathbb{X}^i\mathbb{Y}^j$ of $W$ to be a row of zeros. We know that $B_{n+1} = \mathcal{M}_n W$, and due to the column dependencies in $[\mathcal{M}_n, B_{n+1}]$, we have that $B_{n+1}^T W = [B_{n+1}]_{\mathcal{B}}^T \widehat{W}$. It follows

$$\widehat{C} = [B_{n+1}]_{\mathcal{B}}^T \widehat{W}. \tag{5.25}$$

For the remainder of this section, the compression $[\mathbb{X}^i\mathbb{Y}^j]_{\mathcal{B}}$ represents the column in $[B_{n+1}]_{\mathcal{B}}$. Lets start with (5.24). The column $[\mathbb{X}^2\mathbb{Y}^{n-1}]_{\mathcal{B}}$ is of the form

$$\begin{bmatrix} w \\ \theta \end{bmatrix}$$

(from the form of $B_{n+1} \equiv B_{n+1}(\theta, \phi, \psi)$), where $[w_1, \dots, w_{3n-1}]$ consists of 'old' moments. Let $r_1, \dots, r_{3n-1}$ be succesive row vectors of $P$ (in $\mathcal{J}^{-1}$) and $v^T = [v_1, \dots, v_{3n-1}]$. So

$$\mathcal{J}^{-1}[\mathbb{X}^2\mathbb{Y}^{n-1}]_{\mathcal{B}} = [c_1(\theta), \dots, c_{3n}(\theta)]^T$$

where $c_i(\theta) = \langle r_i, w\rangle + v_i\theta$ for $1 \le i \le 3n-1$, and $c_{3n}(\theta) = \langle v, w\rangle + \varepsilon\theta$. We can now compute

$$\begin{aligned}
\left\langle \widehat{C}\widetilde{x^2y^{n-1}}, \widetilde{x^2y^{n-1}} \right\rangle &= \left([B_{n+1}]_{\mathcal{B}}^T \mathcal{J}^{-1}[B_{n+1}]_{\mathcal{B}}\right)_{n,n} \\
&= [\mathbb{X}^2\mathbb{Y}^{n-1}]_{\mathcal{B}}^T \mathcal{J}^{-1}[\mathbb{X}^2\mathbb{Y}^{n-1}]_{\mathcal{B}} \\
&= [w_1, \dots, w_{3n-1}, \theta] \begin{bmatrix} c_1(\theta) \\ \vdots \\ c_{3n}(\theta) \end{bmatrix} \\
&= \sum_i^{3n-1} w_i c_i(\theta) + \theta\left(\langle v, w\rangle + \varepsilon\theta\right) \\
&= \varepsilon\theta^2 + 2\langle v, w\rangle\theta + \omega
\end{aligned}$$

where $\omega = \sum_i^{3n-1}\langle r_i, w\rangle w_i = \langle Pw, w\rangle$. Let $f(\theta) = \varepsilon\theta^2 + 2\langle v, w\rangle\theta + \omega$, then $\widehat{C}_{n,n} = f(\theta)$.

We also have

$$
\begin{aligned}
\text{(RG in } \mathcal{M}_{n+1}) \qquad \left\langle C_{n+1}\widetilde{x^2y^{n-1}}, \widetilde{x^2y^{n-1}} \right\rangle &= \left\langle C_{n+1}\widetilde{x^3y^{n-2}}, \widetilde{xy^n} \right\rangle \\
&= \left\langle \mathcal{M}_{n+1}\widetilde{y^n}, \widetilde{xy^n} \right\rangle \\
&\quad -a\left\langle \mathcal{M}_{n+1}\widetilde{xy^{n-2}}, \widetilde{xy^n} \right\rangle \\
&\quad -b\left\langle \mathcal{M}_{n+1}\widetilde{y^{n-2}}, \widetilde{xy^n} \right\rangle \\
&= \beta_{1,2n} - a\beta_{2,2n-2} - b\beta_{1,2n-2} \\
&= \phi - a\beta_{2,2n-2} - b\beta_{1,2n-2}
\end{aligned}
$$

which reduces (5.24) to

$$
\phi - a\beta_{2,2n-2} - b\beta_{1,2n-2} \geq f(\theta).
$$

Let us examine (5.21) more closely. We know that $\mathbb{X}^3\mathbb{Y}^{n-2} = \mathbb{Y}^n - a\mathbb{X}\mathbb{Y}^{n-2} - b\mathbb{Y}^{n-2}$ in $\mathcal{C}_{\mathcal{M}_n}$, this implies

