Nonnegative Polynomials and Sums of Squares

— Boundary Structure, Symmetries and Sparsity —

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Deutsche Zusammenfassung

Die konvexen Kegel der nichtnegativen Polynome und Summen von Quadraten sind zentrale Objekte in der konvexen algebraischen Geometrie. Ihr Ursprung liegt in der bedeutenden Arbeit von Hilbert ([Hil88]). Darin werden bezüglich der Anzahl der Variablen n und dem Grad d der Polynome alle Fälle charakterisiert, in denen die Kegel übereinstimmen. Diese Übereinstimmung liegt nur für binäre Formen, quadratische Formen und für ternäre Quartiken vor. Seit dieser klassischen Arbeit ist die Frage nach der Differenz zwischen den beiden Kegeln auch heute noch ein sehr wichtiges und aktuelles Problem. Sie ist für viele Anwendungen von zentraler Bedeutung. Das sicherlich prominenteste Anwendungsgebiet liegt in polynomiellen Optimierungsproblemen, deren Lösung äquivalent dazu ist, die Nichtnegativität von Polynomen zu entscheiden. Diese Optimierungsprobleme lassen sich insbesondere dann effizient lösen, wenn sich spezielle nichtnegative Polynome in diesem Rahmen als Summe von Quadraten schreiben lassen. Der Grund hierfür liegt in der Tatsache, dass die Entscheidung, ob ein gegebenes Polynom nichtnegativ ist, im Allgemeinen NP-schwer ist ([BCSS98]). Die Frage, ob ein Polynom aber eine Summe von Quadraten ist, lässt sich mittels eines *semidefiniten Zugehörigkeitsproblems* lösen. Die Komplexität semidefiniter Zugehörigkeitsprobleme ist zwar im Allgemeinen ungeklärt, sie ist aber polynomiell für eine feste Anzahl an Variablen des Polynoms. Dementsprechend ist eine fundierte Kenntnis über die Differenz des Kegels der nichtnegativen Polynome und des Kegels der Summen von Quadraten sowohl auf der theoretischen als auch auf der praktischen Seite sehr wünschenswert.

Das Ziel dieser Arbeit ist die Untersuchung dieser beiden Kegel und ihres Zusammenspiels mit der reellen algebraischen und konvexen algebraischen Geometrie. Viele der erzielten Resultate gehen dabei explizit auf die Differenz dieser Kegel ein und charakterisieren diese für reichhaltige Klassen von Polynomen sogar explizit. Eine vollständige Beschreibung der Differenz dieser beiden Kegel ist aber aufgrund der komplexen Struktur der Kegel äußerst schwierig und unwahrscheinlich. Die Frage, ob und welche reichhaltigen Teilmengen oder Durchschnitte dieser Kegel vollständig beschrieben werden können, ist ein zentraler Ausgangspunkt vieler vorangegangener Arbeiten. Die neuen Resultate der vorliegenden Arbeit können in die folgenden Gebiete eingegliedert werden:

1. Die Untersuchung der Randstruktur der Kegel der nichtnegativen Polynome und Summen von Quadraten, insbesondere die Konstruktion trennender Hyperebenen und die Frage nach möglichen Dimensionen der Seiten dieser Kegel.

2. Die Frage nach der Nichtnegativität von Polynomen unter Ausnutzung von Symmetrien.

3. Die Untersuchung von dünnbesetzten Polynomen hinsichtlich der Nichtnegativität und Summen von Quadraten.

4. Die Anwendung der Dünnbesetztheit zur Berechnung unterer Schranken von Polynomen mittels geometrischer Programmierung.

Bevor die Resultate dieser Arbeit ausführlicher erläutert werden, wird im Folgenden eine kurze Übersicht über eine Auswahl an Referenzen gegeben, deren Inhalte unmittelbar in Zusammenhang zu dieser Arbeit stehen. In [CL78, CLR87, CLR80, Rez78] werden konkrete Beispiele und Konstruktionen nichtnegativer Polynome betrachtet, die sich nicht als Summe von Quadraten zerlegen lassen. Ein wesentlicher Bestandteil der Untersuchungen in diesen Arbeiten ist der Rand des Kegels der nichtnegativen Polynome sowie die maximale Anzahl an Nullstellen von nichtnegativen Polynomen. In [Ble06] liefert Blekherman Schranken für das Volumenverhältnis eines kompakten Schnitts des Kegels der nichtnegativen Polynome und des Kegels der Summen von Quadraten. Diese Schranken zeigen, dass für einen festgehaltenen Grad der Polynome, der mindestens vier ist, und wachsender Anzahl an Variablen, das Volumenverhältnis beliebig groß wird. Folglich gibt es bedeutend mehr nichtnegative Polynome als Summen von Quadraten. Hilberts klassische Konstruktion für die Existenz nichtnegativer Polynome, die keine Summe von Quadraten sind, wird in der Arbeit [Rez07] beschrieben und erweitert. Wesentliche Bestandteile dieser Untersuchungen sind erneut die Randstrukturen der Kegel sowie die möglichen Dimensionen ihrer zugehörigen Seiten. Die wichtigen Verbindungen von nichtnegativen Polynomen und Summen von Quadraten zu dem Gebiet der polynomiellen Optimierung sind in der Arbeit von Lasserre ([Las01]) sowie in der Arbeit von Parrilo und Sturmfels zu finden ([PS03]). Darüber hinaus gibt es mittlerweile reichlich Übersichtsartikel und Bücher zu diesen Themen ([DP01, Lau09, Mar08, Rez00, BPT13]). Viele weitere Resultate und Artikel finden sich in den zuvor referenzierten Arbeiten oder im weiteren Verlauf dieser Arbeit wieder. Die Resultate der vorliegenden Arbeit werden nun im Detail beschrieben.

Separierende Ungleichungen für nichtnegative Polynome, die keine Summe von Quadraten sind. Eines der wichtigsten Resultate in der konvexen Geometrie ist das Separationstheorem. In seiner einfachsten Form besagt es, dass es für eine abgeschlossene konvexe Menge $C \subset \mathbb{R}^n$ und einen Punkt $x \notin C$ ein lineares Funktional l gibt mit der Eigenschaft $l(x) < 0$ und

$l(C) \geq 0$. Da die Menge der nichtnegativen Polynome und die Menge der Summen von Quadraten abgeschlossene konvexe Kegel bilden, ist es ein interessantes Problem, separierende Ungleichungen für nichtnegative Polynome zu finden, die keine Summe von Quadraten sind. Ein zentrales Hilfsmittel für dieses Problem ist die Dualitätstheorie und die Untersuchung der zugehörigen dualen Kegel. Es ist wohlbekannt, dass solche separierenden Ungleichungen numerisch effizient mittels semidefiniter Programme (SDP) gefunden werden können ([Las01]). Da die Frage, ob ein Polynom eine Summe von Quadraten ist, über ein SDP entschieden werden kann, lässt sich eine separierende Ungleichung für ein nichtnegatives Polynom, das keine Summe von Quadraten ist, wie folgt bestimmen: Durch Formulierung des Problems mittels eines SDP's ist klar, dass dieses SDP unzulässig ist (da das Polynom per Annahme keine Summe von Quadraten ist). Dann liefert aber eine zugehörige Lösung des dualen SDP's ein (numerisches) lineares Funktional als Zertifikat, dass das Polynom keine Summe von Quadraten ist. Will man nun aber exakte (algebraische) Zertifikate haben, wird dieses Problem deutlich schwieriger. In der Tat ist kein allgemeines Verfahren hierfür soweit bekannt.

In den minimalen Fällen, in denen die Kegel der nichtnegativen Polynome und Summen von Quadraten nicht übereinstimmen ($(n, 2d) \in \{(3,6),(4,4)\}$), gibt Blekherman in seiner Arbeit [Ble12a] eine vollständige Charakterisierung der Extremalstrahlen des dualen Kegels der Summen von Quadraten. Diese sind nämlich über Summen von Punktevaluationsfunktionalen eines Polynoms p gegeben und besitzen die folgende Struktur:

$$l(p) = \sum_{i=1}^{m} a_i p(v_i), \; m \in \{8, 9\}, \tag{0.0.1}$$

wobei $a_i \in \mathbb{C}$ und die Punkte $v_i \in \mathbb{C}^n$ der Schnitt von zwei ternären Kubiken ($m = 9$) bzw. drei quaternären Quadriken ($m = 8$) sind. Ist nun p ein nichtnegatives Polynom, das keine Summe von Quadraten ist, so ist man interessiert an der Bestimmung von zwei ternären Kubiken ($m = 9$) bzw. drei quaternären Quadriken ($m = 8$) (sowie deren Schnittpunkte v_i), sodass $l(p) < 0$ ist. Für alle Quadratsummen q gilt dann $l(q) \geq 0$ nach Blekeherman's Resultaten in [Ble12a]. Die exakte Bestimmung und das Finden von *geeigneten* Schnittpunkten für ein festes Polynom p ist allerdings ein offenes Problem.

Basierend auf den Resultaten von Blekherman werden hinreichende Bedingungen für nichtnegative Polynome am Rand des Kegels geliefert, um solche separierenden Ungleichungen der Form (0.0.1) effizient zu konstruieren (Theoreme 3.3.1 und 3.3.3). Diese Kriterien können symbolisch und effizient getestet werden. Die Idee basiert darin, die Nullstellen dieser Polynome als Teil der Schnittpunkte v_i zu wählen. Dabei wird sich herausstellen, dass die vorgestellten Verfahren insbesondere dann effizient sind, wenn die Polynome hinreichend viele Nullstellen besitzen. Dies wird auf große Klassen von Polynomen zutreffen. In vielen Fällen lassen sich sogar rationale Zertifikate recht einfach konstruieren. Als unmittelbare Folgerung lassen sich dann sofort strikt positive Polynome konstruieren, die keine Summe von Quadraten sind. In seiner Arbeit [Ble12a] vermutet Blekherman, dass die Extremalstrahlen in (0.0.1) sogar rein reell beschrieben werden können, in der Hinsicht, dass man immer Schnittpunkte v_i findet, die reell sind. Diese Vermutung wird in der vorliegenden Arbeit von einem berechnungsbasierten Aspekt behandelt, der im wesentlichen äquivalent zu der Originalvermutung von Blekherman ist. Basierend auf den erzielten Resultaten kann vom berechnungsbasierten Standpunkt diese Vermutung für reichhaltige Klassen von Polynomen am Rand des Kegels der nichtnegativen Polynome bestätigt werden (Korollar 3.4.2). Durch einige Experimente und Beispiele wird zusätzlich das Problem der Konstruktion separierender Ungleichungen der Form (0.0.1) mit der Approximation semialgebraischer Mengen in Verbindung gebracht.

Seitenstruktur der Kegel der nichtnegativen Polynome und Summen von Quadraten. Die meisten wohlbekannten Beispiele nichtnegativer Polynome, die keine Summe von Quadraten sind, liegen auf dem Rand des Kegels der nichtnegativen Polynome, der aus all den nichtnegativen Polynomen mit mindestens einer reellen Nullstelle besteht. Der Grund hierfür ist, dass die meisten Konstruktionen solcher Polynome auf der klassischen Konstruktion von Hilbert basieren oder eine Verallgemeinerung dieser sind. Diese Methoden beruhen jedoch alle darauf, dass aus einer vorgegebenen Nullstellenmenge, nichtnegative Polynome konstruiert werden, die keine Summe von Quadraten sind. Die Untersuchung der Randstruktur dieser beiden Kegel ist noch in einem sehr frühen Stadium und sogar in den minimalen Ungleichheitsfällen der Kegel weitgehend offen. In den Gleichheitsfällen der Kegel ist wiederum deutlich mehr bekannt und das Problem zum Teil vollständig gelöst ([Bar02]). Aktuelle Resultate, die beispielsweise den algebraischen Rand dieser Kegel betreffen, liefern bereits ein Indiz für die komplexe Randstruktur der Kegel, da die Komponenten, die den Kegel der Summen von Quadraten von dem Kegel der nichtnegativen Polynome trennen, sehr hohen Grad besitzen ([BHO$^+$12]).

Motiviert durch diese Resultate und Techniken in [Rez07] werden folgende Ergebnisse bezüglich der Randstruktur der Kegel präsentiert. Betrachtet werden exponierte Seiten dieser Kegel, die gegeben sind durch eine Menge von nichtnegativen Polynomen bzw. Summen von Quadraten, die alle auf einer vorgegebenen, endlichen Punktmenge $\Gamma \subset \mathbb{R}^n$ verschwinden. Für ternäre Formen (drei Variablen) und quaternäre Quartiken (vier Variablen und Grad vier) wird als Hauptresultat die Frage nach Dimensionsdifferenzen zwischen den Seiten vollständig charakterisiert (Theoreme 4.2.1 und 4.3.1, Korollare 4.2.2 und 4.3.2). Präziser formuliert, wird in all diesen Fällen die minimale Kardinalität von Γ bestimmt, die eine Dimensionsdifferenz auf den zugehörigen exponierten Seiten bewirkt. Die Resultate gelten dabei unter schwachen Voraussetzungen an die Punkte (wie zum Beispiel die Forderung, dass die Punkte in allgemeiner Lage sind). Diese Dimensionsdifferenzen können dann ausgenutzt werden, um nichtnegative Polynome zu konstruieren, die keine

Summe von Quadraten sind. In den minimalen Ungleichheitsfällen der beiden Kegel wird gezeigt, dass die maximale Dimensionsdifferenz eins ist und diese 1-dimensionale Differenz sogar explizit charakterisiert (Propositionen 4.4.1 und 4.4.5). Dies liefert gleichzeitig eine Konstruktionsmethode für nichtnegative Polynome, die keine Summe von Quadraten sind.

Die Resultate nutzen dabei zum Teil stark kommutativ-algebraische Methoden aus. Wesentliche Bestandteile der Beweise für ternäre Formen basieren auf der Gleichheit von symbolischen Potenzen und gewöhnlichen Potenzen von Verschwindungsidealen. Da diese Potenzen im Allgemeinen über algebraisch abgeschlossenen Körpern betrachtet werden, ist es nötig, einige dieser Aussagen über den reellen Zahlen zu beweisen. Dies geschieht in den entsprechenden Abschnitten. Um die Dimensionen der Seiten explizit zu bestimmen, wird eine Generizitätsbedingung für endliche Punktmengen $\Gamma \subset \mathbb{R}^n$ eingeführt, die als *d-unabhängig* bezeichnet wird. Es stellt sich heraus, dass diese Bedingung Zariski offen ist. Durch die Konstruktion eines expliziten Beispiels einer d-unabhängigen Menge $\Gamma \subset \mathbb{R}^n$ der Größe $|\Gamma| = \binom{n+d-1}{d} - n$ wird gezeigt, dass fast jede endliche Menge Γ mit $|\Gamma| \leq \binom{n+d-1}{d} - n$ ebenfalls d-unabhängig ist (Proposition 4.1.7). In der Tat ist diese obere Schranke sogar optimal.

Das Problem, die Dimensionen der Seiten zu untersuchen, ist insbesondere deshalb interessant, weil man die Existenz nichtnegativer Polynome, die keine Summe von Quadraten sind, sofort aufgrund von einfachen Dimensionszählungen beweisen kann. Die vorgestellten Methoden basieren auf Perturbationstechniken, die in der Tat auf Hilberts klassische Konstruktion zurückgeführt werden können. Als Abschluss wird eine mögliche Erweiterung dieser Techniken für Polynome präsentiert, die nichtnegativ auf einer beliebigen, reellen projektiven Varietät sind.

Nichtnegativität von geraden symmetrischen Polynomen. Die Frage nach der Nichtnegativität von Polynomen ist besonders dann interessant, wenn die Polynome eine spezielle Struktur besitzen. Ein wesentliches Problem des allgemeinen Falls ist dadurch gegeben, dass die Dimension des Kegels der nichtnegativen Polynome und des Kegels der Summen von Quadraten sehr groß ist und sehr schnell anwächst, sobald der Grad oder die Anzahl der Variablen zunehmen. Für *symmetrische* Polynome sind diese Dimensionen deutlich kleiner und vor allem konstant, sobald die Anzahl der Variablen den Grad übersteigt. Die Untersuchung der Nichtnegativitätsfrage für symmetrische Polynome begann mit der Arbeit von Choi, Lam und Reznick in [CLR87], in welcher gerade symmetrische Sextiken untersucht werden. Das zentrale Resultat besagt, dass solche Polynome im $\mathbb{R}^n$ genau dann nichtnegativ sind, wenn sie auf allen Punkten $x \in \mathbb{R}^n$ mit maximal *einer* von Null verschiedenen Komponente nichtnegativ sind. In seinen Arbeiten [Har92b, Har99] erweitert Harris diese Resultate auf gerade symmetrische Oktiken (Grad acht Polynome) und gerade symmetrische ternäre Deziken (drei Variablen und Grad zehn). In diesen Fällen sind für die globale Nichtnegativität Punkte $x \in \mathbb{R}^n$ mit maximal *zwei* von Null verschiedenen Komponenten entscheidend. Zusätzlich wird gezeigt, dass es gerade symmetrische Polynome vom Grad zwölf gibt, deren Nichtnegativität nicht durch Punkte mit maximal zwei von Null verschiedenen Komponenten entscheidbar ist ([Har92b, Har99]). In seiner Arbeit [Tim03] lässt Timofte alle vorhergehenden Resultate als einfache Spezialfälle erscheinen und beweist, dass ein symmetrisches Polynom vom Grad $2d$ im $\mathbb{R}^n$ genau dann nichtnegativ ist, wenn es nichtnegativ auf allen Punkten $x \in \mathbb{R}^n$ mit maximal d verschiedenen Komponenten ist. Zusätzlich wird gezeigt, dass ein *gerade* symmetrisches Polynom vom Grad $2d$ genau dann nichtnegativ im $\mathbb{R}^n$ ist, wenn es nichtnegativ auf allen Punkten $x \in \mathbb{R}^n$ mit maximal $\lfloor \frac{d}{2} \rfloor$ verschiedenen Komponenten ist. Diese Resultate werden von Riener in den Arbeiten [Rie11, Rie12] in deutlich vereinfachter Form bewiesen.

In der vorliegenden Arbeit werden Resultate von Harris verallgemeinert. Dabei werden Polynome betrachtet, die in Unterräumen des Vektorraums der symmetrischen Polynome liegen. Als Hauptresultat werden für die Nichtnegativität solcher symmetrischen Polynome Schranken an die Anzahl der von Null verschiedenen Komponenten eines Punktes $x \in \mathbb{R}^n$ entwickelt. Diese sind einerseits sehr oft besser als die Schranken von Timofte und andererseits gar nicht vom Grad der Polynome, sondern nur von der Dimension der Unterräume abhängig und stehen demnach in starkem Kontrast zu Timoftes Resultat (Theorem 5.2.5). Sie sind insbesondere dann interessant, wenn der Grad der Polynome deutlich größer ist als die Anzahl der Variablen. Unter dieser Voraussetzung ist das Resultat von Timofte nämlich nutzlos und bringt keine Vereinfachung der Nichtnegativitätsfrage eines symmetrischen Polynoms mit sich. Ferner zeigen die vorgestellten Resultate, dass das bessere Maß für die Anzahl der verschiedenen Komponenten eines Punktes $x \in \mathbb{R}^n$ nicht der Grad der Polynome ist (wie in Timoftes Resultat), sondern die Dimension der Unterräume, in denen die Polynome liegen.

Dünnbesetzte nichtnegative Polynome, konvexe Polynome und Summen von Quadraten. Eine Teilmenge $A \subset \mathbb{N}^n$ heißt ein *Kreis* (engl. circuit), wenn A affin abhängig, aber jede echte Teilmenge von A affin unabhängig ist. Als ersten nichttrivialen Fall im Zusammenhang mit nichtnegativen Polynomen und Summen von Quadraten werden Polynome betrachtet, deren Newton Polytope Simplizes sind und deren Trägermengen genau aus den Ecken und einem zusätzlichen inneren Gitterpunkt der Simplizes bestehen. Diese Trägermengen sind dann ein Kreis im Sinne der obigen Definition. In Kapitel 6 werden nichtnegative Polynome und Summen von Quadraten auf solchen Trägermengen vollständig charakterisiert (Theoreme 6.2.6 und 6.3.2). Wie sich herausstellt, hängt speziell die Frage nach der Quadratsummeneigenschaft ausschließlich von der Gitterpunktkonfiguration im Simplex ab und nicht von den Koeffizienten des Polynoms, was auf dem ersten Blick sehr überraschend ist. Diese Bedingung stellt zudem interessante Verbindungen zu dem Gebiet der torischen Geometrie und der Theorie der Gitterpolytope her. Durch Ausnutzung dieser Verbindungen werden große Teilmengen im Vektorraum der

Polynome in n Variablen vom Grad $2d$ gefunden, auf denen der Kegel der nichtnegativen Polynome mit dem Kegel der Summen von Quadraten übereinstimmt (Theorem 6.4.1, Korollare 6.4.2 und 6.4.4). Das vielleicht prominenteste Beispiel eines nichtnegativen Polynoms mit solch einer Trägermenge ist die *arithmetisch-geometrische Ungleichung*, die sich als einfacher Spezialfall eines nichtnegativen Polynoms auf dem Rand des Kegels der nichtnegativen Polynome herausstellen wird. In dieser Hinsicht können die vorgestellten Resultate über die Nichtnegativität solcher Polynome als Verallgemeinerung der arithmetisch-geometrischen Ungleichung angesehen werden. Motiviert durch das noch heute ungelöste Problem ein konvexes homogenes Polynom zu finden, das keine Summe von Quadraten ist, wird daher auch der Schnitt des Kegels der konvexen Polynome auf solchen Trägermengen vollständig charakterisiert (Theorem 6.5.4). Wie sich etwas überraschend herausstellt, gibt es bis auf wenige Spezialfälle (univariate Polynome und deren Homogenisierung) keine konvexen Polynome mit solchen Trägermengen. Da sich besonders die Untersuchung des Kegels der konvexen Polynome noch in einem sehr frühen Stadium befindet, können diese Resultate als Indiz dafür gedeutet werden, dass die Dünnbesetztheit von Polynomen eine Struktur ist, welche die Konvexität von Polynomen verhindert. Basierend auf den Resultaten bezüglich der Nichtnegativität und Summen von Quadraten wird ein neuer konvexer Kegel eingeführt, der *Kegel der Summen von nichtnegativen Kreispolynomen*. Dieser liefert, ähnlich wie die Summen von Quadraten, ein Nichtnegativitätszertifikat, ist allerdings grundsätzlich verschieden von dem Kegel der Summen von Quadraten. Dieser neue Kegel wird sich speziell in der polynomiellen Optimierung im weiteren Verlauf der Arbeit als sehr wichtig erweisen. Es werden viele neue Fragestellungen bezüglich dieses Kegels formuliert und anhand von Beispielen demonstriert. Abschließend werden die Resultate auf beliebige Newton Polytope erweitert und einige offene Probleme in [Rez89] gelöst (Proposition 6.7.1 und Theorem 6.7.2). Hierbei entsteht ein interessanter Zusammenhang zu Triangulierungsproblemen von Polytopen.

Untere Schranken von Polynomen mittels geometrischer Programmierung. Geometrische Programme für die Berechnung unterer Schranken von Polynomen bilden eine Alternative zu unteren Schranken mittels semidefiniter Programmierung. In aktuellen Arbeiten [GM12, GM13] wird dabei ein wichtiger Trade-Off zwischen geometrischen Programmen (GP) und semidefiniten Programmen (SDP) beobachtet: Einerseits können in den obigen Arbeiten GP-basierte untere Schranken nicht besser sein als SDP-basierte untere Schranken. Andererseits können mit geometrischen Programmen weitaus höherdimensionalere Beispiele in kurzer Zeit berechnet werden, während semidefinite Programme aufgrund der schnell und stark anwachsenden Matrizengrößen in dem Programm keinerlei Ergebnisse liefern, oder sehr lange für die Berechnung brauchen.

Motiviert durch die Resultate über dünnbesetzte Polynome in Kapitel 6 werden die in der Literatur bestehenden Klassen der geometrischen Programme für die Bestimmung unterer Schranken von Polynomen signifikant erweitert. Dabei wird gefordert, dass die Newton Polytope der Polynome Simplizes sind, was z.B. für allgemeine Polynome in n Variablen vom Grad d mit voller Trägermenge immer der Fall ist. Diese Erweiterung basiert auf hinreichenden Bedingungen an die Koeffizienten eines Polynoms, damit sich das Polynom als Summe von nichtnegativen Kreispolynomen schreiben lässt, die in Kapitel 6 neu eingeführt werden (Theoreme 7.1.1 und 7.1.2). Ein fundamentales Resultat wird dabei die Eigenschaft sein, dass die unteren Schranken mittels geometrischer Programmierung in vielen Fällen sogar *besser* sind als die semidefiniten Schranken, obwohl sie sich speziell für höherdimensionalere Beispiele deutlich schneller berechnen lassen (Korollar 7.1.4). Es liegt hier also eine win-win Situation vor. Diese Situation lässt sich in den bestehenden Arbeiten [GM12, GM13] nicht beobachten, weil die dort betrachteten Programme sich als Spezialfälle der in dieser Arbeit betrachteten Programme herausstellen. Der Grund für diese Beobachtungen liegt in der Tatsache, dass die in der vorliegenden Arbeit vorgestellten geometrischen Programme nicht auf Quadratsummenzertifikaten basieren, sondern auf der Darstellung nichtnegativer Polynome als Summe von nichtnegativen Kreispolynomen. In vielen Fällen folgt daraus aber auch bereits die Quadratsummeneigenschaft, auf der die Programme in [GM12, GM13] basieren. Zusammengefasst ist daher offensichtlich, dass der neu eingeführte konvexe Kegel der Summen von nichtnegativen Kreispolynomen einen völlig neuen Blickwinkel sowohl für die schwierige Entscheidung der Nichtnegativität eines Polynoms als auch für das Optimieren von Polynomen liefert.

Bereits veröffentlichte Inhalte. Die Inhalte dieser Dissertation sind in den Arbeiten [BIK13, IdW13, IdW14a, IdW14b, IdW14c] veröffentlicht bzw. zur Veröffentlichung eingereicht.

Contents

Chapter 1

Introduction

The cones of nonnegative polynomials and sums of squares arise as central objects in convex algebraic geometry and have their origin in the seminal work of Hilbert ([Hil88]). Depending on the number of variables n and the degree d of the polynomials, Hilbert famously characterizes all cases of equality between the cone of nonnegative polynomials and the cone of sums of squares. This equality precisely holds for bivariate forms, quadratic forms and ternary quartics ([Hil88]). Since then, a lot of work has been done in understanding the difference between these two cones, which has major consequences for many practical applications such as for polynomial optimization problems. Roughly speaking, minimizing polynomial functions (constrained as well as unconstrained) can be done efficiently whenever certain nonnegative polynomials can be written as sums of squares (see Section 2.3 for the precise relationship). The underlying reason is the fundamental difference that checking nonnegativity of polynomials is an NP-hard problem whenever the degree is greater or equal than four ([BCSS98]), whereas checking whether a polynomial can be written as a sum of squares is a *semidefinite feasibility problem* (see Section 2.2). Although the complexity status of the semidefinite feasibility problem is still an open problem, it is polynomial for fixed number of variables. Hence, understanding the difference between nonnegative polynomials and sums of squares is highly desirable both from a theoretical and a practical viewpoint.

The aim of this thesis is the discussion of nonnegative polynomials and sums of squares and their interplay with real algebraic and convex algebraic geometry. We also describe applications in polynomial optimization. Many of our results address the difference between these two cones and characterize it explicitly for rich classes of polynomials. In general, a complete and explicit description of the difference between these two cones is a highly complicated problem, due to the complex structure of these cones. However, the problem to find large subsets or intersections of these cones that can be described explicitly, is the origin of many articles concerning nonnegative polynomials and sums of squares. We add to these works and present several other results, which can be integrated in the following areas:

1. The investigation of the *boundary structure* of the cones of nonnegative polynomials and sums of squares, especially concerning the question of possible dimensions of the faces of these cones and the construction of separating inequalities.

2. The question of nonnegativity of polynomials under the additional structure of *symmetries*.

3. The investigation of *sparsity* structures of polynomials concerning nonnegativity and sums of squares.

4. The application of sparsity structures in *geometric programming* for computing lower bounds for polynomials.

Before describing the new results in this thesis in more detail, we briefly give an overview about some references, which are related to the contents of this thesis. In [CL78, CLR87, CLR80, Rez78] the authors investigate some special constructions of nonnegative polynomials that are not sums of squares. They are mainly based on the boundary structure and the number of possible zeros a nonnegative (resp. a sum of squares) polynomial can have. In [Ble06] Blekherman provides volume bounds for the volume ratio of some compact sections of these cones. He proves that for fixed degree $2d \geq 4$, there are significantly more nonnegative polynomials than sums of squares as the number of variables runs off to infinity. The classical Hilbert construction to prove existence of nonnegative polynomials that are not sums of squares is reviewed and significantly extended in [Rez07] by providing more general perturbation methods to construct such polynomials in low dimensions. These methods rely on studying the boundary structure and dimensions of some faces of the cones. The seminal relationship between nonnegative polynomials and sums of squares as well as polynomial optimization is described in the work of Lasserre in [Las01] and in the work of Parrilo and Sturmfels in [PS03]. For some surveys about nonnegative polynomials and sums of squares as well as their interplay with polynomial optimization we refer to [DP01, Lau09, Mar08, Rez00, BPT13]. There are many other results in this area concerning several special cases and exploiting structures in the problems such as, e.g., symmetry and sparsity of polynomials. Many of these results can be found in the references of the articles described above as well as in later sections of this thesis. We now describe the results in this thesis in more detail.

Separating inequalities for nonnegative polynomials that are not sums of squares. One of the most basic theorems in convex geometry is the separation theorem for convex sets. In its easiest form it says that if $C \subset \mathbb{R}^n$ is a closed convex set and $x \notin C$, then there exists a linear functional l such that $l(x) < 0$ and $l(C) \geq 0$. Since both nonnegative polynomials and sums of squares are full dimensional closed convex cones, one basic problem is the determination of such separating hyperplanes for nonnegative polynomials that are not sums of squares. The major tool for studying questions of this type is given by duality theory and the corresponding dual cones. It is well known that such linear functionals can be obtained efficiently in a numerical way via semidefinite programming ([Las01]). Since testing for the property of being a sum of squares is a semidefinite program (SDP), one of the most common methods to obtain a separating functional for a nonnegative polynomial p that is not a sum of squares is to formulate an SDP requiring the polynomial p to be a sum of squares. Since this SDP is clearly infeasible, any feasible solution of the corresponding dual SDP yields a separating functional. However, the problem gets significantly harder when these functionals (serving as certificates for not being a sum of squares) have to be exact. In fact, no general symbolic method for solving this problem is known so far.

In the smallest cases where there exist nonnegative polynomials that are not sums of squares (i.e., $(n, 2d) \in \{(3, 6), (4, 4)\}$), in [Ble12a] Blekherman completely describes the extreme rays of the dual sums of squares cones. These extreme rays l are given by sums of certain point evaluations of a polynomial p and are of the form

$$l(p) = \sum_{i=1}^{m} a_i p(v_i), \;\; m \in \{8, 9\} \tag{1.0.1}$$

where $a_i \in \mathbb{C}$ and the points $v_i \in \mathbb{C}^n$ come from the intersection of two ternary cubics ($m = 9$) resp. three quaternary quadrics ($m = 8$). However, the determination of such intersection points in order to build separating inequalities for a polynomial p is still an open problem from a symbolic viewpoint. Using these results, we provide sufficient criteria to efficiently obtain such separating functionals for nonnegative polynomials on the boundary of the cones (Theorems 3.3.1 and 3.3.3). These criteria can be checked in a completely symbolic and efficient way. The key idea of this approach is to use the zeros of the polynomials to construct the cubics and quadrics leading to the separating inequalities of the Form (1.0.1). The more zeros the polynomials have, the more efficient this procedure works. Furthermore, for several important classes we can provide exact functionals that are even rational whenever the zeros of the polynomials involved are rational. As a direct consequence, in these cases we can also construct strictly positive polynomials that are not sums of squares with the same separating functional. In [Ble12a] Blekherman conjectures that all the extreme rays of the dual sums of squares cones can be described in a totally real manner, meaning, that all points v_i in the representation (1.0.1) of the extreme rays can be chosen to be real. We consider this conjecture from a more computational viewpoint, which is basically equivalent to the original conjecture. As a corollary, we obtain that our modified conjecture holds (at least) for all boundary polynomials with sufficiently many zeros (see Corollary

3.4.2). We provide examples yielding connections between satisfiability of the criteria in Theorems 3.3.1 and 3.3.3 and approximation of semialgebraic sets.

Facial structure of nonnegative polynomials and sums of squares. Most of the known and prominent nonnegative polynomials that are not sums of squares lie on the boundary of the cone of nonnegative polynomials, which consists of all those polynomials that have at least one real zero. The reason for this is that most of the methods used to construct explicit examples of nonnegative polynomials that are not sums of squares are based on Hilbert's construction or generalizations of it ([Rez07]). These methods yield polynomials with many zeros. The problem of understanding the boundary and the faces of the cones of nonnegative polynomials and sums of squares is widely open, except in the cases of binary forms and quadratic forms ([Bar02]). But already in the smallest cases where the two cones differ, a complete characterization of possible dimensions of the faces is open. Recent results concerning the algebraic boundary of the cone of sums of squares indicate the very complicated structure, since the components discriminating sums of squares from nonnegative polynomials have very large degree ([BHO$^+$12]).

Motivated by results and techniques in [Rez07] we present the following results concerning the facial structure of the cones of nonnegative polynomials and sums of squares. In this thesis we consider exposed faces that are given by polynomials vanishing on a finite set of points $\Gamma \subset \mathbb{R}^n$. For ternary forms as well as for quaternary quartics (four variables and degree four) we provide a complete characterization of the question whether and when there exist dimensional differences between the faces of these cones and when they occur for the first time (Theorems 4.2.1 and 4.3.1, Corollaries 4.2.2 and 4.3.2). More precisely, we determine the smallest cardinality of $\Gamma \subset \mathbb{R}^n$ to observe dimensional gaps between the faces that are given by nonnegative resp. sums of squares polynomials vanishing on Γ. These results hold under some mild conditions (such as, e.g., the condition for the points in Γ to be in general position). For both ternary forms and quaternary quartics we explicitly describe a 1-dimensional difference between these faces yielding a systematic way of constructing nonnegative polynomials on these faces that are not sums of squares (Propositions 4.4.1 and 4.4.5). Indeed, this 1-dimensional difference is actually optimal in the smallest cases where nonnegative polynomials are not sums of squares (i.e., $(n, 2d) \in \{(3, 6), (4, 4)\}$).

Our results for ternary forms are strongly based on commutative algebraic methods. In fact, major steps in some proofs follow by dimensional equality between symbolic powers and ordinary powers of vanishing ideals of certain point sets. Since the theory about symbolic powers and ordinary powers of ideals is mainly considered over algebraically closed fields, we translate some results to the case of real numbers. Furthermore, in order to determine the dimension of the exposed faces, we introduce a genericity condition called *d-independence* for finite sets of points in $\mathbb{R}^n$. This condition will be shown to be Zariski open. By constructing an explicit example of such a set of size $\binom{n+d-1}{d} - n$, this yields that almost every finite set of points $\Gamma \subset \mathbb{R}^n$ is d-independent for $|\Gamma| \leq \binom{n+d-1}{d} - n$ (Proposition 4.1.7). In fact, one can actually show that $\binom{n+d-1}{d} - n$ is an upper bound for the cardinality of a d-independent set and hence it is optimal.

The problem of studying dimensions of the faces of the cones of nonnegative polynomials and sums of squares is particularly interesting, since it allows to prove existence of nonnegative polynomials that are not sums of squares by simple dimension counting. In fact, our results rely on perturbation methods, which can be traced back to Hilbert's classical construction. We end the chapter with an outlook for generalizing these ideas to faces of nonnegative polynomials and sums of squares on arbitrary real projective varieties.

Nonnegativity of even symmetric polynomials. The problem of deciding nonnegativity of polynomials is particularly interesting whenever the polynomials involved have some structure. One obstacle in considering the full cones of nonnegative polynomials and sums of squares relies on the fact that these cones have very large dimensions with growing number of variables or degree. By considering *symmetric* polynomials, the dimensions of these cones are much smaller and, more importantly, they are fixed once the number of variables exceeds the degree of the polynomials. The problem of deciding nonnegativity of symmetric polynomials began with the work of Choi, Lam and Reznick in [CLR87], in which the authors consider even symmetric sextics. They provide a complete semialgebraic description of nonnegative even symmetric sextics and even symmetric sextics that are sums of squares. The key result is that checking nonnegativity in this case can be reduced to checking nonnegativity of univariate polynomials, since it suffices to prove nonnegativity of even symmetric sextics at all points $x \in \mathbb{R}^n$ with at most *one* nonzero component. In [Har92b, Har99] Harris adds to this work by establishing that even symmetric octics (degree $2d = 8$) and even symmetric ternary decics ($n = 3, 2d = 10$) are nonnegative if and only if they are nonnegative at all points $x \in \mathbb{R}^n$ with at most *two* distinct nonzero components. In the case of even symmetric ternary octics it is actually shown that nonnegativity coincides with the property of being a sum of squares. However, he also proves that nonnegativity of even symmetric ternary forms of degree $2d \geq 12$ cannot be checked by considering points with at most two nonzero components.
In [Tim03] Timofte proves a very powerful result, namely, that a symmetric polynomial of degree $2d$ is nonnegative if and only if it is nonnegative at all points $x \in \mathbb{R}^n$ with at most d distinct components. Additionally, an *even* symmetric polynomial of degree $2d$ is nonnegative if and only if it is nonnegative at all points $x \in \mathbb{R}^n$ with at most $\lfloor \frac{d}{2} \rfloor$ distinct components. Later, Riener was

able to reprove these results in a much more elementary fashion than in the original work, where most techniques are based on the theory of differential equations (see [Rie11, Rie12]). Generalizing results in [Har99] we consider even symmetric forms contained in subspaces of even symmetric forms of degree $4d$ in n variables. Concerning the question of nonnegativity of these forms, we develop a uniform bound on the number of distinct components of a point $x \in \mathbb{R}^n$. This bound is independent of the degree of the forms and is often better than Timofte's bound (Theorem 5.2.5). This is in sharp contrast to Timofte's theorem in [Tim03], which states that the number of distinct components depends on the degree of the polynomials. Hence, our result serves as an indication that it is not the degree that is essential for the number of distinct components of points $x \in \mathbb{R}^n$ that have to be checked for nonnegativity. In fact, the proper measure for the number of distinct components seems to be the dimension of the subspaces containing the forms. Our construction is particularly interesting when the degree of the polynomials is significantly larger than the number of variables. In this case, Timofte's bound is useless, since the number of distinct components that have to be checked is larger than the number of variables of the forms.

Nonnegative, Convex, and Sums of Squares Polynomials Supported on Circuits. A subset $A \subset \mathbb{N}^n$ is called a *circuit* if A is affinely dependent but any proper subset of A is affinely independent. We consider polynomials f such that the Newton polytope of f is a simplex and the support of f consists of all the vertices of the simplex with an additional interior lattice point in the simplex. Such polynomials can be regarded as polynomials *supported on a circuit*. We completely characterize the question when such polynomials are nonnegative resp. sums of squares (Theorems 6.2.6 and 6.3.2). As will be seen, the latter question heavily depends on the combinatorial structure of the simplex and, surprisingly enough, it is independent of the coefficients of the polynomials. It yields a very interesting connection to toric geometry and lattice polytopes. By using this connection in more detail, we provide sufficient conditions for simplices to imply equality between nonnegative polynomials and sums of squares. In particular, this characterization yields large subsets of the vector space of polynomials in n variables of even degree $2d$ on which nonnegative polynomials are sums of squares (Theorem 6.4.1, Corollaries 6.4.2 und 6.4.4). The most prominent example in this context is the well known *arithmetic-geometric mean inequality*, which can be considered as a special case of a polynomial supported on a circuit and lying on the boundary of the cone of nonnegative polynomials. Motivated by the open problem to find a convex homogeneous polynomial that is not a sum of squares, we investigate convexity of polynomials supported on circuits and prove the surprising result that there are no convex polynomials supported on circuits, except in the simple univariate case and its homogenization (Theorem 6.5.4). Based on our results about nonnegativity and sums of squares, we introduce a new convex cone, the cone of *sums of nonnegative circuit polynomials*. This convex cone serves as a nonnegativity certificate, which is very different than sums of squares certificates. It also plays a crucial role in polynomial optimization as described in Chapter 7. As a final step, we extend our results to polynomials with arbitrary Newton polytopes and supports given by the vertices of the polytopes and one additional lattice point in the interior. This extension yields interesting connections to triangulation problems of polytopes and solves some open problems in [Rez89] (Proposition 6.7.1 and Theorem 6.7.2).

Lower Bounds for Polynomials with Simplex Newton Polytopes Based on Geometric Programming. Besides the well known techniques based on semidefinite programming, recently, there is much interest in finding lower bounds for polynomials using *geometric programming*. In recent works [GM12, GM13] there is an interesting trade-off that can be observed when comparing the bounds based on semidefinite programming (SDP) and geometric programming (GP). On the one hand, bounds based on GP are not as good as bounds based on SDP. On the other hand, even higher dimensional examples (e.g., polynomials with large degree) can be solved quite fast with GP, whereas SDP methods yield no output at all (or require a very long running time) due to the growing size of the involved matrices.

Motivated by our results about sparse nonnegative polynomials in Chapter 6 we propose new geometric programs that significantly extend the existing ones in the literature in order to find lower bounds for polynomials. Therefore, we require the Newton polytopes of the polynomials to be simplices, which is, e.g., the case for general polynomials in n variables of degree d with full support. These geometric programs are based on conditions on the coefficients of a polynomial that are sufficient to imply that the polynomial is a sum of nonnegative circuit polynomials, which we introduce in Chapter 6 (Theorems 7.1.1 und 7.1.2). One fundamental result is the fact that for many instances the GP based lower bounds are *better* than the SDP based lower bounds, in spite of the fact that they can be computed much faster for higher dimensional examples (Corollary 7.1.4). This is a win-win situation that cannot be observed in other recent works in [GM12, GM13]. The underlying reason for this is the fact that our results rely on the decomposition of nonnegative polynomials as sums of nonnegative circuit polynomials rather than sums of squares, which are part of the geometric programs in [GM12, GM13]. However, for the polynomials considered in [GM12, GM13], these two properties coincide. In this case the SDP based bounds are at least as good as the GP based bounds. Hence, it is obvious that our introduced convex cone of sums of nonnegative circuit polynomials yields a completely new viewpoint both for deciding nonnegativity of polynomials and to optimize polynomials with geometric programming.

Thesis Overview. This thesis is organized as follows. In Chapter 2 we introduce the basic concepts of this thesis. It contains basic facts about nonnegative polynomials and sums of squares, connections to semidefinite programming, duality theory based on the problem of moments and some facts and definitions about the quantitative relationship between nonnegative polynomials and sums of squares as well as about the facial structure of these cones.

In Chapter 3 we state and prove sufficient conditions and construction methods for separating inequalities for nonnegative polynomials that are not sums of squares and that lie on the boundary of the cone of nonnegative polynomials. In this case, it is (relatively) easy to generate strictly positive polynomials that are not sums of squares. We provide some examples and conjectures, which connect the satisfiability problem of the sufficient conditions to the approximation of semialgebraic sets.

Chapter 4 is dedicated to the boundary structure of the cone of nonnegative polynomials and sums of squares. We describe exposed faces of both cones and establish dimensional differences between their faces yielding a procedure to construct nonnegative polynomials that are not sums of squares. In particular, we investigate the question when these dimensional differences occur for the first time and provide bounds that are actually optimal in many cases. By characterizing some dimensional differences explicitly, we provide exact methods in order to construct nonnegative polynomials that are not sums of squares.

In Chapter 5 we investigate nonnegativity of even symmetric forms of degree $4d$ in subspaces of arbitrary dimension in the vector space of even symmetric forms of degree $4d$. We provide subspaces on which nonnegativity can be certified at points $x \in \mathbb{R}^n$, whose number of distinct components is less than in Timofte's theorem and is independent of the degree of the involved polynomials. Furthermore, we introduce a new invariant relating the maximum dimension of a subspace to the property of certifying nonnegativity of polynomials in that subspace at points with a fixed number of distinct components.

In Chapter 6 we discuss polynomials supported on circuits. More precisely, we consider polynomials p such that the Newton polytope of p is a simplex and the support of p consists of all the vertices of the simplex and an additional interior lattice point. For these polynomials we provide a complete solution to the question when these polynomials are nonnegative resp. sums of squares. This will result in many new subsets on which nonnegative polynomials are sums of squares. Additionally, using techniques from toric geometry, we provide conditions on the simplex Newton polytopes to force equality between nonnegative polynomials and sums of squares. Furthermore, we completely characterize convex polynomials in this setting and extend all our results to arbitrary Newton polytopes.

Finally, using results in Chapter 6, in Chapter 7 we introduce a new geometric program in order to produce lower bounds for polynomials. This approach is based on conditions on the coefficients of a polynomial that are sufficient to imply that the polynomial is a sum of nonnegative circuit polynomials.

Published Contents in Advance. The contents of this thesis are published or submitted for publication. They are based on the articles [BIK13, IdW13, IdW14a, IdW14b, IdW14c] together with new examples.

Chapter 2

Preliminaries

This chapter gives a short introduction to the basic concepts of this thesis. We start by introducing the main objects of our thesis, namely the cone of nonnegative polynomials and the cone of sums of squares. We present some key relationships between them and their connection to the widely used technique of semidefinite programming. Furthermore, we introduce some basic concepts of polynomial optimization using sums of squares techniques. Finally, the reader is familiarized with some results concerning the quantitative and qualitative relationship between nonnegative polynomials and sums of squares when taking a convex geometric viewpoint.

2.1 The Cone of Nonnegative Polynomials and Sums of Squares

We consider the vector space of polynomials in n variables of degree at most d and denote it by $\mathbb{R}[\mathbf{x}]_d := \mathbb{R}[x_1, \ldots, x_n]_d$. It is easy to check that $\dim \mathbb{R}[\mathbf{x}]_d = \binom{n+d}{d}$. We will always use the standard multi-index notation: For a polynomial $p \in \mathbb{R}[\mathbf{x}]_d$ and $\alpha \in \mathbb{N}_d^n := \{\alpha \in \mathbb{N}^n : |\alpha| = \alpha_1 + \cdots + \alpha_n \leq d\}$ we use the notation $p = \sum_{\alpha \in \mathbb{N}_d^n} p_\alpha \mathbf{x}^\alpha$ with $p_\alpha \in \mathbb{R}$.

Definition 2.1.1. *A polynomial $p \in \mathbb{R}[\mathbf{x}]_{2d}$ is called* nonnegative *if $p(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$. A nonnegative polynomial $p \in \mathbb{R}[\mathbf{x}]_{2d}$ of even degree $2d$ is a* sum of squares, *if $p = \sum_{i=1}^k q_i^2$ for some polynomials $q_i \in \mathbb{R}[\mathbf{x}]_d$ and $1 \leq i \leq k$.*

Clearly, every sum of squares polynomial is nonnegative. To every polynomial $p \in \mathbb{R}[\mathbf{x}]_d$ we can associate a polytope, the so called *Newton polytope* of p, by considering the exponent vectors of p as lattice points in $\mathbb{R}^n$. Let therefore $A \subset \mathbb{N}_d^n$.

Definition 2.1.2. *Given $p = \sum_{\alpha \in A} p_\alpha \mathbf{x}^\alpha \in \mathbb{R}[\mathbf{x}]_d$, the* Newton polytope *of p is defined as*

$$\mathrm{New}(p) := \mathrm{conv}\{\alpha \in A : p_\alpha \neq 0\}.$$

A necessary condition for a polynomial $p \in \mathbb{R}[\mathbf{x}]_{2d}$ to be nonnegative is that every vertex α of $\mathrm{New}(p)$ has even coordinates and comes with a positive coefficient p_α ([Rez78]). For $p \in \mathbb{R}[\mathbf{x}]_d$ the *homogenization* of p is given by

$$\bar{p}(x_0, x_1, \ldots, x_n) = x_0^d p\left(\frac{x_1}{x_0}, \ldots, \frac{x_n}{x_0}\right).$$

The property of being nonnegative resp. a sum of squares is preserved under homogenizing polynomials, i.e., p is nonnegative resp. a sum of squares if and only if the homogenization $\bar{p}$ is nonnegative resp. a sum of squares ([Mar08]). In this thesis we will mostly work with homogeneous polynomials (also called forms) except when dealing with polynomial optimization or when stated otherwise. Therefore, we fix notation and introduce the convex cone of nonnegative forms and the convex cone of sums of squares forms as follows. Let $H_{n,d}$ be the vector space of real homogeneous polynomials in n variables of degree d. Then we define

$$\begin{aligned} P_{n,2d} &:= \{p \in H_{n,2d} \ : \ p(\mathbf{x}) \geq 0 \text{ for all } \mathbf{x} \in \mathbb{R}^n\}, \\ \Sigma_{n,2d} &:= \left\{p \in P_{n,2d} \ : \ p = \sum\nolimits_i q_i^2 \text{ for some } q_i \in H_{n,d}\right\}. \end{aligned}$$

The investigation of the relationship between the cone of nonnegative forms and the cone of sums of squares has its origin the seminal work of Hilbert when he showed the following remarkable relationship between $P_{n,2d}$ and $\Sigma_{n,2d}$.

Theorem 2.1.3 (Hilbert [Hil88]). *The equality $P_{n,2d} = \Sigma_{n,2d}$ exactly holds for binary forms ($n = 2$), quadratic forms ($2d = 2$) and ternary quartics $(n, 2d) = (3, 4)$.*

The first case states that every univariate (non-homogeneous) nonnegative polynomial is a sum of squares, which follows from the fundamental theorem of Algebra. In fact, every univariate nonnegative polynomial can be written as a sum of two squares by grouping the real and complex roots. For quadratic forms, the proof follows easily by writing the nonnegative quadratic form p as $p(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}$ with a symmetric positive semidefinite matrix A and using Cholesky factorization. The minimum number of squares needed to represent p as a sum of squares is equal to the rank of A. For a proof of $P_{3,4} = \Sigma_{3,4}$ we refer to [CL78]. In this case, every nonnegative ternary quartic can be written as a sum of three squares.

Even though not every nonnegative polynomial can be written as a sum of squares, Hilbert's 17th problem asks for representability of nonnegative polynomials as sums of squares of *rational functions*. In fact, in 1927, Artin provided a solution to this problem.

Theorem 2.1.4 (Artin [Art27]). *Let $p \in P_{n,2d}$. Then there is a sum of squares multiplier $h \in \Sigma_{n,2k}$ such that $h \cdot p$ is a sum of squares.*

If p is a strictly positive form, then there exists a uniform denominator h given by $h = (x_1^2 + \cdots + x_n^2)^k$ for some $k \in \mathbb{N}$ ([Rez00]). However, a main important problem remains to provide efficient degree bounds for the sum of squares multiplier h in this representation. In general, except for ternary forms, even in small dimensions no efficient degree bounds are yet known. For partial recent results about the degree behaviour of such multipliers, see [BGP14].

In order to construct nonnegative polynomials that are not sums of squares in all other cases than in Hilbert's theorem, one can use nonnegative polynomials that are not sums of squares in the smallest cases where the two cones differ, i.e., for $(n, 2d) = (3, 6)$ and $(n, 2d) = (4, 4)$. Using homogenization and the fact that both nonnegativity and the property of being a sum of squares are preserved, one can construct nonnegative polynomials that are not sums of squares easily for an arbitrary number of variables and arbitrary degree. In order to make use of the sparsity of some polynomials, the Newton polytope plays a key role, since it allows to reduce the number of possible monomials that can occur in sums of squares representations.

Theorem 2.1.5 (Reznick [Rez78]). *Let $p = \sum_i q_i^2$ be a sum of squares. Then $\operatorname{New}(q_i) \subset \frac{1}{2}\operatorname{New}(f)$.*

Example 2.1.6. *One of the first explicitly known nonnegative forms that is not a sum of squares is the famous Motzkin form*

$$M(x, y, z) = z^6 + x^4y^2 + x^2y^4 - 3x^2y^2z^2 \in P_{3,6} \setminus \Sigma_{3,6}.$$

Nonnegativity of M follows immediately from the arithmetic-geometric mean inequality. In the other smallest case $(n, 2d) = (4, 4)$, it is proved in [Rez78] that

$$N(w, x, y, z) = w^4 + x^2y^2 + y^2z^2 + z^2x^2 - 4wxyz \in P_{4,4} \setminus \Sigma_{4,4}.$$

Again, nonnegativity follows from the arithmetic-geometric mean inequality. To prove that both M and N are not sums of squares, one can invoke Theorem 2.1.5. Considering the Motzkin form again, one has

$$\frac{1}{2}\operatorname{New}(M) = \operatorname{conv}\{(0, 0, 3)^T, (2, 1, 0)^T, (0, 1, 2)^T\}$$

and the only additional interior lattice point is $(1, 1, 1)^T$. So, the only monomials that can occur in a sum of squares representation are the four monomials z^3, x^2y, xy^2, xyz. But then the coefficient of the monomial $x^2y^2z^2$ has to be nonnegative, in contradiction to the coefficient -3 in M. A similar argument shows that the form N cannot be a sum of squares, since the mixed monomial $xyzw$ cannot be constructed with the monomials corresponding to $\frac{1}{2}\operatorname{New}(N)$. However, one can verify that $(x^2 + y^2 + z^2) \cdot M \in \Sigma_{3,8}$ and $(x^2 + y^2 + z^2 + w^2) \cdot N \in \Sigma_{4,6}$.

Even in the smallest cases $(n, 2d) = (3, 6)$ and $(n, 2d) = (4, 4)$ the question about the precise quantitative relationship between $P_{n,2d}$ and $\Sigma_{n,2d}$ remains an important open problem. There are some special subsets of $H_{n,2d}$, for which precise answers exist. In [CLR87], the authors give a complete description in the case of even symmetric sextics, which form a 3-dimensional subcone of sextic forms for $n \geq 3$. In this case, there are explicit semialgebraic descriptions for the cones of nonnegative even symmetric sextics and of even symmetric sextics that are sums of squares.

2.2 Semidefinite Programming

In this section we provide a brief introduction to semidefinite programming, which is a generalization of linear programming. After presenting some classical results such as weak and strong duality, we look at the relationship between sums of squares and semidefinite programming in more detail. Our presentation follows [Las10, Mar08] unless referenced otherwise. Let $\mathbb{R}^{k\times k}$ denote the algebra of $k \times k$ matrices and $\mathcal{S}_k$ be the subspace of real symmetric $k \times k$ matrices. By $\mathcal{S}_k^+$ we denote the convex cone of $k \times k$ *positive semidefinite matrices*. In semidefinite programming, a linear functional is minimized over the intersection of the cone of positive semidefinite (PSD) matrices with an affine subspace. Before formulating a semidefinite program, we recall some basic conditions for a matrix to be PSD.

Theorem 2.2.1. *Let $A \in \mathcal{S}_k$. Then the following are equivalent.*

1. $A \in \mathcal{S}_k^+$.
2. $\mathbf{x}^T A\mathbf{x} \geq 0$ *for all* $\mathbf{x} \in \mathbb{R}^k$.
3. *All eigenvalues of A are nonnegative.*
4. $A = V^T V$ *for some* $V \in \mathbb{R}^{k\times k}$.
5. *All $2^k - 1$ principal minors of A are nonnegative.*

In the following, we use the notation $A \succeq 0$ for $A \in \mathcal{S}_k^+$ and $A \succ 0$ for A being positive definite. Given $c \in \mathbb{R}^n$ and $A_0, \dots, A_n \in \mathcal{S}_k$, a semidefinite program (SDP) has the following form:

$$p^* := \inf\{c^T\mathbf{x} : A(\mathbf{x}) \succeq 0\}$$

where $A(\mathbf{x}) = A_0 + x_1A_1 + \cdots + x_nA_n$ is a so called *linear pencil.* The feasible region of an SDP

$$S := \{\mathbf{x} \in \mathbb{R}^n : A(\mathbf{x}) \succeq 0\}$$

is called a *spectrahedron.* Recently, there is much interest in studying the geometry of semidefinite programming (see, e.g., [BPT13]). Linear programming problems are just semidefinite programs with diagonal matrices. We note that p^* may not be attained as can be seen by the following example.

Example 2.2.2. *Consider the SDP*

$$p^* := \inf_{\mathbf{x}\in\mathbb{R}^2} \left\{ x_1 : \begin{pmatrix} x_1 & 1 \\ 1 & x_2 \end{pmatrix} \succeq 0 \right\}.$$

Clearly, $p^* = 0$ but there is no feasible point at which $p^* = 0$ is attained.

In order to formulate the corresponding *dual semidefinite program*, we use the standard scalar product on $\mathbb{R}^{k\times k}$ defined by

$$\langle A, B\rangle := \mathrm{Tr}(A^T B) = \sum_{i,j=1}^{k} A_{ij}B_{ij},$$

where $\mathrm{Tr}(A)$ is the trace of A. The dual SDP has the form

$$d^* := \sup_Z \{-\langle A_0, Z\rangle : \langle A_i, Z\rangle = c_i,\ 1 \le i \le n,\ Z \succeq 0\}.$$

Here, the variable is $Z \in \mathcal{S}_k$. A first connection between p^* and d^* is the weak duality theorem (see, e.g., [Mar08]).

Theorem 2.2.3. *Let $\mathbf{x}$ be a feasible point of the primal SDP and Z be a feasible matrix for the dual SDP. Then*

$$-\langle A_0, Z\rangle \le c^T\mathbf{x}.$$

The quantity $p^* - d^*$ is called the *duality gap* and one of the most fundamental differences between linear programming and semidefinite programming is the fact that this gap does not always vanish. In other words, strong duality does not necessarily hold.

Example 2.2.4. *Consider the SDP*

$$p^* := \inf_{\mathbf{x}\in\mathbb{R}^2} \left\{ x_1 : \begin{pmatrix} 0 & x_1 & 0 \\ x_1 & x_2 & 0 \\ 0 & 0 & x_1+1 \end{pmatrix} \succeq 0 \right\}.$$

Looking at all principal minors, one can check immediately that $p^* = 0$. The corresponding dual SDP is given by

$$d^* := \sup\{-Z_{33} : Z_{22} = 0,\, 2Z_{12} + Z_{33} = 1,\, Z \succeq 0\}.$$

Again, checking the principal minors of the matrix Z, we can conclude that $d^* = -1$. Hence, the duality gap is $p^* - d^* = 1$.

However, strong duality holds under special conditions on the existence of strictly feasible points in the corresponding semidefinite programs. The *strong duality theorem* makes this more precise and is one of the most important results in semidefinite programming (see, e.g., [Mar08]).

Theorem 2.2.5. *One has $p^* = d^*$ if*

1. *the primal SDP is strictly feasible, i.e., there exists $\mathbf{x} \in \mathbb{R}^n$ such that $A(\mathbf{x}) \succ 0$, or,*
2. *the dual SDP is strictly feasible, i.e., there exists $Z \succ 0$ such that $\langle A_i, Z \rangle = c_i$, $1 \le i \le n$.*

Furthermore, if both conditions hold, then the optimal values p^* and d^* are attained.

Considering the previous example again, one can see that neither the primal nor the dual problem have a strictly feasible solution. The main reason why semidefinite programming is a very important tool relies on the fact that the optimal value of an SDP can be computed in time polynomial up to an additive error using interior point methods (see, e.g., [dK02]). Connecting this to sums of squares, the main reason why sums of squares techniques are widely used in tackling polynomial optimization problems is the fact that the problem of deciding whether a polynomial is a sum of squares can be reduced to a semidefinite feasibility problem, which, for fixed number of variables, is in P. Let therefore $p \in \mathbb{R}[\mathbf{x}]_{2d}$ be a polynomial of degree $2d$ and $v_d(\mathbf{x}) := (x^\alpha)_{|\alpha| \le d}$ be the vector of monomials up to degree at most d, which has length $s(d) := \binom{n+d}{d}$. The fundamental relationship between sums of squares and semidefinite programming is given by the following result (see, e.g., [Las10]).

Theorem 2.2.6. *A polynomial $p \in \mathbb{R}[\mathbf{x}]_{2d}$ is a sum of squares if and only if there exists $Q \in \mathcal{S}^+_{s(d)}$ such that*

$$p(\mathbf{x}) = v_d(\mathbf{x})^T Q v_d(\mathbf{x}).$$

If $Q \in \mathcal{S}^+_{s(d)}$, then its Cholesky decomposition $Q = V^T V$ yields the representation of p as a sum of squares:

$$p(\mathbf{x}) = v_d(\mathbf{x})^T Q v_d(\mathbf{x}) = v_d(\mathbf{x})^T V^T V v_d(\mathbf{x}) = (V v_d(\mathbf{x}))^T (V v_d(\mathbf{x})).$$

Note that the identity $p(\mathbf{x}) = v_d(\mathbf{x})^T Q v_d(\mathbf{x})$ yields linear equations that the entries of the matrix Q must satisfy (comparing coefficients). Additionally, since, in general, the monomials in $v_d(\mathbf{x})$ are not algebraically independent, the matrix Q will not be unique. So, there will be free parameters in the representation $v_d(\mathbf{x})^T Q v_d(\mathbf{x})$, which have to be chosen such that $Q \in \mathcal{S}^+_{s(d)}$. Therefore, $\Sigma_{n,2d}$ is the *projection of a spectrahedron.* The size of the resulting SDP is polynomial whenever the number of variables or the degree are fixed. However, it is not jointly polynomial. Note furthermore that the size of the SDP often can be reduced significantly by invoking Theorem 2.1.5. Therefore, it suffices to consider monomials contained in $\frac{1}{2}\operatorname{New}(p)$ in order to obtain a sum of squares representation.

Example 2.2.7. *Consider the bivariate polynomial*

$$p = 1 - 2xy + 3x^2y^2 + 4x^4y^2 + x^2y + x^2.$$

Instead of using all $\binom{2+3}{3} = 10$ *monomials of degree at most* 3*, we can reduce this number to four, since the reduced Newton polytope* $\frac{1}{2}New(p)$ *contains the four monomials* $1, x, xy, x^2y$*. Hence,* p *is a sum of squares if and only if*

$$p = (1, x, xy, x^2y)^T \cdot Q \cdot (1, x, xy, x^2y)$$

for some $Q \in \mathcal{S}_4^+$*. Expanding the right hand side and comparing coefficients, the matrix* Q *is given by*

$$Q = \begin{pmatrix} 1 & 0 & -1 & \lambda \\ 0 & 1 & \frac{1-2\lambda}{2} & 0 \\ -1 & \frac{1-2\lambda}{2} & 3 & 0 \\ \lambda & 0 & 0 & 4 \end{pmatrix}.$$

There is one free parameter λ*. Choosing* $\lambda = \frac{1}{2}$*, one can check that* $Q \in \mathcal{S}_4^+$*. In fact, for* $\lambda = \frac{1}{2}$ *the matrix* Q *is even positive definite. Computing a Cholesky decomposition, we find that*

$$p = \left(1 - xy + \frac{1}{2}x^2y\right)^2 + x^2 + \left(\sqrt{2}xy + \frac{\sqrt{2}}{4}x^2y\right)^2 + \left(\sqrt{\frac{29}{8}}x^2y\right)^2.$$

One can show that the number of squares needed in such a representation can always be taken to be equal to the rank of Q ([PW98]). In practice, polynomials often come with certain structures, such as sparsity and symmetry. There are some other techniques that make use of the sparsity and symmetry of polynomials to reduce the number of monomials in sums of squares representations or to handle questions about nonnegativity (see, e.g., [GP04, KKW05] and Chapters 5 and 6).

Since semidefinite programs are solved efficiently in a numerical way, we remark that existence of rational sums of squares representations cannot always be guaranteed. In fact, not every polynomial with rational coefficients that is a sum of squares of real polynomials also admits a sum of squares representation with rational coefficients only ([Sch13]). For example, the form

$$p = x^4 + y^4 + z^4 + xy^3 - 3x^2yz - 4xy^2z + 2x^2z^2 + xz^3 + yz^3 \in \Sigma_{3,4}$$

cannot be written as a sum of squares of forms with rational coefficients only. This is in sharp contrast to the univariate case as the following theorem shows (see, e.g., [Lan06]).

Theorem 2.2.8. *Let* $p \in \mathbb{Q}[x]$ *be a sum of squares. Then* p *is a sum of squares of polynomials with rational coefficients and at most five squares are needed.*

Example 2.2.9. *The polynomial $p(x) = 1 + x + x^2 + x^3 + x^4 + x^5 + x^6$ has four representations as a sum of two squares. Exactly one of them is a rational one:*

$$p(x) = \left(1 + \frac{1}{2}x - \frac{1}{2}x^2 - x^3\right)^2 + 7\left(\frac{1}{2}x + \frac{1}{2}x^2\right)^2.$$

This can be checked by using Theorem 2.2.6. The matrix $Q \in \mathbb{R}^{4\times 4}$ has three parameters and the spectrahedron defining all possible sums of squares representations of p is 3-dimensional (see Figure 2.1). In order to write p as a sum of two squares, one has to choose the three parameters such that the rank of Q is two. Therefore, all 3×3 and higher order minors must vanish. There are four possible solutions (corresponding to the corners of the spectrahedron) of which exactly one is rational, yielding the above representation.

Figure 2.1: On the left: The 3-dimensional spectrahedron describing the possible sums of squares representations. On the right: The projected spectrahedron.

2.3 Polynomial Optimization

One of the most important applications of nonnegative polynomials and sums of squares is in the area of polynomial optimization. We want to sketch the basic ideas of the question why sums of squares techniques play an outstanding role in the optimization of polynomial functions. All presented results are contained in [Las10, Mar08] unless referenced otherwise. We start with the problem of minimizing a polynomial function $p \in \mathbb{R}[\mathbf{x}]_{2d}$ on $\mathbb{R}^n$:

$$p^* := \inf\{p(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^n\}.$$

Computing p^* is an NP-hard problem in general ([BCSS98]). One natural idea to solve this problem is to compute all critical points of p. However, in general, computing critical points by solving systems of polynomial equations is a hard problem as well. Another obstacle in computing p^* is the fact that p^* may not be attained as the bivariate polynomial $p(x, y) = (1 - xy)^2 + x^2$ shows. Here, $p^* = 0$ but there is no point $(x, y) \in \mathbb{R}^2$ such that $p(x, y) = 0$. Looking at the problem of computing p^* from a dual viewpoint, we note that minimizing p is equivalent to maximizing the best lower bound:

$$p^* = \sup\{\lambda \in \mathbb{R} : p - \lambda \geq 0\}.$$

So, minimizing polynomial functions is equivalent to deciding nonnegativity of polynomials, which is NP-hard in general. It lies on the heart of polynomial optimization to relax nonnegativity conditions to conditions requiring polynomials to be sums of squares. In the above case we consider the following *sums of squares relaxation* for minimizing a polynomial function:

$$p^*_{sos} := \sup\left\{\lambda \in \mathbb{R} : p - \lambda = \sum_{i=1}^{k} q_i^2 \text{ for some } q_i \in \mathbb{R}[\mathbf{x}]_d\right\}.$$

Since every sum of squares polynomial is nonnegative, one has the inequality $p^*_{sos} \leq p^*$. An obvious question is when and how often equality holds.

Theorem 2.3.1. *For $p \in \mathbb{R}[\mathbf{x}]_{2d}$ one has $p^*_{sos} = p^*$ if and only if $p - p^*$ is a sum of squares.*

The quantity p^*_{sos} is just the optimal value of a semidefinite program and can be computed efficiently. In fact, using duality theory, sometimes one can even verify whether the relaxation p^*_{sos} is exact, i.e., whether $p^*_{sos} = p^*$. Before defining the dual semidefinite problem we present some known results about the quantities p^*_{sos} and p^*. Let $p \in \mathbb{R}[\mathbf{x}]_{2d}$ be a polynomial with homogeneous decomposition as

$$p = p_0 + \cdots + p_{2d}$$

where p_k is homogeneous of degree k. Of course, one obvious necessary condition for $p^* \neq -\infty$ is that p_{2d} is nonnegative.

Definition 2.3.2. *Let $p \in \mathbb{R}[\mathbf{x}]_{2d}$ be a polynomial with homogeneous decomposition $p = p_0 + \cdots + p_{2d}$. The polynomial p is called* stably bounded from below *on $\mathbb{R}^n$ if p_{2d} is strictly positive on $\mathbb{R}^n$ (or, equivalently, if p_{2d} has no zeros on the unit sphere $\mathbb{S}^{n-1}$).*

Based on the stable boundedness condition there is also a sufficient condition for $p^* \neq -\infty$.

Theorem 2.3.3. *Let $p \in \mathbb{R}[\mathbf{x}]_{2d}$.*

1. *If p is stably bounded from below, then $p^* \neq -\infty$ and p achieves a minimum.*

2. *If $p^*_{sos} \neq -\infty$, then p_{2d} is a sum of squares.*

3. *If p_{2d} is an interior point of $\Sigma_{n,2d}$, then $p^*_{sos} \neq -\infty$.*

Two examples of forms in the interior of $\Sigma_{n,2d}$ are $f_1 = (x_1^2 + \cdots + x_n^2)^d$ and $f_2 = x_1^{2d} + \cdots + x_n^{2d}$. The reverse directions in the last two statements in Theorem 2.3.3 do not hold as the following examples show.

Example 2.3.4. *The Motzkin polynomial $m(x,y) = x^4y^2 + x^2y^4 - 3x^2y^2 + 1$ satisfies $m^* = 0$, $m^*_{sos} = -\infty$ but $m_6 = x^4y^2 + x^2y^4$ is a sum of squares. The polynomial $p = (x-y)^2$ satisfies $p^* = p^*_{sos} = 0$ but $p_2 = (x-y)^2 \in \partial\Sigma_{2,2}$, i.e., p_2 is on the boundary of $\Sigma_{2,2}$, since p_2 has zeros.*

Having collected many interesting connections between the quantities p^* and p^*_{sos}, we now introduce results from the theory of *moments* in order to formulate a dual problem for p^*_{sos} and to check exactness of sums of squares relaxations.

2.4 The Moment Problem

We introduce the *moment problem* in its real form and only in a manner that is essential to understand the key relationship between nonnegative polynomials and moments. We mainly follow [Las10] in our presentation unless referenced otherwise. Let therefore $y = (y_\alpha) \subset \mathbb{R}$ be an infinite sequence of real numbers with $\alpha \in \mathbb{N}^n$. The moment problem asks for the existence of a measure μ supported on $\mathbb{R}^n$ such that

$$y_\alpha = \int_{\mathbb{R}^n} \mathbf{x}^\alpha d\mu.$$

Analougously, one can consider the *truncated moment problem* where $\alpha \in \Delta \subset \mathbb{N}^n$ for a finite set Δ and $y = (y_\alpha)_{\alpha\in\Delta}$ is a finite sequence. The measure μ is called a *representing measure* of the sequence y. Given an infinite sequence $y = (y_\alpha) \subset \mathbb{R}$ consider the linear functional $L_y : \mathbb{R}[\mathbf{x}] \to \mathbb{R}$ with

$$p(\mathbf{x}) = \sum_{\alpha\in\mathbb{N}^n} p_\alpha \mathbf{x}^\alpha \mapsto L_y(p) = \sum_{\alpha\in\mathbb{N}^n} p_\alpha y_\alpha.$$

The following fundamental result relates the moment problem to the problem of deciding nonnegativity of polynomials.

Theorem 2.4.1 (Haviland [Hav36])**.** *Let $y = (y_\alpha)_{\alpha\in\mathbb{N}^n} \subset \mathbb{R}$. There exists a finite Borel measure μ on $\mathbb{R}^n$ such that*

$$y_\alpha = \int_{\mathbb{R}^n} \mathbf{x}^\alpha d\mu \quad \text{for all } \alpha \in \mathbb{N}^n$$

if and only if $L_y(p) \geq 0$ for all nonnegative polynomials p on $\mathbb{R}^n$.

Since every univariate nonnegative polynomial is a sum of squares, the 1-dimensional moment problem is well understood. However, since there is no explicit characterization of nonnegative polynomials in the multivariate case, the multidimensional moment problem is much harder to solve and remains widely open.

Let $p = \sum_\alpha p_\alpha \mathbf{x}^\alpha \in \mathbb{R}[\mathbf{x}]_d$. Recall that

$$v_d(\mathbf{x}) = (1, x_1, x_2, \ldots, x_n, x_1^2, x_1x_2, \ldots, x_1x_n, \ldots, x_1^d, \ldots x_n^d)^T$$

is a basis of the real vector space $\mathbb{R}[\mathbf{x}]_d$, which is of dimension $s(d) = \binom{n+d}{d}$. Then p can be written as

$$p(\mathbf{x}) = \sum_\alpha p_\alpha \mathbf{x}^\alpha = \langle \mathbf{p}, v_d(\mathbf{x}) \rangle$$

where $\mathbf{p} \in \mathbb{R}^{s(d)}$ is the vector of coefficients of p (ordered lexicographically). Given a truncated $s(2d)$-sequence $y = (y_\alpha)$, let $M_d(y)$ be the *moment matrix* of dimension $s(2d)$ with rows and columns labeled by $v_d(\mathbf{x})$ and constructed as follows:

$$M_d(\alpha, \beta) = L_y(\mathbf{x}^\alpha \mathbf{x}^\beta) = y_{\alpha+\beta} \quad \text{for } \alpha, \beta \in \mathbb{N}_d^n.$$

Equivalently, $M_d(y) = L_y(v_d(\mathbf{x}) v_d(\mathbf{x})^T)$. The moment matrix $M_d(y)$ defines a bilinear form on $\mathbb{R}[\mathbf{x}]_d$ as follows:

$$\langle p, q \rangle_y := L_y(pq) = \mathbf{p}^T M_d(y) \mathbf{q} \quad \text{for} \quad \mathbf{p}, \mathbf{q} \in \mathbb{R}^{s(d)}.$$

If the linear functional L_y comes from a measure μ, then, for every $q \in \mathbb{R}[\mathbf{x}]$, it holds that

$$\langle q, q \rangle_y = L_y(q^2) = \int_{\mathbb{R}^n} q^2 d\mu \geq 0$$

implying that $M_d(y) \succeq 0$. However, note that not every sequence y with $M_d(y) \succeq 0$ has a representing measure (in contrast to the 1-dimensional case). By $M(\mathbb{R}^n)_+$ we denote the space of finite Borel measures on $\mathbb{R}^n$. Consider the following problem:

$$p^*_{mom} := \inf_{\mu \in M(\mathbb{R}^n)_+} \int_{\mathbb{R}^n} p \, d\mu$$
$$s.t. \ \mu(\mathbb{R}^n) = 1.$$

Now, we can reformulate the problem of computing p^* as follows.

Theorem 2.4.2. *Let $p \in \mathbb{R}[\mathbf{x}]_{2d}$. Then $p^* = p^*_{mom}$.*

The semidefinite relaxation of p^*_{mom} is based on the non-equivalence between existence of representing measures and positive semidefiniteness of the moment matrix. The relaxation is given by the following program:

$$\sigma_d^* := \inf\{L_y(p) : M_d(y) \succeq 0, y_0 = 1\}.$$

Using duality theory of semidefinite programming one can show that σ_d^* is in fact the dual program of p^*_{sos} with the nice property that there is no duality gap.

Theorem 2.4.3. *Let $p \in \mathbb{R}[\mathbf{x}]_{2d}$. Then $p^*_{sos} = \sigma^*_d$. Additionally, if $\sigma^*_d > -\infty$, then p^*_{sos} has an optimal solution.*

One of the most interesting questions in polynomial optimization concerns exactness of sums of squares relaxations. Suppose p^*_{sos} is computed efficiently via semidefinite programming. Is there a certificate for concluding $p^*_{sos} = p^*$? Using duality theory there are some important results.

Theorem 2.4.4. *Suppose that the optimal solution of the dual problem of p^*_{sos} has rank one, that is, there exists y^* such that $rank(M_d(y^*)) = 1$. Then $p^*_{sos} = p^*$. In this case, factoring $M_d(y^*) = v_d(\mathbf{x}^*)v_d(\mathbf{x}^*)^T$ for some $\mathbf{x} \in \mathbb{R}^n$ yields one global minimizer $\mathbf{x}^*$ that can be read from the subvector of first moments y^*_α with $|\alpha| = 1$.*

Another stopping criterion is based on a so called *flat extension* of moment matrices.

Theorem 2.4.5 (Curto-Fialkow [CF96])**.** *If y^* is the optimal solution of the semidefinite program σ^*_d and $rank(M_{d-1}(y^*)) = rank(M_d(y^*))$, then $\sigma^*_d = p^*_{sos} = p^*$ and there are at least $rank(M_d(y^*))$ global minimizers.*

By Hilbert's theorem, it is clear that $p^*_{sos} = p^*$ whenever p is a univariate polynomial, quadratic polynomial or bivariate polynomial of degree four.

Example 2.4.6. *The global minimum of the univariate polynomial $p(x) = 3x^4 + 4x^3 - 12x^2$ is $p^* = p^*_{sos} = -32$. The dual program σ^*_d is given by*

$$\inf \left\{ 3y_4 + 4y_3 - 12y_2 : M_2(y) = \begin{pmatrix} 1 & y_1 & y_2 \\ y_1 & y_2 & y_3 \\ y_2 & y_3 & y_4 \end{pmatrix} \succeq 0 \right\}.$$

It turns out that the optimal matrix has rank one:

$$M_2(y^*) = \begin{pmatrix} 1 & -2 & 4 \\ -2 & 4 & -8 \\ 4 & -8 & 16 \end{pmatrix}.$$

Hence, we find that $x^* = -2$ is the unique minimizer of p.

We note that all presented ideas and results can be extended to global minimization of polynomials over compact semialgebraic sets. In fact, since there are nice characterizations of nonnegative polynomials over compact semialgebraic sets, there exist some important results concerning the moment problem and hence for constrained sums of squares relaxations (see, e.g., [Las10]).

2.5 Quantitative Aspects

In this subsection we present some key relationships between the cones $P_{n,2d}$ and $\Sigma_{n,2d}$ by taking a convex geometric viewpoint. Considering experimental results in small dimensions, $\Sigma_{n,2d}$ seems to yield a very good approximation of $P_{n,2d}$ in spite of Hilbert's theorem. We present results from [Ble06] about the quantitative relationship between $P_{n,2d}$ and $\Sigma_{n,2d}$ stating that there are, in fact, significantly more nonnegative polynomials than sums of squares.

In order to compare $P_{n,2d}$ and $\Sigma_{n,2d}$, in [Ble06] the idea is to take compact sections of these cones and compare their volume ratio. Let therefore M be the hyperplane of all forms in $H_{n,2d}$ with mean zero on the unit sphere:

$$M = \left\{ p \in H_{n,2d} : \int_{\mathbb{S}^{n-1}} p \, d\sigma = 0 \right\}$$

where σ is the rotation invariant probability measure on $\mathbb{S}^{n-1}$. The dimension of M is $D_M = \binom{n+2d-1}{2d} - 1$. Define the compact sections of $P_{n,2d}$ and $\Sigma_{n,2d}$ with the hyperplane M as

$$\bar{P}_{n,2d} := P_{n,2d} \cap M \qquad \text{and} \qquad \bar{\Sigma}_{n,2d} = \Sigma_{n,2d} \cap M.$$

For an m-dimensional compact set $K \subset \mathbb{R}^m$, the Euclidean volume has the property that

$$\operatorname{vol}((1+\varepsilon) \cdot K) = (1+\varepsilon)^m \cdot \operatorname{vol} K.$$

We would like to think of K and $(1+\varepsilon)K$ as similar in size, but if the ambient dimension m grows, then $(1+\varepsilon)K$ is significantly larger in volume. In order to take this effect into account, the proper measure of the volume here is $\operatorname{vol}(K)^{\frac{1}{m}}$. Then there is the following asymptotic result.

Theorem 2.5.1 ([Ble06])**.** *There exist constants $c_1(d)$ and $c_2(d)$ dependent on d only such that*

$$c_1(d) n^{(d-1)/2} \leq \left(\frac{\operatorname{vol} \bar{P}_{n,2d}}{\operatorname{vol} \bar{\Sigma}_{n,2d}} \right)^{\frac{1}{D_M}} \leq c_2(d) n^{(d-1)/2}.$$

Hence, if the degree is fixed to be $2d \geq 4$, then, asymptotically, there are significantly more nonnegative polynomials than sums of squares. Taking the optimization viewpoint, for sufficiently large n, almost always it holds that $p^*_{sos} < p^*$. However, in spite of this asymptotic result, the picture in small dimensions is still an open research problem as the bounds provided in Theorem 2.5.1 are far from being optimal in these cases. In the following table we demonstrate the values of these bounds for some small dimensions. Here, n^* is the minimal number of variables such that $c_1(d)n^{(d-1)/2} \geq 1$.

n	$2d$	$c_1(d)n^{(d-1)/2}$	$c_2(d)n^{(d-1)/2}$	n^*
3	6	$1.7 \cdot 10^{-7}$	$7.2 \cdot 10^{8}$	$1.8 \cdot 10^{7}$
3	8	$1.1 \cdot 10^{-9}$	$1.9 \cdot 10^{12}$	$2.8 \cdot 10^{6}$
4	4	$2 \cdot 10^{-5}$	442368	9059696640
4	6	$2.2 \cdot 10^{-7}$	$5.6 \cdot 10^{8}$	$1.8 \cdot 10^{7}$

On the positive side, it is shown that nonnegative polynomials can be approximated arbitrarily well by sums of squares.

Theorem 2.5.2 (Lasserre [Las06b]). *Let $p \in \mathbb{R}[\mathbf{x}]$ be nonnegative.*

1. *There exist some $r^* \in \mathbb{N}$ and λ^* such that for all $r \geq r^*$ and $\lambda \geq \lambda^* \geq 0$ the polynomial*

$$p + \lambda \sum_{k=0}^{r} \sum_{j=1}^{n} \frac{x_j^{2k}}{k!} \qquad \text{is a sum of squares.}$$

2. *For every $\varepsilon > 0$ there exists some $r(p, \varepsilon) \in \mathbb{N}$ such that*

$$p_\varepsilon := p + \varepsilon \sum_{k=0}^{r(p,\varepsilon)} \sum_{j=1}^{n} \frac{x_j^{2k}}{k!} \qquad \text{is a sum of squares}$$

and $||p - p_\varepsilon||_1 \to 0$ as $\varepsilon \to 0$, where $||p||_1 = \sum_{\alpha \in \mathbb{N}^n} |p_\alpha|$.

This density result comes with the problem that no explicit bounds for r^*, λ^* and $r(p, \varepsilon)$ are known so far.

2.6 Boundary Structure

A widely open problem in analyzing the convex cones $P_{n,2d}$ and $\Sigma_{n,2d}$ is the study of their facial structure and the possible dimensions of their faces. Whenever these two cones coincide, the facial structure is much better understood ([Bar02]). However, even in the smallest cases where they differ, a complete description of the faces is an open problem. In Chapter 4 we analyze the facial structure of these cones in more detail. In the following, we present some basic results about the boundary structure of $P_{n,2d}$ and $\Sigma_{n,2d}$ as well as their dual cones. All presented results can be found in [BPT13] unless referenced otherwise. We start by recalling some basic definitions and properties from convexity theory.

Definition 2.6.1. *Let $C \subset \mathbb{R}^n$ be a convex cone.*

1. *A subcone $F \subset C$ is called a* face *of C, if for any $x, y \in C$, whenever $x + y \in F$, it holds that $x, y \in F$. The* dimension *of a face F is defined as*

$$\dim F := \dim span(F).$$

2. *An element $p \neq 0$ contained in a 1-dimensional face is called an* extremal element. *Equivalently, if $p = y_1 + y_2$, $y_1, y_2 \in C$, then $p = \lambda_i y_i$ for some $\lambda_i > 0$ and $i \in \{1, 2\}$.*

3. *A face F is called an* exposed face *of C, if $F = C \cap H$ where H is a nontrivial supporting hyperplane to C.*

Every element in a closed convex cone can be written as a finite sum of extremal elements (see, e.g., [Bar02]). Note that we can identify the cones $P_{n,2d}$ and $\Sigma_{n,2d}$ as cones lying in $\mathbb{R}^{\dim H_{n,2d}} = \mathbb{R}^{\binom{n+2d-1}{2d}}$. The description of extremal elements of the cones $P_{n,2d}$ and $\Sigma_{n,2d}$ is a very hard problem. For $\Sigma_{n,2d}$ there is an easy necessary condition, namely, that all extremal elements of $\Sigma_{n,2d}$ are perfect squares ([CLR82]) but this is not sufficient as the example $(x^2+y^2)^2 = (x^2-y^2)^2 + (2xy)^2$ shows.

Example 2.6.2 ([CL78]). *The Motzkin form $M(x,y,z) = z^6 + x^4y^2 + x^2y^4 - 3x^2y^2z^2 \in P_{3,6} \setminus \Sigma_{3,6}$ is extremal in $P_{3,6}$ and the form $N(w,x,y,z) = w^4 + x^2y^2 + y^2z^2 + z^2x^2 - 4wxyz \in P_{4,4} \setminus \Sigma_{4,4}$ is extremal in $P_{4,4}$.*

Let $\mathcal{E}P_{n,2d}$ and $\mathcal{E}\Sigma_{n,2d}$ denote the set of extremal forms of the cones $P_{n,2d}$ and $\Sigma_{n,2d}$.

Theorem 2.6.3 ([CLR82]). *Let $\Sigma_{n,2d} \subsetneq P_{n,2d}$. The inclusion $\mathcal{E}\Sigma_{n,2d} \subset \mathcal{E}P_{n,2d}$ precisely holds in the following cases:*

1. $2d \leq 6$,

2. $(n, 2d) = (3, 8)$,

3. $(n, 2d) = (3, 10)$.

The *dual cone* C^* of a convex cone C in a real vector space V is defined as the set of all linear functionals that are nonnegative on C, i.e.,

$$C^* := \{l \in V^* : l(\mathbf{x}) \geq 0 \text{ for all } \mathbf{x} \in C\}.$$

For closed convex cones the biduality theorem states that $(C^*)^* = C$ ([Bar02]). One of the most important linear functionals when studying faces of $P_{n,2d}$ is the evaluation functional: For $v \in \mathbb{S}^{n-1}$ let $l_v \in H_{n,2d}^*$ be the linear functional given by evaluation at v:

$$l_v(p) = p(v) \quad \text{for} \quad p \in H_{n,2d}.$$

Proposition 2.6.4. *$P_{n,2d}^*$ is the conical hull of functionals l_v for all $v \in \mathbb{S}^{n-1}$:*

$$P_{n,2d}^* = \operatorname{cone}\{l_v : v \in \mathbb{S}^{n-1}\}.$$

In particular, a form f is nonnegative on $\mathbb{R}^n$ if and only if it is nonnegative on the unit sphere $\mathbb{S}^{n-1}$.

Note that testing membership $l \in P^*_{n,2d}$ is just the truncated moment problem, which we introduced earlier by considering duality theory for polynomial optimization problems. In order to give a description of the dual cone of $\Sigma_{n,2d}$, we first note that the dual space $H^*_{n,2d}$ can be identified as a subspace $S_{n,d}$ of the vector space of real quadratic forms in $H_{n,d}$. For a linear functional $l \in H^*_{n,2d}$, the corresponding quadratic form Q_l is defined by $Q_l(f) = l(f^2)$. The cone of positive semidefinite forms in $S_{n,d}$ is then defined as

$$S^+_{n,d} := \{Q \in S_{n,d} : Q(f) \geq 0 \text{ for all } f \in H_{n,d}\}.$$

Proposition 2.6.5 ([Ble12a]). *It holds that*

$$\Sigma^*_{n,2d} = S^+_{n,d} \cap H^*_{n,2d}.$$

In particular, Proposition 2.6.5 implies that $\Sigma^*_{n,2d}$ is a spectrahedron (remember that $\Sigma_{n,2d}$ is a projected spectrahedron, see Section 2.2).

The set of extreme rays of a closed convex cone is very important, since every element in the cone can be written as a sum of finitely many extremal elements. Exposed extreme rays of $P_{n,2d}$ are easy to describe, since their varieties are maximal.

Proposition 2.6.6. *A form $p \in P_{n,2d}$ is an exposed extreme ray of $P_{n,2d}$ if and only if for all $q \in P_{n,2d}$ with $V(p) \subseteq V(q)$ it holds that $q = \lambda p$ for some $\lambda \in \mathbb{R}$.*

Example 2.6.7. *The Motzkin form $M(x, y, z) = z^6 + x^4y^2 + x^2y^4 - 3x^2y^2z^2$ spans an extreme ray of $P_{3,6}$ but it is not exposed. The zeros of M are given by*

$$V(M) = \{(1, 0, 0), (0, 1, 0), (1, 1, 1), (-1, 1, 1), (1, -1, 1), (1, 1, -1)\}.$$

In [CL78], it is proved that $S(x, y, z) = x^4y^2+y^4z^2+z^4x^2-3x^2y^2z^2 \in P_{3,6}\setminus\Sigma_{3,6}$, where nonnegativity of S is given by the arithmetic-geometric mean inequality. One can check easily (since it is known when the arithmetic mean equals the geometric mean) that $V(S) = V(M) \cup \{(0, 0, 1)\}$. But, obviously, $S \neq \lambda M$ for all $\lambda \in \mathbb{R}$. Hence, the Motzkin form does not span an exposed extreme ray of $P_{3,6}$.

Since, by Proposition 2.6.4, every exposed face of $P_{n,2d}$ is given by a set of forms vanishing on a finite set of points, an obvious problem is to determine the maximum number of zeros a nonnegative form $p \in P_{n,2d}$ can have. Following the notation in [CLR80] we define

$$B_{n,2d} := \sup_{\substack{p \in P_{n,2d} \\ |V(p)|<\infty}} |V(p)| \qquad \text{and} \qquad B'_{n,2d} := \sup_{\substack{p \in \Sigma_{n,2d} \\ |V(p)|<\infty}} |V(p)|.$$

An exact determination of these numbers seems to be a rather difficult task. For special cases, these numbers are determined or estimated, as the following theorem shows.

Theorem 2.6.8 ([BHO$^+$12, CLR80, Sha77]). *The numbers $B_{n,2d}$ and $B'_{n,2d}$ satisfy the following relations.*

1. $B_{3,6} = B_{4,4} = 10$,
2. $\frac{(2d)^2}{4} \leq B_{3,2d} \leq \frac{6d(2d-2)}{8} + 1$ *for* $2d \geq 6$,
3. $B_{3,6k} \geq 10k^2$, $B_{3,6k+2} \geq 10k^2 + 1$, $B_{3,6k+4} \geq 10k^2 + 4$,
4. $B'_{n,2d} \geq d^{n-1}$,
5. $B'_{3,2d} = \frac{(2d)^2}{4}$.

Note that the number $B_{3,8}$ satisfying $16 \leq B_{3,8} \leq 19$ is still not exactly determined. In the smallest cases where $P_{n,2d} \neq \Sigma_{n,2d}$, the results are actually more delicate as the following theorem shows.

Theorem 2.6.9 ([BHO$^+$12, CLR80]). *If $p \in P_{3,6}$ and $|V(p)| > 10$, then $p \in \Sigma_{3,6}$ and p is a sum of three squares of cubics. If $p \in P_{4,4}$ and $|V(p)| > 10$, then $p \in \Sigma_{4,4}$ and p is a sum of six squares of quadratics.*

We will strongly make use of this theorem in Chapter 3 when studying separating inequalities for polynomials $p \in \partial P_{3,6}$ and $p \in \partial P_{4,4}$. Forms in $P_{3,6}$ with exactly 10 zeros are in fact extremal.

Theorem 2.6.10 ([Rez07]). *Let $p \in P_{3,6}$ and $|V(p)| = 10$. Then p is extremal, i.e., $p \in \mathcal{E}P_{3,6}$.*

Example 2.6.11. *The Robinson form*

$$R(x, y, z) = x^6 + y^6 + z^6 - (x^4y^2 + x^2y^4 + x^4z^2 + x^2z^4 + y^4z^2 + y^2z^4) + 3x^2y^2z^2$$

satisfies $R \in P_{3,6} \setminus \Sigma_{3,6}$ ([CL78]) and has exactly ten zeros:

$$V(R) = (0, \pm 1, 1), (1, 0, , \pm 1), (\pm 1, 1, 0), (1, 1, 1), (-1, 1, 1), (1, -1, 1), (1, 1, -1).$$

Hence, by Theorem 2.6.10, $R \in \mathcal{E}P_{3,6}$.

Known forms in $P_{3,6}$ with exactly ten zeros are rare (see [Rez07] for some other examples) and it would be a major breakthrough to characterize all possible 10-point configurations $S \subset \mathbb{R}^3$ that arise as varieties of forms $p \in P_{3,6}$. However, in [BHO$^+$12] it is shown that the algebraic boundary of the semialgebraic set $\mathcal{E}P_{3,6} \setminus \Sigma_{3,6}$ is the Severi variety of plane rational sextic curves, which has dimension 17 and degree 26312976 in the set of all plane sextic curves.

Chapter 3

Separating Inequalities for Nonnegative Polynomials that are not Sums of Squares

In this chapter, we tackle the problem of constructing separating inequalities for nonnegative polynomials that are not sums of squares. In the smallest cases where $P_{n,2d} \neq \Sigma_{n,2d}$, i.e., for $(n, 2d) \in \{(3,6),(4,4)\}$, Blekherman showed that it is precisely the *Cayley-Bacharach relation* that prevents sums of squares from filling out the cone of nonnegative polynomials. More precisely, in [Ble12a] it is shown that every separating extreme ray in the dual sums of squares cone for a given nonnegative polynomial that is not a sum of squares depends on an 9-point configuration for $(n, 2d) = (3, 6)$ resp. an 8-point configuration for $(n, 2d) = (4, 4)$ coming from the intersection of two cubic resp. three quadratic forms. Furthermore, given an appropriate 9-point (resp. 8-point) configuration, one can write down an extreme ray of the dual sums of squares cone (see Theorems 3.2.2 and 3.2.1) corresponding to a face of maximal dimension in the sums of squares cone.

A central problem in this area is how to determine the separating inequalities efficiently. This can always be done in a numerical way (see Section 3.2), but is widely open for exact methods currently. Hence, finding constructive methods for computing these inequalities is one main research issue. Blekherman's results do not provide an efficient symbolic way to obtain a proper 9-point (resp. 8-point) configuration to solve this problem (see Section 3.2 for further details).

Our approach to this problem is to construct a proper 9-point (resp. 8-point) configuration out of a given initial set of points. Specifically, we investigate nonnegative polynomials p, which lie on the boundary of the cones $P_{3,6}$ and $P_{4,4}$. Our main result, Theorem 3.3.1, provides a sufficient condition for using some real zeros of p as a subset of a 9-point (resp. 8-point) configuration. The idea is to fill up the set of k zeros with $9 - k$ (resp. $8 - k$) points such that a genericity and a quadratic condition based on the Cayley-Bacharach relation hold (note that $k \leq 10$ for $p \in P_{3,6} \setminus \Sigma_{3,6}$ and $p \in P_{4,4} \setminus \Sigma_{4,4}$; see Theorem 2.6.8). Given these conditions, which are computationally easy to check, we can construct a separating extreme ray immediately. This method reduces the complexity of constructing separating extreme rays via symbolic computation significantly. Furthermore, it yields rational certificates for rational point configurations and even for rational varieties $\mathcal{V}(p) \subset \mathbb{Q}^3$ resp. $\mathcal{V}(p) \subset \mathbb{Q}^4$.

We show that for $p \in P_{3,6} \setminus \Sigma_{3,6}$ and $k \geq 7$ (resp. $p \in P_{4,4} \setminus \Sigma_{4,4}$ and $k \geq 6$) almost every 9-point (resp. 8-point) configuration containing seven (resp. six) zeros leads to a certificate for a nonnegative polynomial p to be not a sum of squares. This proves a slightly modified version of Blekherman's Conjecture 3.3.6 for many instances.

We begin with reviewing some curve theoretical issues as, e.g., the Cayley-Bacharach relation and present Blekherman's results on the dual cones $\Sigma_{3,6}^*$ and $\Sigma_{4,4}^*$. In Section 3.3 we state and prove our main Theorems 3.3.1 and 3.3.3 for ternary sextics and quaternary quartics and discuss exactness and rationality of our methods. Section 3.4 deals with the special case of polynomials with exactly seven (resp. six) zeros. We show that in these cases our method generically yields a separating extreme ray (Theorem 3.4.1), which also proves the special instances in Blekherman's Conjecture 3.3.6. Finally, in Section 3.5 we discuss the difficulties of dropping zeros in our method by applying it to the Motzkin polynomial and investigate some geometric aspects of the set of appropriate point configurations in our method (see Figure 3.1).

3.1 Curve Theoretical Background

We recall some classical results from algebraic geometry. We start with the Cayley-Bacharach relation. It exists in various formulations (see [EGH96]); we use the one given in [Ble12a].

Lemma 3.1.1. *Let $(n, 2d) \in \{(3,6),(4,4)\}$ and $f_1, \dots, f_{n-1} \in H_{n,d}$ be forms intersecting transversely in $s = d^{n-1}$ complex projective points $\gamma_1, \dots, \gamma_s$. Let $v_1, \dots, v_s$ be affine representatives of the projective points γ_i. Then there is a unique linear relation on the values of any $f \in H_{n,d}$ on v_j:*

$$\sum_{j=1}^{s} u_j f(v_j) = 0 \text{ for all } f \in H_{n,d} \tag{3.1.1}$$

with nonzero $u_j \in \mathbb{C}$. Furthermore, if (3.1.1) is satisfied, then the following genericity conditions hold for the cases $(n, 2d) = (3,6)$ resp. $(n, 2d) = (4,4)$.

$$\text{no four of the } v_i \text{ lie on a line and no seven on a quadric,} \tag{3.1.2}$$

$$\text{no five of the } v_i \text{ lie on a plane (i.e., a projective linear 2-space).} \tag{3.1.3}$$

For the genericity condition (3.1.3), see, e.g., [Hil88]. Note that if all points v_j are real, then all Cayley-Bacharach coefficients u_j are real, too (see [Ble12a, Lemma 4.1]) and can be computed by solving a system of linear equations with the coefficients of forms in $H_{3,3}$ resp. $H_{4,2}$ as variables.

Each of the conditions (3.1.2) and (3.1.3) can be checked easily by investigating the minors of the matrix given by the vectors v_j.

For the description of the extreme rays of $\Sigma_{3,6}^*$ one needs to investigate 9-point configurations given as the intersection of two coprime ternary cubics. The following lemma shows that coprimality is the case generically (see [Rez07]).

Lemma 3.1.2. *Suppose $A := \{v_1, \ldots, v_8\}$ is a set of eight distinct points in $\mathbb{R}^3$, no four on a line and no seven on a quadric and let f_1, f_2 be a basis of the vector space of all homogeneous cubics with projective variety affinely represented by A. Then f_1 and f_2 are relatively prime.*

This lemma yields that one can apply Bezout's theorem in order to compute a ninth intersection point v_9 of f_1 and f_2. However, v_9 might not be different from $v_1, \ldots, v_8$ (i.e., the intersection multiplicity might be greater than 1). But, again, generically this will not be the case as the following lemma shows (see [Nie12]).

Lemma 3.1.3. *Let f_1, f_2 be two homogeneous polynomials in n variables (with $n \geq 2$) of degree d and generic coefficients. The discriminant $\Delta(f_1, f_2)$ vanishes if and only if $f_1 = f_2 = 0$ has a singular solution. The set of polynomials for which this is the case is a hypersurface.*

In Section 3.4 we investigate the special case of polynomials $p \in P_{3,6} \setminus \Sigma_{3,6}$ with exactly seven zeros. In this context we use the following lemma (see [Rez07]).