$$
\begin{aligned}
\widehat{C}_{n+1,n-1} &= \left\langle \widehat{C}\widetilde{x^3y^{n-2}}, \widetilde{xy^n} \right\rangle \\
&= \beta_{1,2n} - a\beta_{1,2n-2} - b\beta_{0,2n-2} \\
&= \phi - a\beta_{1,2n-2} - b\beta_{0,2n-2}
\end{aligned}
$$

meaning that (5.21) holds if

$$
\widehat{C}_{n+1,n-1} = \phi - a\beta_{1,2n-2} - b\beta_{0,2n-2} = f(\theta) = \widehat{C}_{n,n}. \tag{5.26}
$$

Considering (5.22) ($\widehat{C}_{n+1,n} = \widehat{C}_{n+2,n-1}$), we start with

$$
\begin{aligned}
\widehat{C}_{n+2,n-1} &= \left\langle \widehat{M}\widetilde{x^3y^{n-2}}, \widetilde{y^{n+1}} \right\rangle \\
&= \left\langle \widehat{M}(\widetilde{y^n} - a\widetilde{xy^{n-2}} - b\widetilde{y^{n-2}}), \widetilde{y^{n+1}} \right\rangle \\
\text{(symmetry in } \widehat{M}) \qquad &= \left\langle \widehat{M}\widetilde{y^{n+1}}, (\widetilde{y^n} - a\widetilde{xy^{n-2}} - b\widetilde{y^{n-2}}) \right\rangle \\
&= \left\langle B_{n+1}\widetilde{y^{n+1}}, (\widetilde{y^n} - a\widetilde{xy^{n-2}} - b\widetilde{y^{n-2}}) \right\rangle \\
&= \psi - a\beta_{1,2n-1} - b\beta_{0,2n-1}.
\end{aligned}
$$

We may compute from (5.25)

$$
\begin{aligned}
\widehat{C}_{n+1,n} &= [\mathbb{X}\mathbb{Y}^n]_{\mathcal{B}}^T \mathcal{J}^{-1}[\mathbb{X}^2\mathbb{Y}^{n-1}]_{\mathcal{B}} \\
&= [\mathbb{X}\mathbb{Y}^n]_{\mathcal{B}}^T \begin{bmatrix} c_1(\theta) \\ \vdots \\ c_{3n}(\theta) \end{bmatrix}
\end{aligned}
$$

where $[\mathbb{X}\mathbb{Y}^n]_{\mathcal{B}}^T = [q_1, \dots, q_{3n-2}, \theta, \phi]$, and $q_i$ are 'old' moments. So

$$\widehat{C}_{n+1,n} = \sum_i^{3n-2} q_i c_i(\theta) + \theta c_{3n-1}(\theta) + \phi c_{3n}(\theta)$$

and (5.22) requires

$$\psi - a\beta_{1,2n-1} - b\beta_{0,2n-1} = \sum_i^{3n-2} q_i c_i(\theta) + \theta c_{3n-1}(\theta) + \phi c_{3n}(\theta). \tag{5.27}$$

Finally, for (5.23) ($\widehat{C}_{n+1,n+1} = \widehat{C}_{n+2,n}$) we have

$$\widehat{C}_{n+2,n} = [\mathbb{Y}^{n+1}]_{\mathcal{B}}^T \mathcal{J}^{-1} [\mathbb{X}^2\mathbb{Y}^{n-1}]_{\mathcal{B}},$$

where $[\mathbb{Y}^{n+1}]_{\mathcal{B}}^T = [p_1, \dots, p_{3n-3}, \theta, \phi, \psi]$, and $p_i$ are 'old' moments. This gives

$$\widehat{C}_{n+2,n} = \sum_i^{3n-3} p_i c_i(\theta) + \theta c_{3n-2}(\theta) + \phi c_{3n-1}(\theta) + \psi c_{3n(\theta)}.$$

To compute $\widehat{C}_{n+1,n+1}$, we set

$$\begin{aligned} [\mathbb{X}\mathbb{Y}^n]_{\mathcal{B}}^T &= [u_1, \dots, u_{3n-2}, \theta, \phi] \\ &= [u(\theta)^T, \phi] \end{aligned}$$

where $u_i$ are old moments. Then similar to before we get

$$\widehat{C}_{n+1,n+1} = \varepsilon\phi^2 + 2\phi\langle u(\theta), v\rangle + \langle Pu(\theta), u(\theta)\rangle$$

and (5.23) is equivalent to

$$\varepsilon\phi^2 + 2\phi\langle u(\theta), v\rangle + \langle Pu(\theta), u(\theta)\rangle = \sum_i^{3n-3} p_i c_i(\theta) + \theta c_{3n-2}(\theta) + \phi c_{3n-1}(\theta) + \psi c_{3n(\theta)}. \tag{5.28}$$

Notice that $\phi = \mathfrak{q}(\theta)$, where $\mathfrak{q}$ is a quadratic function of $\theta$. Substituting this into (5.27) shows that $\psi = \mathfrak{c}(\theta)$, where $\mathfrak{c}$ is a cubic function of theta. Finally, substituting these expressions for $\phi$ and $\psi$ into (5.28) show that it is equivalent to finding the root of a quartic polynomial $\mathcal{Q}(\theta)$. This observation proves the following.

**Theorem 5.14.** *Let $n \geq 3$. Suppose that $\mathcal{M}_n$ is positive and Elliptic-pure. A flat extension $\mathcal{M}_{n+1}$ of $\mathcal{M}_n$ exists if the quartic polynomial $\mathcal{Q}(\theta)$ has a real root.*

Some remarks are in order. Firstly, notice that compared to [38] the requirements for generating a flat extension are more complex. Even in [38] (Remark 2.5) it is noted that the number of constraints for flat extensions increases when $k > 3$ for the variety $y = x^k$. From our analysis, we suspect that when we work with the variety $y^k = x^3$, the number of constraints may remain the same, but their complexity grows with $k$.

Secondly, notice that in the elliptic-pure setting the existence of a flat extension and representing measure are not equivalent conditions. This is not surprising to us, since for $a \geq 0$, the commutative and tracial problems are equivalent, and we have observed this behavior in [10].

**Example 5.15.** Consider now the following example. We take (the unnormalized) $\mathcal{M}_3$ generated by the atoms

$$\{(x_i, y_i), (x_i, -y_i)\} \tag{5.29}$$

where

$$x_i = \frac{1}{i},\ y_i = \sqrt{x_i^3 - \frac{524287}{262144}x_i + 1}, \quad i = 1, \dots, 5. \tag{5.30}$$

It is clear that $\mathcal{M}_3$ satisfies the relation $\mathbb{Y}^2 = \mathbb{X}^3 - \frac{524287}{262144}\mathbb{X} + \mathbb{1}$ (Theorem 4.5 (1)). Moreover, we know that a representing measure exists.

A *numerical* representation of $\mathcal{M}_3$ is given by

$$\begin{pmatrix} 10 & 4.57 & 0 & 2.93 & 0 & 3.24 & 2.37 & 0 & 0.87 & 0 \\ 4.57 & 2.93 & 0 & 2.37 & 0 & 0.87 & 2.16 & 0 & 0.26 & 0 \\ 0 & 0 & 3.24 & 0 & 0.87 & 0 & 0 & 0.26 & 0 & 1.58 \\ 2.93 & 2.37 & 0 & 2.16 & 0 & 0.26 & 2.07 & 0 & 0.08 & 0 \\ 0 & 0 & 0.87 & 0 & 0.26 & 0 & 0 & 0.08 & 0 & 0.39 \\ 3.24 & 0.87 & 0 & 0.26 & 0 & 1.58 & 0.08 & 0 & 0.39 & 0 \\ 2.37 & 2.16 & 0 & 2.07 & 0 & 0.08 & 2.03 & 0 & 0.03 & 0 \\ 0 & 0 & 0.26 & 0 & 0.08 & 0 & 0 & 0.03 & 0 & 0.10 \\ 0.87 & 0.26 & 0 & 0.08 & 0 & 0.39 & 0.03 & 0 & 0.10 & 0 \\ 0 & 0 & 1.58 & 0 & 0.39 & 0 & 0 & 0.10 & 0 & 0.83 \end{pmatrix},$$