Lemma 3.1.4. *Suppose A is a set of seven distinct points in $\mathbb{R}^3$, no four on a line and no seven on a quadric with basis f_1, f_2, f_3 for the vector space of homogeneous cubics with projective variety affinely represented by A. Then f_1, f_2, f_3 have no common zeros outside of A.*

3.2 Blekherman's Results

In [Ble12a] Blekherman fully characterizes the extreme rays of the dual cones $\Sigma_{3,6}^*$ and $\Sigma_{4,4}^*$ via the Cayley-Bacharach relation. We recall his main results.

Theorem 3.2.1. *Let $(n, 2d) \in \{(3,6), (4,4)\}$ and $p \in P_{n,2d} \setminus \Sigma_{n,2d}$. Then there exists forms $q_1, \ldots, q_{n-1} \in H_{n,d}$ intersecting transversely in $s = d^{n-1}$ projective points $\gamma_1, \ldots, \gamma_s$, which yield a certificate for $p \in P_{n,2d} \setminus \Sigma_{n,2d}$. More precisely,* *let $v_1, \dots, v_s$ be affine representatives of $\gamma_1, \dots, \gamma_s$. Then there exists a linear functional $l : H_{n,2d} \to \mathbb{R}$ given by*

$$l(f) \;=\; \sum_{i=1}^{s} a_i f(v_i)$$

for some $a_i \in \mathbb{C}$ such that $l(p) < 0$ and $l(\Sigma_{n,2d}) \geq 0$. Furthermore, at most two of the points γ_i are complex.

Recall that for every $l \in \Sigma_{n,2d}^*$ there is a corresponding quadratic form Q_l defined by $Q_l : H_{n,d} \to \mathbb{R}, f \mapsto l(f^2)$ (see, e.g., [Ble12a, Lau09]). One defines the rank of a linear functional $l \in \Sigma_{n,2d}^*$ by $\operatorname{rank}(l) := \operatorname{rank}(Q_l)$. In [Ble12a] it is shown that for $(n, 2d) \in \{(3, 6), (4, 4)\}$ every extreme ray of $\Sigma_{n,2d}^*$, which does not correspond to a point evaluation (i.e., a rank 1 quadratic form), is given by a rank $(\dim H_{n,d} - n)$ quadratic form, which comes from a 9-point evaluation (resp. 8-point evaluation) in the case $(n, 2d) = (3, 6)$ (resp. $(n, 2d) = (4, 4)$). In particular, $\dim \operatorname{Ker}(Q_l) = n$.

The linear functional l in Theorem 3.2.1 can be described in more detail by the following result.

Theorem 3.2.2 ([Ble12a]). *Let $(n, 2d) \in \{(3, 6), (4, 4)\}$. Suppose l spans an extreme ray of $\Sigma_{n,2d}^*$, which does not correspond to a point evaluation. Let W_l be the kernel of the corresponding quadratic form Q_l and suppose $q_1, \dots, q_{n-1} \in W_l$ intersect transversely in $s = d^{n-1}$ real projective points $\gamma_1, \dots, \gamma_s$ with affine representatives $v_1, \dots, v_s$ such that the unique Cayley-Bacharach relation is given by*

$$u_1 f(v_1) + \cdots + u_9 f(v_s) = 0 \quad for\; f \in H_{n,d}.$$

Then Q_l can be uniquely written as

$$Q_l(f) \;=\; a_1 f(v_1)^2 + \cdots + a_s f(v_s)^2$$

with exactly one single negative coefficient

$$a_k \;=\; \frac{-u_k^2}{\frac{u_1^2}{a_1} + \cdots + \frac{u_s^2}{a_s} - \frac{u_k^2}{a_k}} \tag{3.2.1}$$

and the rest of the a_i being strictly positive. Furthermore, any such form is extreme in $\Sigma_{n,2d}^*$.

Suppose $p \in P_{3,6} \setminus \Sigma_{3,6}$ and we want to construct a separating extreme ray l for p using Theorems 3.2.1 and 3.2.2. Therefore, we need to find two coprime ternary cubics q_1, q_2 intersecting in 9 points. But q_1, q_2 need to be contained in the kernel W_l of the quadratic form Q_l corresponding to l. Hence, one already needs to know l in advance to determine q_1, q_2.

This problem can be avoided by choosing a 9-point configuration $A = \{v_1, \ldots, v_9\}$ coming from an intersection of two real ternary cubics q_1, q_2. So, a separating extreme ray l is obtained by finding an appropriate $\mathbf{a} = (a_1, \ldots, a_9)$ satisfying (3.2.1) with respect to A such that $l_{\mathbf{a}}(p) < 0$. Whether such an $\mathbf{a}$ exists or not is unclear a priori though it can be answered by quantifier elimination methods (see, e.g., [BPR06, BCR98]). But, to the best of our knowledge, no methods are known to compute an appropriate $\mathbf{a}$ in a symbolic and exact way efficiently.

However, one can solve this problem numerically. Let $p \in P_{3,6} \setminus \Sigma_{3,6}$ be a ternary sextic and $r \in \operatorname{int}\left(\Sigma_{3,6}\right)$ (e.g., $r = x^6 + y^6 + z^6$ or $r = (x^2 + y^2 + z^2)^3$). Consider the following semidefinite optimization problem:

$$\min_{\lambda \in \mathbb{R}} \lambda \qquad \text{such that} \quad p + \lambda r \in \Sigma_{3,6}.$$

For λ minimal, the polynomial $p + \lambda r$ is strictly positive and lies on the boundary of $\Sigma_{3,6}$. Hence, $p + \lambda r$ is a sum of exactly three squares $s_1^2 + s_2^2 + s_3^2$ (see [Ble12a]).

The polynomials s_1, s_2, s_3 have no common zeros and an appropriate linear combination of two of these polynomials can be used as q_1 and q_2 in Blekherman's theorem. Of course, the computation of the corresponding nine intersection points will be difficult and not exact, too. Furthermore, getting "nice" values (e.g., a rational minimal λ) depends also highly on the choice of the polynomial $r \in \operatorname{int}\left(\Sigma_{3,6}\right)$. It is not clear how to choose r in dependence of p.

In the case $p \in P_{4,4} \setminus \Sigma_{4,4}$, this approach works the same way. For λ minimal the polynomial $p+\lambda r$ is a sum of exactly four squares $p+\lambda r = s_1^2+s_2^2+s_3^2+s_4^2$. Three of these four s_j have a common zero (see [Ble12a]).

3.3 A Certificate for Boundary Polynomials

Our approach to construct a separating extreme ray for a given boundary polynomial $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ is to investigate certain point sets $A := \{v_1, \ldots, v_9\}$ containing the variety $\mathcal{V}(p)$, satisfying the genericity condition (3.1.2) and for which we can certify that there are coprime polynomials $q_1, q_2 \in H_{3,3}$ with $\mathcal{V}(q_1) \cap \mathcal{V}(q_2) = A$.

Note that if we talk about zeros of homogeneous polynomials in this and the following sections, then we always consider their affine representatives with slight abuse of notation.

The easiest case is when p has at least eight zeros $v_1, \ldots, v_8$ (satisfying (3.1.2)). Lemma 3.1.2 provides the existence of coprime q_1, q_2 vanishing on $v_1, \ldots, v_8$ and thus a ninth point v_9 is given by Bezout's theorem. For a generic set of zeros $v_1, \ldots, v_8$ the corresponding coprime polynomials q_1, q_2 have generic coefficients and hence, due to Lemma 3.1.3, we have $v_9 \notin \{v_1, \ldots, v_8\}$ generically. Thus, $A := \{v_1, \ldots, v_9\}$ satisfies (3.1.2) generically. This yields a certificate l immediately, since for any choice of $a_1, \ldots, a_8$ we obtain an $a_9 < 0$

by (3.2.1) such that

$$l(p) \;=\; \sum_{j=1}^{9} a_j p(v_j) \;=\; a_9 p(v_9) \;<\; 0.$$

In the following, we generalize this idea to any number of zeros between one and seven. We choose the zeros $v_1, \dots, v_k$ of a polynomial $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ as a subset of the nine intersection points $A := \{v_1, \dots, v_9\}$ of two coprime ternary cubics. We provide a symbolic method based on genericity conditions, which yields a separating extreme ray if one finds a $(9-k)$-point configuration satisfying some quadratic relation. Specifically, the following theorem holds.

Theorem 3.3.1. *Let $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$. Let $A := \{v_1, \dots, v_9\} \subset \mathbb{R}^3$ be the intersection of two coprime polynomials $q_1, q_2 \in H_{3,3}$ such that the genericity condition* (3.1.2) *holds and $\mathcal{V}(p) = \{v_1, \dots, v_k\}$ with $1 \leq k \leq 7$. Then one can compute a certificate $l_{\mathbf{a}} : H_{3,6} \to \mathbb{R}, f \mapsto \sum_{j=1}^{9} a_j f(v_j)$, $\mathbf{a} := (a_1, \dots, a_9) \in \mathbb{R}^9$ with respect to A for $p \notin \Sigma_{3,6}$, if the following inequality holds:*

$$(u_{k+1}^2 + \cdots + u_8^2)(p(v_{k+1}) + \cdots + p(v_8)) \;<\; u_9^2 p(v_9). \tag{3.3.1}$$

Here, the u_j are given by the unique Cayley-Bacharach relation on A and $l_{\mathbf{a}}$ is an extreme ray of $\Sigma_{3,6}^*$.

Note that the Cayley-Bacharach coefficients u_j can be computed by solving a system of linear equations (see Section 3.5 for an example). Additionally, all u_j are rational, if every point in A is rational. Note furthermore that, for an arbitrary p, it is not clear whether an A with $\mathcal{V}(p) \subset A$ satisfying (3.3.1) does always exist. We discuss certain special cases in the two following sections.

Proof. Let $p \in \partial P_{3,6}$ with $\mathcal{V}(p) = \{v_1, \dots, v_k\}$, $1 \leq k \leq 7$, such that the genericity condition (3.1.2) holds for $\mathcal{V}(p)$. We choose points $v_{k+1}, \dots, v_8$ such that (3.1.2) is still satisfied. We obtain v_9 as the intersection of two relatively prime, cubic polynomials spanning the vector space of all ternary cubics vanishing on $v_1, \dots, v_8$ (see Lemma 3.1.2). Notice that, generically, we obtain $v_9 \notin \{v_1, \dots, v_8\}$ due to Lemma 3.1.3 and v_9 has to be real, since $v_1, \dots, v_9$ is the intersection of two real polynomials (see e.g., [Rez07]). Let $u_1, \dots, u_9$ be the unique Cayley-Bacharach coefficients for $v_1, \dots, v_9$ in the sense of (3.1.1). Since $v_1, \dots, v_9 \in \mathbb{R}^3$, we have $u_1, \dots, u_9 \in \mathbb{R}$ (see [Ble12a, Lemma 4.1]).

By Theorem 3.2.2, every vector $\mathbf{a} := (a_1, \dots, a_9) \in \mathbb{R}^9$ satisfying (3.2.1) with $a_1, \dots, a_8 > 0$, $a_9 < 0$ yields an extreme ray $l_{\mathbf{a}} : H_{3,6} \to \mathbb{R}, f \mapsto \sum_{j=1}^{9} a_j f(v_j)$ of the dual cone $\Sigma_{3,6}^*$. The linear functional $l_{\mathbf{a}}$ is the dual of a separating hyperplane for p if $l_{\mathbf{a}}(p) < 0$, i.e., if $a_{k+1}p(v_{k+1}) + \cdots + a_9 p(v_9) < 0$, since $\mathcal{V}(p) = \{v_1, \dots, v_k\}$. By (3.2.1), this is equivalent to

$$\begin{aligned} a_{k+1}p(v_{k+1}) + \cdots - \frac{u_9^2}{\frac{u_1^2}{a_1} + \cdots + \frac{u_8^2}{a_8}} p(v_9) \;&<\; 0 \\ \Leftrightarrow (a_{k+1}p(v_{k+1}) + \cdots + a_8 p(v_8)) \cdot \left(\frac{u_1^2}{a_1} + \cdots + \frac{u_8^2}{a_8} \right) \;&<\; u_9^2 p(v_9). \end{aligned}$$

Let $\lambda_{a_1,\dots,a_k} := \sum_{j=1}^{k} \frac{u_j^2}{a_j} \cdot (a_{k+1}p(v_{k+1}) + \cdots + a_8 p(v_8)) > 0$. Thus, $l_{\mathbf{a}}(p) < 0$, if

$$\lambda_{a_1,\dots,a_k} + \sum_{j=k+1}^{8} p(v_j) \left(u_j^2 + \sum_{i \in \{k+1,\dots,8\} \setminus \{j\}} \frac{a_j u_i^2}{a_i} \right) \quad < \quad u_9^2 p(v_9).$$

We choose $a_{k+1} := 1, \dots, a_8 := 1$ and obtain

$$\lambda_{a_1,\dots,a_k} + (u_{k+1}^2 + \cdots + u_8^2)(p(v_{k+1}) + \cdots + p(v_8)) \quad < \quad u_9^2 p(v_9).$$

Since $\lim_{a_1,\dots,a_k \to \infty} \lambda_{a_1,\dots,a_k} \searrow 0$, the relaxation (3.3.1) yields an extreme ray $l_{\mathbf{a}}$ on A separating p from $\Sigma_{3,6}$.

If, on the other hand, any polynomial $g \in \Sigma_{3,6}$ with $\mathcal{V}(g) = \mathcal{V}(p)$ would satisfy (3.3.1), then it follows from the above construction that $l_{\mathbf{a}}(g) < 0$ for $a_1, \dots, a_k$ sufficiently large, $a_{k+1}, \dots, a_8 = 1$ and a_9 given by (3.2.1). This is a contradiction to Theorems 3.2.2 and 3.2.1. Thus, (3.3.1) is indeed a certificate for $p \notin \Sigma_{3,6}$. ■

In order to prove an analogon of Theorem 3.3.1 for $P_{4,4} \setminus \Sigma_{4,4}$, we need to show that Lemma 3.1.2 also holds for a seven point set $A := \{v_1, \dots, v_7\} \subset \mathbb{R}^4$. Generically, the vector space of all quadrics vanishing on A has dimension three (see [Eis05]).

Lemma 3.3.2. *Suppose $A := \{v_1, \dots, v_7\}$ is a set of seven distinct points in $\mathbb{R}^4$, no four on a plane such that q_1, q_2, q_3 is a basis for the vector space of all homogeneous quadrics with projective variety affinely represented by A. Then q_1, q_2, q_3 are relatively prime.*

Proof. Suppose q_1, q_2, q_3 have a common factor g. Then $q_j = g \cdot q_j'$ for $j \in \{1, 2, 3\}$ and g, q_j' have to be linear in $\mathbb{R}[x_1, \dots, x_4]$. Due to the genericity condition at most three zeros (w.l.o.g. v_1, v_2, v_3) are located on $\mathcal{V}(g)$ since otherwise there would exist at least five points contained in a plane. Hence, $\mathcal{V}(q_1'), \mathcal{V}(q_2')$ and $\mathcal{V}(q_3')$ share four points, which is a contradiction, since for each j all points in $\mathcal{V}(q_j')$ are contained in a line. ■

Theorem 3.3.3. *Let $p \in \partial P_{4,4} \setminus \Sigma_{4,4}$. Let $A := \{v_1, \dots, v_8\} \subset \mathbb{R}^4$ be the intersection of three coprime polynomials $q_1, q_2, q_3 \in H_{4,2}$ such that the genericity condition* (3.1.3) *holds and $\mathcal{V}(p) = \{v_1, \dots, v_k\}$ with $1 \leq k \leq 6$. Then there exists a certificate $l_{\mathbf{a}} : H_{4,4} \to \mathbb{R}, f \mapsto \sum_{j=1}^{8} a_j f(v_j)$, $\mathbf{a} := (a_1, \dots, a_8) \in \mathbb{R}^8$ with respect to A for $p \notin \Sigma_{4,4}$, if the following inequality holds*

$$(u_{k+1}^2 + \cdots + u_7^2)(p(v_{k+1}) + \cdots + p(v_7)) \quad < \quad u_8^2 p(v_8). \tag{3.3.2}$$

Here the u_j are given by the unique Cayley-Bacharach relation on A and $l_{\mathbf{a}}$ is an extreme ray of $\Sigma_{4,4}^*$.

The proof works the same way as for Theorem 3.3.1 with the obvious modifications.

In fact, the proof of Theorem 3.3.1 already shows one possible way how to choose $\mathbf{a} = (a_1, \dots, a_9) \in \mathbb{R}^9$ to obtain a separating extreme ray $l_{\mathbf{a}}$.

Corollary 3.3.4. *For $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ and $A = \{v_1, \dots, v_9\} \supset \mathcal{V}(p)$ with* (3.3.1) *satisfied, one valid certificate is given by $a_1 = \dots = a_k = N \in \mathbb{R}$ (for N sufficiently large), $a_{k+1} = \dots = a_8 = 1$ and a_9 given by* (3.2.1). *For $p \in \partial P_{4,4} \setminus \Sigma_{4,4}$ and $A = \{v_1, \dots, v_8\} \supset \mathcal{V}(p)$ with* (3.3.2) *satisfied, one valid certificate is given by $a_1 = \dots = a_k = N \in \mathbb{R}$ (for N sufficiently large), $a_{k+1} = \dots = a_7 = 1$ and a_8 given by the analogon of* (3.2.1) *for $\Sigma_{4,4}^*$ (see [Ble12a]). In particular, $l_{\mathbf{a}}$ is a rational certificate, i.e., every a_j is rational, if every point $v_j \in A$ is rational.*

If one is interested in computing rational certificates, then, from an application viewpoint, there is the following problem. Suppose, we have a rational variety $\mathcal{V}(p) = \{v_1, \dots, v_k\}$ and we choose $v_{k+1}, \dots, v_8 \in \mathbb{Q}^3$ (resp. $v_{k+1}, \dots, v_7 \in \mathbb{Q}^4$) such that the genericity condition (3.1.2) (resp. (3.1.3)) holds (which is always possible). Then it is not clear a priori that the ninth intersection point $v_9 \in \mathbb{R}^3$ (resp. eighth intersection point $v_8 \in \mathbb{R}^4$) given by Bezout is rational, too.

By results in [PSV11] and [Ren11], for $p \in P_{3,6} \setminus \Sigma_{3,6}$ (resp. $p \in P_{4,4} \setminus \Sigma_{4,4}$), the ninth (resp. eighth) intersection point can always be computed exactly. In particular, it can be deduced that this last point will always be rational whenever the remaining points are rational and hence whenever $\mathcal{V}(p)$ is rational.

Corollary 3.3.5. *Let $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ with $\mathcal{V}(p) = \{v_1, \dots, v_k\} \subset \mathbb{Q}^3$ and $\{v_{k+1}, \dots, v_8\} \subset \mathbb{Q}^3$ such that* (3.1.2) *holds. Then there is a rational certificate $l_{\mathbf{a}}$ on $A = \{v_1, \dots, v_9\}$ with v_9 given by Bezout, whenever* (3.3.1) *holds.*

Obviously, an analogous result also holds in the case $(n, 2d) = (4, 4)$.

Note that in our Theorems 3.3.1 and 3.3.3 we only consider real points $v_1, \dots, v_9$ whereas in Blekherman's Theorem 3.2.1 (at most) one pair of complex conjugated points is allowed. However, in [Ble12a] Blekherman states the following conjecture.

Conjecture 3.3.6. *Every extreme ray $l \in \Sigma_{3,6}^*$, which is not a point evaluation, is given by two ternary cubics intersecting in only real points. Analogously, for $l \in \Sigma_{4,4}^*$.*

Based on our results we formulate a slightly modified conjecture here.

Conjecture 3.3.7. *For $p \in P_{3,6} \setminus \Sigma_{3,6}$ there exist $v_1, \dots, v_9 \in \mathbb{R}^3$ yielding a separating extreme ray for p in the sense of Theorem 3.2.1. Analogously, for $p \in P_{4,4} \setminus \Sigma_{4,4}$.*

Clearly, Conjecture 3.3.6 implies Conjecture 3.3.7, since if every extreme ray is real representable, then every nonnegative polynomial that is not a sum of squares can be separated by a real intersection. It is unclear whether the two conjectures are indeed equivalent, however, we strongly suspect this.

3.4 The Seven Point Case

Let $p \in P_{3,6} \setminus \Sigma_{3,6}$ and assume we are interested in finding a separating extreme ray $l_{\mathbf{a}}$ in $\Sigma_{3,6}^*$ for p. That means we need to find a generic 9-point set A being the intersection of two coprime polynomials $q_1, q_2 \in H_{3,3}$ such that the conditions in Theorem 3.2.1 hold. If p is located on the boundary of $P_{3,6}$, i.e., $\mathcal{V}(p) = \{v_1, \ldots, v_k\} \neq \emptyset$, then Theorem 3.3.1 and Corollary 3.3.4 yield a certificate $l_{\mathbf{a}}$ whenever one can fill up $\mathcal{V}(p)$ with points $v_{k+1}, \ldots, v_9$ such that condition (3.3.1) is satisfied.

However, it is not obvious a priori if and how points $v_{k+1}, \ldots, v_9$ can be chosen such that the sufficient condition (3.3.1) of Theorem 3.3.1 holds (note that v_9 is always given by Bezout in this approach). It turns out that for $k = 7$, i.e., the easiest non-trivial case, the problem of choosing an appropriate v_8 is easy, since almost every v_8 yields an v_9 such that (3.3.1) is satisfied. Note that for $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ the variety $\mathcal{V}(p)$ always satisfies the genericity condition (3.1.2) (see [Rez07]).

One reason why this case is of special interest is that $k = 7$ with $v_1, \ldots, v_7$ satisfying the genericity condition (3.1.2) is the smallest number of zeros of a nonnegative polynomial such that the dimensional difference between exposed faces of $P_{3,6}$ and $\Sigma_{3,6}$ given by vanishing of forms on these zeros is strictly positive (see Chapter 4). In particular, by results in the upcoming Chapter 4, this implies that for every generic configuration of seven points one can always construct nonnegative polynomials that are not sums of squares vanishing at these points.

Theorem 3.4.1. *Let $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ and $A := \{v_1, \ldots, v_9\} \subset \mathbb{R}^3$ be the intersection of two coprime polynomials $q_1, q_2 \in H_{3,3}$ such that the genericity condition (3.1.2) holds and $\mathcal{V}(p) = \{v_1, \ldots, v_7\}$. Then there exists a certificate $l_{\mathbf{a}} : H_{3,6} \to \mathbb{R}, f \mapsto \sum_{j=1}^{9} a_j f(v_j)$, $a_j \in \mathbb{R}$ with respect to A for $p \notin \Sigma_{3,6}$ if*

$$u_8^2 p(v_8) \quad \neq \quad u_9^2 p(v_9). \qquad (3.4.1)$$

Furthermore, $l_{\mathbf{a}}$ is an extreme ray of $\Sigma_{3,6}^*$.

Theorem 3.4.1 holds analogously in the case of $p \in P_{4,4} \setminus \Sigma_{4,4}$ and $k = 6$ with the obvious modifications. We omit to formulate the result for this case separately.

Proof. We choose v_8 such that the genericity condition (3.1.2) still holds for $\{v_1, \ldots, v_8\}$ and obtain a real $v_9 \notin \{v_1, \ldots, v_8\}$ such that (3.1.2) and Cayley-Bacharach hold for A generically (see proof of Theorem 3.3.1). Since all conditions of Theorem 3.3.1 are satisfied, there is a certificate $l \in \Sigma^*_{3,6}$ if $u_8^2 p(v_8) < u_9^2 p(v_9)$. But since $\{v_1, \ldots, v_7, v_9\}$ also yields A with Bezout's theorem, this condition holds w.l.o.g. as long as $u_8^2 p(v_8) \neq u_9^2 p(v_9)$. ■

A nice consequence of this theorem is that it immediately verifies Conjecture 3.3.7 for special instances.

Corollary 3.4.2. *Conjecture 3.3.7 holds for $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ with $\#\mathcal{V}(p) \geq 7$ and $p \in \partial P_{4,4} \setminus \Sigma_{4,4}$ with $\#\mathcal{V}(p) \geq 6$. Furthermore, Conjecture 3.3.7 holds also for every exposed extremal form in $P_{3,6} \setminus \Sigma_{3,6}$.*

Proof. The first part immediately follows from Theorem 3.4.1. Furthermore, in [BHO+12] it is shown that every exposed extremal form in $P_{3,6} \setminus \Sigma_{3,6}$ has exactly ten zeros. By choosing seven of them, the results follow. ■

3.5 An Application: The Motzkin Polynomial

In this section, we demonstrate applications of our method. It turns out that finding a separating extreme ray becomes more difficult for polynomials in $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ with six or less zeros. The condition (3.3.1) provides more degrees of freedom and, in particular, the left hand side of this inequality has more than one term. This fact yields that the set of point configurations $A := \{v_1, \ldots, v_9\} \subset \mathbb{R}^3$ with $\mathcal{V}(p) \subset A$, which do not satisfy (3.3.1), will not be a lower dimensional subset in general, in contrast to the seven point case (independent from which point corresponds to the negative entry a_9 in an extreme ray). The same difficulties arise for $p \in P_{4,4} \setminus \Sigma_{4,4}$ with five or less zeros.

As an example, we investigate the Motzkin polynomial

$$m(x, y, z) = x^4y^2 + x^2y^4 - 3x^2y^2z^2 + z^6.$$

The Motzkin polynomial has six zeros.

$$\begin{aligned} v_1 &:= (1,0,0), & v_2 &:= (0,1,0), & v_3 &:= (1,1,1), \\ v_4 &:= (-1,1,1), & v_5 &:= (1,-1,1), & v_6 &:= (1,1,-1). \end{aligned}$$

As a first instance we choose $v_7 := (0,4,1)$ and $v_8 := (4,0,1)$. These eight points satisfy the genericity condition (3.1.2). This can be checked by looking at the (3×3)-minors of the (8×3)-matrix given by the coordinates (x, y, z) of the points $v_1, \ldots, v_8$ and looking at the (6×6)-minors of the (8×6)-matrix given by the coordinates $(x^2, y^2, z^2, xy, xz, yz)$ of the points $v_1, \ldots, v_8$. Hence we can compute two coprime ternary cubics

$$\begin{aligned} q_1 &= -16z^3 + 15x^2z + y^2z + 56y^2x - 56z^2x \\ q_2 &= -4z^3 - x^2y + 4x^2z + 15y^2x - 15z^2x + z^2y \end{aligned}$$

vanishing on $v_1, \ldots, v_8$ by solving the system of linear equations

$$h(v_1) \;=\; 0, \ldots, h(v_8) \;=\; 0$$

on the coefficients of h. Here,

$$\begin{aligned} h \;&:=\; b_1x^3 + b_2y^3 + b_3z^3 + b_4x^2y + b_5x^2z \\ &+\; b_6y^2z + b_7y^2x + b_8z^2x + b_9z^2y + b_{10}xyz. \end{aligned}$$

We compute the Gröbner basis

$$\{7z - 26z^2 - 15z^3 + 26z^4 + 8z^5, -2z + 8z^2 + 2z^3 - 105y - 8z^4 + 105z^2y,$$
$$8z^4 - 422z^3 + 1575y^2 - 1583z^2 + 422z, x - 1\}$$

of q_1, q_2 and $x - 1$ with respect to lexicographic ordering. We obtain $v_9 = (1, 1, -7/2)$ and compute the Cayley-Bacharach coefficients u_j by solving the system of linear equations

$$u_1h(v_1) + \cdots + u_9h(v_9) \;=\; 0$$

in $u_1, \ldots, u_9$. The solution is (up to scalar multiplication)

$$u \;=\; \left(-64, -64, -\frac{40}{9}, -4, -4, \frac{24}{5}, 1, 1, \frac{118098}{5}\right)^T.$$

We have

$$\begin{aligned} (u_7^2 + u_8^2) \cdot (m(v_7) + m(v_8)) \;&=\; 4, \\ u_9^2 m(v_9) \;&=\; 228. \end{aligned}$$

Hence, condition (3.3.1) of Theorem 3.3.1 is satisfied and we find a separating hyperplane for m on A. According to Corollary 3.3.4, we choose $a_1, \ldots, a_6 := 100$ and $a_7, a_8 := 1$. By (3.2.1), we obtain

$$a_9 \;=\; \frac{-u_9^2}{\frac{u_1^2}{a_1} + \cdots + \frac{u_8^2}{a_8}} \;=\; \frac{-14121476824050}{2143157}.$$

We check the correctness of our result by

$$\begin{aligned} l_{\mathbf{a}}(m) \;&=\; a_1m(v_1) + \cdots + a_9m(v_9) \\ &=\; m(0, 4, 1) + m(4, 0, 1) - \frac{14121476824050}{2143157} \cdot m\left(1, 1, -\frac{7}{2}\right) \\ &=\; -\frac{1484936}{2143157} \;<\; 0. \end{aligned}$$

Thus, by Blekherman's Theorem 3.2.2 ([Ble12a]), $l_{\mathbf{a}}$ is a (rational) extreme ray of $\Sigma_{3,6}^*$ separating the Motzkin polynomial m from $\Sigma_{3,6}$.

In contrast to the seven point case, not every generic point configuration yields a separating certificate. For example, with the same approach it is easy to show that the instance $v_7 := (2/7, 2/3, 1)$ and $v_8 := (2/3, 2/7, 1)$ does not satisfy the condition (3.3.1). We show that for a symmetric choice of v_7, v_8, i.e., $v_7 = (q, s, 1), v_8 = (s, q, 1)$ with $q, s \in \mathbb{R}$, the set

$$S \;:=\; \{(q,s) \in \mathbb{R}^2 \;:\; (u_7^2 + u_8^2) \cdot (m(v_7) + m(v_8)) < u_9^2 m(v_9)\}$$

yieding a 9-point configuration, which satisfies (3.3.1) is full dimensional with some nice geometric structure (see Figure (3.1)).

With the formula in [Ren11] we obtain the ninth Cayley-Bacharach point

$$v_9 \;=\; \frac{1}{n(q,s)} \cdot \begin{pmatrix} q^3s + 2q^2s^2 - q^2 + s^3q - 2sq - s^2 \\ q^3s + 2q^2s^2 - q^2 + s^3q - 2sq - s^2 \\ q^3 + q^2s - 2q + s^2q - 2s + s^3 \end{pmatrix},$$

where

$$\begin{aligned} n(q,s) = 12 \quad &\cdot \quad (q^3s^2 - 2q^3s + q^3 + s^3q^2 - 2q^2s^2 \\ &+ \quad q^2s - 3q + 4sq - 2s^3q + s^2q + 2 - 3s + s^3). \end{aligned}$$

Note that $n(q,s)$ vanishes at $q = -2 - s, q = 1, s = 1$. Furthermore, we obtain a non-generic point set for $q = s, q = -s, q = -1, s = -1$ and $q = 2 - s$. We compute the Cayley-Bacharach coefficients in dependence of q, s and obtain

$$\begin{aligned} (u_7^2 + u_8^2) \cdot (m(v_7) + m(v_8)) \;&=\; \frac{64(1 + s^4q^2 + q^4s^2 - 3q^2s^2)}{(q-s)^4} \\ u_9^2 m(v_9) \;&=\; \frac{16(2q^4s^2 + q^4 + 4s^3q^3 - 4q^3s + 2s^4q^2}{(q-s)^4} \\ &+\; \frac{-6q^2s^2 - 2q^2 - 4s^3q + 4sq + s^4 - 2s^2 + 4)}{(q-s)^4}. \end{aligned}$$

Note that the numerator of $(u_7^2+u_8^2)\cdot(m(v_7)+m(v_8))$ is exactly the dehomogenized Motzkin polynomial in s, q for $z = 1$. We set

$$\begin{aligned} K(q,s)/L(q,s) \;&:=\; (u_7^2 + u_8^2) \cdot (m(v_7) + m(v_8)) - u_9^2 m(v_9) \\ &=\; 16(2q^2s^2 - q^2 + 2sq - s^2 + 2)/(q-s)^2. \end{aligned}$$

Since $q \neq s$ by assumption, we just need to investigate $K(q,s)$. Thus, by (3.3.1) we have $(q,s) \in S$ if and only if $K(q,s) < 0$ and $q \notin \{\pm s, \pm 1, \pm 2 - s\}$. Equivalently, $S = \emptyset$ if and only if $K(q,s)$ is nonnegative and $q \notin \{\pm s, \pm 1, \pm 2 - s\}$. Since $K(q,s)$ is a bivariate polynomial of degree 4, $K(q,s)$ is nonnegative if only if it is a sum of squares. It can be checked easily that this is not the case.

We provide a plot of the set $S := \{(q,s) : K(q,s) < 0\} \setminus \{(q,s) : q = 2 - s \text{ or } q = -2 - s\}$ in Figure 3.1 (note that the other non-generic cases are

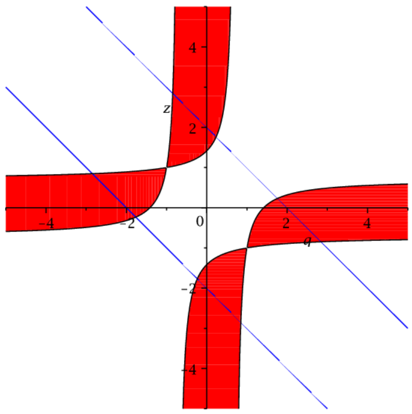

Figure 3.1: The set $S := \{(q,s) : K(q,s) < 0\} \setminus \{(q,s) : q = 2-s \text{ or } q = -2-s\}$ is given by the red area without the blue lines.

not part of S although they are relevant for the computation). Obviously, this set is symmetric in $q = s$ and $q = -s$, semialgebraic and for every q there is an s such that $(q,s) \in S$.

Due to the rich geometric structure of S it would be interesting to investigate the geometric structure of the set of appropriate point configurations satisfying (3.3.1) for general nonnegative polynomials with k zeros.

In contrast, we briefly demonstrate the numerical method for finding a 9-point certificate given in Section 3.2 and the corresponding problems. Let $r = (x^2+y^2+z^2)^3 \in \operatorname{int}(\Sigma_{3,6})$ and consider the following semidefinite optimization problem:

$$\min_{\lambda \in \mathbb{R}} \lambda \qquad \text{such that} \quad m + \lambda(x^2+y^2+z^2)^3 \in \Sigma_{3,6}.$$

The optimal λ is given numerically by $\lambda \approx 0.004596411406567$ and the corresponding sum of squares decomposition of $m + \lambda r \approx s_1^2 + s_2^2 + s_3^2$ is given by

$$m + \lambda(x^2+y^2+z^2)^3 \;\approx\; (-0.8586xz^2 + 0.9414xy^2 + 0.0678x^3)^2 +$$

$$(-0.8586yz^2 + 0.0678y^3 + 0.9414x^2y)^2 + (-1.002z^3 + 0.3608y^2z + 0.3608x^2z)^2.$$

Now, one has to choose an appropriate linear combination of two of the polynomials s_i to obtain the nine intersection points. But it seems unclear how to do this. Since the coefficients of the s_i are given numerically, computing the Gröbner basis of two of the s_i and, say, $x-1$ cannot be expected to work properly.

Finally, we remark that our method allows to generate strictly positive polynomials that are not sums of squares. It also comes with a certificate without optimization, if (3.3.1) is satisfied for a polynomial $p \in \partial P_{3,6} \setminus \Sigma_{3,6}$ (resp. for $(n,2d) = (4,4)$). Let $l_{\mathbf{a}}$ be a separating extreme ray for p and define

$n := p + \lambda \cdot r$ with $\lambda \in \mathbb{R}_{>0}$ and $r \in \text{int}(\Sigma_{3,6})$ (resp. $r \in \text{int}(\Sigma_{4,4})$). Then n is strictly positive and evaluating n on $l_{\mathbf{a}}$ yields

$$l_{\mathbf{a}}(n) \quad = \quad l_{\mathbf{a}}(p) + \lambda \cdot l_{\mathbf{a}}(r)$$

with $l_{\mathbf{a}}(p) < 0$ and $l_{\mathbf{a}}(r) > 0$. Hence, we can immediately solve for λ such that $l_{\mathbf{a}}(n) < 0$.

Chapter 4

Dimensional Differences Between Faces of the Cones of Nonnegative Polynomials and Sums of Squares

In this chapter, we discuss the facial structure of the cones of nonnegative polynomials and sums of squares. Investigating the boundary structure of these cones is a very important and famous tool in analyzing the difference between the cones. This is, because many explicit examples of nonnegative polynomials that are not sums of squares are based on Hilbert's original method, which, roughly speaking, is based on prescribing points and comparing nonnegative polynomials and sums of squares vanishing at these points. In the following, we generalize Hilbert's method by comparing possible dimensions of the faces of these cones. Recently, in small dimensions, several aspects of the difference between these cones, such as the boundary structure of the dual cones and the algebraic boundaries of these cones, are investigated (see [Ble12a, Ble12b, BHO+12]). But it is worth to note that, in spite of these results, we still lack a clear understanding of the quantitative relationship of these cones in small dimensions. In the following, let $\mathbb{RP}^{n-1}$ resp. $\mathbb{CP}^{n-1}$ denote the $(n-1)$-dimensional real resp. complex projective space.

We focus on the study of exposed faces of the cones $P_{n,2d}$ and $\Sigma_{n,2d}$, in particular on the investigation of their possible dimensions. It is easy to describe exposed faces of $P_{n,2d}$. Indeed, the boundary of the cone $P_{n,2d}$ consists of all the forms with at least one real zero, whereas its interior consists of all strictly positive forms. In particular, a maximal proper face of $P_{n,2d}$ consists of all forms with exactly one prescribed zero (see Proposition 2.6.4).

Let Γ be a finite set of points in $\mathbb{RP}^{n-1}$. The forms in $P_{n,2d}$ vanishing at all points of Γ form an exposed face of $P_{n,2d}$, which we call $P_{n,2d}(\Gamma)$:

$$P_{n,2d}(\Gamma) = \{p \in P_{n,2d} : p(s) = 0 \text{ for all } s \in \Gamma\}.$$

Similarly, we let $\Sigma_{n,2d}(\Gamma)$ be the exposed face of $\Sigma_{n,2d}$ consisting of forms that vanish at all points of Γ:

$$\Sigma_{n,2d}(\Gamma) = \{p \in \Sigma_{n,2d} : p(s) = 0 \text{ for all } s \in \Gamma\}.$$

Moreover, any exposed face of $P_{n,2d}$ has a description of the above form and the set Γ can be chosen to be finite [BPT13, Chapter 4]. We note that, despite this simple description of exposed faces, the full facial structure of $P_{n,2d}$ should be very difficult to fully describe, since – as already mentioned – the problem of testing for nonnegativity is known to be NP-hard. Furthermore, even for the exposed faces $P_{n,2d}(\Gamma)$ and $\Sigma_{n,2d}(\Gamma)$, except for the simple cases of $n = 2$ and $2d = 2$, the possible dimensions of these faces have not been investigated yet. We close this gap by deriving estimates for the dimensions of the faces $P_{n,2d}(\Gamma)$ and $\Sigma_{n,2d}(\Gamma)$ and by establishing dimensional differences between those faces in many cases. It is worth remarking that also Hilbert's original proof in [Hil88] of existence of nonnegative polynomials that are not sums of squares can be viewed as establishing a dimensional gap of this type. This dimensional point of view was first made explicit in [Rez07].

For a generic set Γ we reduce the question of dimensions of $P_{n,2d}(\Gamma)$ and $\Sigma_{n,2d}(\Gamma)$ to the question of dimensions of the degree $2d$ components of certain ideals associated with Γ. For an ideal $I \subset \mathbb{R}[\mathbf{x}]$, let I^2 denote the second ordinary power of I, and let $I^{(2)}$ denote the second symbolic power of I. Moreover, let I_d denote the homogeneous degree d part of I.

If $I(\Gamma) \subset \mathbb{R}[\mathbf{x}]$ is the vanishing ideal of a finite set of points $\Gamma \subset \mathbb{RP}^{n-1}$, then the second symbolic power $I^{(2)}(\Gamma)$ of $I(\Gamma)$ is the ideal of all forms in $\mathbb{R}[\mathbf{x}]$ vanishing at every point of Γ to order at least two:

$$I^{(2)}(\Gamma) = \{p \in \mathbb{R}[\mathbf{x}] \;:\; \nabla p(s) = 0 \text{ for all } s \in \Gamma\}.$$

Since every nonnegative form that is zero on $s \in \Gamma$ must vanish to order two on s, it follows that the face $P_{n,2d}(\Gamma)$ is contained in the degree $2d$ part of $I^{(2)}(\Gamma)$:

$$P_{n,2d}(\Gamma) \subset I^{(2)}_{2d}(\Gamma).$$

On the other hand, we know that the face $\Sigma_{n,2d}(\Gamma)$ is contained in the following set:

$$\begin{aligned} \Sigma_{n,2d}(\Gamma) \subset (I_d(\Gamma))^2 &= \left\{ \sum_i \alpha_i f_i g_i \;:\; f_i, g_i \in I_d(\Gamma), \alpha_i \in \mathbb{R} \right\} \\ &= \left\{ \sum_i \alpha_i q_i^2 \;:\; q_i \in I_d(\Gamma), \alpha_i \in \mathbb{R} \right\}. \end{aligned}$$

It is easy to see that this inclusion is actually full dimensional, since we can pick a basis of $(I_d(\Gamma))^2$ consisting of squares and nonnegative linear combinations of these squares will lie in $\Sigma_{n,2d}(\Gamma)$.

Proposition 4.0.1. *Let $\Gamma \subset \mathbb{RP}^{n-1}$ be a finite set. Then $\Sigma_{n,2d}(\Gamma)$ is a full dimensional convex cone in the vector space of all forms of degree $2d$ in $(I_d(\Gamma))^2$:*

$$\dim \Sigma_{n,2d}(\Gamma) = \dim(I_d(\Gamma))^2.$$

4.1 Dimensions of Faces of $P_{n,2d}$

In this section, as for sums of squares, we pose the question under which assumptions $P_{n,2d}(\Gamma)$ is a full dimensional subcone of $I_{2d}^{(2)}(\Gamma)$. In order to answer this question, the following crucial definition is required.

Definition 4.1.1. *Let $\Gamma \subset \mathbb{RP}^{n-1}$ be a finite set of points and $I = I(\Gamma) \subset \mathbb{R}[\mathbf{x}]$ be the vanishing ideal of Γ. We call $\Gamma \subset \mathbb{RP}^{n-1}$* d-independent *if Γ satisfies the following two conditions:*

1. *The forms in I_d share no common zeros in $\mathbb{CP}^{n-1}$ outside of Γ. In other words, the conditions of vanishing on Γ force no additional zeros on forms of degree d in $H_{n,d}$,*
2. *For any $s \in \Gamma$ the forms that vanish to order two on s and vanish at the rest of Γ to order one form a vector space of codimension $|\Gamma| + n - 1$ in $H_{n,d}$.*

The second condition in the above definition simply states that the constraints of vanishing on Γ and additionally double vanishing at any point $s \in \Gamma$ are all linearly independent. We provide the following equivalent characterization of d-independence based on Hilbert functions.

Proposition 4.1.2. *Let $\Gamma \subset \mathbb{RP}^{n-1}$ be a finite set of points and let $J \subset \mathbb{R}[\mathbf{x}]$ be the ideal generated by $I_d(\Gamma)$. Then Γ is d-independent if and only if the Hilbert polynomial of $\mathbb{R}[\mathbf{x}]/J$ is equal to $|\Gamma|$.*

Proof. Let J be the ideal generated by $I_d(\Gamma)$. Let $I_{\mathbb{C},d}(\Gamma)$ be the set of all degree d *complex* forms vanishing on Γ. We first observe that linear combinations of forms in $I_d(\Gamma)$ taken with complex coefficients generate $I_{\mathbb{C},d}(\Gamma)$. Therefore, if we let $J_{\mathbb{C}}$ be the complex ideal generated $I_{\mathbb{C},d}(\Gamma)$, then it suffices to show that the Hilbert polynomial of $\mathbb{C}[\mathbf{x}]/J_{\mathbb{C}}$ is $|\Gamma|$.

We now apply Bertini's theorem (see, e.g., [Har92a, Theorem 17.16]) to the linear system of divisors $I_{\mathbb{C},d}(\Gamma)$. Since Γ is d-independent, it follows that a general element of $I_{\mathbb{C},d}(\Gamma)$ is non-singular at every point of Γ and thus we may find a smooth hypersurface $f_1 \in I_{\mathbb{C},d}(\Gamma)$. Now, d-independence guarantees that a general form in $I_{\mathbb{C},d}(\Gamma)$ intersects f_1 smoothly and therefore we apply Bertini's theorem again to find $f_2 \in I_{\mathbb{C},d}(\Gamma)$ such that $f_1 \cap f_2$ is smooth. We proceed in this way repeatedly applying Bertini's theorem until we end up with a transverse zero-dimensional intersection $V = f_1 \cap \cdots \cap f_{n-1}$. By construction, we have $\Gamma \subseteq V$.

Since $J_{\mathbb{C}}$ defines a zero-dimensional ideal and all forms in $J_{\mathbb{C}}$ vanish on Γ, it follows that the Hilbert polynomial of $\mathbb{C}[\mathbf{x}]/J_{\mathbb{C}}$ is a constant and it is greater or equal than $|\Gamma|$. Since we have $\langle f_1, \ldots, f_{n-1} \rangle \subset J_{\mathbb{C}}$ and the ideal generated by $f_1, \ldots, f_{n-1}$ is radical, it follows that we just need to show that for all $s \in V \setminus \Gamma$ there exists $g \in J_{\mathbb{C}}$ such that $g(s) \neq 0$ and $g(z) = 0$ for all $z \in V \setminus \{s\}$. Since Γ

is d-independent, it suffices to show that for all $s \in V \setminus \Gamma$ there exists $h \in I_d(\Gamma)$ such that $h(s) \neq 0$. Also there exists $h' \in \mathbb{C}[x_1, \ldots, x_n]$ such that $h'(s) = 1$ and $h'(z) = 0$ for all $z \in V \setminus \{s\}$. Therefore $hh' \in J_{\mathbb{C}}$ and one direction of the proposition follows.

Now suppose that Γ is not d-independent. First, if all forms in $I_d(\Gamma)$ vanish at a point not in Γ, then all forms in J vanish on at least $|\Gamma| + 1$ points and therefore the Hilbert function of $\mathbb{R}[\mathbf{x}]/J$ is at least $|\Gamma| + 1$ for all large enough degrees. Therefore, the Hilbert polynomial of $\mathbb{R}[\mathbf{x}]/J$ is not $|\Gamma|$. Now suppose that for some $s \in \Gamma$ and for some $w \in \mathbb{R}^n \setminus \operatorname{span}\{s\}$ we have $\langle \nabla p(s), w \rangle = 0$ for all $p \in I_d(\Gamma)$. Then again we find that the Hilbert function of $\mathbb{R}[\mathbf{x}]/J$ is at least $|\Gamma| + 1$ for all high enough degrees. ■

We remark that in the above proof h' may be chosen such that $\deg h' \leq (n-1)(d-1)$. Therefore, we have $\deg hh' \leq (n-1)(d-1) + d$ and for all degrees $k \geq (n-1)(d-1) + d$ the Hilbert function of $\mathbb{C}[\mathbf{x}]/J_{\mathbb{C}}$ (and of $\mathbb{R}[\mathbf{x}]/J$) evaluated at k must be equal to $|\Gamma|$. Thus, using standard methods (vanishing determinants) we can express the set of all configurations of k points in $\mathbb{RP}^{n-1}$ that are d-independent as a complement of a closed algebraic set. Hence, the set of configurations Γ of k points in $\mathbb{RP}^{n-1}$ that are d-independent is Zariski open, which proves the following corollary:

Corollary 4.1.3. *The set of d-independent configurations of k points in $\mathbb{RP}^{n-1}$ is a Zariski open subset of $(\mathbb{RP}^{n-1})^k$.*

4.1.1 Sum of Squares Certificate.

In this subsection, we provide the proof of the following proposition, which ensures full dimensionality of $P_{n,2d}(\Gamma)$ in $I_{2d}^{(2)}(\Gamma)$.

Proposition 4.1.4. *Let $\Gamma \subset \mathbb{RP}^{n-1}$ be a d-independent set. Then $P_{n,2d}(\Gamma)$ is a full dimensional convex cone in $I_{2d}^{(2)}(\Gamma)$:*

$$\dim P_{n,2d}(\Gamma) = \dim I_{2d}^{(2)}(\Gamma).$$

Let Γ be a finite set of points in $\mathbb{RP}^{n-1}$ and consider $I_{2d}^{(2)}(\Gamma)$, the vector space of forms of degree $2d$ vanishing on Γ with multiplicity at least two. Every double zero forces n linear conditions on forms vanishing on Γ. Since not all of these conditions are necessarily independent, the following inequality always holds:

$$\dim I_{2d}^{(2)}(\Gamma) \geq \dim H_{n,2d} - n|\Gamma|. \tag{4.1.1}$$

However, generically – with a small list of exceptions concerning n, d – the Alexander-Hirschowitz Theorem [Mir99] tells us that equality holds in (4.1.1).

We establish full dimensionality of $P_{n,2d}(\Gamma)$ in $I_{2d}^{(2)}(\Gamma)$ by finding a form $p \in P_{n,2d}(\Gamma)$ to which we can add a suitably small multiple of any double vanishing form such that it will remain nonnegative:

$$p + \epsilon_q q \in P_{n,2d}(\Gamma) \text{ for any } q \in I_{2d}^{(2)}(\Gamma) \text{ and for some sufficiently small } \epsilon_q.$$

The form p can be viewed as a certificate of full dimensionality of $P_{n,2d}(\Gamma)$ in $I_{2d}^{(2)}(\Gamma)$. The important point is that p can be any form, in particular, we will focus on finding such p that is a sum of squares. This approach follows that of [Rez07] and, indeed, it can be traced to the original proof of Hilbert in [Hil88].

For a form p, let the Hessian H_p of p be the matrix of second derivatives of p:

$$H_p = (h_{ij}), \quad \text{where} \quad h_{ij} = \frac{\partial^2 p}{\partial x_i \partial x_j}.$$

We note that if a form p vanishes at a point $s \in \mathbb{R}^n$, then, by homogeneity, p needs to vanish at a line through s. Therefore, s lies in the kernel of the Hessian of p at s: $H_p(s)s = 0$.

If a form p is nonnegative, then its Hessian at any zero s is positive semidefinite, since zero is a minimum for p. We call a nonnegative form p *round* at a zero $s \in \mathbb{RP}^{n-1}$ if the Hessian of p at s is positive definite on the subspace $s^\perp$ of vectors perpendicular to s, i. e.,

$$p \text{ is round at a zero } s \quad \Leftrightarrow \quad y^T H_p(s) y > 0 \ \text{ for all } y \in s^\perp \setminus \{0\} \ .$$

For a form p, we let $V(p)$ denote the real projective variety of p. We need the following "extension lemma", which follows from [Rez07, Lemma 3.1].

Lemma 4.1.5. *Let $p \in P_{n,2d}$ be a nonnegative form with a finite zero set $V(p)$ and suppose that p is round at every point in $V(p)$. Furthermore, let q be a form such that q vanishes to order two on $V(p)$. Then, for a sufficiently small ϵ, the form $p + \epsilon q$ is nonnegative.*

From this, we infer the following immediate corollary, which will be crucial for the proof of Proposition 4.1.4.

Corollary 4.1.6. *Let Γ be a finite set in $\mathbb{RP}^{n-1}$. Suppose that there exists a nonnegative form p in $P_{n,2d}(\Gamma)$ such that $V(p) = \Gamma$ and p is round at every point $s \in \Gamma$. Then the face $P_{n,2d}(\Gamma)$ is full dimensional in the vector space $I_{2d}^{(2)}(\Gamma)$.*

Proof. Let $p \in P_{n,2d}(\Gamma)$ be as in the assumptions. Then, by Lemma 4.1.5, for any $q \in I_{2d}^{(2)}(\Gamma)$ we have $p + \epsilon q \in P_{n,2d}(\Gamma)$ for sufficiently small ϵ. Since $P_{n,2d}(\Gamma)$ is a convex set, it follows that it is full dimensional in $I_{2d}^{(2)}(\Gamma)$. ∎

We can finally provide the proof of Proposition 4.1.4.

Proof of Proposition 4.1.4. Let $q_1, \ldots, q_k$ be a basis of $I_d(\Gamma)$. We claim that $p = \sum_{i=1}^k q_i^2$ has the properties of Corollary 4.1.6 and therefore, the convex cone $P_{n,2d}(\Gamma)$ is full dimensional in $I_{2d}^{(2)}(\Gamma)$.

Since Γ forces no additional zeros and since $q_1, \ldots, q_k$ is a basis of $I_d(\Gamma)$, it follows that the forms q_i have no common zeros outside of Γ and thus $V(p) = \Gamma$.

Now, choose $s \in \Gamma$. It remains to show that p is round at s, i. e., $H_p(s)$ is positive definite on $s^\perp$. Since the forms in $I_d(\Gamma)$ that double vanish at s form a vector space of codimension $n-1$ in $I_d(\Gamma)$, we see that for $1 \leq i \leq k$ the gradients of q_i at s must span a vector space of dimension $n-1$. Since, by Euler's identity (see, e. g., [Has07, Lemma 11.4]), $\langle \nabla q_i, s\rangle = 0$ for all i, this implies that the gradients actually span $s^\perp$.

Note that the Hessian of p is the sum of the Hessians of q_i^2, i. e.,

$$H_p = \sum_{i=1}^{k} H_{q_i^2}.$$

Since $q_i(s) = 0$ for all i and $s \in \Gamma$, we conclude that

$$\frac{\partial^2 q_i^2}{\partial x_l \partial x_j}(s) = 2\frac{\partial q_i}{\partial x_l}(s)\frac{\partial q_i}{\partial x_j}(s).$$

Therefore, we see that the Hessian of q_i^2 at any $s \in \Gamma$ is actually double the tensor of the gradient of q_i at s with itself:

$$H_{q_i^2}(s) = 2\nabla q_i \otimes \nabla q_i(s).$$

It is now straightforward to verify that

$$\nabla q_i(s)^T H_{q_i^2}(s) \nabla q_i(s) > 0$$

for all $1 \leq i \leq k$ and $s \in \Gamma$, which shows the claim. ■

From now on, we will focus on the study of the degree $2d$ part of the second symbolic power $I_{2d}^{(2)}(\Gamma)$ since, by Proposition 4.1.4, we have the equality

$$\dim P_{n,2d}(\Gamma) = \dim I_{2d}^{(2)}(\Gamma),$$

whenever Γ is a finite d-independent set. However, note that, though Corollary 4.1.3 ensures that d-independence is a Zariski open condition, we still have to construct an explicit example of a d-independent set to make the previous results more powerful. We close this gap in the following subsection.

4.1.2 A d-independent Set of Size $\binom{n+d-1}{d} - n$

The aim of this section is to prove the following result.

Proposition 4.1.7. *Let Γ be a generic collection of points in $\mathbb{RP}^{n-1}$ such that $|\Gamma| \leq \binom{n+d-1}{d} - n$. Then Γ is d-independent.*

For this goal, we will construct an example of a d-independent set of cardinality $\binom{n+d-1}{d} - n$. Since, by Corollary 4.1.3, being d-independent is a Zariski open condition, this will already show the claim. In our upcoming article [BIKV14] we prove that $\binom{n+d-1}{d} - n$ is an upper bound for the cardinality of a d-independent set. Hence, the bound from Proposition 4.1.7 is optimal.

Define $\bar{S}_{n,d}$ to be the set of points in $\mathbb{RP}^{n-1}$ that correspond to nonnegative integer partitions of d:

$$\bar{S}_{n,d} = \left\{ [\alpha_1 : \ldots : \alpha_n] \in \mathbb{RP}^{n-1} \ : \ \alpha_i \in \mathbb{Z},\, \alpha_i \geq 0,\, \sum_{i=1}^{n} \alpha_i = d \right\}.$$

We can think of the points in $\bar{S}_{n,d}$ as all the possible exponent choices for monomials in n variables of degree d. Therefore, $\bar{S}_{n,d}$ contains $\binom{n+d-1}{d}$ points.

Now let $S_{n,d}$ be the set of points in $\mathbb{RP}^{n-1}$ that correspond to partitions of d with at least two nonzero parts. The points in $S_{n,d}$ again correspond to monomials of degree d but we exclude the monomials of the form x_i^d. Therefore, $S_{n,d}$ contains $\binom{n+d-1}{d} - n$ points.

Proposition 4.1.8. *The set $S_{n,d}$ is d-independent.*

The proof of the above proposition requires some additional results. The following proposition is taken from [Rez92, p. 31] and has been known for at least a hundred years. We reproduce the proof below.

Proposition 4.1.9. *There are no nontrivial forms in $H_{n,d}$ that vanish on $\bar{S}_{n,d}$. In other words, $I_d(\bar{S}_{n,d}) = 0$.*

Proof. For every point $s = [s_1 : \ldots : s_n] \in \bar{S}_{n,d}$ we will construct a form $p_s \in H_{n,d}$ that vanishes at all points in $\bar{S}_{n,d}$ except for s. This shows that the conditions of vanishing at any point in $\bar{S}_{n,d}$ are linearly independent and since $|\bar{S}_{n,d}| = \dim H_{n,d}$, we see that $\dim I_d(\bar{S}_{n,d}) = 0$.

Let $M = x_1 + \ldots + x_n$. For $i = 1, \ldots, n$, let h_i be the form defined as follows:

$$h_i = \prod_{k=0}^{s_i - 1} (dx_i - kM).$$

It is clear that the degree of h_i is s_i and h_i vanishes at all partitions in $\bar{S}_{n,d}$ with i-th part less than s_i. Now, let p_s be defined as

$$p_s = \prod_{i=1}^{n} h_i.$$

The form p_s has degree $\sum_{i=1}^{n} s_i = d$, and it does not vanish at s. However, for any other partition of d, there exists i such that the i-th part is less than s_i. Then h_i will vanish for that i and, thus, p_s will vanish at any partition of d except for s. ∎

As in the proof of Proposition 4.1.9, let $M = x_1 + \ldots + x_n$. For $i = 1, \ldots, n$ define a form Q_i as follows:

$$Q_i = \prod_{k=0}^{d-1} (dx_i - kM). \tag{4.1.2}$$

We observe that each Q_i vanishes on $S_{n,d}$. Indeed, let $s = [s_1 : \ldots : s_n] \in S_{n,d}$ and consider $Q_i(s)$. We know that $M(s) = d$, because points in $S_{n,d}$ are partitions of d, and, therefore, the factor of Q_i that corresponds to $k = s_i$ will vanish at s, forcing $Q_i(s) = 0$. Hence, $Q_i \in I_d(S_{n,d})$ for all $i = 1, \ldots, n$.

We will now show that the forms Q_i actually form a basis of $I_d(S_{n,d})$. The fact that we have such a nicely factoring basis is what, eventually, allows us to prove that $S_{n,d}$ is d-independent.

Proposition 4.1.10. *The forms Q_i form a basis of $I_d(S_{n,d})$.*

Proof. We first show that the forms Q_i are linearly independent. Let $e_1, \ldots, e_n$ be the standard basis vectors of $\mathbb{RP}^{n-1}$. It is easy to see that $Q_i(e_j) = 0$ for $i \neq j$, since x_i divides Q_i. On the other hand, $Q_i(e_i) = d!$. Therefore, if there exists $\alpha_i \in \mathbb{R}$ such that $\alpha_1 Q_1 + \ldots + \alpha_n Q_n = 0$, then, by evaluating this linear combination at e_i, we see that $\alpha_i = 0$ and this works for all i. Thus, the forms Q_i are linearly independent.

We now show that the forms Q_i span $I_d(S_{n,d})$. Let $p \in I_d(S_{n,d})$ and let $\beta_i = p(e_i)$. Consider the form

$$\bar{p} = p - \sum_{i=1}^{n} \frac{\beta_i}{d!} Q_i.$$

It is clear that $\bar{p}$ vanishes at the standard basis vectors e_i. Therefore, $\bar{p}$ vanishes not only on $S_{n,d}$ but also on $\bar{S}_{n,d}$. By Proposition 4.1.9, it follows that $\bar{p} = 0$ and, therefore, p is in the span of Q_i.

■

We now show that the set $S_{n,d}$ satisfies the two conditions of d-independence from Definition 4.1.1.

Lemma 4.1.11. *The set $S_{n,d}$ forces no additional zeros for forms of degree d.*

Proof. Since, by Proposition 4.1.10, the forms Q_i form a basis of $I_d(S_{n,d})$, the statement of the lemma is equivalent to showing that $S_{n,d}$ is projectively equal to $\cap_{i=1}^n V(Q_i)$.

Let $v = [v_1 : \ldots : v_n] \in \cap_{i=1}^n V(Q_i)$ be a nonzero point and first suppose that $v_1 + \ldots + v_n = 0$, i. e., $M(v) = 0$. Therefore, by Equation (4.1.2), we see that $Q_i(v) = d^d v_i^d$. Since, by assumption, $Q_i(v) = 0$ for all i, it follows that $v = 0$, which is a contradiction.

Now suppose that $v_1 + \ldots + v_n \neq 0$. By homogeneity, we can assume that $v_1 + \ldots + v_n = d$. In this case, from Equation (4.1.2), it follows that $Q_i(v) = d^d v_i(v_i - 1) \cdots (v_i - d + 1)$. Since $Q_i(v) = 0$ for all i, we infer that each v_i is a nonnegative integer between 0 and $d-1$ and $v_1 + \ldots + v_n = d$. In other words, $v \in S_{n,d}$. ■

We know that $|S_{n,d}| = \binom{n+d-1}{d} - n$. For the second condition of the d-independence property we need to show that for any $s \in S_{n,d}$ the vector space of forms double vanishing at s and vanishing at the rest of $S_{n,d}$ with multiplicity one has codimension $|S_{n,d}| + n - 1 = \binom{n+d-1}{d} - 1$ in $H_{n,d}$. Since $\dim H_{n,d} = \binom{n+d-1}{d}$, we thus need to show that the vector space of forms double vanishing at any $s \in S_{n,d}$ and vanishing at the rest of $S_{n,d}$ with multiplicity one is 1-dimensional. This will follow from the next lemma.

Lemma 4.1.12. *For every point $s \in S_{n,d}$ there is a unique (up to a constant multiple) form in $I_d(S_{n,d})$ being singular at s.*

Proof. Let $s = [s_1 : \ldots : s_n] \in S_{n,d}$ and let $p \in I_d(S_{n,d})$ be a form singular at s.

Since, by Proposition 4.1.10, the forms Q_i form a basis of $I_d(S_{n,d})$, we may assume that $p = \alpha_1 Q_1 + \ldots + \alpha_n Q_n$ for certain $\alpha_i \in \mathbb{R}$. Now, let $A = (a_{ij})$ be the $(n \times n)$-matrix with entries

$$a_{ij} = \frac{\partial Q_i}{\partial x_j}(s).$$

The statement of the lemma is equivalent to showing that $\operatorname{rank} A = n - 1$. Recall from Equation (4.1.2) the definition of Q_i:

$$Q_i = \prod_{k=0}^{d-1}(dx_i - kM).$$

The form Q_i vanishes at s, because the term $dx_i - s_i M$ corresponding to $k = s_i$ vanishes at s. Therefore, the only nonzero term in $\dfrac{\partial Q_i}{\partial x_j}$ evaluated at s will come from differentiating out $dx_i - s_i M$. Now, for $1 \le i \le n$ let

$$P_{s_i} = \frac{Q_i}{dx_i - s_i M}.$$

We observe that $P_{s_i}(s) \neq 0$, since we removed from Q_i the only factor that vanishes at s.

Recall that $M = x_1 + \ldots + x_n$ and, therefore, if we differentiate out $dx_i - s_i M$ from Q_i with respect to x_j and evaluate it at s, we see that

$$\frac{\partial Q_i}{\partial x_j}(s) = \begin{cases} P_{s_i}(s)\,(d - s_j) & \text{if } i = j \\ -P_{s_i}(s) s_j & \text{if } i \neq j. \end{cases}$$

Since $P_{s_i}(s) \neq 0$, we can divide the i-th row of A by $P_{s_i}(s)$ to obtain a matrix $B = (b_{ij})$, where

$$b_{ij} = \begin{cases} d - s_j & \text{if } i = j \\ -s_j & \text{if } i \neq j. \end{cases}$$

By construction, $\operatorname{rank} B = \operatorname{rank} A$. Since s is a partition of d, it is clear that the all ones vector $\mathbf{1}$ is in the kernel of B. Now, let $C = (c_{ij})$ be the matrix with j-th column having the same entry s_j, i.e., $c_{ij} = s_j$. We observe that the rank of C is one and $B = dI - C$, where I is the identity matrix. Therefore, we know that $\operatorname{rank} B \geq \operatorname{rank} I - \operatorname{rank} C = n - 1$. Since we already found a vector in the kernel of B, it follows that the rank of B is $n - 1$. ■

We have now shown that the set $S_{n,d}$ is d-independent and together with Corollary 4.1.3 this shows that d-independence is a generic condition for sets of k points in $\mathbb{RP}^{n-1}$ with $k \leq \binom{n+d-1}{d} - n$. In particular, this proves Proposition 4.1.7.

In view of Propositions 4.0.1, 4.1.4, and 4.1.7, our original question of finding a dimensional difference between the faces $P_{n,2d}(\Gamma)$ and $\Sigma_{n,2d}(\Gamma)$ can be reduced to the following:

Question 4.1.13. *Let $\Gamma \subset \mathbb{RP}^{n-1}$ (or equivalently $\mathbb{CP}^{n-1}$) be a generic set of points such that $|\Gamma| \leq \binom{n+d-1}{d} - n$, and let $I(\Gamma)$ be the vanishing ideal of Γ. For what values of $|\Gamma|$ does equality*

$$\dim I_{2d}^{(2)}(\Gamma) = \dim(I_d(\Gamma))^2$$

hold?

4.2 Dimensional Differences for Ternary Forms

In this section, we study the case of ternary forms and provide a complete characterization for the occurence of dimensional differences between exposed faces of the cones $P_{3,2d}$ and $\Sigma_{3,2d}$. Again, we first state our main results of this section.

Theorem 4.2.1. *Let $d \geq 3$ and Γ be a d-independent set of points in $\mathbb{RP}^2$ such that $|\Gamma| \leq \binom{d+1}{2}$. Then*

$$\dim I_{2d}^{(2)}(\Gamma) = \dim(I_d(\Gamma))^2.$$

Moreover, if $\binom{d+1}{2} + 1 \leq |\Gamma| \leq \binom{d+1}{2} + (d-2)$, then $\dim I_{2d}^{(2)}(\Gamma) > \dim(I_d(\Gamma))^2$.

Based on our previous results, the next corollary is an immediate consequence of Theorem 4.2.1.

Corollary 4.2.2. *Let $d \geq 3$ and $\Gamma \subset \mathbb{RP}^2$ be d-independent with $|\Gamma| \leq \binom{d+1}{2}$. Then*

$$\dim P_{3,2d}(\Gamma) = \dim \Sigma_{3,2d}(\Gamma).$$

Furthermore, for $\binom{d+1}{2} + 1 \leq |\Gamma| \leq \binom{d+1}{2} + (d-2)$ we have

$$\dim P_{3,2d}(\Gamma) > \dim \Sigma_{3,2d}(\Gamma).$$

We remark that we often prove the stronger result that $I_{2d}^{(2)}(\Gamma) = (I_d(\Gamma))^2$, which implies that, in degree $2d$, the symbolic square of I is equal to the ordinary square of I, since we have

$$(I_d(\Gamma))^2 \subset (I^2(\Gamma))_{2d} \subset I_{2d}^{(2)}(\Gamma).$$

In order to prove the main results, we need some preparatory lemmas using techniques from commutative algebra and always assuming $d \geq 3$.

Lemma 4.2.3. *Let $\Gamma \subset \mathbb{RP}^{n-1}$ be a finite set and $I = I(\Gamma) \subset \mathbb{R}[\mathbf{x}]$ be the vanishing ideal. Let $\overline{I^m}$ be the saturation of the ordinary m-th power of I. Then*

$$\overline{I^m} = I^{(m)}.$$

Proof. Consider the primary decomposition $I = \bigcap_{s\in\Gamma} I(s)$, where $I(s) = \{f \in \mathbb{R}[\mathbf{x}] \ : \ f(s) = 0\}$. Then, by definition of symbolic powers, we have $I^{(m)} = \bigcap_{s\in\Gamma} I(s)^m$. Moreover, the primary decomposition of I^m contains $I(s)^m$ for all $s \in \Gamma$ and an additional component Q associated to the maximal homogeneous ideal $\mathfrak{m} = (x_1, \dots, x_n)$. By definition, $\overline{I^m} = \bigcup_{j\geq 0} I^m : \mathfrak{m}^j$. From the previous discussion we obtain

$$\begin{aligned} I^m : \mathfrak{m}^j &= \left(\bigcap_{s\in\Gamma} I(s)^m \cap Q\right) : \mathfrak{m}^j \\ &= \left(\bigcap_{s\in\Gamma} I(s)^m : \mathfrak{m}^j\right) \cap Q : \mathfrak{m}^j \\ &= (I^{(m)} : \mathfrak{m}^j) \cap (Q : \mathfrak{m}^j). \end{aligned}$$

Since Q is $\mathfrak{m}$-primary, for sufficiently large j, it follows that $Q : \mathfrak{m}^j = \mathbb{R}[\mathbf{x}]$. Moreover, $I^{(m)} : \mathfrak{m}^j = I^{(m)}$, thus, $I^m : \mathfrak{m}^j = I^{(m)}$ for sufficiently large j. ■

Note that, as a consequence of the above lemma, we clearly have that $(\overline{I^2})_{2d} = (I^{(2)})_{2d}$.

Given an ideal $I \subset \mathbb{R}[\mathbf{x}]$, let $\alpha(I)$ be the minimum degree of a generator of I. We make the following simple observation.

Lemma 4.2.4. *Let $I \subset \mathbb{R}[\mathbf{x}]$ be a homogeneous ideal and let $m = \alpha(I)$. Then $(I^2)_{2m} = (I_m)^2$.*

Proof. Since $I_m \subset I$, we always have the inclusion $(I_m)^2 \subset (I^2)_{2m}$. On the other hand, if $f \in (I^2)_{2m}$, then we can write $f = \sum_{a\in J} g_a \cdot h_a$ for certain polynomials $g_a, h_a \in I$ and $J \subset \mathbb{N}$ being finite. Moreover, since $2m = \deg(f) = \deg(g_a) + \deg(h_a)$ and $\alpha(I) = m$, we conclude $\deg(f_a) = \deg(g_a) = m$ for all $a \in J$. Hence, $g_a, h_a \in I_m$ for all $a \in J$. ■

Recall that for an ideal $I \subset \mathbb{R}[\mathbf{x}]$ the *saturation degree* of I is defined as

$$\operatorname{satdeg}(I) = \min\{t \ : \ \overline{I}_t = I_t\}$$

(see, e. g., [Eis95]). Moreover, we use $\operatorname{reg}(I)$ to denote the (Castelnuovo-Mumford) regularity of I.

Lemma 4.2.5. *Let $\Gamma \subset \mathbb{RP}^{n-1}$ be a finite set and let $I = I(\Gamma) \subset \mathbb{R}[\mathbf{x}]$ be the vanishing ideal. If $\alpha(I) = \operatorname{reg}(I)$, then $\operatorname{satdeg}(I^2) \leq \alpha(I^2) = 2\alpha(I)$.*

Proof. As we have seen in the proof of Lemma 4.2.3, it holds that $I^2 = I^{(2)} \cap Q$, where Q is $\mathfrak{m}$-primary. More precisely, one has $Q = \mathfrak{m}^{2\alpha(I)}$. So, for $j \in \mathbb{N}$, one has $(I^2)_j = (I^{(2)} \cap \mathfrak{m}^{2\alpha(I)})_j$. For $j \geq 2\alpha(I)$ the ideal $\mathfrak{m}^{2\alpha(I)}$ contains all monomials of degree j. Therefore, $(I^2)_j = I^{(2)}_j$ in this case and, by Lemma 4.2.3, it follows that $(I^2)_j = (\overline{I^2})_j$, i.e., $\operatorname{satdeg}(I^2) \leq 2\alpha(I)$. The equality $\alpha(I^2) = 2\alpha(I)$ is true in general. ■

We need the following definition of a set $\Gamma \subset \mathbb{R}^n$ being in general linear position, which naturally extends to $\mathbb{RP}^{n-1}$.

Definition 4.2.6. *Let $\Gamma \subset \mathbb{R}^n$ be a finite set. Γ is in* general linear position *if one of the following conditions holds*

(i) $|\Gamma| \leq n$ *and* $\dim \operatorname{Aff}(\Gamma) = |\Gamma| - 1$

(ii) $|\Gamma| \geq n+1$ *and no n of the points in Γ lie on a common hyperplane.*

Note that any set Γ with $|\Gamma| \leq n$ that is in general linear position can be extended to a set in general linear position of greater cardinality.

Lemma 4.2.7. *Let $\Gamma \subset \mathbb{RP}^2$ be in general linear position with $|\Gamma| = \binom{d+1}{2}$. Then $\operatorname{reg}(I(\Gamma)) = d$.*

Proof. Due to the minimal resolution conjecture for $\mathbb{RP}^2$ (see, e.g., [BG86, Wal95]), for $\Gamma \subset \mathbb{RP}^2$ it holds that $\operatorname{reg}(I(\Gamma)) \in \{d, d+1\}$. For $|\Gamma| = \binom{d+1}{2}$ it is shown in [Lor90, Section 3] that, indeed, $\operatorname{reg}(I(\Gamma)) = d$. ■

We can now prove Theorem 4.2.1.

Proof of Theorem 4.2.1. Let $\Gamma \subset \mathbb{RP}^2$ be such that $|\Gamma| = \binom{d+1}{2} - k$ for $0 \leq k \leq \binom{d+1}{2} - 1$. We first prove that $\dim(I_d(\Gamma))^2 = \dim I^{(2)}_{2d}(\Gamma)$. We show the claim by induction on k. First assume $k = 0$, i.e., $|\Gamma| = \binom{d+1}{2}$. By Lemma 4.2.7, we have $\alpha(I(\Gamma)) = \operatorname{reg}(I(\Gamma)) = d$ and, from Lemma 4.2.4, we infer that $(I^2(\Gamma))_{2d} = (I_d(\Gamma))^2$. Hence, by Lemma 4.2.3 and 4.2.5, we obtain $I^{(2)}_{2d}(\Gamma) = (I_d(\Gamma))^2$.

Now suppose that the claim holds for fixed k and we have $\dim(I_d(\Gamma))^2 = \dim I^{(2)}_{2d}(\Gamma) = \binom{d+2}{2} + 3k$ for any d-independent set $\Gamma \subset \mathbb{RP}^2$ with $|\Gamma| = \binom{d+1}{2} - k$. For the induction step $k \mapsto k+1$, let $\Gamma \subset \mathbb{RP}^2$ be d-independent with $|\Gamma| = \binom{d+1}{2} - (k+1)$. Let $s \in \mathbb{RP}^2$ be such that the set $T = \Gamma \cup \{s\}$ is d-independent and in general linear position. Note that $|T| = \binom{d+1}{2} - k$. Since Γ and T are d-independent, we have

$$\dim I_d(T) = d + 1 + k \text{ and } \dim I_d(\Gamma) = d + 2 + k.$$

Furthermore, we know that $\dim I_{2d}^{(2)}(T) = \binom{d+2}{2} + 3k$ by hypothesis. Now, let $Q_1 \in I_d(T)$ with the additional property that one of its partial derivatives vanishes at s. Without loss of generality, assume $\frac{\partial Q_1}{\partial x_1}(s) = 0$. We can extend Q_1 to a basis $B = \{Q_1, Q_2, \ldots, Q_{d+1+k}\}$ of $I_d(T)$. Note that there must be at least one basis element Q_j, $j \neq 1$, such that $\frac{\partial Q_j}{\partial x_1}(s) \neq 0$. Otherwise, we arrive at a contradiction in regard to d-independence of T. By assumption, there exist $\binom{d+2}{2} + 3k$ pairwise products of elements of B forming a basis of $(I_d(T))^2$. Let $\widetilde{B}$ denote this basis of $(I_d(T))^2$. Furthermore, extend B to a basis of $I_d(\Gamma)$ by adding a suitable form $Q \in H_{3,d}$. Observe that $Q(s) \neq 0$, since Γ is d-independent. We claim that there exist two forms $Q_l, Q_m \in B$ such that the set

$$L = \widetilde{B} \cup \{Q_l Q, Q_m Q, Q^2\}$$

forms a basis of $(I_d(\Gamma))^2$. Suppose that this set L is linearly dependent for any choice of $Q_l, Q_m \in B$. Hence, we have

$$\sum_{Q_i Q_j \in \widetilde{B}} \alpha_{ij} Q_i Q_j + \alpha_{l,m}^{(l)} Q_l Q + \alpha_{l,m}^{(m)} Q_m Q + \alpha Q^2 = 0$$

for a nontrivial set of coefficients $(\alpha_{ij}, \alpha_{l,m}^{(l)}, \alpha_{l,m}^{(m)}, \alpha)$. To simplify notation we use $P_{l,m}$ to denote the above linear combination. Clearly, we have $P_{l,m}(s) = \alpha Q^2(s)$. Since $Q(s) \neq 0$, it follows that $\alpha = 0$. We remark that the forms in $\widetilde{B}$ vanish to order two at s, whereas the forms $Q_l Q$ and $Q_m Q$ vanish to order one at s. Therefore, by taking partial derivatives, we get

$$0 = \frac{\partial P_{l,m}}{\partial x_i}(s) = \alpha_{l,m}^{(l)} \frac{\partial Q_l Q}{\partial x_i}(s) + \alpha_{l,m}^{(m)} \frac{\partial Q_m Q}{\partial x_i}(s)$$

for $1 \leq i \leq 3$. Assume that there exists i such that $\frac{\partial Q_l Q}{\partial x_i}(s) = 0$ and $\frac{\partial Q_m Q}{\partial x_i}(s) \neq 0$. This implies $\alpha_{l,m}^{(m)} = 0$. On the other hand, since $Q_l Q$ only vanishes to order one at s, there exists $j \neq i$ such that $\frac{\partial Q_l Q}{\partial x_j}(s) \neq 0$. This forces $\alpha_{l,m}^{(l)} = 0$. Since, we assumed that L is linearly dependent for all pairs $(Q_l, Q_m) \in B$, the just conducted reasoning shows that the following relation holds:

$$\frac{\partial Q_l Q}{\partial x_i}(s) = 0 \Leftrightarrow \frac{\partial Q_m Q}{\partial x_i}(s) = 0 \quad \text{for all} \quad i, l, m$$

and, hence,

$$\frac{\partial Q_l}{\partial x_i}(s) = 0 \Leftrightarrow \frac{\partial Q_m}{\partial x_i}(s) = 0 \quad \text{for all} \quad i, l, m. \tag{4.2.1}$$

Recall that the basis B was constructed in the way that $\frac{\partial Q_1}{\partial x_1}(s) = 0$. Furthermore, as already remarked, due to d-independence of T, there must exist $j \neq 1$ such that $\frac{\partial Q_j}{\partial x_1}(s) \neq 0$. Setting $l = 1$, $m = j$ and $i = 1$, this yields a contradiction to (4.2.1). Hence, there must exist two forms $Q_l, Q_m \in B$ such that L is a linearly independent set. We have $|L| = \binom{d+2}{2} + 3(k+1) = \dim I_{2d}^{(2)}(\Gamma)$.

It remains to consider the case $\binom{d+1}{2} + 1 \leq |\Gamma| \leq \binom{d+1}{2} + (d-2)$. It is routine to check that in this case

$$\dim I_{2d}^{(2)}(\Gamma) - \dim(I_d(\Gamma))^2 = \left(\binom{d+2}{2} - 3|\Gamma|\right) - \left(\binom{\binom{d+2}{2} - |\Gamma| + 1}{2}\right) > 0.$$

∎

In particular, for d-independent sets Γ with $|\Gamma| \leq \binom{d+1}{2}$ the theorem also implies that $\dim(I^2(\Gamma))_{2d} = \dim I_{2d}^{(2)}(\Gamma)$.

From Theorem 4.2.1 we can immediately infer Corollary 4.2.2. Observe that the maximal size of a d-independent set $\Gamma \subset \mathbb{RP}^2$ is equal to $\binom{d+2}{2} - 3 = \binom{d+1}{2} + (d-2)$. Hence, Theorem 4.2.1 covers all d-independent sets concerning the occurence of dimensional differences.

4.3 The Case $(n, 2d) = (4, 4)$

We now fully describe the situation with respect to $P_{n,2d}(\Gamma)$ and $\Sigma_{n,2d}(\Gamma)$ in the case $(n, 2d) = (4, 4)$ for sets Γ in $\mathbb{R}^4$ with $|\Gamma| \leq 6$. In the following, we will work with affine representatives in $\mathbb{R}^4$ rather than projective points in $\mathbb{RP}^3$. Let $\Gamma = \{s_1, \ldots, s_6\}$ be a set of six points in $\mathbb{R}^4$ in general linear position so that any four of them span $\mathbb{R}^4$. We will show that Γ is 2-independent. In particular, this implies that the conditions of vanishing at $s_i \in \Gamma$ are linearly independent and therefore $\dim I_2(\Gamma) = \binom{5}{2} - 6 = 4$. It follows that the dimension of the vector space $(I_2(\Gamma))^2$ spanned by squares from $I_2(\Gamma)$ is at most $\binom{5}{2} = 10$. We will show that it is equal to 10.

On the other hand, the Alexander-Hirschowitz Theorem tells us that, generically, the dimension of $I_4^{(2)}(\Gamma)$ is $\binom{7}{4} - 6 \cdot 4 = 11$. It is not hard to show that for six points in $\mathbb{R}^4$ in general linear position this dimension count is actually correct. Therefore, we should have a gap of one dimension between $P_{4,4}(\Gamma)$ and $\Sigma_{4,4}(\Gamma)$.

We now state the main result of this section.

Theorem 4.3.1. *Let $\Gamma \subset \mathbb{RP}^3$ be a finite set in general linear position. Then the following hold.*

(i) If $|\Gamma| = 6$, then

$$\dim(I_2(\Gamma))^2 = 10 < 11 = \dim I_4^{(2)}(\Gamma).$$

(ii) If $|\Gamma| \leq 5$, then

$$\dim(I_2(\Gamma))^2 = \dim I_4^{(2)}(\Gamma).$$

Again, as a direct consequence, we obtain the following corollary.

Corollary 4.3.2. *Let $\Gamma \subset \mathbb{RP}^3$ be a finite set in general linear position. Then the following hold:*

(i) If $|\Gamma| = 6$, then

$$\dim \Sigma_{4,4}(\Gamma) = 10 < 11 = \dim P_{4,4}(\Gamma).$$

(ii) If $|\Gamma| \leq 5$, then

$$\dim \Sigma_{4,4}(\Gamma) = \dim P_{4,4}(\Gamma).$$

The proof of the above theorem will require several preparatory results. We start with a special construction for (i). Let $\Gamma = \{s_1, \ldots, s_6\}$. To every three element subset $T = \{t_1, t_2, t_3\}$ of $\{1, \ldots, 6\}$ we can associate the hyperplane L_T spanned by the vectors s_{t_1}, s_{t_2} and s_{t_3}. We want to construct a double covering of $s_1, \ldots, s_6$ by four hyperplanes of the form L_T with some nice combinatorial properties. We select four triples T_i such that any two of them intersect in exactly one element of $\{1, \ldots, 6\}$ and each element is contained in precisely two triples. Here is an example of such a covering, which is not unique:

$$T_1 = \{1, 2, 3\}, \quad T_2 = \{1, 4, 5\}, \quad T_3 = \{2, 4, 6\}, \quad T_4 = \{3, 5, 6\}.$$

To every such covering we can associate the complementary covering, where we replace the triple T_i with its complement $\overline{T}_i$. So, in the given example, $\overline{T}_1 = \{4, 5, 6\}$, $\overline{T}_2 = \{2, 3, 6\}$, $\overline{T}_3 = \{1, 3, 5\}$ and $\overline{T}_4 = \{1, 2, 4\}$. We observe that the complementary covering also shares the property that any two triples intersect in exactly one element and that every element is contained in exactly two triples.

To each triple T we associate the linear functional with kernel L_T. We can think of this functional as the inner product with the unit normal vector to L_T, which is unique up to a sign. The choice of sign will not make any difference to us. We let u_i and v_i be a unit normal vector to L_{T_i} and $L_{\overline{T}_i}$, respectively.

The vectors u_i and v_i form a pair of bases of $\mathbb{R}^4$. The key is to work with the dual configurations. We define u_i^* to be vectors such that

$$\langle u_i^*, u_j \rangle = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases}$$

One way to think about u_i^* is that if we form the matrix U with rows u_i, then u_i^* form the columns of U^{-1}. We define vectors v_i^* in the same way for v_i.

We will show that the four forms

$$\begin{aligned} Q_1(\mathbf{x}) &= \langle \mathbf{x}, u_1 \rangle \langle \mathbf{x}, v_1 \rangle, \quad Q_2(\mathbf{x}) = \langle \mathbf{x}, u_2 \rangle \langle \mathbf{x}, v_2 \rangle, \\ Q_3(\mathbf{x}) &= \langle \mathbf{x}, u_3 \rangle \langle \mathbf{x}, v_3 \rangle, \quad Q_4(\mathbf{x}) = \langle \mathbf{x}, u_4 \rangle \langle \mathbf{x}, v_4 \rangle \end{aligned}$$

form a basis of $I_2(\Gamma)$. This factoring basis will allow us to prove 2-independence of Γ, and pairwise products Q_iQ_j with $1 \leq i \leq j \leq 4$ will form a basis of $(I_2(\Gamma))^2$.

The vectors u_i and v_i are not just two arbitrary sets of bases of $\mathbb{R}^4$. Since they come from a configuration of six points in general linear position, they carry some structure. The following simple lemma will be crucial to our proofs.

Lemma 4.3.3. *For all $1 \leq i, j \leq 4$ the following hold:*

$$\langle u_i, v_j^* \rangle \neq 0 \ \textit{ and } \ \langle v_i, u_j^* \rangle \neq 0.$$

Proof. By symmetry, it suffices to prove only one of the two assertions. Again, by symmetry, it will be enough to show that $\langle u_1^*, v_1 \rangle \neq 0$ and $\langle u_1^*, v_2 \rangle \neq 0$.

Suppose that $\langle u_1^*, v_1 \rangle = 0$. Then, it follows that v_1 is in the span of u_2, u_3, u_4. Let

$$v_1 = \alpha_2 u_2 + \alpha_3 u_3 + \alpha_4 u_4.$$

Now consider the inner product $\langle v_1, s_4 \rangle$. Recall that v_1 came from the triple $\{4, 5, 6\}$, u_2 from $\{1, 4, 5\}$, u_3 from $\{2, 4, 6\}$ and u_4 from $\{3, 5, 6\}$. It follows that

$$\langle v_1, s_4 \rangle = 0 = \alpha_4 \langle s_4, u_4 \rangle.$$

The points s_i being in general linear position implies that $\langle s_4, u_4 \rangle \neq 0$ and, therefore, $\alpha_4 = 0$. By considering inner products of v_1 with s_5 and s_6, we can also show that $\alpha_2 = \alpha_3 = 0$, which yields a contradiction.

Similarly, if $\langle u_1^*, v_2 \rangle = 0$, then v_2 is in the span of u_2, u_3, u_4. Let

$$v_2 = \alpha_2 u_2 + \alpha_3 u_3 + \alpha_4 u_4.$$

Recall that v_2 came from the triple $\{2, 3, 6\}$, u_2 from $\{1, 4, 5\}$, u_3 from $\{2, 4, 6\}$ and u_4 from $\{3, 5, 6\}$. By an analogous argument as before, we can establish that $\alpha_2 = 0$ by taking inner products with s_6. Then, we use the inner product with s_2 to show that $\alpha_4 = 0$ and we will arrive at a contradiction. ∎

Lemma 4.3.4. *The forms Q_i, $1 \leq i \leq 4$ form a basis of $I_2(\Gamma)$. Furthermore, the pairwise products Q_iQ_j with $1 \leq i \leq j \leq 4$ form a basis of $(I_2(\Gamma))^2$ and* $\dim(I_2(\Gamma))^2 = 10$.

Proof. It is not hard to show that $I_2(\Gamma)$ has dimension 4. To show this claim, it suffices to prove that the polynomials Q_i are linearly independent. Consider the values of Q_i at the points u_i^*.

From the definition of the dual points u_i^* and Lemma 4.3.3, it follows that $Q_i(u_i^*) = \langle u_i^*, v_i \rangle \neq 0$ and $Q_i(u_j^*) = 0$ if $i \neq j$. Therefore, if $P = \alpha_1 Q_1 + \alpha_2 Q_2 + \alpha_3 Q_3 + \alpha_4 Q_4 = 0$ for $\alpha_i \in \mathbb{R}$, then, by considering $P(u_i^*)$, we can see that $\alpha_i = 0$ for each i and, therefore, the Q_i are linearly independent.

Now consider pairwise products Q_iQ_j for $1 \leq i \leq j \leq 4$. These forms clearly belong to $(I_2(\Gamma))^2$, and we need to show their linear independence. Of all the pairwise products only Q_i^2 does not vanish at u_i^*. Therefore, the squares

Q_i^2 are linearly independent from all other pairwise products and it remains to show linear independence of Q_iQ_j for $1 \le i < j \le 4$.

By Lemma 4.3.3, only the products Q_iQ_j vanish at u_i^* to order one. If both indices are distinct from i, then the product vanishes to order two. Suppose that these products are linearly dependent, i. e., there exists a linear combination such that

$$\sum_{1\le i<j\le 4} \alpha_{ij} Q_i Q_j = 0,$$

where not all α_{ij} are zero. Differentiating and subsequently evaluating this equation at u_1^*, we obtain

$$\sum_{1<j\le 4} \alpha_{1j} \frac{\partial Q_1 Q_j}{\partial x_k}(u_1^*) = 0, \quad 1 \le k \le 4,$$

which is equivalent to

$$\sum_{1<j\le 4} \alpha_{1j} \frac{\partial Q_j}{\partial x_k}(u_1^*) = 0, \quad 1 \le k \le 4.$$

This is a (4×3)-system of linear equations in the variables $\alpha_{12}, \alpha_{13}, \alpha_{14}$. Denote the corresponding coefficient matrix by A. Assume that this system has a nontrivial solution, meaning that all (3×3)-minors of A must vanish. Considering the cross product of the three vectors $u_2, u_3, u_4 \in \mathbb{R}^4$ (see, e. g., [Mas83]), we can see that the entries of the cross product are exactly equal to an alternating (3×3)-minor of A. Hence, we conclude that the cross product is the zero vector, implying that the three vectors u_2, u_3, u_4 are linearly dependent, which is a contradiction, since u_1, u_2, u_3, u_4 form a basis of $\mathbb{R}^4$. Hence, we conclude that $\alpha_{12} = \alpha_{13} = \alpha_{14} = 0$. Analogously, by following this procedure with u_2^*, u_3^* and u_4^*, we can infer that $\alpha_{23} = \alpha_{24} = \alpha_{34} = 0$ and hence all pairwise products are linearly independent. Since pairwise products Q_iQ_j span $(I_2(\Gamma))^2$ and are linearly independent, it finally follows that $\dim(I_2(\Gamma))^2 = 10$. ∎

We are now ready to show 2-independence of Γ.

Proposition 4.3.5. *Let Γ be a set of 6 points in $\mathbb{R}^4$ in general linear position. Then Γ is 2-independent.*

Proof. We first show that Γ forces no additional zeros on quadratic forms. Recall that $Q_i = \langle \mathbf{x}, u_i\rangle\langle \mathbf{x}, v_i\rangle$ and the forms Q_i form a basis of $I_2(\Gamma)$. It suffices to show that the forms Q_i have no common zeros outside of Γ.

Let $V_{\mathbb{C}}(Q_i)$ denote the complex zero set of the forms Q_i, $1 \le i \le 4$ and let z be a nonzero point in the intersection $\cap_{i=1}^4 V_{\mathbb{C}}(Q_i)$. First assume that $z \in \cap_{i=1}^4 V_{\mathbb{R}}(Q_i)$. It follows that, for each i, we either have $\langle z, u_i\rangle = 0$ or $\langle z, v_i\rangle = 0$. Since u_i and v_i form a basis of $\mathbb{R}^4$, the vector z cannot be orthogonal to all four u_i or v_i. If $\langle z, u_i\rangle = 0$ for three indices i, which we may assume, without loss of generality, to be 1, 2 and 3, then it follows that z is a multiple of u_4^*. But then $\langle z, u_4 \rangle \neq 0$ and, from Lemma 4.3.3, we know that $\langle z, v_4 \rangle \neq 0$. Therefore, $Q_4(z) \neq 0$, which is a contradiction.

It thus must happen that z is orthogonal to at most two of the vectors u_i and to two of the vectors v_i. Again, without loss of generality, we may assume that z is orthogonal to u_1, u_2, v_3 and v_4. Since u_1 comes from the triple $\{1,2,3\}$, u_2 comes from $\{1,4,5\}$, v_3 comes from $\{1,3,5\}$ and v_4 comes from $\{1,2,4\}$, it follows that z lies in the intersection of the spans of $\{s_1, s_2, s_3\}$, $\{s_1, s_4, s_5\}$, $\{s_1, s_3, s_5\}$ and $\{s_1, s_2, s_4\}$. Since the points s_i are in general linear position, we infer that s_1 spans this intersection. The other points s_i arise in the same manner from choosing different pairs of u_i's and v_i's. If z is complex, then the same arguments as before applied to the real and imaginary part of z imply the claim.

For the second condition of 2-independence, we need to show that for any $s_i \in S$ there exists a unique (up to a constant multiple) form in $I_2(\Gamma)$ that is singular at s_i. Again, by symmetry, we only need to prove this for s_1. By construction, s_1 is orthogonal to u_1, u_2, v_3 and v_4. Therefore, it follows that $\nabla Q_1(s_1) = \langle v_1, s_1 \rangle u_1$, $\nabla Q_2(s_1) = \langle v_2, s_1 \rangle u_2$, $\nabla Q_3(s) = \langle u_3, s_1 \rangle v_3$ and $\nabla Q_4(s) = \langle u_4, s_1 \rangle v_4$. The coefficients of the vectors u_1, u_2, v_3 and v_4 are nonzero, and since the points s_i are in general linear position, it follows that u_1,u_2, v_3 and v_4 span the vector space $s_1^\perp$. Therefore, there is only one (up to a constant multiple) linear combination of gradients of Q_i that vanishes at s_1. ■

Note that from the above proofs, it follows that $\dim \Sigma_{4,4}(\Gamma) = 10$. On the other hand, the Alexander-Hirschowitz Theorem implies $\dim P_{4,4}(\Gamma) = 11$. We have thus shown part (i) of Theorem 4.3.1. In the remaining part of this section, we will provide the proof of Theorem 4.3.1 (ii).

Proposition 4.3.6. *Let $\Gamma \subset \mathbb{R}^4$ be in general linear position with $|\Gamma| \leq 6$. Then Γ is 2-independent.*

Proof. For $|\Gamma| = 6$, the statement is already proven in Proposition 4.3.5. Let now $|\Gamma| \leq 5$. It is easy to see that the first condition of 2-independence is still satisfied whenever points are in general linear position. Indeed, we already know that the forms $Q_1, \ldots, Q_4$ do not have any zeros outside of $\{s_1, \ldots, s_6\}$. We define $Q_5(\mathbf{x}) = \langle \mathbf{x}, u_1 \rangle \langle \mathbf{x}, u_2 \rangle$, which extends $Q_1, \ldots, Q_4$ to a basis of $I_2(\Gamma)$. Since the points are in general linear position, we have $Q_5(s_6) \neq 0$. Hence, we see that the first condition of 2-independence is satisfied for $|\Gamma| = 5$. If Γ is of smaller cardinality, we can always extend Γ to a set $\widetilde{\Gamma}$ of cardinality five that is in general linear position. In the next step, one can extend a basis $Q_1, \ldots, Q_5$ for $I_2(\widetilde{\Gamma})$ to a basis of $I_2(\Gamma)$. Using that those new polynomials do not vanish at all of $\widetilde{\Gamma}$ and using that $\widetilde{\Gamma}$ satisfies the first condition of 2-independence, one can infer that also Γ satisfies this condition.
It remains to verify the second condition of 2-independence, i. e., we need to show that the vector space of quadratic forms vanishing on Γ and that are

singular at exactly one point of Γ is of dimension $7 - |\Gamma|$. We proceed by induction on $|\Gamma|$. For $|\Gamma| = 6$, the claim follows from Proposition 4.3.5. For $|\Gamma| < 6$, we extend Γ to a set $\widetilde{\Gamma}$ with $|\widetilde{\Gamma}| = 6$ in general linear position. By induction, we know that the vector space of quadratic forms vanishing on $\widetilde{\Gamma}$ and that are singular at one point of Γ is of dimension one. This already implies that the dimension of the vector space of quadratic forms vanishing only on Γ and that are singular at exactly one point of Γ is of dimension at most $1 + |\widetilde{\Gamma} \setminus \Gamma|$. Hence, it suffices to show that, when decreasing the number of points in Γ, we gain one new linearly independent relation per point. We demonstrate this explicitly only for $|\Gamma| = 5$, since all the other cases follow the same line of arguments. Let $P = \sum_{i=1}^{5} \alpha_i Q_i$ be singular at s_1, where $\alpha_i \in \mathbb{R}$. Then $\nabla P(s_1) = \sum_{i=1}^{4} \alpha_i \nabla Q_i(s_1)$. As in the proof of Proposition 4.3.5 (up to multiples), there is only one possible solution of this equation. Moreover, Q_5 is clearly double vanishing at s_1 and linearly independent of the former linear combination, which shows that the dimension of the vector space of quadratic forms vanishing at $s_1, \dots, s_5$ and being singular at s_1 is two. For $s_2, \dots, s_5$, the situation is a bit different, since $\nabla Q_5(s_i) \neq 0$ for $2 \leq i \leq 5$. If P is singular at s_2, then

$$\nabla P(s_2) = (\alpha_1 \langle s_2, v_1\rangle + \alpha_5 \langle s_2, u_2\rangle) u_1 + \alpha_2 \langle s_2, u_2\rangle v_2 + \alpha_3 \langle s_2, v_3\rangle u_3 + \alpha_4 \langle s_2, u_4\rangle v_4.$$

The same arguments as before show that $\alpha_1\langle s_2, v_1\rangle + \alpha_5\langle s_2, u_2\rangle, \alpha_2, \alpha_3, \alpha_4$ are uniquely determined (up to multiples). This gives one additional degree of freedom for choosing α_1 and α_5. Hence, again, the required dimension is two. For the other cases, one proceeds in an analogous way. ■

We remark that for $(n, 2d) = (4, 4)$ the above proposition is stronger than the consequence of Proposition 4.1.7, since it explicitly classifies which generic point configurations in $\mathbb{R}^4$ are 2-independent.

Consider the following forms

$$\begin{aligned} Q_5(\mathbf{x}) &= \langle \mathbf{x}, u_1\rangle\langle \mathbf{x}, u_2\rangle, \quad Q_6(\mathbf{x}) = \langle \mathbf{x}, u_1\rangle\langle \mathbf{x}, u_3\rangle, \\ Q_7(\mathbf{x}) &= \langle \mathbf{x}, u_2\rangle\langle \mathbf{x}, u_4\rangle, \quad Q_8(\mathbf{x}) = \langle \mathbf{x}, u_1\rangle\langle \mathbf{x}, u_4\rangle. \end{aligned}$$

Finally, we can provide the proof of Theorem 4.3.1 (ii).