while $B_4$ takes the (numerical) form

$$\begin{pmatrix} 2.16 & 0 & 0.26 & 0 & 1.58 \\ 2.07 & 0 & 0.08 & 0 & 0.39 \\ 0 & 0.08 & 0 & 0.39 & 0 \\ 2.03 & 0 & 0.03 & 0 & 0.10 \\ 0 & 0.03 & 0 & 0.10 & 0 \\ 0.03 & 0 & 0.10 & 0 & 0.83 \\ 2.02 & 0 & 0.01 & 0 & 0.03 \\ 0 & 0.01 & 0 & 0.03 & 10\theta \\ 0.01 & 0 & 0.03 & 10\theta & 10\phi \\ 0 & 0.03 & 10\theta & 10\phi & 10\psi \end{pmatrix}.$$

A *Mathematica* computation reveals $\mathcal{Q}(\theta)$ (5.28) to be a quadratic equation

$$\theta^2 + c = 0, \tag{5.31}$$

in which $c$ is a positive rational. From this it is easy to see that no real solutions for $\theta$ exists, and hence, by the converse of Theorem 5.14, no flat extension to $\mathcal{M}_4$. The exact forms of $\mathcal{M}_3, B_4$ and $\mathcal{Q}(\theta)$ can be found in the associated *Mathematica* notebook https://github.com/

Abhishek-B/PhD-Thesis-Supplementary-Material.

**Remark 5.16.** It is interesting to note that (5.31) is a quadratic polynomial and not quartic. Through discussions with Zalar, we know that this can be understood by looking closer at the generating atoms (5.29) for Example 5.15. Since we use $y_i$ and $-y_i$ in (5.29), the odd degree moments of $y$ are equal to zero. Hence, the change of variables $z = y^2$, reduces Example 5.15 to the moment problem with $z = x^3$. A solution of which is dependent on a quadratic polynomial as shown in [38].

Chapter 6

# Conclusions and Future Work

To conclude, we summarize the thesis and our results. As is natural in mathematics, solutions to certain problems tend to raise more questions. We present several conjectures, questions and future research directions in this chapter. Many of these seem to be quite difficult problems, but we hope to study these in the near future.

## 6.1 Summary

This thesis studied aspects of the polynomial optimization problem

$$p^{min} = \min_{x \in \mathbb{R}^n} p(x),$$
$$s.t.\ g_1(x) \geq 0, \ldots, g_k(x) \geq 0.$$

In Chapter 2 we gave necessary background for approximations of $p^{min}$ via sum of squares. We discussed elementary properties of polynomials, formulating the SOS programs as semi-definite programs, and presented major results for SOS representations, such as Artin's solution to Hilbert's $17^{th}$ problem and the many Positivstellensätze. We discussed specializations of these results to strictly positive polynomials, and some recent advances towards understanding SOS representations for non-negative polynomials.

In Chapter 3 we compared state-of-the-art SOS relaxations for constructing non-negative, bihomogeneous, biquadratic polynomials which are not SOS. Our results are collected in the MATLAB package PnCP, an entanglement detection tool for quantum states. PnCP is the first computational package which not only employs entanglement criteria which are applicable for quantum states in arbitrary dimensions, it does so with state-of-the-art optimization algorithms.

The Truncated Tracial Moment Problem (dual to optimization of non-commutative polynomials) was presented in Chapter 4. We presented excerpts from the published, peer reviewed, journal article "The singular bivariate quartic tracial moment problem" [10], a collaborative project with Dr. Aljaž Zalar. It was shown that the bivariate quartic tracial moment problem reduces to four canonical cases when $\mathcal{M}_2$ has ranks 5 and 6. Furthermore, we presented results that in some rank 6 cases, the bivariate quartic tracial moment problem is equivalent to the feasibility of 3 LMI's and a rank condition.

Chapter 5 extends the study of the Tracial Moment Problem to arbitrary truncation orders, with the representing measure contained in an elliptic variety. We reduced the Tracial problem to the classic Moment Problem in two out of three canonical cases. Moreover, in the commutative setting we gave sufficient conditions for a representing measure to exist.

## 6.2 Open Questions

### 6.2.1 SOS Representations

As we saw in Chapter 2, for non-negative polynomials $p \in \mathbb{R}[x]$ and $\ell \in \mathbb{N}$, $(x_1^2+\cdots+x_n^2)^\ell p$ is not guaranteed to be SOS. However, the results of Chapter 3 indicate that for randomly generated polynomials, the denominator $(x_1^2+\cdots+x_n^2)^\ell$ generally works, i.e., Theorem 2.14 works for generic non-negative polynomials. It would be interesting to formalize this understanding. We conjecture the following on bad points (cf. Chapter 2).