Proof of Theorem 4.3.1 (ii). First, consider the case $|\Gamma| = 5$. Then, by 2-independence of Γ, we have $\dim I_2(\Gamma) = 5$ and the forms $Q_1, \dots, Q_5$ form a basis of $I_2(\Gamma)$ (to see this, evaluate at $u_1^*, \dots, u_4^*$ and s_6). We claim that all $\binom{5+1}{2} = 15$ pairwise products Q_iQ_j, $1 \leq i, j \leq 5$ are linearly independent, which is the right dimension count, since $\dim I_4^{(2)}(\Gamma) = 35 - 20 = 15$. Again, by evaluating at the points $u_1^*, \dots, u_4^*$ and s_6, we see that the pairwise products Q_i^2, $1 \leq i \leq 5$ are linearly independent from the pairwise products Q_iQ_j with $1 \leq i < j \leq 5$. Hence, it remains to prove linear independence of the latter ones. For this aim, we use similar techniques as before. Suppose that those forms are linearly dependent, i. e., there exists a linear combination

$$\sum_{1\le i<j\le 5} \alpha_{ij} Q_i Q_j = 0, \tag{4.3.1}$$

where not all α_{ij} are zero. Consider the evaluation of (4.3.1) at the point u_4^*. The only forms that vanish to order one at u_4^* are Q_1Q_4, Q_2Q_4 and Q_3Q_4. The remaining ones vanish to higher order. Hence, differentiating P and subsequently evaluating at u_4^* yields the following (4×3)-system of linear equations (note that $Q_i(u_i^*) \neq 0$):

$$\alpha_{14}\frac{\partial Q_1}{\partial x_k}(u_4^*) + \alpha_{24}\frac{\partial Q_2}{\partial x_k}(u_4^*) + \alpha_{34}\frac{\partial Q_3}{\partial x_k}(u_4^*) = 0, \quad 1 \le k \le 4.$$

By the same arguments as in the proof of Lemma 4.3.4, we can conclude that $\alpha_{14} = \alpha_{24} = \alpha_{34} = 0$. Now evaluate (4.3.1) at u_3^*. This time, the forms Q_1Q_3, Q_2Q_3 are the only pairwise products vanishing to order one. This yields a (4×2)-system of linear equations, from which we infer $\alpha_{13} = \alpha_{23} = 0$, since, in this case, vanishing of all (2×2)-minors implies linear dependence of u_1, u_2 contradicting the fact that $u_1, \dots, u_4$ form a basis of $\mathbb{R}^4$. Analogously, evaluating (4.3.1) at u_1^* yields $\alpha_{12} = \alpha_{15} = 0$ by exactly the same arguments as before. So, we are left with the pairwise products Q_2Q_5, Q_3Q_5, Q_4Q_5. These forms are clearly linearly independent, since the forms Q_i, $2 \le i \le 4$ are linearly independent. Hence, the claim follows.

Now, assume $|\Gamma| < 5$. In this case, note that there is always an overcount in the pairwise products. For example, in the case $|\Gamma| = 4$, there are $\binom{6+1}{2} = 21$ pairwise products. Since $\dim I_4^{(2)}(\Gamma) = 35 - 16 = 19$, we need to prove that, out of these 21 pairwise products, there exist 19 pairwise products that are linearly independent. Since the proof uses exactly the same strategy as in the case $|\Gamma| = 5$ and does not contain new arguments, in the next table, we only provide a basis for $(I_2(\Gamma))^2$ for $|\Gamma| < 5$. For $|\Gamma| = m$, the forms Q_i, $1 \le i \le 10 - m$ form a basis of $I_2(\Gamma)$. We set $L = \{Q_iQ_j : i \le j\}$ and use $B(\Gamma) \subset L$ to denote a basis of $(I_2(\Gamma))^2$.

$\lvert\Gamma\rvert$	$\dim(I_2(\Gamma))^2$	$\dim I_4^{(2)}(\Gamma)$	$B(\Gamma)$
4	19	19	$L \setminus \{Q_2Q_6, Q_3Q_5\}$
3	23	23	$L \setminus \{Q_1Q_7, Q_2Q_6, Q_3Q_5, Q_4Q_5, Q_5Q_6\}$
2	27	27	$L \setminus M$

where

$$M = \{Q_1Q_7, Q_2Q_6, Q_2Q_8, Q_3Q_8, Q_4Q_6, Q_5Q_7, Q_6Q_7, Q_6Q_8, Q_7Q_8\}.$$

Note that for $|\Gamma| = 1$ it always holds that $\dim(I_2(\Gamma))^2 = \dim I_4^{(2)}(\Gamma)$ and hence the proof is finished. ■

From Theorem 4.3.1 we can immediately infer Corollary 4.3.2.

4.4 Explicit Characterization of 1-dimensional Differences

The aim of this section is to explicitly characterize a dimensional difference between $P_{n,2d}(\Gamma)$ and $\Sigma_{n,2d}(\Gamma)$ for $(n,2d) = (4,4)$ and $(n,2d) = (3,6)$. By Theorems 4.3.1 and 4.2.1, the first time those differences occur is exactly for $|\Gamma| = 6$, respectively, $|\Gamma| = 7$, and it follows by dimension counting that the dimensional difference in these cases is exactly one. Hence, constructing forms in $I_{2d}^{(2)}(\Gamma) \setminus (I_d(\Gamma))^2$ already yields a complete characterization of the occuring dimensional differences in the two smallest cases, in which nonnegative forms that are not sums of squares exist.

4.4.1 The case $(n,2d) = (4,4)$

In order to describe the dimensional difference, we need to construct a form R of degree four such that $R \in I_4^{(2)}(\Gamma) \setminus (I_2(\Gamma))^2$.

Proposition 4.4.1. *Let $\Gamma \subset \mathbb{R}^4$ be in general linear position with $|\Gamma| = 6$. Set $R = \langle \mathbf{x}, u_1\rangle\langle \mathbf{x}, u_2\rangle\langle \mathbf{x}, u_3\rangle\langle \mathbf{x}, u_4\rangle$. Then $R \in I_4^{(2)}(\Gamma) \setminus (I_2(\Gamma))^2$.*

Proof. We know that products Q_iQ_j with $1 \leq i \leq j \leq 4$ form a basis of $(I_2(\Gamma))^2$. We observe that $R(u_i^*) = 0$ for all i, and the only form from the spanning set that does not vanish at u_i^* is Q_i^2. Therefore, if we assume that R is spanned by Q_iQ_j, then R needs to be spanned by products Q_iQ_j with $i \neq j$.

Now consider $R(v_k^*)$. By Lemma 4.3.3, we know that $R(v_k^*) \neq 0$. However, $Q_iQ_j(v_k^*) = 0$, since $\langle v_i^*, v_k\rangle = 0$ for $i \neq k$. Therefore, we arrive at a contradiction. ■

Corollary 4.4.2. *Let $\Gamma \subset \mathbb{R}^4$ be in general linear position with $|\Gamma| = 6$. There exists $p \in P_{4,4}(\Gamma) \setminus \Sigma_{4,4}(\Gamma)$ with $\Gamma \subset V(p)$. These forms can be constructed via $Q_1^2 + Q_2^2 + Q_3^2 + Q_4^2 + \varepsilon R$ for sufficiently small $\varepsilon > 0$.*

We now provide an explicit example for a form as described in the above corollary.

Example 4.4.3. *Let $s_1 = (0,0,1,1)$, $s_2 = (0,1,0,1)$, $s_3 = (0,1,1,0)$, $s_4 = (1,0,0,1)$, $s_5 = (1,0,1,0)$ and $s_6 = (1,1,0,0)$ and $\Gamma = \{s_1,\ldots,s_6\}$. The following polynomials form a basis of $I_2(\Gamma)$:*

$$Q_1(\mathbf{x}) = x_1(x_1 - x_2 - x_3 - x_4), \quad Q_2(\mathbf{x}) = x_2(x_2 - x_1 - x_3 - x_4),$$
$$Q_3(\mathbf{x}) = x_3(x_3 - x_1 - x_2 - x_4), \quad Q_4(\mathbf{x}) = x_4(x_4 - x_1 - x_2 - x_3).$$

The form $R = \langle \mathbf{x}, u_1\rangle\langle \mathbf{x}, u_2\rangle\langle \mathbf{x}, u_3\rangle\langle \mathbf{x}, u_4\rangle$ from Proposition 4.4.1 becomes

$$R = \langle \mathbf{x}, e_1\rangle\langle \mathbf{x}, e_2\rangle\langle \mathbf{x}, e_3\rangle\langle \mathbf{x}, e_4\rangle = x_1x_2x_3x_4.$$

One can verify that $Q_1^2 + Q_2^2 + Q_3^2 + Q_4^2 + R \in P_{4,4}(\Gamma) \setminus \Sigma_{4,4}(\Gamma)$.

4.4.2 The case $(n, 2d) = (3, 6)$

We consider the case $(n, 2d) = (3, 6)$ and $\Gamma \subset \mathbb{R}^3$ with $|\Gamma| = 7$. Compared to the case $(n, 2d) = (4, 4)$ from the previous section, the situation becomes more involved. Let $\Gamma = \{s_1, \ldots, s_7\}$. Let u_1, u_2, u_3 be the normal vectors to the hyperplanes passing through s_1, s_2, respectively, s_3, s_4, respectively, s_5, s_6. Note that, generically, u_1, u_2, u_3 form a basis of $\mathbb{R}^3$. Let u_1^*, u_2^*, u_3^* be the dual basis to u_1, u_2, u_3. Furthermore, we define K_1, K_2, K_3 to be the conics passing through the points s_i with $i \in \{3, 4, 5, 6, 7\}$, respectively $i \in \{1, 2, 5, 6, 7\}$, respectively $i \in \{1, 2, 3, 4, 7\}$. Generically, we can assume that $K_i(u_j^*) \neq 0$ for $1 \leq i \neq j \leq 3$.

Lemma 4.4.4. *Let $Q_1(\mathbf{x}) = \langle \mathbf{x}, u_1 \rangle K_1$, $Q_2(\mathbf{x}) = \langle \mathbf{x}, u_2 \rangle K_2$ and $Q_3(\mathbf{x}) = \langle \mathbf{x}, u_3 \rangle K_3$. Then $\{Q_1(\mathbf{x}), Q_2(\mathbf{x}), Q_3(\mathbf{x})\}$ is a basis of $I_3(\Gamma)$.*

Proof. Assume that $Q_1(\mathbf{x}), Q_2(\mathbf{x})$ and $Q_3(\mathbf{x})$ are linearly dependent, i. e., there exist $(\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3 \setminus \{(0, 0, 0)\}$ such that

$$0 = \alpha_1 Q_1(\mathbf{x}) + \alpha_2 Q_2(\mathbf{x}) + \alpha_3 Q_3(\mathbf{x}). \tag{4.4.1}$$

Evaluating (4.4.1) at u_i^* and using that $\langle u_i^*, u_j \rangle = 0$, for $i \neq j$, and $K_i(u_j^*) \neq 0$, for all $1 \leq i, j \leq 3$, we infer $(\alpha_1, \alpha_2, \alpha_3) = (0, 0, 0)$. ■

We now construct an explicit form $R \in I_6^{(2)}(\Gamma) \setminus (I_3(\Gamma))^2$.

Proposition 4.4.5. *Let $R = K\langle \mathbf{x}, u_1 \rangle \langle \mathbf{x}, u_2 \rangle \langle \mathbf{x}, u_3 \rangle$, where K is the unique cubic double vanishing at the point s_7 and vanishing at $s_1, \ldots, s_6$ with multiplicity one such that $K(u_i^*) \neq 0$ for $1 \leq i \leq 3$. Then $R \in I_6^{(2)}(\Gamma) \setminus (I_3(\Gamma))^2$.*

Proof. By construction, it is clear that $R \in I_6^{(2)}(\Gamma)$. We have to prove that R together with all pairwise products Q_iQ_j, $1 \leq i \leq j \leq 3$ form a linearly independent set of polynomials. Suppose these forms were linearly dependent, i. e., there exists a nontrivial linear combination $\alpha_R R + \sum_{1 \leq i \leq j \leq 3} \alpha_{ij} Q_i Q_j = 0$. By evaluating this relation at u_i^*, we get that $\alpha_{ii} = 0$ for $1 \leq i \leq 3$. It remains to prove linear independence of the forms Q_iQ_j and R with $1 \leq i < j \leq 3$. Suppose that these forms are linearly dependent. The forms Q_1Q_2 and Q_1Q_3 vanish to order one at u_1^*, whereas the forms Q_2Q_3 and R vanish to order two. Hence, by taking the partial derivatives and subsequently evaluating them at u_1^*, we get for $k \in \{2, 3\}$ and $1 \leq j \leq 3$

$$\alpha_{1k} \frac{\partial Q_1 Q_k}{\partial x_j}(u_1^*) = \alpha_{1k} \left(\frac{\partial Q_1}{\partial x_j} \cdot Q_k + Q_1 \cdot \frac{\partial Q_k}{\partial x_j} \right)(u_1^*) = \alpha_{1k} Q_1(u_1^*) \cdot \frac{\partial Q_k}{\partial x_j}(u_1^*) = 0$$

and hereby the following (3×2)-system of linear equations:

$$\alpha_{12} Q_1(u_1^*) \cdot \frac{\partial Q_2}{\partial x_j}(u_1^*) + \alpha_{13} Q_1(u_1^*) \cdot \frac{\partial Q_3}{\partial x_j}(u_1^*) = 0 \;, \quad 1 \leq j \leq 3.$$

Suppose that this system has a nontrivial solution. This is the case if and only if the rank of the corresponding coefficient matrix is one. Hence, all (2×2)-minors must vanish. One can check (by taking the partial derivatives and considering $K_i(u_j^*) \neq 0$) that the rank is one if and only if the cross product of the two vectors u_2 and u_3 is zero, implying that u_2 and u_3 are linearly dependent. But this is a contradiction, since u_1, u_2 and u_3 form a basis of $\mathbb{R}^3$. Hence, the above system can only have the trivial solution $\alpha_{12} = \alpha_{13} = 0$, and we are now left with the equation $\alpha_{23}Q_2Q_3 + \alpha_R R = 0$. However, since the form Q_2Q_3 vanishes to order one at u_2^* and the form R with order two at u_2^*, we get $\alpha_{23} = 0$ by taking the partial derivatives and hence $\alpha_R = 0$, which finishes the proof. ■

Corollary 4.4.6. *Let $\Gamma \subset \mathbb{R}^3$ be 3-independent and $|\Gamma| = 7$. Under the assumptions of the previous lemma there exists $p \in P_{3,6}(\Gamma) \setminus \Sigma_{3,6}(\Gamma)$ with $\Gamma \subset V(p)$. These forms can be constructed via $Q_1^2 + Q_2^2 + Q_3^2 + \varepsilon R$ for sufficiently small $\varepsilon > 0$.*

Example 4.4.7. *Note that the condition $K_i(u_j^*) \neq 0$ is essential. Let $\Gamma = \{s_1, \dots, s_7\}$ with*

$$s_1 = (1,0,0), s_2 = (0,1,0), s_3 = (0,0,1), s_4 = (1,1,0), s_5 = (1,0,1),$$
$$s_6 = (0,1,1), s_7 = (1,1,1).$$

It can be checked that this set of points is 3-independent. However, one can verify that $u_3^* = \left(\frac{1}{2}, \frac{1}{2}, 0\right)$ and hence it represents the same projective point as s_4. In particular, we always have $K_1(u_3^*) = 0$ by construction. However, we can perturb the point s_4 to $\tilde{s}_4 = (1,-2,2)$. The new set of points remains 3-independent, and we have $K_i(u_j^*) \neq 0$ for $1 \leq i \leq j \leq 3$. The three basis polynomials are then given by

$$\begin{aligned} Q_1(x_1,x_2,x_3) &= (3x_1x_2 - x_1x_3 - 2x_2x_3)(-x_3 + x_2 + x_1), \\ Q_2(x_1,x_2,x_3) &= (x_2 - x_3)(x_1 - x_3)(2x_1 + x_2), \\ Q_3(x_1,x_2,x_3) &= x_3(8x_1^2 + x_2^2 - 8x_1x_3 - x_2x_3). \end{aligned}$$

Furthermore, we have

$$R = -x_3(2x_1 + x_2)^2(x_1 + x_2 - x_3)(x_2 - x_3)(-x_3 + x_1).$$

One can check that

$$Q_1^2 + Q_2^2 + Q_3^2 + R \in P_{3,6}(\Gamma) \setminus \Sigma_{3,6}(\Gamma).$$

4.5 General (Naive) Bounds for Dimensional Differences

We now want to derive some naive dimension counts for the dimensions of $P_{n,2d}(\Gamma)$ and $\Sigma_{n,2d}(\Gamma)$, which help to understand when, theoretically, dimensional gaps between these faces can occur. Moreover, these counts yield some a priori bounds on the minimal size of Γ such that dimensional gaps between these faces can be observed. A first step in this direction is the following lemma.

Lemma 4.5.1. *Let Γ be a d-independent set of k points in $\mathbb{RP}^{n-1}$. Then* $\dim P_{n,2d}(\Gamma) \geq \binom{n+2d-1}{2d} - kn$ *and* $\dim \Sigma_{n,2d}(\Gamma) \leq \binom{\binom{n+d-1}{d}-k+1}{2}$.

Proof. The dimension of $I_{2d}^{(2)}(\Gamma)$ is at least $\binom{n+2d-1}{2d} - kn$, since we are imposing at most kn linearly independent conditions by forcing forms to double vanish at all points of Γ. From Proposition 4.1.4 we know that $P_{n,2d}(\Gamma)$ is full dimensional in $I_{2d}^{(2)}(\Gamma)$ and, thus, the bound for the dimension of $P_{n,2d}(\Gamma)$ follows.

Since Γ is d-independent, we know that the dimension of $I_d(\Gamma)$ is $\binom{n+d-1}{d} - k$. We can have at most $\binom{\dim I_d(\Gamma)+1}{2}$ linearly independent pairwise products coming from $I_d(\Gamma)$ and, therefore, the dimension of $(I_d(\Gamma))^2$ is at most $\binom{\binom{n+d-1}{d}-k+1}{2}$. Since, by Proposition 4.0.1, $\Sigma_{n,2d}(\Gamma) \subset (I_d(\Gamma))^2$ is a full dimensional containment, the bound for $\Sigma_{n,2d}(\Gamma)$ follows. ■

For a d-independent set Γ of size k let $G_{n,2d}(k)$ be the size of the minimal gap between the dimensions of $P_{n,2d}(\Gamma)$ and $\Sigma_{n,2d}(\Gamma)$ over all d-independent sets of size k, which, by Lemma 4.5.1, is given by

$$G_{n,2d}(k) = \binom{n+2d-1}{2d} - kn - \binom{\binom{n+d-1}{d} - k + 1}{2}. \tag{4.5.1}$$

From Section 4.1.2 we know that there exist d-independent sets of any cardinality $k \leq \binom{n+d-1}{d} - n$. We want to determine the smallest positive integer k for which $G_{n,2d}(k) > 0$ and we want to find the maximum of $G_{n,2d}(k)$.

Proposition 4.5.2. *The function $G_{n,2d}(k)$ is maximized at $k = \binom{n+d-1}{d} - n$. Its value and the largest gap are*

$$\binom{n+2d-1}{2d} - n\binom{n+d-1}{d} + \binom{n}{2}. \tag{4.5.2}$$

The smallest value of k such that $G_{n,2d}(k) > 0$ is the smallest integer strictly greater than:

$$\binom{n+d-1}{d} - n + \frac{1}{2} - \sqrt{\left(n - \frac{1}{2}\right)^2 + 2\binom{n+2d-1}{2d} - 2n\binom{n+d-1}{d}}. \tag{4.5.3}$$

Proof. We observe that $G_{n,d}(k)$ is a quadratic function of k with a negative leading coefficient. It is easy to show that $G_{n,d}(k)$ attains its maximum value at $k = \binom{n+d-1}{d} - n + \frac{1}{2}$. Therefore, the maximum value of $G_{n,2d}(k)$ for an integer k will occur with $k = \binom{n+d-1}{d} - n$ and it is a matter of easy manipulation to obtain equation (4.5.2).

The bound in equation (4.5.3) comes from simply calculating the smallest root of $G_{n,2d}(k)$. We skip the routine application of the quadratic formula. ■

We make several remarks. First we observe that the largest gap from Proposition 4.5.2

$$\binom{n+2d-1}{2d} - n\binom{n+d-1}{d} + \binom{n}{2}$$

is zero in all cases, where the cones $P_{n,2d}$ and $\Sigma_{n,2d}$ coincide. However, this number is strictly positive in the cases, where there are nonnegative forms that are not sums of squares. In the smallest cases $(n, 2d) = (4, 4)$ and $(n, 2d) = (3, 6)$, in which $P_{n,2d}$ is strictly larger than $\Sigma_{n,2d}$, the gap is one.

However, as either n or d grows, we can see that the dimensional gap between exposed faces of $P_{n,2d}$ and $\Sigma_{n,2d}$ grows and, asymptotically, it approaches the full dimension of the vector space $P_{n,2d}$.

We note that the bound from Equation 4.5.3 simplifies remarkably for $n = 3$. In this case, we get the bound of $\binom{d+2}{2} - d - 1$, and we need to take the smallest integer above that, which leads to

$$k = \binom{d+2}{2} - d = \binom{d+1}{2} + 1.$$

This is actually the correct bound for the case of $n = 3$ as we proved in Theorem 4.2.1.

Though, in general, for $n \geq 4$ the formula does not appear to simplify and the bound given is not going to be optimal, Theorem 4.3.1 implies optimality of the naive dimension count also in the case $(n, 2d) = (4, 4)$. The non-optimality in the general case is caused by an overcount for the dimension of the vector space $(I_d(\Gamma))^2$.

We note that for $k = \binom{n+d-1}{d} - n$, which leads to the largest gap, the bound on the dimension of $(I_d(\Gamma))^2$ is also optimal, generically. We can see this from the example of the d-independent set $S_{n,d}$ from Section 4.1.2, which has exactly this cardinality. Indeed, for $S_{n,d}$, it is not hard to show that all pairwise products of the forms Q_i, which form a basis of $I_d(S_{n,d})$, are linearly independent in $H_{n,2d}$. This shows that the dimension of $(I_d(S_{n,d}))^2$ is $\binom{n+1}{2}$, which is exactly equal to the bound we use.

Question 4.5.3. *From the above discussion it is natural to ask the following questions.*

(i) In addition to the known cases ($(n, 2d) \in \{(3, 2d), (4, 4)\}$), are there other cases, in which the naive bound from Proposition 4.5.2 for the smallest cardinality of a set Γ forcing a dimensional gap between the corresponding faces is correct?

(ii) Given n, d, is it possible to characterize the set of integers S such that $\dim P_{n,2d}(\Gamma) > \dim \Sigma_{n,2d}(\Gamma)$ if and only if $|\Gamma| \in S$?

(iii) Can the naive bounds from Proposition 4.5.2 be further improved?

(iv) Is it possible to characterize more cases for which

$$\dim P_{n,2d}(\Gamma) - \dim \Sigma_{n,2d}(\Gamma) = 1?$$

4.6 Extension to Arbitrary Real Projective Varieties

Motivated by the question whether there exist more cases for which the gap $\dim P_{n,2d}(\Gamma) - \dim \Sigma_{n,2d}(\Gamma)$ is equal to one, we consider the following question: Given a form that is nonnegative on a real projective variety $X \subset \mathbb{P}^{n-1}$, when is every such nonnegative form a sum of squares on X? By $P_{X,2d}$ resp. $\Sigma_{X,2d}$ we denote the set of nonnegative resp. sums of squares forms of degree $2d$ on X. In this setting, Hilbert's theorem is just the case $X = \mathbb{P}^{n-1}$. In [BSV13] it is proved that $P_{X,2d}$ and $\Sigma_{X,2d}$ are, indeed, closed convex cones. We call a projective variety $X \subset \mathbb{P}^{n-1}$ *nondegenerate*, if it is not contained in a hyperplane. The main result in [BSV13] is given by the following theorem.

Theorem 4.6.1 (Blekherman, Smith, Velasco [BSV13])**.** *Let $X \subset \mathbb{P}^{n-1}$ be a real irreducible nondegenerate projective subvariety such that the set $X(\mathbb{R})$ of real points is Zariski dense. Then $P_{X,2} = \Sigma_{X,2}$ if and only if X is a variety of minimal degree.*

Remember that X is a variety of minimal degree, if $\deg(X) = 1 + \operatorname{codim}(X)$. Varieties of minimal degree are completely charaterized (see, e.g., [EH87]). There are exactly three families:

1. totally-real irreducible quadratic hypersurfaces,
2. cones over the Veronese surface,
3. rational normal scrolls.

In order to extend the result to forms of arbitrary even degree $2d$, the Veronese embedding $v_d : \mathbb{P}^n \to \mathbb{P}^{\binom{n+d}{n}-1}$, mapping a point to all monomials of degree d, plays a key role. Then every nonnegative form of degree $2d$ on X is a sum of squares if and only if the d-th Veronese embedding of $X \subset \mathbb{P}^n$ is a variety of minimal degree.

Example 4.6.2 ([BSV13])**.** *The rational quartic curve $C \subset \mathbb{P}^3$ defined by $[y_0 : y_1] \mapsto [y_0^4 : y_0^3 y_1 : y_0 y_1^3 : y_1^4]$ is not a variety of minimal degree but $v_2(C) \subset \mathbb{P}^8$ is the rational normal curve of degree eight, which is a variety of minimal degree. Hence, every nonnegative quartic form on C is a sum of squares.*

We are interested in the exposed faces of the convex cones $P_{X,2d}$ and $\Sigma_{X,2d}$. For this, let $\Gamma \subset X$ be a finite set of points in X. For any positive integer d we define the cones

$$\begin{aligned} P_{X,2d}(\Gamma) &:= \{p \in P_{X,2d} : p(s) = 0 \text{ for all } s \in \Gamma\}, \\ \Sigma_{X,2d}(\Gamma) &:= \{p \in \Sigma_{X,2d} : p(s) = 0 \text{ for all } s \in \Gamma\}. \end{aligned}$$

It is immediate that these cones are exposed faces of $P_{X,2d}$ and of $\Sigma_{X,2d}$ and that $\Sigma_{X,2d}(\Gamma) \subset P_{X,2d}(\Gamma)$. In the previous section, we analyzed the case $X = \mathbb{P}^{n-1}$ and proved some powerful results using the Alexander-Hirschowitz Theorem, especially for $n = 3$. In our upcoming article [BIKV14], we generalize concepts in the previous section to the above setting of arbitrary projective varieties. Again, in order to determine the dimension of $P_{X,2d}(\Gamma)$, one can look at the dimension of the vector space of double vanishing forms on X and introduce a concept of d-independence in this setting. Even more, one can prove that d-independence is a sufficient condition for full dimensionality of $P_{X,2d}(\Gamma)$ in the set of double vanishing forms. However, a major drawback is that there is no Alexander-Hirschowitz type result for arbitrary real projective varieties X. For some concrete results, we refer to [LP13, Theorem 2.1].

Rather than completely describing the results in [BIKV14] we look at a specific case in more detail in order to shed light on these general extensions. Let $X = \mathbb{P}^1 \times \mathbb{P}^1$ be the product of two projective spaces. The coordinate ring of X is just the set of *multihomogeneous* polynomials in two sets of variables $\mathbf{x} = (x_1, x_2)$ and $\mathbf{y} = (y_1, y_2)$. As an example, we consider the degree vector $2d = (4, 4)$, hence, the considered polynomials are quartics in $\mathbf{x}$ and $\mathbf{y}$. Forms of this type form a vector space of dimension $\binom{2+4-1}{4}\binom{2+4-1}{4} = 25$. Now, let $\Gamma = \{s_1, \ldots, s_6\} \subset \mathbb{P}^1 \times \mathbb{P}^1$ with $|\Gamma| = 6$ and

$$s_1 = (1, 0; 1, 0), s_2 = (0, 1; 0, 1), s_3 = (1, 1; 1, 1), s_4 = (1, 1; 1, 0),$$

$$s_5 = (1, -1; 0, 1), s_6 = (0, 1; 1, 1).$$

It can be proved (with analagous methods as before) that

$$\dim P_{X,(4,4)} = 25 - 6 \cdot 3 = 7 > 6 = \dim \Sigma_{X,(4,4)}.$$

Using similar techniques as in the previous sections, we can compute three forms f_1, f_2, f_3 vanishing on Γ and a double vanishing form q on Γ that is not in the span of the pairwise products $f_i f_j$ for $1 \leq i \leq j \leq 3$. Note that the forms f_1, f_2, f_3 are quadratic in $\mathbf{x}$ and $\mathbf{y}$. Then, for a sufficiently small $\varepsilon > 0$, the form $f_1^2 + f_2^2 + f_3^2 + \varepsilon q$ is nonnegative but not a sum of squares. We used the package SyNRAC for Maple (see [AY03]) to verify that the following form lies in $P_{X,(4,4)} \setminus \Sigma_{X,(4,4)}$:

$$
\begin{gathered}
p = f_1^2 + f_2^2 + f_3^2 + \frac{1}{2}q \\
= \\
(x_1y_1y_2(-x_2+x_1))^2+(x_2y_1(y_1-y_2)(-x_2+x_1))^2+(x_1y_2(x_1y_2+x_2y_2-2x_2y_1))^2+ \\
\frac{1}{2}[(9y_1^2y_2^2+y_2^4-5y_1y_2^3)x_1^4+(y_1^3y_2-5y_1y_2^3+2y_2^4-8y_1^2y_2^2)x_2x_1^3+ \\
(y_1^2y_2^2+y_1^3y_2+y_2^4+y_1y_2^3+y_1^4)x_2^2x_1^2+(y_1y_2^3-2y_1^4+y_1^2y_2^2)x_2^3x_1+(-2y_1^3y_2+y_1^2y_2^2+y_1^4)x_2^4)] \\
\in P_{X,(4,4)} \setminus \Sigma_{X,(4,4)}.
\end{gathered}
$$

Chapter 5

Low Dimensional Test Sets for Nonnegativity of Even Symmetric Forms

Since checking nonnegativity of polynomials is an NP-hard problem in general, one might ask whether additional structure on polynomials reduces the complexity of checking nonnegativity. Therefore, an alternative approach in order to simplify the question whether a real polynomial p of even degree $2d$ is nonnegative, is to look for *test sets* $\Omega \subset \mathbb{R}^n$ for nonnegativity of polynomials. Here, we call $\Omega \subset \mathbb{R}^n$ a test set for a polynomial p if $p(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$ if and only if $p(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \Omega$. For example, if p is a homogeneous polynomial, then $\Omega = \mathbb{S}^{n-1}$ is a test set for p. Classifying polynomials, for which there exist test sets simplifying the question of nonnegativity, is seemingly a difficult problem. However, for *symmetric* polynomials such test sets exist. Symmetric polynomials play an outstanding role in practice as many problems come with symmetric structure.

In [Tim03], Timofte proves a very powerful result, namely that a symmetric polynomial in n variables of degree $2d$ is nonnegative if and only if it is nonnegative at all points $\mathbf{x} \in \mathbb{R}^n$ with at most d distinct components. Additionally, an *even* symmetric polynomial of degree $2d$ is nonnegative if and only if it is nonnegative at all points $x \in \mathbb{R}^n$ with at most $\lfloor \frac{d}{2} \rfloor$ distinct components. Later, Riener was able to reprove this result in a much more elementary fashion than in the original work, where most techniques are based on the theory of differential equations (see [Rie12]; see also [Rie11]).

In this chapter, we are interested in even symmetric forms. We consider the question of how to identify test sets for such forms and investigate their properties. In particular, we analyze under which additional conditions on even symmetric forms the bound of at most $\lfloor \frac{d}{2} \rfloor$ distinct components given by Timofte can be further improved. Polynomials with such interesting structures are those lying in certain subspaces. We analyze the question of whether it is even possible that there exist uniform bounds better than Timofte's one and independent of the degree of the polynomials. In fact, our results imply that very often it is not the degree of the polynomials that is essential for the number of components to be checked, but the dimension of the corresponding subspaces. This is in sharp contrast to Timofte's theorem.

This chapter is organized as follows: In Section 5.1 we provide some basic tools and definitions from the theory of symmetric polynomials. In Section 5.2 we introduce test sets and present core problems on them we are interested in. Furthermore, we recall some previous work, such as Timofte's theorem and summarize our main results (Theorem 5.2.5). In Section 5.3 we consider 4-dimensional subspaces of even symmetric forms of degree $4d$ and prove our first main result. We end this section by applying our results on some examples and provide some conjectures based on these experiments. In Section 5.4 we consider subspaces of arbitrary dimension. We prove our second main result (Theorem 5.4.2) by adjusting the number of variables and generalizing techniques from Section 5.3. In Section 5.5 we tackle problems concerning the maximum dimension of such subspaces resp. the geometrical and topological structure of the set of all forms, whose nonnegativity can be decided at all points with a fixed number of distinct components. Here, we prove our remaining main results, which are Theorem 5.5.2 and Corollary 5.5.4. Finally, we discuss some open problems.

5.1 Preliminaries

In this section, we introduce some notations and facts that are essential for upcoming results. We begin with some classical facts about symmetric polynomials. Let $\mathbb{R}[\mathbf{x}]_d^S$ be the vector space of symmetric polynomials of degree $d \in \mathbb{N}$. A homogeneous symmetric polynomial is called an *even symmetric form* if all exponents are even. A vector $\lambda = (\lambda_1, \dots, \lambda_n) \in \mathbb{N}^n$ is called a *partition* of d if $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ and $\lambda_1 + \cdots + \lambda_n = d$. The vector space dimension of $\mathbb{R}[\mathbf{x}]_d^S$ is given by the number of partitions of d with length at most n. Note that the dimension of $\mathbb{R}[\mathbf{x}]_d^S$ is fixed, i.e., independent of n, whenever $n \geq d$. A fundamental theorem in the theory of symmetric polynomials states that every symmetric polynomial $p \in \mathbb{R}[\mathbf{x}]_d^S$ can be written as a polynomial in the power sums $M_r(\mathbf{x}) = \sum_{i=1}^n x_i^r$ for $0 \leq r \leq n$. For an overview and introduction see, e.g., [Sag01].

We now introduce *Schur polynomials* that also form a basis of $\mathbb{R}[\mathbf{x}]^S$. Let $d \neq 0$ be a natural number with a partition $d = \sum_{j=1}^l d_j$, $d_1 \geq \cdots \geq d_l$ where all d_j are positive integers. For a fixed partition $(d_1, \dots, d_l)$ the *l-variate* *monomial symmetric function* $m_{(d_1,\dots,d_l)}$ is given by

$$m_{(d_1,\dots,d_l)} := \sum_{\sigma \in S_l} x_{\sigma(1)}^{d_1} \cdots x_{\sigma(l)}^{d_l},$$

where S_l is the symmetric group in l elements and σ denotes a permutation in S_l. We define

$$D_{(d_1,\dots,d_l)} := \det \begin{pmatrix} x_1^{d_1+l-1} & x_1^{d_2+l-2} & \cdots & x_1^{d_l} \\ \vdots & \vdots & \ddots & \vdots \\ x_l^{d_1+l-1} & x_l^{d_2+l-2} & \cdots & x_l^{d_l} \end{pmatrix}. \quad (5.1.1)$$

Furthermore, we denote the determinant $\prod_{1 \leq i,j \leq l}(x_i - x_j)$ of the $(l \times l)$-Vandermonde Matrix by Δ_l, i.e.,

$$\Delta_l := \det \begin{pmatrix} x_1^{l-1} & x_1^{l-2} & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ x_l^{l-1} & x_l^{l-2} & \cdots & 1 \end{pmatrix}. \quad (5.1.2)$$

The *Schur function* $S_{(d_1,\dots,d_l)}$ is defined as

$$S_{(d_1,\dots,d_l)} := \frac{D_{(d_1,\dots,d_l)}}{\Delta_l}. \quad (5.1.3)$$

It is a well known fact that Schur functions are, indeed, symmetric polynomials, which have an amazing combinatorial structure. For example, the monomials of the Schur polynomial $S_{(d_1,\dots,d_l)}$ are in one to one correspondence to all semistandard $(d_1, \dots, d_l)$-tableaux. For our needs, the following proposition is crucial (see, e.g., [Sag01]).

Proposition 5.1.1. *Let $d_1 \geq \cdots \geq d_l \in \mathbb{N}$. The Schur polynomial $S_{(d_1,\dots,d_l)}$ can be expressed as*

$$S_{(d_1,\dots,d_l)} = \sum_{\{(c_1,\dots,c_l) \in \mathbb{N}^l \,:\, \sum_{j=1}^r c_j \leq \sum_{j=1}^r d_j \text{ for all } 1 \leq r \leq l\}} \kappa_{(c_1,\dots,c_l),(d_1,\dots,d_l)} m_{(c_1,\dots,c_l)},$$

where all $\kappa_{(c_1,\dots,c_l),(d_1,\dots,d_l)}$ are nonnegative integers and all $m_{(c_1,\dots,c_l)}$ are monomial symmetric functions.

The coefficients $\kappa_{(c_1,\dots,c_l),(d_1,\dots,d_l)}$ are called *Kostka numbers*. They count the cardinality of the set of all semistandard $(c_1, \dots, c_l)$-tableaux of type $(d_1, \dots, d_l)$ and are thus nonnegative integers.

5.2 The Structure of Test Sets

In the following, we provide a brief discussion of the structure of test sets. We define *test sets* and *k-points*, state Timofte's theorem, and set up the major notations and problems for the remainder of this chapter.

Definition 5.2.1. *We say that a set $\Omega \subset \mathbb{R}^n$ is a* test set *for $p \in \mathbb{R}[\mathbf{x}]$ if the following does hold: $p \geq 0$ if and only if $p(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \Omega$.*

Based on existing results about nonnegativity of symmetric polynomials, natural test sets to consider are given by *k-points*. In the following definition, we make this more precise.

Definition 5.2.2.

1. *Let Ω_k denote the set of all points $(x_1, \dots, x_n) \in \mathbb{R}^n$ such that there exist $a_1 < \dots < a_k \in \mathbb{R}$ with $x_i \in \{a_1, \dots, a_k\}$ for every $1 \leq i \leq n$.*
2. *Let Ω_k^+ denote the set of all points $(x_1, \dots, x_n) \in \mathbb{R}^n_{\geq 0}$ such that there exist $a_1 < \dots < a_k \in \mathbb{R}_{>0}$ with $x_i \in \{0, a_1, \dots, a_k\}$ for every $1 \leq i \leq n$. In this case, we call a point $x \in \mathbb{R}^n$ a k-*point.

The problem of constructing test sets for symmetric forms began with the work of Choi, Lam and Reznick in [CLR87], and was followed in [Har99]. We summarize the main results in these articles, remarking that the authors dealed with forms. However, the results are obviously true also in the non-homogeneous case.

Theorem 5.2.3 ([CLR87, Har99])**.** *For even symmetric forms the following hold.*

1. *Ω_1^+ is a test set for even symmetric sextics $(2d = 6)$.*
2. *Ω_2^+ is a test set for even symmetric octics $(2d = 8)$ and ternary even symmetric decics $(n = 3, 2d = 10)$*
3. *Nonnegative even symmetric ternary octics are sums of squares.*

All these results are completely generalized in the work of Timofte. His main theorem can be stated as follows.

Theorem 5.2.4 (Timofte [Tim03])**.** *Let $p \in \mathbb{R}[\mathbf{x}]^S_{2d}$ with $d \geq 2$. Then*

1. *Ω_d is a test set for p.*
2. *If p is even symmetric, then $\Omega^+_{\lfloor \frac{d}{2} \rfloor}$ is a test set for p.*

As an example, since we are dealing with even symmetric forms, the following does hold: Nonnegativity of even symmetric octics $(2d = 8)$ and even symmetric decics $(2d = 10)$ can be reduced to semidefinite feasibility problems, since, by Timofte's theorem, one has to check whether these forms are nonnegative at all 2-points. Hence, the problem reduces to check whether a finite number of binary forms are nonnegative. By Hilbert's theorem ([Hil88]), this can be decided by checking whether these forms are sums of squares.

Our main goal is to characterize symmetric forms for which there exist test sets based on k-points that are independent of the degree of the investigated forms. Let $\mathbb{R}[\mathbf{x}]_{4d}^{S,e}$ be the vector space of *even* symmetric forms in n variables of degree $4d$ and

$$\begin{aligned} B \;:=\; & \{M_{j_{(i,1)}}^{k_{(i,1)}} \cdots M_{j_{(i,r_i)}}^{k_{(i,r_i)}} \;:\; r_i \in \mathbb{N},\; j_{(i,1)}, \ldots, j_{(i,r_i)} \in 2\mathbb{N}, \\ & k_{(i,1)}, \ldots, k_{(i,r_i)} \in \mathbb{N},\; \sum_{l=1}^{r_i} j_{(i,l)} k_{(i,l)} = 4d\} \;\subset\; \mathbb{R}[\mathbf{x}]_{4d}^{S,e}. \end{aligned} \tag{5.2.1}$$

Recall that $M_j = (x_1^j + \ldots + x_n^j)$. In the following, we always assume that $n \geq 3$, since the question of nonnegativity of binary forms is obvious by Hilbert's theorem. The key idea is to restrict to subspaces of $\mathbb{R}[\mathbf{x}]_{4d}^{S,e}$ given by forms

$$p \;:=\; \sum_{i=1}^{m} \alpha_i f_i(\mathbf{x}) + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d, \tag{5.2.2}$$

where $\alpha_i, \beta, \gamma, \delta \in \mathbb{R}^*$ and $f_i(\mathbf{x}) \in B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$ for $1 \leq i \leq m$. In particular, we are interested in the constant

$$\begin{aligned} M_{n,4d}^{(k)} \;:=\; & \max\{m \;:\; p \geq 0 \Leftrightarrow p \geq 0 \text{ at all } k\text{-points, for all } p \text{ with} \\ & \{f_1, \ldots, f_m\} \subseteq B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\} \text{ and } \alpha_i, \beta, \gamma, \delta \in \mathbb{R}^*\}. \end{aligned}$$

To the best of our knowledge, nothing is known about these numbers so far. Note that $M_{n,4d}^{(k)}$ can be interpreted as a measure for the maximum dimension $m+3$ such that at all $(m+3)$-subspaces of forms given as in (5.2.2) (for arbitrary $\{f_1, \ldots, f_m\} \subseteq B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$) nonnegativity can be decided at all k-points. Furthermore, we are interested in the set

$$A_{n,4d}^{(k)} \;:=\; \{p \in \mathbb{R}[\mathbf{x}]_{4d}^{S,e} \;:\; p \geq 0 \Leftrightarrow p \geq 0 \text{ at all } k\text{-points}\},$$

i.e., the set of all forms in $\mathbb{R}[\mathbf{x}]_{4d}^{S,e}$ for which nonnegativity can be decided at all k-points. Less is known about geometrical and topological properties of these sets. For example, a priori it is unclear whether these sets are connected or even convex.

We summarize our upcoming results (Theorems 5.3.1, 5.4.2, 5.5.2, Corollary 5.5.4) in the following theorem.

Theorem 5.2.5. *Let* $p := \sum_{i=1}^m \alpha_i f_i(\mathbf{x}) + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$ *with* $\alpha_i, \beta, \gamma, \delta \in \mathbb{R}^*$ *and* $n \geq 3$. *Furthermore, let* $f_i(\mathbf{x}) \in B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$ *for* $1 \leq i \leq m$.

1. *For* $m + 2 \leq n$ *and* p *satisfying some extra conditions (see* (5.4.2)*) the set of* $(m+1)$*-points is a test set for* p,
2. *For* $4d \geq 12$, $n \in \{d-1, d\}$ *we have* $M_{n,4d}^{(2)} = 1$,

3. For $4d \geq 12$, $n \in \{d-1, d\}$ the set $A^{(2)}_{n,4d}$ is not convex.

Note that the statement can be extended to the case of forms p with $\alpha_i, \beta, \gamma, \delta \in \mathbb{R}$. One can construct a sequence of forms as in (5.2.2) and converging to p coefficient-wise. Since nonnegativity of all elements is decidable at k-points, this will also hold for p due to continuity of polynomials in their coefficients.

An important motivation to restrict attention to subspaces of even symmetric forms is given by the fact that they contain *sparse* even symmetric forms. Since every symmetric form can be written as a polynomial in the power sum polynomials, an interesting class to look at is given by symmetric forms with sparsity structure in this representation, i.e., where only a small number of power sums are present. Hence, considering subspaces of even symmetric forms also correspond to sparsity aspects of even symmetric forms.

5.3 Subspaces of Even Symmetric Forms of Dimension Four

We start with the study of some 4-dimensional subspaces. The main result in this section is the following theorem.

Theorem 5.3.1. *Let $n \geq 3$. The set of 2-points is a test set for real even symmetric forms of the form*

$$p \;:=\; \alpha M_{j_1}^{k_1} \cdots M_{j_r}^{k_r} + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d, \tag{5.3.1}$$

where $\alpha, \beta, \gamma, \delta \in \mathbb{R}^*$ and the following conditions are satisfied:

$$j_1, \ldots, j_r \in 2\mathbb{N},\ k_1, \ldots, k_r \in \mathbb{N},\ \sum_{i=1}^{r} j_i k_i = 4d, j_1 \notin \{2, 2d\}, \tag{5.3.2}$$

and either $j_1, \ldots, j_r \leq 2d$ or $j_2, \ldots, j_r \in \{2, 2d\}$.

Hence, we can conclude the following corollary.

Corollary 5.3.2. *Let p be of the form* (5.3.1) *satisfying* (5.3.2). *Then nonnegativity of p can be reduced to a finite number of semidefinite feasibility problems.*

Proof. By Theorem 5.3.1, p is nonnegative if and only if it is nonnegative at all 2-points. Hence, p is nonnegative if and only if a finite number of binary forms are nonnegative. By Hilbert's theorem, this is the case if and only if these binary forms are sums of squares, which can be decided by semidefinite programs (see [Las10]). ∎

Note that the special case of $(n, 2d) = (3, 8)$ in the main Theorem 5.3.1 is considered by Harris in [Har99]. In order to prove Theorem 5.3.1, we need some further results that follow a similar line as the results in [Har99]. For given p of the form (5.3.1) satisfying (5.3.2) let $J(y)$ be the Jacobian of $\{M_{j_1}^{k_1} \cdots M_{j_r}^{k_r}, M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$ at the point y, i.e.,

$$J(y) : \mathbb{R}^4 \to \mathbb{R}^n, \quad (\alpha, \beta, \gamma, \delta) \mapsto \left(\frac{\partial p}{\partial x_1}(y), \ldots, \frac{\partial p}{\partial x_n}(y) \right)^T.$$

$J(y)$ is an $(n \times 4)$-matrix, where every column is given by the gradient of an element in $\{M_{j_1}^{k_1} \cdots M_{j_r}^{k_r}, M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$. The following proposition is very crucial for the proofs in the remainder of this chapter, but is also interesting itself, since it connects rank deficiency with k-points.

Proposition 5.3.3. *The following does hold for $y \in \mathbb{R}^n_{\geq 0}$: $\operatorname{rank} J(y) < 3$ if and only if y is a k-point with $k \leq 2$.*

Proof. First, we prove the proposition for the case that $r = 1$, i.e., the first column of J is given by the partial derivatives of $M_{j_1}^{k_1}$ with $j_1 k_1 = 4d$, $j_1 \in 2\mathbb{N}$ and $j_1 \notin \{2, 2d\}$ (see (5.3.2)). Thus, the Jacobian J is given by the following matrix

$$J = \begin{bmatrix} k_1 j_1 M_{j_1}^{k_1-1} x_1^{j_1-1} & 4\,d x_1 M_2^{2d-1} & 4\,d x_1^{2d-1} M_{2d} & 2\,d x_1 M_2^{d-1} \left(M_{2d} + x_1^{2d-2} M_2\right) \\ \vdots & \vdots & \vdots & \vdots \\ k_1 j_1 M_{j_1}^{k_1-1} x_n^{j_1-1} & 4\,d x_n M_2^{2d-1} & 4\,d x_n^{2d-1} M_{2d} & 2\,d x_n M_2^{d-1} \left(M_{2d} + x_n^{2d-2} M_2\right) \end{bmatrix}.$$

We investigate all (3×3)-minors of J. Due to the symmetry of p (and therefore also J) in the variables $x_1, \ldots, x_n$ it suffices to restrict to x_1, x_2, x_3. Note that every (3×3)-minor containing the fourth column of J is irrelevant, since the fourth column is in the span of the second and the third column. Hence, if there exists a nonzero (3×3)-minor containing the fourth column, then there also exists a nonzero (3×3)-minor containing the first three columns. Thus, it only remains to investigate the leading principal (3×3)-minor of J, which is due to calculation rules of determinants given by

$$(4d)^3 M_{j_1}^{k_1-1} M_{2d} M_2^{2d-1} q(x_1, x_2, x_3)$$

with

$$q(x_1, x_2, x_3) \quad := \quad \det \begin{bmatrix} x_1^{j_1-1} & x_1 & x_1^{2d-1} \\ x_2^{j_1-1} & x_2 & x_2^{2d-1} \\ x_3^{j_1-1} & x_3 & x_3^{2d-1} \end{bmatrix}. \tag{5.3.3}$$

Note that q does not equal the zero polynomial, since $j_1 \notin \{2, 2d\}$ by assumption. Obviously, $q(x_1, x_2, x_3)$ vanishes if one entry is zero and, by (5.1.1), (5.1.2), and (5.1.3), we have

$$q(x_1, x_2, x_3) \quad = \quad \Delta_3 \cdot (\pm 1) \cdot S_{(d_1, d_2, d_3)}$$

with $(d_1, d_2, d_3) = (j_1-3, 2d-2, 1)$ for $j_1 > 2d$ and $(d_1, d_2, d_3) = (2d-3, j_1-2, 1)$ for $j_1 < 2d$. Since $\Delta_3 = (x_1 - x_2)(x_1 - x_3)(x_2 - x_3)$, $q(x_1, x_2, x_3)$ vanishes if two entries are equal or if any entry is zero (since in this case the matrix in (5.3.3) is singular). By Proposition 5.1.1, $q(x_1, x_2, x_3)$ has no further zeros on $\mathbb{R}^3_{>0}$, because $S_{(d_1,d_2,d_3)}$ is a sum of monomial symmetric functions with nonnegative coefficients (the Kostka-numbers) and therefore $S_{(d_1,d_2,d_3)}(y) > 0$ for every $y \in \mathbb{R}^3_{>0}$.

Since finally $M_{j_1}^{k_1-1}$, M_{2d}, and M_2^{2d-1} are sums of squares, the leading principal (3×3)-minor of J does not vanish for a 3-point $y \in \mathbb{R}^3_{>0}$. Hence, the minor vanishes if and only if one of $\{y_1, y_2, y_3\}$ is zero or at least two of them are equal, which is exactly the case if and only if (y_1, y_2, y_3) is a 2-point.

But this already implies that the rank of J is less than three if and only if $y = (y_1, \ldots, y_n)$ is a 2-point. Assume that $J(y)$ has rank three. Then there exists a non-vanishing (3×3)-minor of $J(y)$ given by the first three columns and three rows i_1, i_2 and i_3. Hence, by the previous argumentation, we have $y_{i_1} > y_{i_2} > y_{i_3} > 0$, i.e., y is not a 2-point. On the other hand, assume that $J(y)$ has rank two. Then every (3×3)-minor of $J(y)$ given by the first three columns and three arbitrary rows i_1, i_2, and i_3 vanishes, i.e., by the previous argumentation, $(y_{i_1}, y_{i_2}, y_{i_3})$ is a 2-point. Since $\{i_1, i_2, i_3\}$ is an arbitrary subset of cardinality three of $\{1, \ldots, n\}$, we can conclude that y is a 2-point in total.

Now, we step over to the general case. Here, the first column of J is given by the partial derivatives of $M_{j_1}^{k_1} \cdots M_{j_r}^{k_r}$ satisfying (5.3.2), i.e., the first column is given by

$$\left(\sum_{i=1}^{r} k_i j_i x_1^{j_i-1} M_{j_i}^{k_i-1} \prod_{l \in \{1,\ldots,r\} \setminus \{i\}} M_{j_l}^{k_l}, \; \ldots, \; \sum_{i=1}^{r} k_i j_i x_n^{j_i-1} M_{j_i}^{k_i-1} \prod_{l \in \{1,\ldots,r\} \setminus \{i\}} M_{j_l}^{k_l} \right)^T.$$

With the same argument as in the case $r = 1$, it suffices to investigate the leading principal (3×3)-minor. By the calculation rules of the determinant this minor is given by

$$(4d)^2 M_{2d} M_2^{2d-1} \left(\sum_{i=1}^{r} k_i j_i q_i(x_1, x_2, x_3) M_{j_i}^{k_i-1} \prod_{l \in \{1,\ldots,r\} \setminus \{i\}} M_{j_l}^{k_l} \right), \qquad (5.3.4)$$

where

$$q_i(x_1, x_2, x_3) \;:=\; \det \begin{bmatrix} x_1^{j_i-1} & x_1 & x_1^{2d-1} \\ x_2^{j_i-1} & x_2 & x_2^{2d-1} \\ x_3^{j_i-1} & x_3 & x_3^{2d-1} \end{bmatrix} \;=\; \Delta_3 \cdot (\pm 1) \cdot S_{(d_1,d_2,d_3)} \qquad (5.3.5)$$

with $(d_1, d_2, d_3) = (j_i-3, 2d-2, 1)$ for $j_i > 2d$ and $(d_1, d_2, d_3) = (2d-3, j_i-2, 1)$ for $j_i < 2d$. Since all j_i are even numbers (see (5.3.2)), all M_{j_i} are sums of squares, which due to symmetry in the variables only vanish at the origin.

Hence, the zero set of (5.3.4) only depends on the polynomials q_i. Note that q_i is the zero polynomial if and only if $j_i \in \{2, 2d\}$. With the same argument as in the case $r = 1$, we know furthermore that all $q_i \neq 0$ vanish at $(y_1, y_2, y_3) \in \mathbb{R}^3_{\geq 0}$ if and only if (y_1, y_2, y_3) is a 2-point. Hence, we are done if we can show that there exists an $q_i \neq 0$ and all q_i have the same sign. But this follows from the conditions (5.3.2). They guarantee that $q_1 \neq 0$ and either all other $q_i = 0$ (and thus the sign of q_1 does not matter) or all $j_i \leq 2d$, which implies that the number of column changes needed to transform the defining matrix of each q_i to the standard form (5.1.1) is equal for all i and thus the signs of all q_i coincides.

Thus, the principal (3×3)-minor indeed vanishes if and only if $(y_1, y_2, y_3) \in \mathbb{R}^3_{\geq 0}$ is a 2-point and, analogously as in the case $r = 1$, this implies that the rank of J is less than three if and only if $(y_1, \dots, y_n)$ is a 2-point. ■

If y is not a 2-point, Proposition 5.3.3 says that the solution space of $J(y) \cdot v = 0$ where $v := (\alpha, \beta, \gamma, \delta)$ is 1-dimensional and, in fact, is obviously spanned by the following form that is clearly singular at y:

$$T_y(\mathbf{x}) \quad := \quad (\overline{M_2}^d M_{2d}(\mathbf{x}) - \overline{M_{2d}} M_2(\mathbf{x})^d)^2, \tag{5.3.6}$$

where $\overline{M_r} := M_r(y)$.

As a next step, we prove that for any sum of $2k$-th powers the image on the unit sphere is already given by the image of the set of all 2-points on the unit sphere. This generalizes Lemma 2.6 in [Har99] where this is shown to be true for $2k = 4$. However, the proof follows the same line.

Lemma 5.3.4. *Let $\mathbf{x} \in \mathbb{R}^n_+$ be such that $M_2(\mathbf{x}) = 1$ and $M_{2k}(\mathbf{x}) = r$. Then there exists a 2-point $z = (a, \dots, a, b) \in \mathbb{R}^n_+$ such that $M_2(z) = 1$ and $M_{2k}(z) = r$.*

Proof. We first note that the inequality $\frac{1}{n^{k-1}} \leq M_{2k}(\mathbf{x}) \leq 1$ is true, since we are dealing with points $\mathbf{x} \in \mathbb{R}^n_+$ such that $M_2(\mathbf{x}) = 1$ and by the equivalence of norms. Let

$$z_\alpha \quad := \quad \left(\frac{\cos\alpha}{\sqrt{n-1}}, \dots, \frac{\cos\alpha}{\sqrt{n-1}}, \sin\alpha \right).$$

Then $f(\alpha) := M_{2k}(z_\alpha) = \frac{\cos^{2k}\alpha}{(n-1)^{k-1}} + \sin^{2k}\alpha$. In particular, $M_2(z_\alpha) = 1$ for all α as well as $f(\frac{\pi}{2}) = 1$ and, since $\cos(\arcsin(x)) = \sqrt{1-x^2}$, it follows that

$$f\left(\arcsin\left(\frac{1}{\sqrt{n}}\right)\right) \quad = \quad \frac{(1-1/n)^k}{(n-1)^{k-1}} + \frac{1}{n^k} \quad = \quad \frac{1}{n^{k-1}}.$$

Hence, by the intermediate value theorem, for all r with $\frac{1}{n^{k-1}} \leq r \leq 1$ there exists $\alpha^* \in [\arcsin(\frac{1}{\sqrt{n}}), \frac{\pi}{2}]$ such that $f(\alpha^*) = r$ and $z_{\alpha^*} = (a, \dots, a, b)$. ■

Now we can prove our main theorem.

Proof. (Theorem 5.3.1) We need to prove that if $\alpha M_{j_1}^{k_1}\cdots M_{j_r}^{k_r}+\beta M_2^{2d}+\gamma M_{2d}^2+\delta M_{2d}M_2^d$ is nonnegative at all 2-points, then it is also nonnegative globally. Suppose p is nonnegative at all 2-points but not nonnegative. Let $-\lambda := \min_{x\in\mathbb{S}^{n-1}} p < 0$ denote the minimum value of p over the unit sphere and let $y = (y_1,\ldots,y_n) \in \mathbb{S}^{n-1}$ be a minimizer such that $p(y) = -\lambda$ (note that it suffices to restrict to the unit sphere due to homogeneity). Since the degree of every variable in every monomial of p is even, we can assume w.l.o.g. that $y \in \mathbb{S}_+^{n-1}$. Then $q(\mathbf{x}) := p(\mathbf{x}) + \lambda M_2^{2d}(\mathbf{x}) \geq 0$ and $q(y) = 0$. By assumption, y is not a k-point with $k \leq 2$ (because p is nonnegative at these points). By Proposition 5.3.3, we have rank $J(y) = 3$ and hence $q = k\cdot T_y(\mathbf{x}), k > 0$ with T_y as in (5.3.6), since q is in the kernel of $J(y)$. Thus, $q(\mathbf{x}) = 0$ whenever $M_{2d} = \overline{M_{2d}}$, i.e., $x_1^{2d}+\cdots+x_n^{2d} = y_1^{2d}+\cdots+y_n^{2d}$. By Lemma 5.3.4, there exists a 2-point $z = (a,a,\ldots,a,b)$ such that $(n-1)a^2+b^2 = 1$ and $(n-1)a^{2d}+b^{2d} = \overline{M_{2d}}$. But this implies $p(z) = -\lambda$, which is a contradiction, since p is nonnegative at all 2-points. ∎

5.3.1 Applications

In this subsection we briefly want to demonstrate how our Theorem 5.3.1 can be applied to test nonnegativity of an example class and even how to derive a semialgebraic description of a certain subcone of the cone of nonnegative even symmetric forms.

The key fact from an application side is that checking whether forms are nonnegative at 2-points can be reduced to checking nonnegativity of univariate polynomials, which can be done efficiently by checking numerically (i.e., under usage of SDP-methods) whether these polynomials are sums of squares (due to Hilbert's theorem). Alternatively, this can also be done by using quantifier elimination methods, which happen to work quite efficiently for univariate polynomials of sufficiently low degree.

Our first two examples show that the same set of coefficients yields different results concerning nonnegativity when the number of variables increases.

Example 5.3.5. *Consider the form*

$$p(x_1,x_2,x_3) \;\; := \;\; M_4^3 - \frac{1}{10}M_2^6 + M_6^2 + M_6 M_2^3.$$

By Theorem 5.3.1, $p \geq 0$ if and only if the two binary forms $p(x_1,x_2,0)$ and $p(x_1,x_1,x_2)$ are nonnegative. By dehomogenizing the binary forms, this is the case if and only if the following two univariate polynomials are nonnegative:

$$\begin{aligned} f_1 &= \frac{29}{10}\,x^{12} + \frac{12}{5}\,x^{10} + \frac{9}{2}\,x^8 + 2\,x^6 + \frac{9}{2}\,x^4 + \frac{12}{5}\,x^2 + \frac{29}{10}, \\ f_2 &= \frac{108}{5}\,x^{12} + \frac{24}{5}\,x^{10} - 2\,x^6 + 12\,x^4 + \frac{24}{5}\,x^2 + \frac{29}{10}. \end{aligned} \qquad (5.3.7)$$

Since these polynomials are obviously nonnegative, we conclude $p \geq 0$.

Example 5.3.6. *Now, we consider the same form in four variables, i.e.,*

$$p(x_1, x_2, x_3, x_4) \;:=\; M_4^3 - \frac{1}{10} M_2^6 + M_6^2 + M_6 M_2^3.$$

By Theorem 5.3.1, $p \geq 0$ if and only if the four binary forms $p(x_1, x_2, 0, 0)$, $p(x_1, x_1, x_2, 0)$, $p(x_1, x_1, x_1, x_2)$ and $p(x_1, x_1, x_2, x_2)$ are nonnegative. By dehomogenizing, the first two binary forms are exactly the polynomials f_1, f_2 in (5.3.7) *from which we already know that they are nonnegative. Hence, p is nonnegative if and only if the following two univariate polynomials are nonnegative:*

$$f_3 = \frac{441}{10}\,x^{12} - \frac{324}{5}\,x^{10} - \frac{135}{2}\,x^8 - 18\,x^6 + \frac{45}{2}\,x^4 + \frac{36}{5}\,x^2 + \frac{29}{10},$$
$$f_4 = \frac{108}{5}\,x^{12} + \frac{48}{5}\,x^{10} - 24\,x^8 - 88\,x^6 - 24\,x^4 + \frac{48}{5}\,x^2 + \frac{108}{5}.$$

It is easy to check that these polynomials are indefinite. Hence, p is not a nonnegative form.

Example 5.3.7. *Now, we investigate the 4-variate dodecics given by*

$$p(x_1, x_2, x_3, x_4) \;:=\; \alpha M_4^3 + \beta M_2^6 + \gamma M_6^2 + M_6 M_2^3. \qquad (5.3.8)$$

It turns out that quantifier elimination methods are not suitable to decide for which $(\alpha, \beta, \gamma) \in \mathbb{R}^3$ the form p is nonnegative, since the problem is too complex. Here, we used the quantifier elimination package SynRAC *for* Maple *(see [AY03]), which terminated without a solution after round about* 18 *minutes.*

But application of Theorem 5.3.1 allows to quickly derive a description of the desired semialgebraic set. We successively apply Theorem 5.3.1 on polynomials p given by the parameter sets $\{(\alpha, \beta, \gamma) \;:\; \alpha \in \{1, 2\}, (\beta, \gamma) \in [-10, 10]^2 \cap \mathbb{Z}^2\}$ and $\{(\alpha, \beta, \gamma) \in [-4, 4] \cap \mathbb{Z}^3\}$. The nonnegativity regions of the corresponding polynomials in the parameter sets are depicted in the three pictures of Figure 5.1.

The computed region of nonnegativity obviously is polyhedral. In fact, the approximated set of parameters, which yield nonnegative polynomials p, can easily be identified as

$$\{(\alpha, \beta, \gamma) \in \mathbb{R}^3 \;:\; \beta \geq 0, \alpha + \beta + \gamma + 1 \geq 0\}.$$

We furthermore checked with SOSTools *(see [PPSP05]) for various examples (e.g., $\alpha = 1$, $\beta = 0$, $\gamma \in \{-1, -2\}$) located on the boundary of the polyhedra described by the upper set, whether the corresponding polynomials p are sums of squares. Indeed, this was always the case. Hence, by convexity, one would expect that every nonnegative form is a sum of squares in this particular subcone.*

These examples demonstrate that our results allow computer based approximations of the nonnegativity cone of even symmetric forms, for which nonnegativity is equivalent to nonnegativity at all 2-points.

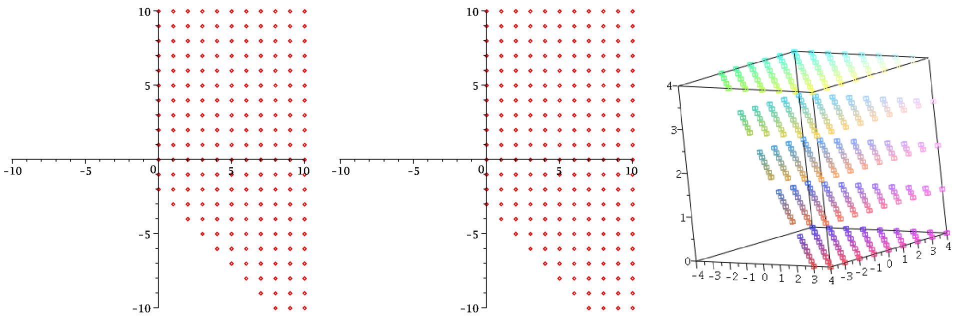

Figure 5.1: The nonnegativity region of polynomials of the form (5.3.8) in the parameter sets $\{(\alpha,\beta,\gamma)\ :\ \alpha\in\{1,2\},(\beta,\gamma)\in[-10,10]^2\cap\mathbb{Z}^2\}$ and $\{(\alpha,\beta,\gamma)\in[-4,4]\cap\mathbb{Z}^3\}$.

5.4 Subspaces of Arbitrary Dimension

A natural question is how far the constructions in Section 5.3 can be generalized to higher dimensional subspaces in the vector space of even symmetric forms of degree $4d$ in n variables. We show that with some obvious modifications such generalizations are indeed possible. However, the price to pay is an adjustment of the number of variables to the ambient dimension of the investigated subspaces of forms of degree $4d$.

Before we can introduce the formal setting for this section, we need to give one more definition. Let $V\subset\mathbb{N}^k$. For every vector $(v_1,\ldots,v_k)\in V$, which is not a $(k-1)$-point, we denote by σ_v the permutation, which maps v to the unique vector $\sigma_v(v)$ with $\sigma_v(v_1)>\cdots>\sigma_v(v_k)$. For every $v,w\in V$ with v,w not being $(k-1)$-points, we say that v and w are *identically oriented ordered*, if $\operatorname{sign}(\sigma_v)\cdot\operatorname{sign}(\sigma_w)=1$. We say that V is *identically oriented ordered* (abbrev. ioo), if every pair $v,w\in V$ with v,w not being $(k-1)$-points, is identically oriented ordered. In order to generalize our approach from the 4-dimensional case to arbitrary dimensions, we need an analagous statement about rank deficiency of the Jacobian matrix of an even symmetric form. Based on the property of a set being identically oriented ordered, we first provide some technical conditions for the polynomials in the investigated subspaces. The unique motivation for these very technical conditions is to guarantee that a certain minor of a Jacobian $J(y)$ does not vanish. Thus, in the proof of Lemma 5.4.1, it will become clear why they have to be chosen in this way (and we suggest the reader not to worry too much about them up to this proof).

So, we consider the following class of even symmetric forms: Let for $m\le n$

$$p(\mathbf{x}) \ := \ \sum_{i=1}^{m-2}\alpha_i f_i(\mathbf{x})+\beta M_2^{2d}+\gamma M_{2d}^2+\delta M_{2d}M_2^d, \qquad (5.4.1)$$

where $\alpha_1,\ldots,\alpha_{m-2},\beta,\gamma,\delta\in\mathbb{R}^*$ and $f_i(\mathbf{x})\in B\setminus\{M_2^{2d},M_{2d}^2,M_{2d}M_2^d\}$ be such that the following conditions (which are a natural generalization of (5.3.2)) hold:

$$\begin{aligned}
&j_{(i,1)},\ldots,j_{(i,r_i)} \in 2\mathbb{N},\ k_{(i,1)},\ldots,k_{(i,r_i)} \in \mathbb{N},\ \sum_{l=1}^{r_i} j_{(i,l)}k_{(i,l)} = 4d,\\
&j_{(i,1)} \notin \{2,2d\} \cup \bigcup_{l=1}^{i-1}\{j_{(l,1)},\ldots,j_{(l,r_l)}\} \text{ for every } 1 \le i \le m-2, \qquad (5.4.2)\\
&\Psi^{ioo} := \{(j_{(1,l_1)}, j_{(2,l_2)},\ldots,j_{(m-2,l_{m-2})},2,2d) \ :\ 1 \le l_i \le r_i, 1 \le i \le m-2\}.
\end{aligned}$$

Here, Ψ^{ioo} is a set that is identically oriented ordered. Again, as in Section 5.3, we denote the Jacobian of p at the point y by $J(y)$, which is an $n \times (m+1)$-matrix. Note that for $m = 3$ the fact that Ψ is identically oriented ordered is equivalent to the conditions (5.3.2). The extension of the conditions (5.4.2) w.r.t. the conditions (5.3.2) become necessary for a generalization to arbitrary dimensions of the subspace for two reasons: Firstly, we need to guarantee that specific $(m \times m)$-minors of interest in $J(y)$ do not equal the zero polynomial. Recall that we similarly had to guarantee that the investigated leading principal (3×3)-minor in the proof of Proposition 5.3.3 did not equal the zero polynomial. Secondly, in the case that our investigated minor can (by calculation rules of the determinant) be rewritten as a sum of simpler determinants, we need to guarantee that all these determinants have the same sign. Recall that we also had to do this in the 4-dimensional case when the first term was a product of different power sums (see proof of Proposition 5.3.3).

Lemma 5.4.1. *The following does hold for $y \in \mathbb{R}^n_{\ge 0}$: $\operatorname{rank} J(y) < m$ if and only if y is a k-point with $k \le m-1$.*

Proof. Basically, the proof works analogously to the one in Proposition 5.3.3 up to the fact that we investigate $(m \times m)$-minors instead of (3×3)-minors.

The last three columns of J agree with those in the dimension four case (see proof of Proposition 5.3.3). For $1 \le i \le m-2$ the i-th column of J is given by

$$\begin{pmatrix} \sum_{l=1}^{r_i} k_{(i,l)} j_{(i,l)} x_1^{j_{(i,l)}-1} M_{j_{(i,l)}}^{k_{(i,l)}-1} \prod_{s\in\{1,\ldots,r_i\}\setminus\{l\}} M_{j_{(i,s)}}^{k_{(i,s)}} \\ \vdots \\ \sum_{l=1}^{r_i} k_{(i,l)} j_{(i,l)} x_n^{j_{(i,l)}-1} M_{j_{(i,l)}}^{k_{(i,l)}-1} \prod_{s\in\{1,\ldots,r_i\}\setminus\{l\}} M_{j_{(i,s)}}^{k_{(i,s)}} \end{pmatrix}.$$

Our goal is to find an $(m \times m)$-minor, which vanishes only on k-points with $k \le m-1$. With the same arguments on the last column of J and the symmetry of the variables, we can restrict to the leading principal $(m \times m)$-minor of J, as in the proof of Proposition 5.3.3. By calculation rules of the determinant this minor is given by $(4d)^2 M_{2d} M_2^{2d-1}$ times

$$\sum_{1\le l_1\le r_1,\cdots,1\le l_m\le r_m} q_{(l_1,\ldots,l_{m-2})}(\mathbf{x}) \cdot \sum_{i=1}^{m-2} k_{(i,l_i)} j_{(i,l_i)} M_{j_{(i,l_i)}}^{k_{(i,l_i)}-1} \prod_{s\in K_i} M_{j_{(i,s)}}^{k_{(i,s)}}, \quad (5.4.3)$$

where $K_i := \{1, \ldots, r_i\} \setminus \{l_i\}$ and

$$\begin{aligned}
& q_{(l_1,\ldots,l_{m-2})}(\mathbf{x}) \\
:= \; & \det \begin{bmatrix} x_1^{j_{(1,l_1)}-1} & \cdots & x_1^{j_{(m-2,l_{m-2})}-1} & x_1 & x_1^{2d-1} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ x_m^{j_{(1,l_1)}-1} & \cdots & x_m^{j_{(m-2,l_{m-2})}-1} & x_m & x_m^{2d-1} \end{bmatrix} \\
= \; & \Delta_m \cdot (\pm 1) \cdot S_{(d_1,\ldots,d_m)},
\end{aligned} \tag{5.4.4}$$

for appropriate choices of d_i, which we discuss in more detail later. First, notice that all power sums involved in (5.4.3) are sums of squares, since all $j_{(i,l_i)}$ are even by condition (5.4.2). Hence, the zero set of (5.4.3) only depends on the polynomials $q_{(l_1,\ldots,l_{m-2})}$, as in the dimension four case. Note that $q_{(l_1,\ldots,l_{m-2})}$ is the zero polynomial if and only if two columns of the matrix (5.4.4) coincide, which is the case precisely if and only if $(j_{(1,l_1)}, \ldots, j_{(m-2,l_{m-2})}, 2, 2d)$ is an $(m-1)$-point. In particular, the minor (5.4.3) is not the zero polynomial, since the condition $j_{(i,1)} \notin \{2, 2d\} \cup \bigcup_{l=1}^{i-1} \{j_{(l,1)}, \ldots, j_{(l,r_l)}\}$ guarantees that at least $q_{(1,\ldots,1)}$ is not the zero polynomial.

Note that for all nonzero polynomials $q_{(l_1,\ldots,l_{m-2})}$ the factor ± 1 is given by

$$\operatorname{sign}(\sigma_{(j_{(1,l_1)},\ldots,j_{(m-2,l_{m-2})},2,2d)}(j_{(1,l_1)}, \ldots, j_{(m-2,l_{m-2})}, 2, 2d))$$

and each d_i equals the i-th entry of the image vector of this permutation minus $(m-i)$ (see (5.1.1)). Since we assumed in (5.4.2) that Ψ is identically oriented ordered, we know in particular that all signs of permutations corresponding to $(j_{(1,l_1)}, \ldots, j_{(m-2,l_{m-2})}, 2, 2d)$ coincide. Thus, we are done if we can show that every nonzero $q_{(l_1,\ldots,l_{m-2})}$ vanishes exactly at all $(m-1)$-points. But this is obviously the case, since Δ_m vanishes if and only if two entries x_i and x_j coincide and the whole matrix given in (5.4.4) vanishes for $x_j = 0$, since it has a zero-column in this case. By Proposition 5.1.1, we can write $S_{(d_1,\ldots,d_m)}$ as a sum of monomial symmetric functions times a nonnegative Kostka-number, which guarantees that $q_{(l_1,\ldots,l_{m-2})}$ does not vanish on a non-$(m-1)$-point in the strictly positive orthant. The rest of the argumentation is analogously to the proof of Proposition 5.3.3. ■

With this lemma, we can prove an analogous version of Theorem 5.3.1

Theorem 5.4.2. *Let $m \leq n$. The set of $(m-1)$-points is a test set for all even symmetric forms of the form $p := \sum_{i=1}^{m-2} \alpha_i f_i(\mathbf{x}) + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$ as in (5.4.1) such that the conditions (5.4.2) are satisfied.*

Proof. We need to prove that if $p = \sum_{i=1}^{m-2} \alpha_i f_i(\mathbf{x}) + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$ is nonnegative at all $(m-1)$-points, it is also nonnegative globally. Suppose this is not the case. Let $-\lambda := \min_{x \in \mathbb{S}^{n-1}} p < 0$ denote the minimum value of p over the unit sphere and let $y = (y_1, \ldots, y_n) \in \mathbb{S}^{n-1}$ be a minimizer such that $p(y) = -\lambda$. Since the degree of every variable in every monomial of p is even, we can assume w.l.o.g. that $y \in \mathbb{S}_+^{n-1}$. Then $q(\mathbf{x}) := p(\mathbf{x}) + \lambda M_2^{2d}(\mathbf{x}) \geq 0$ and $q(y) = 0$. Since, by assumption, y is not a k-point with $k \leq (m-1)$ (because p is nonnegative at these points), y must have at least m distinct entries. By Lemma 5.4.1, we have $\operatorname{rank} J(y) = m$ and hence $q = k \cdot T_y(\mathbf{x})$ with T_y as in (5.3.6) and $k > 0$. Thus $q(\mathbf{x}) = 0$ whenever $x_1^{2d} + \cdots + x_n^{2d} = y_1^{2d} + \cdots + y_n^{2d}$. By Lemma 5.3.4, there exists a 2-point $z = (a, \ldots, a, b)$ such that $(n-1)a^2 + b^2 = 1$ and $(n-1)a^{2d} + b^{2d} = \overline{M_{2d}}$. But this implies $p(z) = -\lambda$, which is a contradiction, since p is nonnegative at all 2-points. ■

Example 5.4.3. *Consider even symmetric forms in $n = 6$ variables of degree $4d = 32$. By Timofte's theorem, these forms are nonnegative if and only if they are nonnegative at all 8-points, which obviously is a useless information in this case. However, considering appropriate subspaces of dimension $m + 1 \leq 7$, Theorem 5.4.2 states that nonnegativity on these subspaces can be checked at $(m-1)$-points.*

5.5 k-point Certificates at Maximal Subspaces

We have seen that the number of components to check for nonnegativity of even symmetric forms can be reduced by considering appropriate subspaces containing the three power sums

$$M_2^{2d}, M_{2d}^2, M_{2d}M_2^d.$$

Recall that $\mathbb{R}[\mathbf{x}]_{4d}^{S,e}$ is the vector space of *even* symmetric forms in n variables of degree $4d$ and let B be as in (5.2.1). In this section, we analyze the problem to determine for fixed $k \in \mathbb{N}$ the maximum dimension of all subspaces of forms given as

$$p \;:=\; \sum_{i=1}^{m} \alpha_i f_i(\mathbf{x}) + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$$

where $f_i(\mathbf{x}) \in B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$ for $1 \leq i \leq m$ and where nonnegativity can be checked at all k-points. Recall that

$$\begin{aligned} M_{n,4d}^{(k)} \;:=\; & \max\{m \;:\; p \geq 0 \Leftrightarrow p \geq 0 \text{ at all } k\text{-points, for all } p \text{ with} \\ & \{f_1, \ldots, f_m\} \subseteq B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\} \text{ and } \alpha_i, \beta, \gamma, \delta \in \mathbb{R}^*\}. \end{aligned}$$

Note that $M_{s,4d}^{(k)} = M_{L(n,4d),4d}^{(k)}$ for $s > L(n, 4d)$, where

$$L(n, 4d) := \dim \mathbb{R}[\mathbf{x}]_{4d}^{S,e}.$$

As an illustrative example, consider the quantity $M_{3,12}^{(2)}$. In this case, we have $\dim \mathbb{R}[x_1, x_2, x_3]_{12}^{S,e} = 7$. An element $p \in \mathbb{R}[x_1, x_2, x_3]_{12}^{S,e}$ can be represented as

$$p \;=\; \alpha_1 M_6 M_4 M_2 + \alpha_2 M_4^3 + \alpha_3 M_4^2 M_2^2 + \alpha_4 M_4 M_2^4 + \beta M_2^6 + \gamma M_6^2 + \delta M_6 M_2^3.$$

Fixing the last three terms, the question is, how many of the first four terms can be used in the representation of p to decide nonnegativity of p via nonnegativity at all 2-points for any choice of the remaining four power sums. For example, if $M_{3,12}^{(2)} = 1$, then the forms

$$p = \alpha_1 q + \beta M_2^6 + \gamma M_6^2 + \delta M_6 M_2^3 \text{ with } q \in \{M_6M_4M_2, M_4^3, M_4^2M_2^2, M_4M_2^4\}$$

would be nonnegative if and only if they are nonnegative at all 2-points, and there exist $f_1, f_2 \in \{M_6M_4M_2, M_4^3, M_4^2M_2^2, M_4M_2^4\}$ such that

$$p = \alpha_1 f_1 + \alpha_2 f_2 + \beta M_2^6 + \gamma M_6^2 + \delta M_6 M_2^3$$

is nonnegative at all 2-points but not globally nonnegative. In fact, we prove that $M_{3,12}^{(2)} = 1$ by a much stronger result, which partially follows from Theorem 5.3.1. The next Lemma is a generalization of Lemma 3.3 in [Har99].

Lemma 5.5.1. *Let $d \geq 3$, $y \in \mathbb{R}^n_{\geq 0}$ and $\varphi : \mathbb{R}^n \to \mathbb{R}^3$ defined by*

$$\varphi : (x_1, \ldots, x_n) \mapsto (M_2, M_{2d-2}, M_{2d}).$$

Then $y \in \partial\varphi(\mathbb{R}^3)$ if and only if y is a 2-point.

Proof. The Jacobian $\mathrm{Jac}(y)$ of φ at a point y is a $(3 \times n)$-matrix. Then $y \in \partial\varphi(\mathbb{R}^3)$ if and only if $\operatorname{rank} \mathrm{Jac}(y) < 3$. By symmetry, it suffices to investigate the leading principal (3×3)-minor corresponding to the first three rows and columns. By (5.1.1), (5.1.2), and (5.1.3), this minor is given by $2 \cdot (2d-2) \cdot 2d \cdot \Delta_3 \cdot S_{2d-2,2d-3,2}$. As in the proof of Proposition 5.3.3, this minor vanishes if and only if y is a 2-point. ∎

Theorem 5.5.2. *Let $p := \sum_{i=1}^m \alpha_i f_i(\mathbf{x}) + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d \in \mathbb{R}[\mathbf{x}]_{4d}^{S,e}$ with $\alpha_1, \ldots, \alpha_m, \beta, \gamma, \delta \in \mathbb{R}^*$ and $f_i(\mathbf{x}) \in B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$. Then for $4d \geq 12$ we have*

$$M_{n,4d}^{(2)} = 1 \quad \text{for} \quad n \in \{d-1, d\}.$$

Proof. Let $4d \geq 12$. Furthermore, since $n \in \{d-1, d\}$, the additional power sums $f_j(\mathbf{x}) = M_{j_1}^{k_1} \cdots M_{j_r}^{k_r} \in B$ have the property that $j_k \leq 2d$ for $1 \leq k \leq r$. This is because every even symmetric form in n variables can uniquely be represented in the first n power sums of even power (see Section 5.1). Hence, by Theorem 5.3.1, we have $M_{n,4d}^{(2)} \geq 1$. It remains to show that there is a choice of two power sums $f_1, f_2 \in B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$ such that

$$p = \alpha_1 f_1 + \alpha_2 f_2 + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$$

is nonnegative at all 2-points but not nonnegative globally. For this we generalize the construction in [Har99] where the author proves this for even symmetric ternary forms of degree 12. For $y \in \mathbb{R}^n$ define

$$p_y(\mathbf{x}) := (\overline{M_2}^d M_{2d} - \overline{M_{2d}} M_2^d)^2 + (\overline{M_2}^d M_{2d-2} M_2 - \overline{M_{2d-2}}\,\overline{M_2} M_2^d)^2.$$

The form p_y is precisely of our desired form $p = \alpha_1 f_1 + \alpha_2 f_2 + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$ with $f_1 = M_{2d-2}^2 M_2^2$ and $f_2 = M_{2d-2} M_2 M_2^d$. Note that $f_1, f_2 \in B$ if $n \in \{d-1, d\}$. By construction, for $x \in \mathbb{S}^{n-1}$ we have $M_2(\mathbf{x}) = 1$ and hence $p_y(\mathbf{x}) = 0$ if and only if $M_{2d} = \overline{M_{2d}}$ and $M_{2d-2} = \overline{M_{2d-2}}$. Note that $\frac{1}{n^{d-2}} \leq M_{2d-2} \leq 1$ and $\frac{1}{n^{d-1}} \leq M_{2d} \leq 1$ (see proof of Lemma 5.3.4). Fix $\Theta \in (\frac{1}{n^{d-2}}, 1)$ and define $Y_\Theta := \{x \in \mathbb{S}^{n-1} : M_{2d-2}(\mathbf{x}) = \Theta\}$. We then have $\varepsilon_2(\Theta) \leq M_{2d}(t) \leq \varepsilon_1(\Theta)$ for some $\varepsilon_1, \varepsilon_2$ as t ranges over Y_Θ. Note that $\frac{1}{n^{d-1}} < \varepsilon_2 < \varepsilon_1 < 1$, since for $x \in \mathbb{S}^{n-1}$ $\frac{1}{n^{d-2}} < M_{2d-2}(\mathbf{x}) < 1$ implies $\frac{1}{n^{d-1}} < M_{2d}(\mathbf{x}) < 1$. Now, choose some $v \in Y_\Theta$ such that $\varepsilon_2(\Theta) < M_{2d}(v) < \varepsilon_1(\Theta)$. Since we are dealing with even symmetric forms, we can additionally assume w.l.o.g. that $v \in \mathbb{S}_+^{n-1}$. By Lemma 5.5.1, v is not a k-point for $k \leq 2$. Hence, if $z \in \mathbb{S}_+^{n-1}$ is a 2-point, then we claim (due to $v \in Y_\Theta \subset \mathbb{S}^{n-1}$) that

$$p_v(z) \;=\; (M_{2d}(z) - M_{2d}(v))^2 + (M_{2d-2}(z) - \Theta)^2 \;\geq\; \kappa \;>\; 0.$$

For $M_{2d-2}(z) \neq \Theta$ this is obvious. If $M_{2d-2}(z) = \Theta$, then we use Lemma 5.5.1. On the one hand, $\varphi(z)$ and $\varphi(v)$ can only differ in the last component. On the other hand, $z \in \partial\varphi(\mathbb{R}^3)$ and $v \notin \partial\varphi(\mathbb{R}^3)$. Thus, $M_{2d}(z) \neq M_{2d}(v)$. Note that also $p_v(z) \geq \kappa > 0$ at all 2-points $z \in \mathbb{S}^{n-1} \setminus \mathbb{S}_+^{n-1}$, since p is even symmetric.

Choosing $0 < \lambda < \kappa$, we conclude that $p_{v,\lambda} := p_v - \lambda M_2^{2d}$ is nonnegative at all 2-points but not nonnegative globally, since $p_{v,\lambda}(v) = -\lambda < 0$. So, we have constructed a form $p = \alpha_1 f_1 + \alpha_2 f_2 + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$ that is nonnegative at all 2-points but not nonnegative globally and hence $M_{n,4d}^{(2)} = 1$ for $n \in \{d-1, d\}$. ■

Note that we have $M_{n,4}^{(2)} = 0$ and $M_{n,8}^{(2)} = 2$ by Timofte's theorem. We conclude the following corollary generalizing [Har99, Theorem 3.3], which covers $n = 3$.

Corollary 5.5.3. *Let $4d \geq 12$. The set of 2-points is not a test set for $\mathbb{R}[\mathbf{x}]_{4d}^{S,e}$ for $n \leq d$.*

Proof. Theorem 5.5.2 proves the corollary for $n \in \{d-1, d\}$. For the general case, we can multiply the form p in Theorem 5.5.2 by an appropriate power sum in order to increase the degree. ■

Another consequence of Theorem 5.5.2 is that for $n \in \{d-1, d\}$ the set of all n-forms of degree $4d$ for which the set of 2-points is a test set is not convex. For this, we recall that

$$A_{n,4d}^{(k)} \;=\; \{p \in \mathbb{R}[\mathbf{x}]_{4d}^{S,e} \;:\; p \geq 0 \Leftrightarrow p \geq 0 \text{ at all } k\text{-points}\}.$$

Note that $A_{n,4d}^{(k)} \subseteq A_{n,4d}^{(k+1)}$ and $A_{n+1,4d}^{(k)} \subseteq A_{n,4d}^{(k)}$ for all $n, d, k \in \mathbb{N}$. Furthermore, by Timofte's theorem, we always have $A_{n,4d}^{(d)} = \mathbb{R}[\mathbf{x}]_{4d}^{S,e}$ for $n \geq d$.

Corollary 5.5.4. *Let $4d \geq 12$ and $n \in \{d-1, d\}$. The set $A_{n,4d}^{(2)}$ is not convex.*

Proof. By Theorem 5.5.2, there exists a form

$$p \;=\; \alpha_1 f_1 + \alpha_2 f_2 + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d \;\notin\; A_{n,4d}^{(2)}$$

for some $f_1, f_2 \in B \setminus \{M_2^{2d}, M_{2d}^2, M_{2d}M_2^d\}$. Obviously, $p = \frac{1}{2}p_1 + \frac{1}{2}p_2$ with $p_1 := 2\alpha_1 f_1 + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$ and $p_2 := 2\alpha_2 f_2 + \beta M_2^{2d} + \gamma M_{2d}^2 + \delta M_{2d} M_2^d$. By Theorem 5.3.1, we have $p_1, p_2 \in A_{n,4d}^{(2)}$. ■

Note that due to the inclusion $A_{n+1,4d}^{(k)} \subseteq A_{n,4d}^{(k)}$ it is not obvious that for $n < d-1$ the above corollary still holds. We note furthermore that the number $M_{n,4d}^{(2)}$ for $n > d$ seems to be more challenging to determine than for $n \leq d$. For example, for $n = 4$ and $4d = 12$ we have $\dim \mathbb{R}[x_1, x_2, x_3, x_4]_{12}^{S,e} = 9$. The Jacobian of the form $p := \alpha_1 M_8 M_4 + \beta M_2^6 + \gamma M_6^2 + \delta M_6 M_2^3$ does not satisfy Proposition 5.3.3 and therefore it seems unclear whether p is nonnegative if and only if it is nonnegative at all 2-points. However, we conjecture that this is true as well as $M_{n,4d}^{(2)} = 1$ for $n > d$.

5.6 Outlook

Since it seems a very difficult problem to determine conditions for forms in our investigated subspaces to be sums of squares, it would be an interesting task to analyze the difference between nonnegative forms and sums of squares in these cases. Experimentally, we were not able to construct nonnegative forms that are not sums of squares. Furthermore, we note that in the setting of Theorem 5.4.2 the bound of $(m-1)$ is not optimal in general. Consider the case of nonnegative even symmetric octics in at least four variables, which is a 5-dimensional convex cone. Following Theorem 5.2.4, such forms are nonnegative if and only if they are nonnegative at all 3-points. But using Timofte's theorem, we know that nonnegativity can be decided at 2-points in this case. However, if the degree $4d$ is sufficiently larger than the number of variables, our bound of $(m-1)$ components is significantly more useful than the bound in Timofte's theorem. An interesting future prospect would be to analyze these bounds in an asymptotic sense.

Additionally, from a computational viewpoint it would be interesting to extend the experimental approach used in Section 5.3 in order to achieve more understanding of the semialgebraic structure of the cone of nonnegative even symmetric forms of degree $4d$ and its subcones.

Maybe the most interesting follow-up task is to shed light on the numbers $M_{n,4d}^{(k)}$ for $k \geq 3$ as well as a deeper understanding of the geometrical and topological structure of the sets $A_{n,4d}^{(k)}$.

Chapter 6

Nonnegative Polynomials and Sums of Squares Supported on Circuits

Forcing additional structure on polynomials often simplifies certain problems in theory and practice. One of the most prominent examples is given by *sparse* polynomials, which arise in different areas in mathematics. Exploiting sparsity of problems often reduces the complexity of solving hard problems. An important example is, e.g., given by sparse polynomial optimization problems (see, e.g., [Las06a]). In this chapter, we consider sparse polynomials having a special structure in terms of their Newton polytopes and supports. More precisely, we consider polynomials $f \in \mathbb{R}[\mathbf{x}]$, whose Newton polytopes are simplices and the supports are given by all the vertices of the simplices and one additional interior lattice point in the simplices. Such polynomials have exactly $n+2$ monomials and can be regarded as *supported on a circuit*. Note that $A \subset \mathbb{N}^n$ is called a *circuit*, if A is affinely dependent, but any proper subset of A is affinely independent (see, e.g., [GKZ08]). We write these polynomials as

$$f \quad = \quad \sum_{j=0}^{n} b_j \mathbf{x}^{\alpha(j)} + c\mathbf{x}^y \tag{6.0.1}$$

where the Newton polytope $\Delta := \mathrm{New}(f) = \mathrm{conv}\{\alpha(0), \ldots, \alpha(n)\} \subset \mathbb{R}^n$ is a lattice simplex, $y \in \mathrm{int}(\Delta)$, $b_j \in \mathbb{R}_{>0}$ and $c \in \mathbb{R}^*$. We denote this class of polynomials as P_Δ^y.

For nonnegative polynomials and sums of squares, work has been done for special configurations in the above setting, namely, in [FK11, Rez89] the authors tackle these problems for very special coefficients and simplices in the above sparse setting. We aim to extend results in all of these papers and establish connections between them for polynomials $f \in P_\Delta^y$.

For $f \in P_{\Delta}^{y}$ we define the *circuit number* Θ_f as

$$\Theta_f \quad := \quad \prod_{j=0}^{n} \left(\frac{b_j}{\lambda_j}\right)^{\lambda_j},$$

where the λ_j are uniquely given by the convex combination $\sum_{j=0}^{n} \lambda_j \alpha(j) = y, \lambda_j \geq 0, \sum_{j=0}^{n} \lambda_j = 1$.

This chapter is organized as follows. In Section 6.1 we introduce some notations and recall some results that are essential for the upcoming sections and proofs of the main theorems. Section 6.2 deals with invariants and properties of polynomials $f \in P_{\Delta}^{y}$. It is shown that for every polynomial $f \in P_{\Delta}^{y}$ there is an associated *standard form* g, which is supported on a scaled standard simplex and one interior lattice point such that all invariants are preserved. Furthermore, we completely characterize nonnegativity of polynomials in P_{Δ}^{y}. Section 6.3 is devoted to the section of the cone of sums of squares with P_{Δ}^{y}. This section will also be completely characterized and extended to the case of multiple interior lattice points in the support of $f \in P_{\Delta}^{y}$. In Section 6.4 we derive interesting connections between our results and some classical/recent problems in toric geometry and lattice polytopes. Using these connections in more detail, we provide sufficient conditions for equality between nonnegative polynomials and sums of squares supported on circuits. Additionally, in Section 6.5 we completely characterize convex polynomials in P_{Δ}^{y}. Based on our main theorems, in Section 6.6 we introduce a new certificate for nonnegativity of polynomials, namely, the cone of *sums of nonnegative circuit polynomials*. Finally, in Section 6.7 we consider extensions to arbitrary Newton polytopes and sparse support sets, thereby providing some counterexamples and solutions to open questions in [Rez89]. An outlook for future possibilities is given in Section 6.8.

6.1 Preliminaries and Known Results

Let $\mathbb{R}[\mathbf{x}]_d$ be the vector space of polynomials in n variables of degree d. For the remainder of this chapter we work with non-homogeneous polynomials. With slight abuse of notation, we denote the convex cone of nonnegative polynomials resp. sums of squares again as

$$\begin{aligned} P_{n,2d} &:= \{p \in \mathbb{R}[\mathbf{x}]_{2d} : p(\mathbf{x}) \geq 0 \text{ for all } x \in \mathbb{R}^n\}, \\ \Sigma_{n,2d} &:= \left\{p \in P_{n,2d} : p = \sum_{i=1}^{k} q_i^2 \text{ for } \ q_i \in \mathbb{R}[\mathbf{x}]_d\right\}. \end{aligned}$$

Since we are interested in nonnegative polynomials and sums of squares in the class P_{Δ}^{y}, we consider the sections

$$P_{n,2d}^{y} := P_{n,2d} \cap P_{\Delta}^{y} \quad \text{and} \quad \Sigma_{n,2d}^{y} := \Sigma_{n,2d} \cap P_{\Delta}^{y}.$$

When asking for nonnegativity of polynomials with a simplex Newton polytope and an additional interior lattice point in the support, this is closely related to what is called an *agiform* in [Rez89]. Given a simplex $\Delta \subset \mathbb{R}^n$ and an interior lattice point $y \in \operatorname{int}(\Delta)$, the corresponding agiform to Δ and y is given by

$$f(\Delta, \lambda, y) = \sum_{i=0}^{n} \lambda_i \mathbf{x}^{\alpha(i)} - \mathbf{x}^y$$

where $y = \sum_{i=0}^n \lambda_i \alpha(i), \sum_{i=0}^n \lambda_i = 1, \lambda_i \geq 0$. The term *agiform* is implied by the fact that the form $f(\Delta, \lambda, y) = \sum_{i=0}^n \lambda_i \mathbf{x}^{\alpha(i)} - \mathbf{x}^y$ is nonnegative by the *arithmetic-geometric mean inequality.* Note that an agiform has a zero at the all ones vector $\mathbf{1}$, implying that agiforms lie on the boundary of the cone of nonnegative polynomials. A natural question is to characterize those agiforms that can be written as sums of squares. In [Rez89] it is shown that this depends heavily on the combinatorial structure of the simplex Δ and the location of y in the interior. We need some definitions and results adapted from [Rez89].

Definition 6.1.1. *Let* $\hat{\Delta} := \{0, \alpha(1), \ldots, \alpha(n)\} \subset (2\mathbb{N})^n$ *be such that* $\operatorname{conv}(\hat{\Delta})$ *is a simplex and let* $L \subset \operatorname{conv}(\hat{\Delta}) \cap \mathbb{Z}^n$.

1. *Define* $A(L) := \{\frac{1}{2}(s+t) \in \mathbb{Z}^n : s, t \in L \cap (2\mathbb{Z})^n\}$ *and* $\overline{A}(L) := \{\frac{1}{2}(s+t) \in \mathbb{Z}^n : s \neq t, s, t \in L \cap (2\mathbb{Z})\}$ *as the set of averages of even resp. distinct even points in* L.

2. *We say that* L *is* $\hat{\Delta}$*-mediated, if*

$$\hat{\Delta} \ \subset \ L \ \subset \ \overline{A}(L) \cup \hat{\Delta},$$

i.e., every $\beta \in L \setminus \hat{\Delta}$ *is an average of two distinct even points in* L.

Theorem 6.1.2 (Reznick [Rez89]). *There is a* $\hat{\Delta}$*-mediated set* Δ^* *satisfying* $A(\hat{\Delta}) \subseteq \Delta^* \subseteq (\Delta \cap \mathbb{Z}^n)$*, which contains every* $\hat{\Delta}$*-mediated set.*

If $A(\hat{\Delta}) = \Delta^*$ resp. $\Delta^* = (\Delta \cap \mathbb{Z}^n)$, we say that Δ is an *M-simplex* resp. *H-simplex.*

Example 6.1.3. *The standard simplex given by* $\operatorname{conv}\{0, 2d \cdot e_1, \ldots, 2d \cdot e_n\} \subset \mathbb{R}^n$ *for* $d \in \mathbb{N}$ *is an* H*-simplex. The Newton polytope* $\operatorname{conv}\{(0,0),(2,4),(4,2)\} \subset \mathbb{R}^2$ *of the Motzkin polynomial* $f = 1 + x^4y^2 + x^2y^4 - 3x^2y^2$ *is an* M*-simplex (see Figure 6.1).*

The main result in [Rez89] concerning the question when agiforms are sums of squares is given by the following theorem.

Theorem 6.1.4 (Reznick [Rez89]). *Let* $f(\Delta, \lambda, y)$ *be an agiform. Then it holds that* $f(\Delta, \lambda, y) \in \Sigma_{n,2d}^y$ *if and only if* $y \in \Delta^*$.

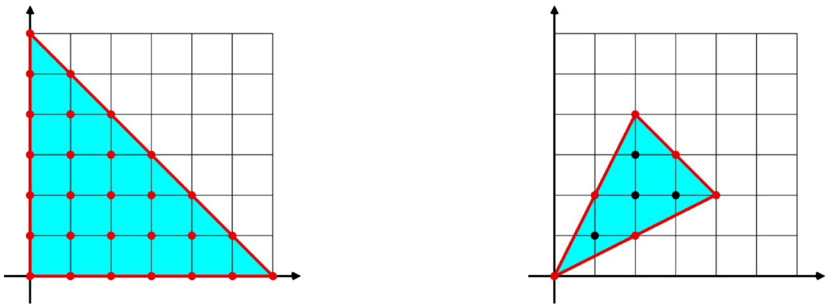

Figure 6.1: On the left: The H-simplex $\operatorname{conv}\{(0,0),(6,0),(0,6)\} \subset \mathbb{R}^2$. On the right: The M-simplex $\operatorname{conv}\{(0,0),(2,4),(4,2)\} \subset \mathbb{R}^2$. The red points are the lattice points contained in the corresponding sets Δ^*.