**Conjecture 6.1.** *The set $\mathcal{B} = \{p \in \mathbb{R}[x] : p$ has a bad point at the origin$\}$ is closed.*

An affirmation of this conjecture would allow us to guarantee the theoretical success of the CNR relaxation of Chapter 3 and greatly improve the reliability of PnCP. Furthermore, if true Conjecture 6.1 would allow existing SOS and optimization software to also use the CNR relaxation.

A natural approach to Conjecture 6.1 is to examine the cone

$$C_{n,d}^N = \left\{ f \in \mathbb{R}[x_1,\ldots,x_n]_d : \left(\sum_{i=1}^n x_i^2\right)^N f = SOS \right\},$$

and to understand the asymptotic relationship between $C_{n,d}^N$ and the cone of non-negative polynomials $\mathcal{P}_{n,d}$. In [11] Blekherman studies a similar problem, and analyses the volumes of $\mathcal{P}_{n,m}$ and $\Sigma_{n,m}$. He showed that (asymptotically) there are many more non-negative forms, than there are SOS forms. It is readily seen that

$$\Sigma_{n,m} \subseteq C_{n,m}^0 \subseteq \cdots \subseteq C_{n,m}^N \subseteq \cdots \subseteq \mathcal{P}_{n,m},$$

and while it is known that $\bigcup_N C_{n,m}^N \neq \mathcal{P}_{n,m}$, the density of $C_{n,m}^N$ (for a fixed $N$) has not yet been studied. Specifically, we ask the following.

**Question 6.2.** *What is the aysmptotic relationship between the volumes of $C_{n,m}^N$ and $\mathcal{P}_{n,m}$? In particular, given some fixed $\varepsilon > 0$, is there some (possibly large) $N_\varepsilon$ such that (in an appropriate topology) $C_{n,m}^N$ is dense in $\mathcal{P}_{n,m}$ for $N > N_\varepsilon$?*

### 6.2.2 Tracial Moment Problem

We have made many advances in understanding the Tracial Moment Problem, particularly in the bivariate quartic setting, in [10]. In future works we would like to resolve the non-singular bivariate quartic tracial moment problem with rank 6 and column relation $\mathbb{Y}^2 = \mathbb{1}$. While this appears to be a difficult task, we believe techniques from [34] can help. We ask in the particular the following question.

**Question 6.3.** *Given an generalized nc Hankel matrix $\mathcal{M}_2(\beta)$ how can we check if there is an extension $\mathcal{M}_3(\beta)$ such that $\mathcal{M}_3(\beta)$ has a flat extension? More generally, how can we check if a given generalized Hankel matrix $\mathcal{M}_n(\beta)$ admits an extension to $\mathcal{M}_{n+1}(\beta)$ which then admits a flat extension $\mathcal{M}_{n+2}(\beta)$?*

It is also shown in Chapter 4, that in two of the rank 6 cases, the minimal measure consists of atoms of size at most 2. After reviewing some examples in [10], we conjecture that this is true for all quartic tracial sequences $\beta^{(4)}$.

**Conjecture 6.4.** *Given a quartic moment sequence $\beta^{(4)}$ (equivalently $\mathcal{M}_2(\beta)$) with a finitely atomic representative measure $\mu$, the atoms have size at most $2$, i.e., $2\times 2$ matrices can generate the moment sequence.*

While we have also made advances for the Tracial Moment Problem on elliptic varieties, the case of the relation $\mathbb{Y}^2 = \mathbb{X}^3 - \mathbb{X} + b\mathbb{1}$ is not well understood. We would like to examine the atoms in this case more closely, with the aim of find sufficient conditions for the existence of a measure.

Our immediate aim for the commutative elliptic-pure Moment Problem, is to find necessary conditions for the existence of a measure. The work of [94] may prove useful for this. It is known that if $\beta^{(2n)}$ admits a representing measure, then there is some $k \in \mathbb{N}$ such that $\mathcal{M}_{n+k}$ admits a flat extension $\mathcal{M}_{n+k+1}$. Our first approach to obtaining necessary conditions is to find an upper bound on $k$.

Chapter 6

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