6.2 Invariants and Nonnegativity of Polynomials Supported on Circuits

The main contribution of this section is to introduce a *norm relaxation strategy* and use it to characterize $P_{n,2d}^y$, i.e., the set of nonnegative polynomials supported on a circuit (Theorem 6.2.6). Along the way we provide standard forms and invariants, which reflect the nice structural properties of the class P_Δ^y.

In Section 6.2.1 we outline the norm relaxation strategy. In Section 6.2.2 we introduce standard forms for polynomials in P_Δ^y and prove the existence of a particular norm minimizer for polynomials, where the coefficient c equals the negative circuit number Θ_f (Proposition 6.2.4). In Section 6.2.3 we put all pieces together and characterize nonnegativity for polynomials in P_Δ^y (Theorem 6.2.6). In Section 6.2.4 we discuss connections to Gale duals and A-discriminants.

6.2.1 The Norm Relaxation Strategy

We start with a short outline of the new strategy, which we introduce and apply here in order to tackle the problem of nonnegativity of polynomials. Let $f = \sum_{\alpha \in A} b_\alpha \mathbf{x}^\alpha \in \mathbb{R}[\mathbf{x}]$ be a polynomial with $A \subset \mathbb{N}^n$ being finite, $0 \in A$ and $\alpha \in (2\mathbb{N})^n$ as well as $b_\alpha > 0$ if α is contained in the vertex set $\operatorname{vert}(A)$ of $\operatorname{conv}(A)$. Instead of trying to answer the question whether $f(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$, we investigate the relaxed problem

$$\text{Is } f(|\mathbf{x}|) \;=\; \sum_{\alpha \in \operatorname{vert}(A)} b_\alpha \cdot |\mathbf{x}^\alpha| - \sum_{\alpha \in A \setminus \operatorname{vert}(A)} |b_\alpha| \cdot |\mathbf{x}^\alpha| \geq 0 \text{ for all } \mathbf{x} \in \mathbb{R}_{\geq 0}^n\ ?$$

Since the strictly positive orthant $\mathbb{R}_{>0}^n$ is an open dense set in $\mathbb{R}_{\geq 0}^n$ and the componentwise exponential function

$$\operatorname{Exp} : \mathbb{R}^n \to \mathbb{R}_{>0}^n, (x_1, \ldots, x_n) \mapsto (\exp(x_1), \ldots, \exp(x_n))$$

is a bijection, the previos problem is equivalent to the question

$$\text{Is } f(e^{\mathbf{w}}) \;=\; \sum_{\alpha \in \mathrm{vert}(A)} b_\alpha \cdot e^{\langle \mathbf{w}, \alpha \rangle} - \sum_{\alpha \in A \setminus \mathrm{vert}(A)} |b_\alpha| \cdot e^{\langle \mathbf{w}, \alpha \rangle} \geq 0 \ \text{ for all } \ \mathbf{w} \in \mathbb{R}^n \text{ ?}$$

Clearly, an affirmative answer of this question implies nonnegativity of f. The philosophy behind the relaxation is that, on the one hand, the question of $f(e^{\mathbf{w}}) \geq 0$ is eventually easier to answer, since we have *linear* operations on the exponents and, on the other hand, the gap between $f(e^{\mathbf{w}}) \geq 0$ and nonnegativity hopefully is not too big, in particular for *sparse* polynomials. We show that for polynomials supported on a circuit (and some more general classes of sparse polynomials) both is true: In fact, for circuit polynomials it holds that $f(e^{\mathbf{w}}) \geq 0$ if and only if $f(\mathbf{x}) \geq 0$ and this equivalence can be characterized exactly, explicitly and easily in terms of the coefficients of f and the combinatorial structure of A.

6.2.2 Standard Forms and Norm Minimizers of Polynomials Supported on Circuits

Let $f \in \mathbb{R}[\mathbf{x}]$ be of the Form (6.0.1) defined on a circuit $A = \{\alpha(0), \ldots, \alpha(n), y\} \subset \mathbb{Z}^n$. Observe that there exists a unique convex combination $\sum_{j=0}^{n} \lambda_j \alpha(j) = y$. In the following, we assume w.l.o.g. that $\alpha(0) = 0$, which is always possible, since otherwise we can factor out a monomial $\mathbf{x}^{\alpha(0)}$ with $\alpha(0) \in (2\mathbb{N})^n$. We define the *support matrix* M^A by

$$M^A \;=\; \begin{pmatrix} 1 & 1 & \cdots & 1 & 1 \\ 0 & \alpha(1)_1 & \cdots & \alpha(n)_1 & y_1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \alpha(1)_n & \cdots & \alpha(n)_n & y_n \end{pmatrix} \;\in\; \mathbb{Z}^{(n+1)\times(n+2)}$$

and M_j^A as the matrix obtained by deleting the j-th column of M^A, where we start to count at 0. Furthermore, we always assume that $b_0 = \lambda_0$, which is always possible, since multiplication with a scalar does not change the variety. We denote the canonical basis of $\mathbb{R}^n$ with $e_1, \ldots, e_n$.

Proposition 6.2.1. *Let f be a polynomial of the Form* (6.0.1) *supported on a circuit $A = \{\alpha(0), \ldots, \alpha(n), y\} \subset \mathbb{Z}^n$ and $y = \sum_{j=0}^{n} \lambda_j \alpha(j)$ with $\sum_{j=0}^{n} \lambda_j = 1$, $0 < \lambda_j < 1$ for all j. Let $\mu \in \mathbb{N}_{>0}$ denote the least common multiple of the denominators of the λ_j. Then there exists a unique polynomial g of the Form* (6.0.1) *with* $\mathrm{supp}(g) = A' = \{0, \alpha(1)', \ldots, \alpha(n)', y'\} \subset \mathbb{Z}^n$ *such that the following properties hold.*

(1) $M^A = \begin{pmatrix} 1 & 0 \\ 0 & T \end{pmatrix} M^{A'}$ *for some $T \in GL_n(\mathbb{Q})$,*

(2) f and g have the same coefficients,

(3) $\alpha(j)' = \mu \cdot e_j$ *for every* $1 \leq j \leq n$,

(4) $y' = \sum_{j=1}^{n} \lambda_j \alpha(j)'$,

(5) $f(e^{\mathbf{w}}) = g(e^{T^t \mathbf{w}})$ *for all* $\mathbf{w} \in \mathbb{R}^n$.

For every f of the Form (6.0.1) we call the polynomial g, which satisfies all the conditions of the proposition, the *standard form* of f. Note that the support matrix $M^{A'}$ of the standard form of f is of the shape

$$M^{A'} = \begin{pmatrix} 1 & 1 & \cdots & \cdots & 1 & 1 \\ 0 & \mu & 0 & \cdots & 0 & \mu\lambda_1 \\ \vdots & 0 & \ddots & & \vdots & \vdots \\ \vdots & \vdots & & \ddots & 0 & \vdots \\ 0 & 0 & \cdots & 0 & \mu & \mu\lambda_n \end{pmatrix} \in \mathbb{Z}^{(n+1)\times(n+2)}. \tag{6.2.1}$$

Proof. We assume w.l.o.g. that $\alpha(0) = 0$. Let $\overline{M}_{n+1}^{A}$ be the submatrix of M_{n+1}^{A} obtained by deleting the first row and column; analogously for $\overline{M}_{n+1}^{A'}$. By definition, we have $\alpha(j) = \overline{M}_{n+1}^{A} e_j$ and $\alpha(j)' = \overline{M}_{n+1}^{A'} e_j$ for $1 \leq j \leq n$. We construct the polynomial g. We choose the same coefficients for g as for f. Since $\{0, \alpha(1), \ldots, \alpha(n)\}$ form a simplex, there exists a unique matrix $T \in GL_n(\mathbb{Q})$ such that

$$M_{n+1}^{A} = \begin{pmatrix} 1 & 0 \\ 0 & T \end{pmatrix} M_{n+1}^{A'}$$

with $M^{A'}$ being of the form (6.2.1) and given by $\mu T = (\overline{M}_{n+1}^{A})^{-1}$. Thus, (1) – (3) holds. Since $y = \sum_{j=0}^{n} \lambda_j \alpha(j)$, it follows that, in affine coordinates, we have $y_j' = T^{-1}\lambda_j(\overline{M}_{n+1}^{A} e_j)$, i.e., $y' = \mu(\lambda_0, \ldots, \lambda_n)$. This is (4).

We show that $f(e^{\mathbf{w}}) = g(e^{T^t \mathbf{w}})$ for every $\mathbf{w} \in \mathbb{R}^n$. We investigate the monomial $\mathbf{x}^{\alpha(j)}$:

$$b_j e^{\langle \alpha(j), \mathbf{w} \rangle} = b_j e^{\langle \overline{M}_{n+1}^{A} e_j, \mathbf{w} \rangle} = b_j e^{\langle T \overline{M}_{n+1}^{A'} e_j, \mathbf{w} \rangle} = b_j e^{\langle \alpha(j)', T^t \mathbf{w} \rangle}$$

For the inner monomials y and y' we know that $y = Ty'$ and thus for $y' = \sum_{j=0}^{n} \lambda_j \alpha(j)'$ we have $y = T(\sum_{j=0}^{n} \lambda_j \alpha(j)') = \sum_{j=0}^{n} \lambda_j T\alpha(j)' = \sum_{j=0}^{n} \lambda_j \alpha(j)$. Therefore,

$$\begin{aligned} c e^{\langle y, \mathbf{w} \rangle} &= c e^{\langle \sum_{j=0}^{n} \lambda_j \alpha(j), \mathbf{w} \rangle} = c e^{\sum_{j=0}^{n} \lambda_j \langle \alpha(j), \mathbf{w} \rangle} = c e^{\sum_{j=0}^{n} \lambda_j \langle \alpha(j)', T^t \mathbf{w} \rangle} \\ &= c e^{\langle y', T^t \mathbf{w} \rangle}. \end{aligned}$$

This is (5). ∎

Proposition 6.2.1 can easily be generalized to polynomials

$$f \quad = \quad b_0 + \sum_{j=1}^{n} b_j \mathbf{x}^{\alpha(j)} + \sum_{y(i) \in I} a_i \mathbf{x}^{y(i)} \in \mathbb{R}[\mathbf{x}], \tag{6.2.2}$$

with $\mathrm{New}(f) = \Delta = \mathrm{conv}\{0, \alpha(1), \ldots, \alpha(n)\}$ being a simplex and $I \subset (\mathrm{int}(\Delta) \cap \mathbb{Z}^n)$. Every $y(i)$ has a unique convex combination $y(i) = \lambda_0^{(i)} + \sum_{j=1}^{n} \lambda_j^{(i)} \alpha(j)$ with $\lambda_j^{(i)} > 0$ for all i, j.

Corollary 6.2.2. *Let f be defined as in* (6.2.2)*. Then Proposition 6.2.1 holds literally if we apply (4) for every $y(i)$ and define μ as the least common multiple of the denominators of all $\lambda_j^{(i)}$.*

Proof. By definition of μ, the support matrix $M^{A'}$ is integral again. Since in the proof of Proposition 6.2.1 neither uniqueness of y is used nor special assumptions about y are made, the statement follows. ■

Proposition 6.2.3. *Let $f = \lambda_0 + \sum_{j=1}^{n} b_j \mathbf{x}^{\alpha(j)} + c\mathbf{x}^y \in P_\Delta^y$ be such that $c < 0$ and $y = \sum_{j=1}^{n} \lambda_j \alpha(j)$ with $\sum_{j=0}^{n} \lambda_j = 1$, $\lambda_j \geq 0$. Then $f(e^{\mathbf{w}})$ with $\mathbf{w} \in \mathbb{R}^n$ has a unique extremal point, which is always a minimum.*

This proposition was used in [TdW13] (see Lemma 4.2 and Theorem 5.4). For convenience, we provide an own and easier proof here.

Proof. We investigate the standard form g of f. For the partial derivative $x_j \partial g / \partial x_j$ (we can multiply with x_j, since $e^{\mathbf{w}} \geq 0$) we have

$$x_j \frac{\partial g}{\partial x_j} = b_j \mu x_j^{\mu} + c \lambda_j \mu x_j^{\lambda_j \mu} \prod_{k=2}^{n} x_k^{\lambda_k \mu}.$$

Hence, the partial derivative vanishes for some $e^{\mathbf{w}}$ if and only if

$$\exp\left(w_j \mu - \sum_{k=1}^{n} \lambda_k \mu w_k \right) \quad = \quad -\frac{c \lambda_j}{b_j}.$$

Since the right hand side is strictly positive, we can apply $\log|\cdot|$ on both sides for every partial derivative and obtain the following linear system of equations:

$$\left(E_n - \begin{pmatrix} \lambda_1 & \cdots & \lambda_n \\ \vdots & \ddots & \vdots \\ \lambda_1 & \cdots & \lambda_n \end{pmatrix} \right) \cdot \begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} \quad = \quad \begin{pmatrix} 1/\mu(\log(\lambda_1) + \log(-c) - \log(b_1)) \\ \vdots \\ 1/\mu(\log(\lambda_n) + \log(-c) - \log(b_n)) \end{pmatrix}$$

Since the matrix on the left hand side has full rank, we have a unique solution.

For arbitrary f, we have $f(e^{\mathbf{w}}) = g(e^{T^t \mathbf{w}})$ by Proposition 6.2.1 and, hence, if $\mathbf{w}^*$ is the unique extremal point for $g(e^{\mathbf{w}})$, then $(T^t)^{-1} \mathbf{w}^*$ is the unique extremal point for $f(e^{\mathbf{w}})$.

For every $\mathbf{w} \in \mathbb{R}^n$ with $||\mathbf{w}|| \to \infty$ the polynomial f converges against the terms, which are contained in a particular proper face of $\mathrm{New}(f)$. Since all these terms are strictly positive, $f(e^{\mathbf{w}})$ converges against a number in $\mathbb{R}_{>0} \cup \{\infty\}$. Thus, the unique extremal point has to be a global minimum. ■

For $f \in P_\Delta^y$ we define $\mathbf{s}_f^* \in \mathbb{R}^n$ as the unique vector satisfying

$$\prod_{k=1}^{n} (e^{s_{k,f}^*})^{\alpha(j)_k} \;=\; e^{\langle \mathbf{s}_f^*, \alpha(j)\rangle} \;=\; \frac{\lambda_j}{b_j} \quad \text{for all} \quad 1 \leq j \leq n.$$

$\mathbf{s}_f^*$ indeed is well defined, since application of $\log|\cdot|$ on both sides yields a linear system of equations with variables $s_{k,f}^*$ and the rank of this system has to be n, since $\mathrm{conv}(A)$ is a simplex. If the context is clear, then we simply write $\mathbf{s}^*$ instead of $\mathbf{s}_f^*$ resp. $e^{\mathbf{s}^*}$ instead of $e^{\mathbf{s}_f^*}$. We recall that the circuit number associated to a polynomial $f \in P_\Delta^y$ is given by

$$\Theta_f = \prod_{j=0}^{n} \left(\frac{b_j}{\lambda_j}\right)^{\lambda_j} = \prod_{j=1}^{n} \left(\frac{b_j}{\lambda_j}\right)^{\lambda_j}.$$

Note that we scaled such that $b_0 = \lambda_0$.

Proposition 6.2.4. *For $f \in P_\Delta^y$ and $c = -\Theta_f$ the point $\mathbf{s}^* \in \mathbb{R}^n$ is a root and the unique global minimizer of $f(e^{\mathbf{w}})$.*

Due to this proposition, we call the point $\mathbf{s}^*$ the *norm minimizer* of f. We remark that this proposition was already shown for polynomials in P_Δ^y in standard form in [FK11] and for arbitrary simplices but in a more complicated way in [TdW13].

Proof. For $f(e^{\mathbf{s}^*})$ we have

$$\begin{aligned} f\left(e^{\mathbf{s}^*}\right) &= \lambda_0 + \sum_{j=1}^{n} b_j e^{\langle \mathbf{s}^*, \alpha(j)\rangle} - \Theta_f e^{\langle \mathbf{s}^*, y\rangle} \;=\; \sum_{j=0}^{n} \lambda_j - \Theta_f \cdot \prod_{j=1}^{n} \left(\frac{\lambda_j}{b_j}\right)^{\lambda_j} \\ &= 1 - 1 \;=\; 0. \end{aligned}$$

For the minimizer statement we investigate the partial derivatives $x_j \partial f / \partial x_j$ (we can multiply with x_j, since $e^{\mathbf{w}} \geq 0$). Since $y_j = \sum_{k=1}^n \lambda_j \alpha_j(k)$, we obtain

$$x_j \frac{\partial f}{\partial x_j} \;=\; \sum_{k=1}^{n} b_k \alpha_j(k) \mathbf{x}^{\alpha(k)} - \Theta_f \cdot \left(\sum_{k=1}^{n} \lambda_j \alpha_j(k)\right) \mathbf{x}^y.$$

Evaluation of the partial derivative at $e^{\mathbf{s}^*}$ yields

$$\begin{aligned} x_j \frac{\partial f}{\partial x_j}(e^{\mathbf{s}^*}) &= \sum_{k=1}^{n} b_k \alpha_j(k) \left(\frac{\lambda_k}{b_k}\right) - \Theta_f \left(\sum_{k=1}^{n} \lambda_j \alpha_j(k)\right) \cdot \prod_{j=1}^{n} \left(\frac{\lambda_j}{b_j}\right)^{\lambda_j} \\ &= \sum_{k=1}^{n} \lambda_j \alpha_j(k) - \sum_{k=1}^{n} \lambda_j \alpha_j(k) \;=\; 0. \end{aligned}$$

Finally, by Proposition 6.2.3, $e^{\mathbf{s}^*}$ is the unique global minimizer of $f(e^{\mathbf{w}})$. ■

6.2.3 Nonnegativity of Polynomials Supported on a Circuit

In this section, we characterize nonnegativity of polynomials in P_Δ^y. The following lemma allows us to reduce the case of $y \in \partial\Delta$ to the case $y \in \text{int}(\Delta)$.

Lemma 6.2.5. *Let $f = b_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha(j)} + c \cdot \mathbf{x}^y$ be such that $\Delta = \text{New}(f) = \text{conv}\{0, \alpha(1), \ldots, \alpha(n)\}$ is a simplex and $y \in \partial\Delta$. Let furthermore F be the face of Δ containing y. Then f is nonnegative if and only if the restriction of f to the face F is nonnegative.*

Proof. For the necessity of nonnegativity of the restricted polynomial, see [Rez89]. Otherwise, the restriction to the face F contains the monomial $\mathbf{x}^y$ and this restriction is nonnegative. Since all other terms in f correspond to the (even) vertices of Δ and have nonnegative coefficients, the claim follows. ■

Now, we can completely characterize the section $P_{n,2d}^y$. Note that the following theorem covers the known special cases of agiforms in [Rez89] and circuit polynomials in standard form in [FK11].

Theorem 6.2.6. *Let $f = \lambda_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha(j)} + c \cdot \mathbf{x}^y \in P_\Delta^y$ be of the Form (6.0.1) with $\alpha(j) \in (2\mathbb{N})^n$. Then the following are equivalent.*

1. *$f \in P_{n,2d}^y$, i.e., f is nonnegative.*
2. *$|c| \leq \Theta_f$ and $y \notin (2\mathbb{N})^n$ or $c \geq -\Theta_f$ and $y \in (2\mathbb{N})^n$.*

Proof. First, observe that $f \geq 0$ is trivial for $c \geq 0$ and $y \in (2\mathbb{N})^n$, since f is a sum of monomial squares in this case.

We apply the norm relaxation strategy introduced in Section 6.2.1. Initially, we show that $f(\mathbf{x}) \geq 0$ if and only if $f(e^{\mathbf{w}}) \geq 0$ for all $f \in P_\Delta^y$. Let w.l.o.g. $y_1, \ldots, y_k$ be the odd entries of the exponent vector y. Thus, for every $1 \leq j \leq k$, replacing x_j by $-x_j$ changes the sign of the term $c \cdot \mathbf{x}^y$. Since all other terms of f are nonnegative for every choice of $\mathbf{x} \in \mathbb{R}^n$, we have $f(\mathbf{x}) \geq 0$ if $\text{sgn}(c) \cdot \text{sgn}(x_1) \cdots \text{sgn}(x_k) = 1$. Since furthermore, for $\text{sgn}(c) \cdot \text{sgn}(x_1) \cdots \text{sgn}(x_k) = -1$ we have $c \cdot \mathbf{x}^y = -|c| \cdot |x_1|^{y_1} \cdots |x_n|^{y_n}$, we can assume $c \leq 0$ and $\mathbf{x} \geq 0$ without loss of generality. Then $\lambda_0 + \sum_{j=0}^n b_j \mathbf{x}^{\alpha(j)} - |c||\mathbf{x}|^y$ is nonnegative for all $\mathbf{x} \in \mathbb{R}^n$ if and only if this is the case for all $\mathbf{x} \in \mathbb{R}_{\geq 0}^n$. And since $\mathbb{R}_{>0}^n$ is an open dense set in $\mathbb{R}_{\geq 0}^n$, we can restrict ourselves to the strictly positive orthant. With the componentwise bijection between $\mathbb{R}_{>0}^n$ and $\mathbb{R}^n$ given by the Exp-map, it follows that $f(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$ if and only if $f(e^{\mathbf{w}}) \geq 0$ for all $\mathbf{w} \in \mathbb{R}^n$. Hence, the theorem is shown if we prove that this is the case if and only if $c \in [-\Theta_f, 0]$.

Let $b_1, \ldots, b_n \in \mathbb{R}_{>0}$ be fixed arbitrarily and $(f_c)_{c \in \mathbb{R}}$ be the corresponding family of polynomials in P_Δ^y. By Proposition 6.2.4, $f_c(e^{\mathbf{w}})$ has a unique global minimum for $c = -\Theta_f$ attained at $\mathbf{s}^* \in \mathbb{R}^n$ satisfying $f_{-\Theta_f}(e^{\mathbf{s}^*}) = 0$. Since $e^{\mathbf{s}^*}$ is a *global* (norm) minimum, this implies in particular that $f_c(e^{\mathbf{w}}) \geq 0$ for all $\mathbf{w} \in \mathbb{R}^n$ if $c = -\Theta_f$.

But this fact also completes the proof for general $c < 0$: Since $c \cdot e^{\langle \mathbf{w}, y\rangle}$ is the unique negative term in $f_c(e^{\mathbf{w}})$ for all $\mathbf{w} \in \mathbb{R}^n$, a term by term inspection yields that $f_c(e^{\mathbf{w}}) < f_{-\Theta_f}(e^{\mathbf{w}})$ if and only if $c < -\Theta_f$. Hence, $f_c(e^{\mathbf{w}}) < 0$ for some $\mathbf{w} \in \mathbb{R}^n$ if and only if $c < -\Theta_f$. ∎

An immediate consequence of the theorem is an upper bound for the number of zeros of polynomials $f \in P^y_{n,2d}$.

Corollary 6.2.7. *Let $f \in P^y_{n,2d}$. Then f has at most 2^n affine real zeros $\mathbf{x} \in \mathbb{R}^n$, all of which satisfy $|x_j| = e^{s^*_j}$ for $1 \leq j \leq n$.*

Proof. Assume $f \in \partial P^y_{n,2d}$ and $f(\mathbf{x}) = 0$ for some $\mathbf{x} \in \mathbb{R}^n$. Then we know by the proof of Theorem 6.2.6 that $|x_j| = e^{s^*_j}$. Thus, $\mathbf{x} = (\pm e^{s^*_1}, \ldots, \pm e^{s^*_n})$. ∎

The bound in Corollary 6.2.7 is sharp as demonstrated by the well known Motzkin polynomial $f = 1 + x_1^2x_2^4 + x_1^4x_2^2 - 3x_1^2x_2^2 \in P^y_{2,6}$. The zeros are given by $\mathbf{x} = (\pm 1, \pm 1)$. Furthermore, it is important to note that the maximum number of zeros does not depend on the degree of the polynomials, which is in sharp contrast to previously known results concerning the maximum number of zeros of nonnegative polynomials and sums of squares (see [CLR80]).

In order to illustrate the achievements of this section, we give some examples. Let $f = 1 + x_1^2x_2^4 + x_1^4x_2^2 - 3x_1^2x_2^2$ be the Motzkin polynomial, which is supported on a circuit A with $y = \sum_{j=0}^2 \frac{1}{3}\alpha(j)$. We apply Proposition 6.2.1 and compute the standard form g of $1/3 \cdot f$. Then g is the polynomial, which is supported on a circuit $A' = \{0, \alpha(1)', \alpha(2)'\}$ satisfying $M^A = \begin{pmatrix} 1 & 0 \\ 0 & T \end{pmatrix} M^{A'}$ for some $T \in GL_n(\mathbb{Q})$ with $\alpha(1)' = (\mu, 0)^t$, $\alpha(2)' = (0, \mu)^t$ and $y' = 1/3\alpha(1)' + 1/3\alpha(2)'$, where $\mu = \operatorname{lcm}\{1/\lambda_0, 1/\lambda_1, 1/\lambda_2\} = \operatorname{lcm}\{3,3,3\} = 3$. Additionally, g has the same coefficients as f. It is easy to see that

$$T = \begin{pmatrix} 4/3 & 2/3 \\ 2/3 & 4/3 \end{pmatrix}$$

and thus

$$g = 1/3 + 1/3x_1^3 + 1/3x_2^3 - x_1x_2.$$

By Proposition 6.2.1, we have $f(e^{\mathbf{w}}) = g(e^{T^t\mathbf{w}})$. The circuit number Θ_f is invariant w.r.t. transformation to the standard form, since it only depends on the coefficients of f and the convex combination of y. Thus, we have

$$\Theta_f = \Theta_g = \prod_{j=0}^{2}\left(\frac{\lambda_j}{b_j}\right)^{\lambda_j} = \left(\frac{1/3}{1/3}\right)^{1/3} \cdot \left(\frac{1/3}{1/3}\right)^{1/3} \cdot \left(\frac{1/3}{1/3}\right)^{1/3} = 1.$$

Since $y = (2,2) \in (2\mathbb{N})^2$, by Theorem 6.2.6, $f \geq 0$ if and only if the inner coefficient c of f satisfies $c \geq -\Theta_f = -1$. But the inner coefficient c of the Motzkin polynomial equals its negative circuit number. Hence, the Motzkin polynomial is contained in the boundary of the cone of nonnegative polynomials.

If $c = -\Theta_f$, then we know by Proposition 6.2.4 that $f(e^{\mathbf{w}}) = 0$ at the unique point $\mathbf{s}^*$ with

$$1/3 \cdot e^{4s_1^*+2s_2^*} \;=\; 1/3 \quad \text{and} \quad 1/3 \cdot e^{2s_1^*+4s_2^*} \;=\; 1/3.$$

Thus, $\mathbf{s}^* = (0,0)$. Since, by the proof of Theorem 6.2.6, $f(\mathbf{x}) = 0$ only if $f(|x_1|,|x_2|) = 0$, we can conclude that every affine root $\mathbf{v} \in \mathbb{R}^n$ of the Motzkin polynomial satisfies $|v_j| = 1$.

We give a second example where nonnegativity is not already known. Let $f = 1/4 + 2 \cdot x_1^2 x_2^4 + x_1^4 x_2^4 - 2.5 \cdot x_1^2 x_2^3$. Again, it is easy to see that $\lambda_1 = 1/2$ and $\lambda_2 = 1/4$. Hence,

$$\Theta_f \;=\; \left(\frac{b_1}{\lambda_1}\right)^{\lambda_1} \cdot \left(\frac{b_2}{\lambda_2}\right)^{\lambda_2} \;=\; (2 \cdot 2)^{1/2} \cdot (1 \cdot 4)^{1/4} \;=\; 2 \cdot \sqrt{2} \;\approx\; 2.828.$$

Since $|c| < \Theta_f$, we can conclude that f is a strictly positive polynomial.

6.2.4 A-Discriminants and Gale Duals

For a given $(n+1) \times m$ support matrix M^A with $A \subset \mathbb{Z}^n$ and $\text{conv}(A)$ being full dimensional, a *Gale dual* or *Gale transformation* is an integral $m \times (m-n-1)$ matrix M^B such that its rows span the $\mathbb{Z}$-kernel of M^A, i.e., for every integral vector $v \in \mathbb{Z}^m$ with $M^A v = 0$ it holds that v is an integral linear combination of the rows of M^B (see, e.g., [GKZ08, PT]).

If A is a circuit, then M^B is a vector with $n+2$ entries. It turns out that this vector is closely related to the global minimum $e^{\mathbf{s}^*} \in \mathbb{R}^n$ and the circuit number Θ_f.

Corollary 6.2.8. *Let $f = \sum_{j=0}^n b_j \mathbf{x}^{\alpha(j)} + c\mathbf{x}^y$ be a polynomial supported on a circuit A of the Form* (6.0.1). *Let $e^{\mathbf{s}^*} \in \mathbb{R}^n$ be the global minimizer and Θ_f be the circuit number. Then the Gale dual M^B of the support matrix M^A is an integral multiple of the vector*

$$\left(b_0 e^{\langle \mathbf{s}^*, \alpha(0)\rangle}, \ldots, b_n e^{\langle \mathbf{s}^*, \alpha(n)\rangle}, -\Theta_f e^{\langle \mathbf{s}^*, y\rangle}\right) \;\in\; \mathbb{R}^{n+2}.$$

Proof. The Gale dual M^B needs to satisfy $M^A(M^B)^t = 0$. Since A is a circuit, M^B spans a 1-dimensional vector space. From $y = \sum_{j=0}^n \lambda_j \alpha(j)$ it follows by construction of $e^{\mathbf{s}^*}$ and Θ_f (see proof of Proposition 6.2.4) that

$$\left(b_0 e^{\langle \mathbf{s}^*, \alpha(0)\rangle}, \ldots, b_n e^{\langle \mathbf{s}^*, \alpha(n)\rangle}, -\Theta_f e^{\langle \mathbf{s}^*, y\rangle}\right) \;=\; (\lambda_0, \ldots, \lambda_n, -1)$$

and the statement follows by definition of M^A and y. ■

We furthermore want to point out that the circuit number Θ_f and the question of nonnegativity is closely related to A-discriminants. Let $A = \{\alpha(1), \ldots, \alpha(d)\} \subset \mathbb{Z}^n$ and denote by $\mathbb{C}^A$ the space of all polynomials of the form $\sum_{j=1}^{d} b_j \mathbf{z}^{\alpha(j)}$ with $b_j \in \mathbb{C}^*$. Since every polynomial in $\mathbb{C}^A$ is uniquely determined by its coefficients, $\mathbb{C}^A$ can be identified with a $(\mathbb{C}^*)^d$ space. Let ∇_A be the closure of the subset of all polynomials f in $\mathbb{C}^A$ for which there exists a point $\mathbf{z} \in (\mathbb{C}^*)^n$ such that

$$f(\mathbf{z}) \;=\; 0 \;\text{ and }\; \frac{\partial f}{\partial z_j}(\mathbf{z}) \;=\; 0 \;\text{ for all } 1 \leq j \leq n.$$

It is well known that ∇_A is an irreducible $\mathbb{Q}$-variety. If ∇_A is of codimension 1, then the *A-discriminant* Δ_A is the integral irreducible polynomial in $\mathbb{C}[b_1, \ldots, b_d]$, which has variety ∇_A (see, e.g., [GKZ08]).

The discriminant of a polynomial is a very important tool, since it describes the algebraic boundary of the cone of nonnegative polynomials ([Nie12]). The following statement is an immediate consequence of Proposition 6.2.4 and Theorem 6.2.6. Without the nonnegativity aspect, it was already known before and can also be derived from [GKZ08], [TdW13].

Corollary 6.2.9. *A polynomial $f \in P_{\Delta}^{y}$ vanishes under the A-discriminant if and only if $f \in \partial P_{n,2d}^{y}$ if and only if $|c| = \Theta_f$ and $y \notin (2\mathbb{N})^n$ or $c = -\Theta_f$ and $y \in (2\mathbb{N})^n$.*

6.3 Sums of Squares Supported on a Circuit

In this section, we completely characterize the section $\Sigma_{n,2d}^{y}$. It is particularly interesting that this section depends heavily on the lattice point configuration in Δ, thereby yielding a connection to the theory of lattice polytopes and toric geometry. By investigating this connection in more detail, we will prove that the sections $P_{2,2d}^{y}$ and $\Sigma_{2,2d}^{y}$ almost always coincide and encounter large sections, on which nonnegative polynomials are equal to sums of squares (see Corollaries 6.4.2 and 6.4.4).

Surprisingly, the sums of squares condition is exactly the same as for the corresponding agiforms in [Rez89]. For this, we briefly review the Gram matrix method for sums of squares polynomials. Let $\mathbb{N}_d^n = \{\alpha \in \mathbb{N}^n : \alpha_1 + \cdots + \alpha_n \leq d\}$ and $p = \sum_{k=1}^{r} h_k^2$ where $p(\mathbf{x}) = \sum_{\alpha \in \mathbb{N}_{2d}^n} a(\alpha)\mathbf{x}^{\alpha}$ and $h_k(\mathbf{x}) = \sum_{\beta \in \mathbb{N}_d^n} b_k(\beta)\mathbf{x}^{\beta}$. Let $B(\beta) := (b_1(\beta), \ldots, b_r(\beta))$ and $G(\beta, \beta') = B(\beta) \cdot B(\beta') = \sum_k b_k(\beta) b_k(\beta')$. Comparing coefficients one has

$$a(\alpha) = \sum_{\beta + \beta' = \alpha} G(\beta, \beta') = \sum_{\beta} G(\beta, \alpha - \beta).$$

In this case $[B(\beta) \cdot B(\beta')]_{\beta, \beta' \in \mathbb{N}_d^n}$ is a positive semidefinite matrix. Furthermore, we need the following well known lemma (see, e.g., [BPT13]).

Lemma 6.3.1. *Let $f \in \Sigma_{n,2d}$ be a sum of squares and $T \in GL_n$ be a matrix yielding a variable transformation $\mathbf{x} \mapsto T\mathbf{x}$. Then $f(T\mathbf{x})$ also is a sum of squares.*

Theorem 6.3.2. *Let $f := \lambda_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha(j)} + c \cdot \mathbf{x}^y \in P_{n,2d}^y$. Then*

$$f \in \Sigma_{n,2d}^y \quad \text{if and only if} \quad y \in \Delta^* \quad \text{or} \quad c > 0 \quad \text{as well as} \quad y \in (2\mathbb{N})^n.$$

Furthermore, if $f \in \Sigma_{n,2d}^y$, then f is a sum of binomial squares.

Proof. First, assume that $f \in \Sigma_{n,2d}^y$. We can assume that $c < 0$ by the following argument: If $y \in (2\mathbb{N})^n$ then f is obviously a sum of (monomial) squares for $c > 0$. If $y \notin (2\mathbb{N})^n$ and $c > 0$, then, by Lemma 6.3.1, and a suitable variable transformation as in the proof of Theorem 6.2.6, we can reduce to the case $c < 0$. Let $f = \sum h_k^2$ and define $M := \{\beta : b_k(\beta) \neq 0 \text{ for some } k\}$. Following [Rez89, Theorem 3.3], we claim that the set $L := 2M \cup \hat{\Delta} \cup \{y\}$ is $\hat{\Delta}$-mediated and hence $y \in \Delta^*$. For this we write every $\beta \in L \setminus \hat{\Delta}$ as a sum of two distinct points in M, which implies that β is an average of two distinct points in $2M \subset L$. Note that if $G(\alpha, \alpha') < 0$ then $b_k(\alpha) b_k(\alpha') < 0$ for some k and hence $\alpha \neq \alpha'$ and $\alpha' \in M$. Hence, it suffices to show that for $\beta \in L \setminus \hat{\Delta}$ there exists α with $G(\alpha, \beta - \alpha) < 0$. We have $a(y) = c < 0$, so $G(\alpha_0, y - \alpha_0) < 0$ for some α_0. If $\beta \neq y$ then $\beta \in L \setminus (\hat{\Delta} \cup \{y\})$ and $a(\beta) = 0 = \sum G(\alpha, \beta - \alpha)$. But $\beta \in 2M$, so $G(\frac{1}{2}\beta, \frac{1}{2}\beta) > 0$ and there must exist α with $G(\alpha, \beta - \alpha) < 0$ to make the sum vanish.

Let now $y \in \Delta^*$. We investigate two cases. Firstly, $y \notin (2\mathbb{N})^n$. Then it suffices to prove the statement for $c = \pm \Theta_f$ by the following argument: Let $f_1 = \lambda_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha(j)} - c \cdot \mathbf{x}^y \in P_{n,2d}^y$ and $f_2 = \lambda_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha(j)} + c \cdot \mathbf{x}^y \in P_{n,2d}^y$. Let c^* be such that $-c < c^* < c$ and $f_3 = \lambda_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha_j} + c^* \cdot \mathbf{x}^y \in P_{n,2d}^y$. Then we have $f_3 = \lambda_1 f_1 + \lambda_2 f_2$ with $\lambda_1 = \frac{c+c^*}{2c}$, $\lambda_2 = \frac{c-c^*}{2c}$ and $\lambda_1, \lambda_2 > 0$, $\lambda_1 + \lambda_2 = 1$. By the same argument about the variable transformation as above (proof of Theorem 6.2.6, Lemma 6.3.1) it suffices to investigate the case $c = -\Theta_f$. Consider the following linear transformation of the variables $x_1, \ldots, x_n$.

$$T : (x_1, \ldots, x_n) \mapsto \left((e^{s^*})_1 x_1, \ldots, (e^{s^*})_n x_n\right),$$

where $(e^{s^*})_j$ denotes the j-th coordinate of the global minimizer $e^{\mathbf{s}^*}$ of f. By construction, $f \in \Sigma_{n,2d}^y$ if and only if $f(T(\mathbf{x})) \in \Sigma_{n,2d}^y$, where

$$f(T(\mathbf{x})) = \lambda_0 + \sum_{j=1}^n \lambda_j \mathbf{x}^{\alpha(j)} - \mathbf{x}^y. \tag{6.3.1}$$

But $f(T(\mathbf{x}))$ is the dehomogenization of an agiform and, therefore, by Theorem 6.1.4, $f \in \Sigma_{n,2d}^y$ if and only if $y \in \Delta^*$.

If $y \in (2\mathbb{N})^n$, we use the same argument to prove that f is a sum of squares for $c = -\Theta_f$. For $c > -\Theta_f$, the polynomial f is obviously a sum of squares, since the inner monomial can be written as $-\Theta_f \mathbf{x}^y$ plus a sum of squares term $(c + \Theta_f)\mathbf{x}^y$.

In [Rez89, Theorem 4.4] it is shown that the agiforms in (6.3.1) are sums of *binomial* squares. Thus, for $y \in \Delta^*$, the nonnegative polynomials $f \in P^y_{n,2d}$ are also sums of binomial squares, since the binomial structure is preserved under the variable transformation T. ■

Agiforms can be recovered by setting $b_j = \lambda_j$ and hence Theorems 6.2.6 and 6.3.2 generalize results for agiforms in [Rez89]. Furthermore, by setting $\alpha(j) = 2d \cdot e_j$ for $1 \leq j \leq n$, we recover what is called an *elementary diagonal minus tail form* in [FK11], and, again, Theorems 6.2.6 and 6.3.2 generalize one of the main results in [FK11] to arbitrary simplices.

We remark that in [Rez89] an algorithm is given to compute such a sum of squares representation for agiforms in Theorem 6.3.2, which can be generalized to arbitrary circuit polynomials using the variable transformation T. Theorem 6.3.2 also comes with two immediate corollaries.

Corollary 6.3.3. *Let Δ be an H-simplex and $f \in P^y_\Delta$. Then $f \in P^y_{n,2d}$ if and only if $f \in \Sigma^y_{n,2d}$.*

Proof. Since Δ is an H-simplex, it holds that $\Delta^* = (\Delta \cap \mathbb{Z}^n)$ and we always have $y \in \Delta^*$. ■

The second corollary concerns sums of squares relaxations for minimizing polynomial functions. For this, remember that $f^*_{sos} = \sup\{\lambda : f - \lambda \in \Sigma_{n,2d}\}$ is a lower bound for $f^* = \inf\{f : \mathbf{x} \in \mathbb{R}^n\}$ (see Chapter 2).

Corollary 6.3.4. *Let $f \in P^y_\Delta$. Then $f^*_{sos} = f^*$ if and only if $y \in \Delta^*$.*

Proof. We have $f^*_{sos} = f^*$ if and only if $f - f^* \in \Sigma^y_{n,2d}$. However, subtracting the minimum of the polynomial f does not affect the question whether $y \in \Delta^*$ or not. Hence, if $y \in \Delta^*$, this will also hold for the nonnegative polynomial $f - f^*$ and vice versa. ■

Now, we consider the case of multiple interior lattice points in the simplex Δ. In the case that all interior monomials come with a negative coefficient, we can write the polynomial as a sum of nonnegative circuit polynomials if and only if it is nonnegative. Furthermore, we get equivalence between nonnegativity and sums of squares if the whole support is contained in Δ^*. In the following, let $\{\lambda_0^{(i)}, \ldots, \lambda_n^{(i)}\}$ be the (unique) convex combination of $y(i) \in I \subset (\text{int}(\Delta) \cap \mathbb{N}^n)$ and scale such that $b_0 = \sum_{j=1}^{|I|} \lambda_0^{(j)}$.

Theorem 6.3.5. *Let $f = \sum_{j=1}^{|I|} \lambda_0^{(j)} + \sum_{j=1}^{n} b_j \mathbf{x}^{\alpha(j)} - \sum_{y(i) \in I} a_i \mathbf{x}^{y(i)}$ be such that* $\text{New}(f) = \Delta = \text{conv}\{0, \alpha(1), \ldots, \alpha(n)\}$ *is a simplex with $\alpha(j) \in (2\mathbb{N})^n$,* *all* $a_i, b_j > 0$ *and* $I \subset (\text{int}(\Delta) \cap \mathbb{N}^n)$. *Then*

$$f \in P_{n,2d} \quad \textit{if and only if} \quad f \;=\; \sum_{i=1}^{|I|} E_{y(i)},$$

where all $E_{y(i)} \in P_\Delta^{y(i)}$ *are nonnegative circuit polynomials with support sets* $\{0, \alpha(1), \ldots, \alpha(n), y(i)\}$.

If furthermore $I \subseteq \Delta^*$, *then we have*

$$\begin{aligned} f \in P_{n,2d} \quad & \textit{if and only if} \quad f \in \Sigma_{n,2d} \\ & \textit{if and only if} \quad f \textit{ is a sum of binomial squares.} \end{aligned} \tag{6.3.2}$$

In particular, (6.3.2) *always holds, if* Δ *is an* H*-simplex.*

Again, we get an immediate corollary.

Corollary 6.3.6. *Let* f *be as above and* $I \subset \Delta^*$. *Then* $f^*_{sos} = f^*$.

In order to prove Theorem 6.3.5, we need the following lemma.

Lemma 6.3.7. *Let* $f = b_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha(j)} - \sum_{y(i)\in I} a_i \mathbf{x}^{y(i)}$ *be nonnegative with simplex Newton polytope* $\text{New}(f) = \Delta = \text{conv}\{0, \alpha(1), \ldots, \alpha(n)\}$ *for some* $\alpha(j) \in (2\mathbb{N})^n$. *Furthermore, let* $I \subset (\text{int}(\Delta) \cap \mathbb{N}^n)$ *and* $a_i, b_j > 0$. *Then* f *has a global minimizer* $v^* \in \mathbb{R}^n_{>0}$.

Proof. Since all $b_j > 0$ and $\alpha(j) \in (2\mathbb{N})^n$, clearly f has a global minimizer on $\mathbb{R}^n$. Assume that all global minimizers are not contained in $\mathbb{R}^n_{\geq 0}$. We make a term by term inspection for a minimizer v in comparison with $|v| = (|v_1|, \ldots, |v_n|)$: For every vertex of Δ we have $b_j v^{\alpha(j)} = b_j |v^{\alpha(j)}|$; for every interior point we have $-a_i |v|^{y(i)} \leq -a_i v^{y(i)}$ and hence $f(v) \geq f(|v|)$. This is a contradiction and therefore at least one global minimizer v^* is contained in $\mathbb{R}^n_{\geq 0}$.

Assume for at least one component $v^*_j = 0$. We define $g = b_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha(j)} - a_i \mathbf{x}^{y(i)}$ for one $y(i) \in I$. By Proposition 6.2.3, $g(e^{\mathbf{w}})$ has a unique global minimizer on $\mathbb{R}^n$ and hence g has a unique global minimizer on $\mathbb{R}^n_{>0}$. But, by construction of f and g, we have $f(\mathbf{x}) < g(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^n_{>0}$ and $f(\mathbf{x}) = g(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n_{\geq 0} \setminus \mathbb{R}^n_{>0}$. Thus, $v^*_j \neq 0$ for all $1 \leq j \leq n$. ∎

Proof. (Proof of Theorem 6.3.5) Let

$$f = \sum_{j=1}^{|I|} \lambda_0^{(j)} + \sum_{j=1}^{n} b_j \mathbf{x}^{\alpha(j)} - \sum_{y(i)\in I} a_i \mathbf{x}^{y(i)}$$

be nonnegative and, by Lemma 6.3.7, let $v \in \mathbb{R}^n_{>0}$ be a global minimizer of f. First, we investigate the case $\alpha(j) = \alpha_j e_j$ for some $\alpha_j \in 2\mathbb{N}$ and e_j denoting the j-th standard vector. For any $1 \leq k \leq n$ we have

$$\left(x_k \frac{\partial f}{\partial x_k}\right)(v) \;=\; b_k \cdot \alpha(k)_k \cdot v_k^{\alpha_k} - \sum_{y(i)\in I} a_i \cdot y(i)_k \cdot v^{y(i)} \;=\; 0. \tag{6.3.3}$$

Let $\{\lambda_0^{(i)}, \ldots, \lambda_n^{(i)}\}$ be the coefficients of the (unique) convex combination of $y(i) \in I$ and $\lambda^{(i)} = (\lambda_1^{(i)}, \ldots, \lambda_n^{(i)}) \in \mathbb{R}_{>0}^n$. For $y(i) \in I$ we define

$$b_{y(i),k} = \frac{a_i \cdot \lambda_k^{(i)} \cdot v^{y(i)}}{v^{\alpha(k)}} \tag{6.3.4}$$

Since for all i, k it holds that $\sum_{j=1}^n \lambda_k^{(i)} \alpha(j)_k = y(i)_k$ and all $\alpha(j)_k = 0$ unless $j = k$, we get with (6.3.3) that

$$b_k = \sum_{y(i) \in I} b_{y(i),k}.$$

By Proposition 6.2.4 and Theorem 6.2.6, we conclude that

$$E_{y(i)}(\mathbf{x}) = \lambda_0^{(i)} + \sum_{k=1}^n b_{y(i),k} x_k^{\alpha_k} - a_i \mathbf{x}^{y(i)}$$

is a nonnegative circuit polynomial and has its minimum value at v. This yields the desired decomposition:

$$\begin{aligned} f(\mathbf{x}) &= \sum_{j=1}^{|I|} \lambda_0^{(j)} + \sum_{k=1}^n b_k x_k^{\alpha_k} - \sum_{y(i) \in I} a_i \mathbf{x}^{y(i)} \\ &= \sum_{j=1}^{|I|} \lambda_0^{(j)} + \sum_{k=1}^n \left(\sum_{y(i) \in I} b_{y(i),k} \right) x_k^{\alpha_k} - \sum_{y(i) \in I} a_i \mathbf{x}^{y(i)} \\ &= \sum_{y(i) \in I} E_{y(i)}(\mathbf{x}). \end{aligned} \tag{6.3.5}$$

Now, we head over to the case of arbitrary $\alpha(j) \in (2\mathbb{N})^n$. Let $v \in \mathbb{R}_{>0}^n$ be a global minimizer of f. By Corollary 6.2.2 (and Proposition 6.2.1), there exists a unique polynomial g satisfying

$$f(e^{\mathbf{w}}) = g(e^{T^t \mathbf{w}}) \quad \text{for all} \quad \mathbf{w} \in \mathbb{R}^n \tag{6.3.6}$$

such that $T \in GL_n(\mathbb{R})$ and g has a support matrix

$$M^{A'} = \begin{pmatrix} 1 & 1 & \cdots & \cdots & 1 & 1 & \cdots & 1 \\ 0 & \mu & 0 & \cdots & 0 & \mu\lambda_1^{(1)} & \cdots & \mu\lambda_1^{(|I|)} \\ \vdots & 0 & \ddots & & \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & & \ddots & 0 & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & 0 & \mu & \mu\lambda_n^{(1)} & \cdots & \mu\lambda_n^{(|I|)} \end{pmatrix} \in \mathbb{Z}^{(n+1)\times(n+|I|)}$$

where μ is the least common multiple of the denominators of all $\lambda_j^{(i)}$ and 2 (since vertices of $\mathrm{New}(g)$ shall be in $(2\mathbb{N})^n$).

Since $v \in \mathbb{R}^n_{>0}$, we can define $\mathrm{Log}\,|v'| = T^t \,\mathrm{Log}\,|v|$. By (6.3.5) and (6.3.6), it follows that v' is a global minimizer for g and thus in particular

$$f(v) \;=\; f(e^{\mathrm{Log}\,|v|}) \;=\; g(e^{T^t\,\mathrm{Log}\,|v|}) \;=\; \sum_{i=1}^{|I|} E_{\mu\lambda^{(i)}}(e^{\mathrm{Log}\,|v'|})$$

for some nonnegative circuit polynomials $E_{\mu\lambda^{(i)}}$ with global minimizer $v' \in \mathbb{R}^n_{>0}$.

Since $\mathrm{supp}(E_{\mu\lambda^{(i)}}) \subseteq \mathrm{supp}(g)$ and $\mathrm{New}(E_{\mu\lambda^{(i)}}) = \mathrm{New}(g)$, we have, by Proposition 6.2.4,

$$E_{\mu\lambda^{(i)}}(e^{\mathrm{Log}\,|v'|}) \;=\; E_{y(i)}(e^{\mathrm{Log}\,|v|})$$

such that each $E_{y(i)}(e^{\mathrm{Log}\,|v|})$ is a nonnegative circuit polynomial with global minimizer v and support set $\{0, \alpha(1), \ldots, \alpha(n), y(i)\}$ satisfying $f = \sum_{i=1}^{|I|} E_{y(i)}$.

If, additionally, every $y(i) \in \Delta^*$ (e.g., when Δ is an H-simplex), we know, by Theorem 6.3.2, that all $E_{y(i)}(\mathbf{x})$ are sums of (binomial) squares and hence f is a sum of (binomial) squares. ∎

Note that Theorem 6.3.5 generalizes [FK11, Theorem 2.7], where this is shown for so called *diagonal minus tail forms* f with $\alpha(j) = 2d$ for $1 \leq j \leq n$.

We remark that the correct decomposition of the b_j in Theorem 6.3.5 for the case of a general simplex Newton polytope is also given by (6.3.4), since due to

$$e^{\langle \mathrm{Log}\,|v|, y(i)-\alpha(j)\rangle} \;=\; e^{\langle (T^t)^{-1}\,\mathrm{Log}\,|v'|, T^t(\mu(\lambda^{(i)}-e_j))\rangle} \;=\; e^{\langle \mathrm{Log}\,|v'|, \mu(\lambda^{(i)}-e_j)\rangle}$$

these scalars remain invariant under the transformation T from resp. to the standard form.

Example 6.3.8. *The polynomial* $f = 1+\frac{1}{2}x^6+\frac{1}{32}y^4-\frac{1}{2}xy-\frac{1}{2}x^2y$ *is nonnegative and has a zero at* $v = (1,2)$. *By using the constructions in Theorem 6.3.5, we can decompose* f *as sum of two polynomials in* $P^y_{n,2d}$ *with* $y \in \{(1,1),(2,1)\}$ *and vanishing at* v. *More precisely,*

$$f = \left(\frac{7}{12} + \frac{1}{6}x^6 + \frac{1}{64}y^4 - \frac{1}{2}xy\right) + \left(\frac{5}{12} + \frac{1}{3}x^6 + \frac{1}{64}y^4 - \frac{1}{2}x^2y\right).$$

Since Δ *is an* H*-simplex, we have* $f \in \Sigma_{2,6}$. *Using the algorithm in [Rez89] and a suitable variable transformation (see proof of Theorem 6.3.2), we get the following representation for* f *as a sum of binomial squares:*

$$f = \frac{1}{2}(x-x^3)^2 + \frac{1}{2}(1-x^2)^2 + \left(x - \frac{1}{2}y\right)^2 + \frac{1}{2}(1-y^2)^2.$$

6.4 A Sufficient Condition for H-simplices

By Theorem 6.3.2, all nonnegative polynomials in P_Δ^y supported on an H-simplex are sums of squares. Here, we provide a sufficient condition for a lattice simplex Δ to be an H-simplex, meaning, that all lattice points in Δ except the vertices are midpoints of two even distinct lattice points in Δ. In the following, we call a full dimensional lattice polytope $P \subset \mathbb{R}^n$ *normal*, if every lattice point in kP is a sum of exactly k lattice points in P, i.e.,

$$k \in \mathbb{N}, m \in kP \cap \mathbb{Z}^n \Rightarrow m = m_1 + \ldots + m_k, \quad m_1, \ldots, m_k \in P \cap \mathbb{Z}^n.$$

The following theorem uses toric ideals. For an introduction of toric ideals, see, e.g., [Stu97].

Theorem 6.4.1. *Let $\hat{\Delta} := \{\alpha(0), \alpha(1), \ldots, \alpha(n)\} \subset (2\mathbb{N})^n$ and $\Delta = \operatorname{conv}(\hat{\Delta})$ be a lattice simplex. Furthermore, let $B := \frac{1}{2}\Delta \cap \mathbb{N}^n$ and I_B be the corresponding toric ideal of B. If*

1. *I_B is generated in degree two, i.e., $I_B = \langle I_{B,2} \rangle$ and*
2. *the simplex $\frac{1}{2}\Delta$ is normal,*

then Δ is an H-simplex.

Proof. Let $L := (\Delta \cap \mathbb{N}^n) \setminus \hat{\Delta}$. Note that for $u \in L \setminus (2\mathbb{N})^n$ the statement follows from normality of $\frac{1}{2}\Delta$, since we have $u = s + t$ with $s, t \in B$. Therefore, $u = \frac{2s+2t}{2}$. Now, let

$$\left\{\frac{1}{2}\alpha(0), \ldots, \frac{1}{2}\alpha(n)\right\} = \{\alpha(0)', \ldots, \alpha(n)'\}$$

be the vertices of $\frac{1}{2}\hat{\Delta}$ and consider $u \in B \setminus \frac{1}{2}\hat{\Delta}$. By clearing denominators in the unique convex combination of u we get a relation

$$N \cdot u = \lambda_0 \alpha(0)' + \cdots + \lambda_n \alpha(n)', \quad N = \sum_{i=0}^{n} \lambda_i, \quad \lambda_i \geq 0.$$

For the corresponding toric ideal I_B, this yields that $x_u^N - \prod_{i=0}^n x_{\alpha(i)'}^{\lambda_i} \in I_B$. Since I_B is generated in degree two, we have the following representation:

$$x_u^N - \prod_{i=0}^{n} x_{\alpha(i)'}^{\lambda_i} = \sum_{\substack{m,n \in \mathbb{N}^B \\ |m|=|n|=2}} f_{m,n}(x^m - x^n)$$

for some polynomials $f_{m,n}$. Matching monomials, it follows that there exists m such that $x^m = x_u^2$ (note that $f_{m,n}$ contains x_u^{N-2}). Since $|m| = 2$, we have $x_u^2 - x_v x_{v'} \in I_B$ with $v, v' \in B$, yielding the relation $2u = \frac{2v+2v'}{2}$. ∎

Corollary 6.4.2. *Let $\Delta \subset \mathbb{R}^2$ be a lattice simplex as in Theorem 6.4.1 such that $\frac{1}{2}\Delta$ has at least four boundary lattice points. Then Δ is an H-simplex.*

Proof. Since every 2-polytope is normal, we only need to prove that the corresponding toric ideals are generated in degree two. But this is [Koe93, Theorem 2.10]. ∎

Hence, in $\mathbb{R}^2$, almost every simplex Δ with even vertices is an H-simplex, a fact that was claimed in [Rez89] without proof. This yields that the sections $P_{2,2d}^{y}$ and $\Sigma_{2,2d}^{y}$ almost always coincide.

Example 6.4.3. *We demonstrate Theorem 6.4.1 by two interesting examples.*

1. *The Newton polytope of the Motzkin polynomial*

$$m = 1 + x^4y^2 + x^2y^4 - 3x^2y^2 \in P_{2,6} \setminus \Sigma_{2,6}$$

   is an M-simplex $\Delta = \operatorname{conv}\{(0,0),(4,2),(2,4)\}$ such that $\frac{1}{2}\Delta$ has exactly three boundary lattice points. One can check that the corresponding toric ideal I_B is generated by cubics.

2. *Note that the conditions in Theorem 6.4.1 are not equivalent. The simplex $\Delta = \operatorname{conv}\{(0,0),(2,4),(10,6)\}$ is easily checked to be an H-simplex, but $\partial\frac{1}{2}\Delta$ contains exactly three lattice points.*

In higher dimensions things get more involved both in checking the conditions in Theorem 6.4.1 and in determining the maximal $\hat{\Delta}$-mediated set Δ^*. Note that Δ^* can lie strictly between $A(\hat{\Delta})$ and $(\Delta \cap \mathbb{Z}^n)$, which correspond to M-simplices resp. H-simplices. In [Rez89] an algorithm for computing Δ^* is proposed. However, one expects to do better, but to our best knowledge, there is no algorithm known being more efficient. On the other hand, checking normality of polytopes and quadratic generation of toric ideals is an active area of research. It is an open problem to decide whether every *smooth* lattice polytope is normal and the corresponding toric ideal is generated by quadrics (see, e.g., [Gub12, Stu97]). However, for an arbitrary lattice polytope P, the multiples kP are normal for $k \geq \dim P - 1$ and their toric ideals are generated by quadrics for $k \geq \dim P$ ([BGT97]). In light of these results, we can draw another interesting corollary from Theorem 6.4.1.

Corollary 6.4.4. *Let $\Delta \subset \mathbb{R}^n$ be a lattice simplex as in Theorem 6.4.1 such that $\frac{1}{2}\Delta = M\Delta'$ for a lattice simplex $\Delta' \subset \mathbb{R}^n$ and $M \geq n$. Then Δ is an H-simplex.*

Proof. The result follows from the previously quoted results together with Theorem 6.4.1. ∎

Note that Corollaries 6.4.2 and 6.4.4 yield large sections on which nonnegative polynomials and sums of squares coincide.

6.5 Convex Polynomials Supported on Circuits

In this section, we investigate convex polynomials/forms supported on a circuit. Recently, there is much interest in understanding the convex cone of convex polynomials/forms. Since deciding convexity of polynomials is NP-hard in general [AOPT13], but very important in different areas in mathematics, such as, e.g., in convex optimization, it is natural to investigate properties of the cone of convex polynomials/forms.

Definition 6.5.1. *Let $f \in \mathbb{R}[\mathbf{x}]$. Then f is* convex *if the Hessian H_f of f is positive semidefinite for all $\mathbf{x} \in \mathbb{R}^n$, or, equivalently, $\mathbf{v}^t H_f(\mathbf{x})\mathbf{v} \geq 0$ for all $\mathbf{x}, \mathbf{v} \in \mathbb{R}^n$.*

Unlike the property of nonnegativity and sums of squares, convexity of polynomials is not preserved under homogenization. Therefore, we need to distinguish between convex polynomials and convex forms. The relationship between convexity and nonnegativity resp. sums of squares arises when considering homogeneous polynomials, since every convex form is nonnegative. However, the relation between convex forms and sums of squares is not well understood except the fact that these cones are not included in each other. The problem to find a convex form that is not a sum of squares is still open. For an overview and proofs of the previous facts see, e.g., [BPT13, Rez11]. Here, we look for convex polynomials/forms in the class P_Δ^y. We start with the univariate (nonhomogeneous) case.

Proposition 6.5.2. *Let $f = 1 + ax^y + bx^{2d} \in P_\Delta^y$ and $b > 0$. Then f is convex exactly in the following cases.*

1. *$y = 1$,*
2. *$a > 0$ and $y = 2l$ for $y > 1$ and $l \in \mathbb{N}$.*

Proof. Let $f = 1 + ax^y + bx^{2d}$. Note that the degree is necessarily even and $b > 0$. Then f is convex if and only if $D^2(f) \geq 0$ where $D^2(f) = ay(y-1)x^{y-2} + 2db(2d-1)x^{2d-2}$. For $y = 1$ the polynomial $D^2(f)$ is a square and hence f is convex. Now, consider the case $y > 1$. First, suppose that $a < 0$. Then $D^2(f)$ is always indefinite, since the monomial x^{y-2} in $D^2(f)$ corresponds to a vertex of the corresponding Newton polytope of $D^2(f)$ and has a negative coefficient. Otherwise, if $a > 0$ and $y = 2l$ for $l \in \mathbb{N}$, then $D^2(f) \geq 0$ and f is convex. If $y = 2l + 1$ then x^{y-2} has an odd power and hence $D^2(f)$ is indefinite, implying that f is not convex. ∎

The homogeneous version is much more difficult than the affine version. We just prove the following claims instead of giving a full characterization.

Proposition 6.5.3. *Let $f = z^{2d} + ax^y z^{2d-y} + bx^{2d} \in P_\Delta^y$ be a form and $b > 0$. Then the following hold.*

1. *For $y = 2l - 1$, $l \in \mathbb{N}$, or $a < 0$, the form f is not convex.*
2. *For $y = 2l$ and $0 < a \leq \frac{(y-1)(2d-y-1)}{y(2d-y)}$ the form f is convex.*

Proof. We have

$$\frac{\partial^2 f}{\partial z^2} = 2d(2d-1)z^{2d-2} + (2d-y)(2d-y-1)ax^y z^{2d-y-2}.$$

Evaluating this partial derivative at $z = 1$, in order to be nonnegative, it is obvious that y must be even and $a \geq 0$, proving the first claim. For the second claim, we investigate the principal minors of H_f. We have that $\frac{\partial^2 f}{\partial x^2} \geq 0$ if and only if $D^2(f) \geq 0$ where $D^2(f)$ is the dehomogenized polynomial $\frac{\partial^2 f}{\partial x^2}(x, 1)$. This yields $y = 1$ or $a \geq 0$ and $y = 2l$. From $\frac{\partial^2 f}{\partial z^2}$ we get again that y must be even and $a \geq 0$. Finally, one can check that all exponents of the dehomogenized determinant $\det H_f(x, 1)$ are even and have positive coefficients for $0 < a \leq \frac{(y-1)(2d-y-1)}{y(2d-y)}$. Hence, for $y = 2l$ and $0 < a \leq \frac{(y-1)(2d-y-1)}{y(2d-y)}$ the form f is convex. ∎

Note that for $y = 1$ the form $f = z^{2d} + ax^y z^{2d-y} + bx^{2d} \in P_\Delta^y$ is never convex, whereas, by Proposition 6.5.2, the dehomogenized polynomial is always convex. As a sharp contrast, we prove the surprising result that for $n \geq 2$ there are no convex polynomials in the class P_Δ^y, implying that there are no convex forms in P_Δ^y for $n \geq 3$.

Theorem 6.5.4. *Let $n \geq 2$ and $f \in P_\Delta^y$. Then f is not convex.*

Proof. Let

$$f = 1 + \sum_{j=1}^{n} A_j x_1^{\alpha(j)_1} \cdot \ldots \cdot x_n^{\alpha(j)_n} + B x_1^{y_1} \cdot \ldots \cdot x_n^{y_n}$$

with $A_j > 0$ for $1 \leq j \leq n$ and $B \in \mathbb{R}^*$. We will prove that the principal minor $[1, 2] \times [1, 2]$ (deleting all rows and columns except the first and second one) of the Hessian of f is indefinite, implying that the Hessian of f is not positive semidefinite and hence the polynomial f is not convex. We have

$$\frac{\partial^2 f}{\partial x_1^2}\frac{\partial^2 f}{\partial x_2^2} - \left(\frac{\partial^2 f}{\partial x_1 x_2}\right)^2$$

$$\begin{aligned}
= & \sum_{j=1}^{n}\sum_{i=1}^{n} \left(c_j x_1^{\alpha(j)_1 - 2} x_2^{\alpha(j)_2} \cdot \ldots \cdot x_n^{\alpha(j)_n} + d_1 x_1^{y_1 - 2} x_2^{y_2} \cdot \ldots \cdot x_n^{y_n}\right) \\
\cdot & \left(c_i x_1^{\alpha(i)_1} x_2^{\alpha(i)_2 - 2} \cdot \ldots \cdot x_n^{\alpha(n)_i} + d_2 x_1^{y_1} x_2^{y_2 - 2} x_3^{y_3} \cdot \ldots \cdot x_n^{y_n}\right) \\
- & \left(\sum_{k=1}^{n} c_k x_1^{\alpha(k)_1 - 1} x_2^{\alpha(k)_2 - 1} x_3^{\alpha(k)_3} \cdot \ldots \cdot x_n^{\alpha(k)_n} + d_3 x_1^{y_1 - 1} x_2^{y_2 - 1} x_3^{y_3} \cdot \ldots \cdot x_n^{y_n}\right)^2
\end{aligned}$$

where

$$\begin{aligned} c_j &:= A_j\alpha(j)_1\alpha(j)_1 - 1, \\ c_i &:= A_i\alpha(i)_1\alpha(i)_1 - 1, \\ c_k &:= A_k\alpha(k)_1\alpha(k)_2, \\ d_1 &:= By_1(y_1-1), \\ d_2 &:= By_2(y_2-1), \\ d_3 &:= By_1y_2. \end{aligned}$$

We claim that there is a point $\mathbf{x} \in \mathbb{R}^n$ at which this minor is negative. For this, note that all exponents in $\left(\frac{\partial^2 f}{\partial x_1 x_2}\right)^2$ also appear in $\frac{\partial^2 f}{\partial x_1^2}\frac{\partial^2 f}{\partial x_2^2}$. Hence, we can restrict to the latter ones. The $\binom{n+2}{2}$ different exponents are of the following type:

(1) $(2\alpha(j)_1 - 2, 2\alpha(j)_2 - 2, 2\alpha(j)_3, \ldots, 2\alpha(j)_n)$ for $1 \leq j \leq n$

(2) $(\alpha(i)_1 + \alpha(j)_1 - 2, \alpha(i)_2 + \alpha(j)_2 - 2, \alpha(i)_3 + \alpha(j)_3, \ldots, \alpha(i)_n + \alpha(j)_n)$ for $1 \leq i < j \leq n$.

(3) $(\alpha(j)_1 + y_1 - 2, \alpha(j)_2 + y_2 - 2, \alpha(j)_3 + y_3, \ldots, \alpha(j)_n + y_n)$ for $1 \leq j \leq n$

(4) $(2y_1 - 2, 2y_2 - 2, 2y_3, \ldots, 2y_n)$

We claim that the point $(2y_1-2, 2y_2-2, 2y_3, \ldots, 2y_n)$ is always a vertex in the convex hull of the points (1)-(4), i.e., in the Newton polytope of the investigated minor. The points in (2) are obviously convex combinations from appropriate points in (1) and the points in (3) are convex combinations from points in (1) and (4). Hence, it remains to show that (4) is not a convex combination of the points in (1). Therefore, denote the points in (1) by P_j and the point in (4) by Q. Let

$$Q = \sum_{j=1}^{n} \mu_j P_j \quad \text{with} \quad \sum_{j=1}^{n} \mu_j = 1 \quad \text{and} \quad \mu_j \geq 0 \quad \text{for all} \quad 1 \leq j \leq n.$$

But since $\sum_{j=1}^{n} \mu_j(-2) = -2$, this equation is equivalent to

$$y = \sum_{j=1}^{n} \mu_j \alpha(j) \quad \text{with} \quad \sum_{j=1}^{n} \mu_j = 1 \quad \text{and} \quad \mu_j = \frac{1}{2} \quad \text{for all} \quad 1 \leq j \leq n.$$

But this means that y lies on the boundary of Δ, the Newton polytope of f. This is a contradiction, since $f \in P_\Delta^y$, in particular, $y \in \text{int}(\Delta)$. Hence, (4) is a vertex of the Newton polytope of the investigated minor. Extracting the coefficient of its corresponding monomial in the minor, we get that this coefficient equals $-B^2y_1y_2(y_1+y_2-1) < 0$. Therefore, the Newton polytope of the minor of the Hessian of f has a vertex coming with a negative coefficient and hence it is indefinite, proving the claim. ∎

Note that this already implies that there is also no convex form in P^y_Δ whenever $n \geq 3$, since non-convexity is preserved under homogenization. Since it is mostly unclear which structures prevent polynomials from being convex, Theorem 6.5.4 is an indication that sparsity is among these structures.

6.6 Sums of Nonnegative Circuit Polynomials

Motivated by results in previous sections, we introduce a new family of non-negativity certificates.

Definition 6.6.1. *We define the set of* sums of nonnegative circuits polynomials *(SONC) as*

$$C_{n,2d} := \left\{ f \in \mathbb{R}[\mathbf{x}]_{2d} \ : \ f = \sum_{i=1}^{k} \mu_i g_i, \mu_i \geq 0, g_i \in P^y_{\Delta_i} \cap P_{n,2d} \right\}$$

for some simplices $\Delta_i \subset \mathbb{R}^n$.

Remember that membership in $P^y_{n,2d}$ can be easily checked and is completely characterized by the circuit number Θ_f (Theorem 6.2.6). Obviously, for $\alpha, \beta \in \mathbb{R}_{>0}$ and $f, g \in C_{n,2d}$, it holds that $\alpha f + \beta g \in C_{n,2d}$ and hence $C_{n,2d}$ is a convex cone. Then we have the following relations.

Proposition 6.6.2. *The following relationships hold between the corresponding cones.*

1. $C_{n,2d} \subset P_{n,2d}$,
2. $C_{n,2d} \nsubseteq \Sigma_{n,2d}$ *and* $\Sigma_{n,2d} \nsubseteq C_{n,2d}$,
3. $C_{n,2d} \cap K_{n,2d} = \{0\}$ *for* $n \geq 2$, *where* $K_{n,2d}$ *is the cone of convex polynomials.*

Proof. Since $\mu_i g_i \in P_{n,2d}$, the first inclusion is obvious. Considering sums of squares, the Motzkin polynomial is a sum of nonnegative circuit polynomials but not a sum of squares, proving the first non-inclusion. For the second one, we use the following argument. Let $f \in \Sigma_{2,6}$ be such that f has nine zeros. Concretely, let $f = f_1^2 + f_2^2$, where the two cubics f_1, f_2 intersect in nine distinct real points. If $f = \sum_{i=1}^k \mu_i g_i, \mu_i \geq 0, g_i \in P^y_{\Delta_i} \cap P_{n,2d}$ for some simplices Δ_i, then all $g_i \in P^y_{\Delta_i} \cap P_{n,2d}$ must vanish at the nine intersection points, in contradiction to Corollary 6.2.7, yielding at most $2^2 = 4$ zeros for g_i. The property $C_{n,2d} \nsubseteq K_{n,2d}$ for $n \geq 2$ immediately follows from Theorem 6.5.4. ∎

Hence, the convex cone $C_{n,2d}$ serves as a nonnegativity certificate, which, by Proposition 6.6.2, is very different than sums of squares certificates.

Example 6.6.3. *Let* $f = 3 + 4x^6 + 4y^6 + x^8 + x^4y^4 - 3xy + 5x^3y + 2x^4y^2$. *The Newton polytope* $\mathrm{New}(f) = \mathrm{conv}\{(0,0)^T, (0,4)^T, (4,4)^T, (8,0)^T)\}$ *is not a simplex and* $f \in C_{2,8}$. *An explicit representation is given by*

$$f = (1 + x^6 + 2y^4 - 3xy) + (1 + 3x^6 + 2y^4 + 5x^3y) + (1 + x^8 + x^4y^4 + 2x^4y^2).$$

Of course, it is a priori completely unclear, which type of nonnegative polynomials have a SONC decomposition resp. how big the gap between $C_{n,2d}$ and $P_{n,2d}$ is. Furthermore, it is not obvious how to compute such a decomposition, if it exists. But, as a promising and fruitful first step, we can deduce the following corollary from Theorem 6.3.5.

Corollary 6.6.4. *Let* $f = b_0 + \sum_{j=1}^n b_j \mathbf{x}^{\alpha(j)} + \sum_{i=1}^k a_i \mathbf{x}^{y(i)}$ *be nonnegative with* $b_j \in \mathbb{R}_{>0}$ *and* $a_i \in \mathbb{R}^*$ *such that* $\mathrm{New}(f) = \Delta = \mathrm{conv}\{0, \alpha(1), \ldots, \alpha(n)\}$ *is a simplex and all* $y(i) \in (\mathrm{int}(\Delta) \cap \mathbb{N}^n)$. *If there exists a vector* $v \in (\mathbb{R}^*)^n$ *such that* $a_i v^{y(i)} < 0$ *for all* $1 \leq i \leq k$, *then* f *is SONC.*

Proof. Every monomial square is a strictly positive term as well as a 0-simplex circuit polynomial. Thus, we can ignore these terms. If a particular vector $v \in (\mathbb{R}^*)^n$ with the desired properties exists, then Theorem 6.3.5 immediately yields a SONC decomposition after a variable transformation $x_j \mapsto -x_j$ for all j with $v_j < 0$. ■

6.7 Extension to Arbitrary Polytopes

In Section 6.3, for $f \in P_\Delta^y$, we proved that $f \in \Sigma_{n,2d}^y$ if and only if $y \in \Delta^*$. One might wonder whether this equivalence does also hold for arbitrary polytopes. More precisely, let $Q \subset \mathbb{R}^n$ be an arbitrary lattice polytope with even vertices and denote by AP_Q^y the set of all polynomials of the form $\sum_{\alpha \in \mathrm{vert}(Q)} b_\alpha \mathbf{x}^\alpha + c\mathbf{x}^y$ that are supported on the vertices $\mathrm{vert}(Q)$ of Q and an additional interior lattice point $y \in \mathrm{int}(Q)$. As a generalization of our previous notation, we call $f \in AP_Q^y$ an *agiform* if $\sum_{\alpha \in \mathrm{vert}(Q)} b_\alpha \alpha = y$ and $\sum_{\alpha \in \mathrm{vert}(Q)} b_\alpha = 1$, all $b_\alpha > 0$ and $c = -1$.

In [Rez89] it is asked whether the lattice point criterion $y \in Q^*$ is again an equivalent condition for a polynomial in AP_Q^y to be a sum of squares. Here, we provide a solution to this question. Let P_Q^y resp. Σ_Q^y denote the set of nonnegative resp. sums of squares polynomials in AP_Q^y. As for a simplex Δ, for an arbitrary lattice polytope Q we use the same definition of an M-polytope resp. an H-polytope as for an M-simplex resp. an H-simplex (see Section 6.1).

The implication $f \in \Sigma_Q^y \Rightarrow y \in Q^*$ does always hold. For agiforms, this is proved already in [Rez89]. The proof in the case of arbitrary coefficients follows exactly the same line as the proof of Theorem 6.3.2, since it mainly uses negativity of the interior monomial, which we can assume by suitable variable transformations as before. However, the reverse direction fails to be true in general as we now prove.

Proposition 6.7.1. *There exists $f \in P_Q^y \setminus \Sigma_Q^y$ and $y \in Q^*$.*

Proof. We provide an explicit example. Let

$$Q = \operatorname{conv}\{v_0, v_1, v_2, v_3\} = \operatorname{conv}\{(0,0), (4,0), (4,2), (2,4)\},\ y = (2,2).$$

It is easy to check that Q is an H-polytope (indeed, it can actually be proved that Theorem 6.4.1 is true for arbitrary polytopes). Since Q is not a simplex, there are many convex combinations of y:

$$y = \lambda_0 v_1 + \lambda_1 v_1 + \lambda_2 v_2 + \lambda_3 v_3,\ \sum_{i=0}^{3} \lambda_i = 1,\ \ \lambda_i \geq 0.$$

The set of convex combinations of y is given by

$$\left\{(\lambda_0, \lambda_1, \lambda_2, \lambda_3) = \left(\frac{1}{2} - \frac{1}{2}\lambda_3, -\frac{1}{2} + \frac{3}{2}\lambda_3, 1 - 2\lambda_3, \lambda_3\right) : \frac{1}{3} \leq \lambda_3 \leq \frac{1}{2}\right\}.$$

The corresponding agiform $f(Q, \lambda, y)$ is then given by

$$f(Q, \lambda, y) = \left(\frac{1}{2} - \frac{1}{2}\lambda_3\right) + \left(-\frac{1}{2} + \frac{3}{2}\lambda_3\right) x^4 + (1 - 2\lambda_3)x^4y^2 + \lambda_3 x^2y^4 - x^2y^2.$$

For $\lambda_3 = \frac{2}{5}$, the nonnegative polynomial

$$f = \frac{3}{10} + \frac{1}{10}x^4 + \frac{1}{5}x^4y^2 + \frac{2}{5}x^2y^4 - x^2y^2$$

can easily be checked to be not a sum of squares (in spite of the fact that $y \in Q^*$.) ■

Actually, one can prove that the polynomial $f(Q, \lambda, y)$ in the above proof is a sum of squares if and only if $\lambda_3 = \frac{1}{2}$. In [Rez89] the author suspects that the condition $y \in Q^*$ is not sufficient by looking at similar examples. However, in all of these examples the constructed polynomials that are nonnegative but not a sum of squares are not supported on the vertices of Q and an additional interior lattice point $y \in \operatorname{int}(Q)$. We conclude that in the non-simplex case the problem of deciding the sums of squares property depends on the coefficients of the polynomials, a sharp contrast to the simplex case. However, motivated by a question in [Rez89] for agiforms we are interested in the following sets: Let $C(y)$ denote the set of convex combinations of the interior lattice point $y \in \operatorname{int}(Q)$, i.e.,

$$C(y) = \left\{\lambda = (\lambda_0, \ldots, \lambda_s) : y = \sum_{i=0}^{s} \lambda_i v_i,\ \sum_{i=0}^{s} \lambda_i = 1,\ \ \lambda_i \geq 0\right\}$$

where v_i are the s vertices of Q. Note that $C(y)$ is a polytope. Fixing f and y, we define

$$\mathrm{SOS}(f, y) = \{\lambda \in C(y) : f(Q, \lambda, y) \ \text{ is a sum of squares}\}$$

where $Q = \mathrm{New}(f)$. We have already seen in the proof of Proposition 6.7.1 that the structure of $\mathrm{SOS}(f, y)$ is unclear and highly depends on the convex combinations of y. It is formulated as an open question in [Rez89], whether one can say something about $\mathrm{SOS}(f, y)$ for fixed f and y. For this, let

$$Q = Q_1^{(i)} \cup \cdots \cup Q_{r(i)}^{(i)}$$

be a triangulation of Q for $1 \leq i \leq t$, where t is the number of triangulations of Q without using new vertices. We are interested in those simplices $Q_j^{(i)}$ that contain the point $y \in \mathrm{int}(Q)$ and their maximal mediated sets $(Q_j^{(i)})^*$. Recall that for every lattice simplex Δ with vertex set $\hat{\Delta}$ we denote Δ^* as the maximal $\hat{\Delta}$-mediated set (see Section 6.1).

Theorem 6.7.2. *Let $Q \subset \mathbb{R}^n$ be a lattice n-polytope, $y \in (\mathrm{int}(Q) \cap \mathbb{N}^n)$, and $f \in AP_Q^y$ be an agiform. Then* $\mathrm{SOS}(f, y) = C(y)$*, i.e.,* every *agiform is a sum of squares, if and only if $y \in Q_j^{(i)}$ implies $y \in (Q_j^{(i)})^*$ for every $1 \leq i \leq t$ and $1 \leq j \leq r(i)$.*

Proof. Assume $y \in Q_j^{(i)} \Rightarrow y \in (Q_j^{(i)})^*$ for every $1 \leq i \leq t$ and $1 \leq j \leq r(i)$. Let $\lambda \in C(y)$ with $f(Q, \lambda, y)$ being the corresponding agiform. By [Rez89, Theorem 7.1], every agiform can be written as a convex combination of simplicial agiforms. In fact, following the proof in [Rez89, Theorem 7.1], it can be verified that the vertices of the corresponding simplicial agiforms form a subset of the vertices of Q, since the set $C(y)$ of convex combinations of y is a polytope with vertices being a subset of $\mathrm{vert}(Q)$. Hence, these agiforms come from triangulating the polytope Q into simplices without using new vertices. Since $y \in (Q_y^{(i)})^*$, by Theorem 6.1.4, the corresponding simplicial agiforms are always sums of squares and since $f(Q, \lambda, y)$ is a sum of them, the claim follows.

For the reverse direction, we prove that $y \in Q_{y,k}^{(i)}$ and $y \notin (Q_{y,k}^{(i)})^*$ for some i, k implies that $\mathrm{SOS}(f, y) \neq C(y)$. Therefore, let $Q^{(i)}$ be a triangulation of Q and $k \in \{1, \ldots, r(i)\}$ be such that $y \in Q_{y,k}^{(i)}$ and $y \notin (Q_{y,k}^{(i)})^*$. Suppose $\mathrm{vert}(Q) = \{v_1, \ldots, v_m\}$. Then $C(y)$ is a polytope of dimension $m-(n+1) =: d$. Let

$$f(Q, \lambda, y) = \sum_{i=1}^{m} \lambda_i(\mu_1, \ldots, \mu_d)\mathbf{x}^{v_i} - \mathbf{x}^y$$

be the corresponding agiform. Note that the coefficients λ_i depend on d parameters $\mu_1, \ldots, \mu_d$, since $\dim C(y) = d$. By assumption, there exist $a_1, \ldots, a_d \in \mathbb{R}_{>0}$ such that $f(Q, \lambda, y)_{|(\mu_1,\ldots,\mu_d)=(a_1,\ldots,a_d)} = g$ is a simplicial agiform with respect to the simplex $Q_{y,k}^{(i)}$. Since $y \notin (Q_{y,k}^{(i)})^*$, the agiform g is not a sum of squares. By continuity, we can construct a sequence $(\mu_1, \ldots, \mu_d)$ converging against $(a_1, \ldots, a_d)$ with the properties that $f(Q, \lambda, y)_{|(\mu_1,\ldots,\mu_d)=(a_1+\varepsilon,\ldots,a_d+\varepsilon)}$ is an agiform for some $\varepsilon > 0$ with its support equal to $\{v_1, \ldots, v_m, y\}$ and not being a sum of squares, since, otherwise, if every sequence member is a sum of squares, this will also hold for the limit agiform g corresponding to $(a_1, \ldots, a_d)$ by closedness of the cone of sums of squares. Hence, $\mathrm{SOS}(f, y) \neq C(y)$. ∎

Example 6.7.3. *Let again*

$$Q = \mathrm{conv}\{v_0, v_1, v_2, v_3\} = \mathrm{conv}\{(0,0),(4,0),(4,2),(2,4)\}$$

be as in the proof of Proposition 6.7.1. There are six interior lattice points in Q *given by*

$$\mathrm{int}(Q) \cap \mathbb{N}^n = \{(1,1),(2,1),(3,1),(2,2),(2,3),(3,2)\}.$$

Since Q *has four vertices,* $C(y)$ *for* $y \in (\mathrm{int}(Q) \cap \mathbb{N}^n)$ *has a free parameter* λ_3 *(see proof of Proposition 6.7.1). In the following table, for all* $y \in (\mathrm{int}(Q) \cap \mathbb{N}^n)$*, we provide the range of the free parameter* λ_3 *yielding valid convex combinations for* y *as well as the set* $\mathrm{SOS}(f,y)$*.*

y	λ_3	$\mathrm{SOS}(f,y)$
$(1,1)$	$\frac{1}{6} \leq \lambda_3 \leq \frac{1}{4}$	$\lambda_3 \in [0.191; \frac{1}{4}]$
$(2,1)$	$0 \leq \lambda_3 \leq \frac{1}{4}$	$\lambda_3 \in [0; \frac{1}{4}]$
$(3,1)$	$0 \leq \lambda_3 \leq \frac{1}{4}$	$\lambda_3 \in [0; \frac{1}{4}]$
$(2,2)$	$\frac{1}{3} \leq \lambda_3 \leq \frac{1}{2}$	$\lambda_3 \in \{\frac{1}{2}\}$
$(2,3)$	$\frac{2}{3} \leq \lambda_3 \leq \frac{3}{4}$	$\lambda_3 \in [0.683; \frac{3}{4}]$
$(3,2)$	$\frac{1}{6} \leq \lambda_3 \leq \frac{1}{2}$	$\lambda_3 \in [\frac{1}{4}; \frac{1}{2}]$

The sets $\mathrm{SOS}(f,y)$ *are computed with* SOSTOOLS *([PPSP05]). Note that* Q *has two different triangulations (see Figure 6.7). The lattice points* $(2,1)$ *and* $(3,1)$ *are the only lattice points that satisfy* $y \in Q_j^{(i)} \Rightarrow y \in (Q_j^{(i)})^*$ *for all* $i \in \{1,2\}$ *and* $j \in \{1,\ldots,r(i)\}$*. Hence, exactly for* $y \in \{(2,1),(3,1)\}$*, every agiform is a sum of squares.*

6.8 Outlook

We want to give an outlook for possible future directions of research. Starting with the section $\Sigma_{n,2d}^y$, we renew some open questions in [Rez89]. Is there an algorithm to compute Δ^* that is more efficient as the one in [Rez89]? What can be said about the asymptotics of Δ^*, in particular, what is the "probability" that a simplex is an H-simplex? This is settled in $\mathbb{R}^2$ in Corollary 6.4.2, but seems widely open for $n > 2$. However, every sufficiently large simplex is an H-simplex (see Corollary 6.4.4). Tackling this problem from the viewpoint of toric geometry (see Theorem 6.4.1), it would be a breakthrough to characterize simplices that are normal and their corresponding toric ideals are generated by quadrics. In Section 6.6 we introduced the convex cone $C_{n,2d}$ of sums of nonnegative circuit polynomials, which is different from the

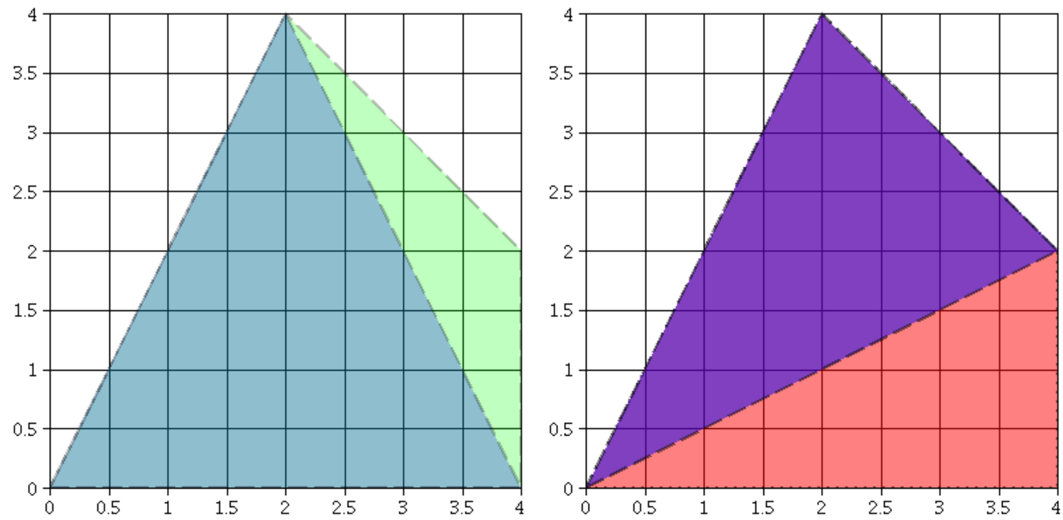

Figure 6.2: The two different triangulations of Q.

convex cone of sums of squares. From a practical point of view, the major problem is to determine the complexity of checking membership in $C_{n,2d}$. In particular, when is every nonnegative polynomial a sum of nonnegative circuit polynomials? In Corollary 6.6.4, we already proved this for a rich class of nonnegative polynomials, but we suspect that the relationship between $P_{n,2d}$ and $C_{n,2d}$ should be more delicate. Another very interesting problem is to look for more classes of polynomials, for which nonnegativity can be derived by the norm relaxation method introduced in subsection 6.2.1.

Chapter 7

Lower Bounds for Polynomials with Simplex Newton Polytopes Based on Geometric Programming

Finding lower bounds for real polynomials is a central problem in polynomial optimization. Several well known approaches to this problem work well in small dimension or with additional structure enforced on the polynomials. The best known lower bounds are provided by *Lasserre relaxations* using semidefinite programming (see Sections 2.3 and 2.4). In spite of the fact that the optimal value of a semidefinite program can be computed in time polynomial up to an additive error, the size of these programs grows rapidly with the number of variables or degree of the polynomials. Therefore, recently, there is much interest in finding lower bounds for polynomials using the alternative approach of *geometric programming* (see (7.2.1) for a formal definition). In recent works [GM12, GM13] several important observations are made for polynomial optimization via geometric programming. The two key observations are the following ones:

1. Lower bounds based on geometric programming are not as good as bounds obtained by semidefinite programming.
2. Even higher dimensional examples can be solved quite fast with geometric programming whereas semidefinite programs do not yield an output at all due to the too high dimension resp. degree of polynomials.

For $f \in \mathbb{R}[\mathbf{x}]_{2d}$ of degree $2d$ we consider again the polynomial optimization problem

$$f^* \ := \ \inf\{f(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^n\} \ = \ \sup\{\lambda \in \mathbb{R} : f - \lambda \geq 0\}$$

with the lower bound f^*_{sos} given by the semidefinite relaxation of f^* as

$$f^*_{sos} \ = \ \sup\left\{\lambda \in \mathbb{R} \ : \ f - \lambda = \sum_{i=1}^{k} q_i^2 \ \text{ for some } \ q_i \in \mathbb{R}[x]\right\}.$$

Based on our results in Chapter 6, in this chapter we extend results in [GM12] in order to provide lower bounds for polynomials using geometric programs, which can be solved in time polynomial in the input using interior point methods ([NN94]). We denote these lower bounds by f_{gp}^*.

In fact, this extension relies on the key observation that nonnegativity can not only be certified via sums of squares, but also via *sums of nonnegative circuit polynomials* (abbrev. SONC), which we introduced in Chapter 6, Section 6.6. In [FK11] Fidalgo and Kovacec provide nonnegativity resp. sums of squares certificates for a class of polynomials, which have the scaled standard simplex $\mathrm{conv}\{0, 2d \cdot e_1, \ldots, 2d \cdot e_n\}$ as Newton polytopes. In [GM12] Ghasemi and Marshall show that these certificates can be translated into geometric programs in order to find lower bounds for polynomials. But since the certificates in [FK11] are special instances of the ones in Chapter 6, it is self-evident to ask, whether the translation into geometric programs can also be generalized. The purpose of this chapter is to show that this is indeed the case.

As main theoretical results we contribute in this chapter some easily checkable criteria on the coefficients of a polynomial, which imply that the polynomial is a sum of nonnegative circuit polynomials (Theorems 7.1.1 and 7.1.2). In many cases this implies that the polynomial is also a sum of binomial squares. The key observation is that, as in [GM12], these criteria can be translated into geometric optimization problems (Corollary 7.2.2), which are naturally connected to SONC certificates (Theorem 7.1.3). As a surprising fact we show in Corollary 7.1.4 that for very rich classes of polynomials with simplex Newton polytope, the optimal value f_{gp}^* satisfies $f_{gp}^* \geq f_{sos}^*$, in contrast to the general observation by Ghasemi and Marshall in [GM12, GM13], which we outlined in the beginning. Additionally, the computation of f_{gp}^* is much faster than in the corresponding semidefinite optimization problem. This is a win-win situation and establishes a very interesting connection between sums of nonnegative circuits and geometric programming.

Let $f \in \mathbb{R}[\mathbf{x}]_{2d}$ be of the form $f = \sum_{\alpha \in \mathbb{N}_{2d}^n} f_\alpha \mathbf{x}^\alpha$. Throughout this chapter we assume that $\mathrm{New}(f) = \Delta$ is a simplex with even vertex set $\{0, \alpha(1), \ldots, \alpha(n)\} \subset \mathbb{N}_{2d}^n$ and corresponding coefficients $f_0, f_{\alpha(j)} > 0$ for $1 \leq j \leq n$. Following existing literature [FK11, GM12, Las07], we define

$$\Omega(f) \quad = \quad \{\alpha \in \mathbb{N}_{2d}^n : f_\alpha \neq 0\} \setminus \{0, \alpha(1), \ldots, \alpha(n)\}.$$

Hence, we have a decomposition

$$f \quad = \quad f_0 + \sum_{\alpha \in \Omega(f)} f_\alpha \mathbf{x}^\alpha + \sum_{j=1}^{n} f_{\alpha(j)} \mathbf{x}^{\alpha(j)}$$

where f_0 is the constant term in f. Let

$$\begin{aligned} \Delta(f) \quad &= \quad \{\alpha \in \Omega(f) : f_\alpha \mathbf{x}^\alpha \text{ is not a square}\} \\ &= \quad \{\alpha \in \Omega(f) : f_\alpha < 0 \text{ or } \alpha_i \text{ is odd for some } 1 \leq i \leq n\}. \end{aligned}$$

The degree of our extension of the work [GM12] is strongly based on our results in Chapter 6. It relies on decompositions of nonnegative polynomials as sums of nonnegative circuit polynomials. When considering the scaled standard simplex $2d\Delta_{n-1}$ as the Newton polytope of a polynomial, our results coincide with the results in [GM12]. Therefore, considering arbitrary simplices yields a significant extension of [GM12] and contains the scaled standard simplex $2d\Delta_{n-1}$ as one special instance.

7.1 A Sufficient Condition on the Coefficients of a Polynomial for the SONC Property

In this section, we provide sufficient criteria on the coefficients of a polynomial that imply the SONC property of a polynomial (see Definition 6.6.1), thereby generalizing many existing results in the literature along the way. For the remainder of this chapter we make the following assumption.

Asssumption: Let $f \in \mathbb{R}[\mathbf{x}]_{2d}$ be a polynomial such that its Newton polytope $\mathrm{New}(f) = \Delta$ with vertices $\{0, \alpha(1), \ldots, \alpha(n)\} \subset (2\mathbb{N})^n$ is a simplex.

Note that every $\alpha \in \Omega(f)$ can be written as a unique convex combination of the vertex set $\{0, \alpha(1), \ldots, \alpha(n)\}$:

$$\alpha \quad = \quad \sum_{i=0}^{n} \lambda_i^{(\alpha)} \alpha(i) \quad \text{with} \quad \sum_{i=0}^{n} \lambda_i^{(\alpha)} \quad = \quad 1 \quad \text{and} \quad \lambda_i^{(\alpha)} \quad \geq \quad 0 \qquad (7.1.1)$$

where $\lambda_0^{(\alpha)}, \ldots, \lambda_n^{(\alpha)} \in \mathbb{R}_{\geq 0}$ denote the scalars in the convex combination of $\alpha \in \Omega(f)$ in terms of the vertices of $\mathrm{New}(f)$. Thus, we can write the polynomial f as

$$f \quad = \quad \sum_{\alpha \in \Omega(f)} \lambda_0^{(\alpha)} + \sum_{j=1}^{n} f_{\alpha(j)} \mathbf{x}^{\alpha(j)} + \sum_{\alpha \in \Omega(f)} f_\alpha \mathbf{x}^\alpha \qquad (7.1.2)$$

with $f_{\alpha(j)} > 0$ for $1 \leq j \leq n$ and $f_\alpha \in \mathbb{R}$. Scaling the polynomial by a new constant positive term $f_0 = \sum_{\alpha \in \Omega(f)} \lambda_0^{(\alpha)}$ is obviously irrelevant for nonnegativity of f and for polynomial optimization. The chosen scaling will turn out to be very suitable for our statements. In order to further simplify connections to the results in [FK11, GM12] we consider the homogenized polynomial

$$F \quad = \quad \sum_{j=0}^{n} f_{\alpha(j)} \mathbf{x}^{\alpha(j)} x_0^{2d-|\alpha(j)|} + \sum_{\alpha \in \Omega(f)} f_\alpha \mathbf{x}^\alpha x_0^{2d-|\alpha|}$$

with $\alpha(0) = 0 \in \mathbb{N}^n$, $f_{\alpha(0)} = \sum_{\alpha \in \Omega(f)} \lambda_0^{(\alpha)}$ and $|\alpha| = \sum_{j=1}^{n} |\alpha_j| \in [0, 2d] \cap \mathbb{N}$ for all $\alpha \in \mathrm{New}(f) \cap \mathbb{N}^n$.

Theorem 7.1.1. *Let F be a homogeneous polynomial as above and suppose there exist $a_{\alpha,j} \geq 0$ for all $\alpha \in \Delta(F)$ and $0 \leq j \leq n$ such that*

(1) $|f_\alpha| = \prod_{j=0}^n \left(\frac{a_{\alpha,j}}{\lambda_j^{(\alpha)}}\right)^{\lambda_j^{(\alpha)}}$ *for all $\alpha \in \Delta(F)$.*

(2) $f_{\alpha(j)} \geq \sum_{\alpha\in\Delta(F)} a_{\alpha,j}$ *for all $0 \leq j \leq n$.*

Then $F - \sum_{\alpha\in\Omega(f)\setminus\Delta(f)} f_\alpha \cdot \mathbf{x}^\alpha \cdot x_0^{2d-|\alpha|}$ and hence also F is a SONC. If, additionally, $\Delta(F) \subseteq \Delta^*$, then F is a sum of binomial squares.

Proof. Using Theorems 6.2.6 and (1) we conclude that

$$\sum_{j=0}^{n} a_{\alpha,j}\mathbf{x}^{\alpha(j)}x_0^{2d-|\alpha(j)|} + f_\alpha \mathbf{x}^\alpha x_0^{2d-|\alpha|}$$

is a SONC for every $\alpha \in \Delta(F)$. By summing over all $\alpha \in \Delta(F)$ it holds that

$$\sum_{j=0}^{n}\left(\sum_{\alpha\in\Delta(F)} a_{\alpha,j}\right)\mathbf{x}^{\alpha(j)}x_0^{2d-|\alpha(j)|} + \sum_{\alpha\in\Delta(F)} f_\alpha \mathbf{x}^\alpha x_0^{2d-|\alpha|} \tag{7.1.3}$$

is a SONC. Then condition (2) yields that

$$\sum_{j=0}^{n} f_{\alpha(j)}\mathbf{x}^{\alpha(j)}x_0^{2d-|\alpha(j)|} + \sum_{\alpha\in\Delta(F)} f_\alpha \mathbf{x}^\alpha x_0^{2d-|\alpha|}$$

is a SONC. Since for every $\alpha \in \Omega(F) \setminus \Delta(F)$ the term $f_\alpha \mathbf{x}^\alpha$ is a monomial square, F is a SONC. The sum of binomial square property follows from Theorem 6.3.2. ■

Setting $\alpha(j) = 2d$ for $0 \leq j \leq n$ the sum of binomial squares statement recovers [GM12, Theorem 2.3]. Additionally, e.g., by [GM12, Remark 2.4], we can assume that $a_{\alpha,j} = 0$ if and only if $\lambda_j^{(\alpha)} = 0$. Theorem 7.1.1 yields a new sufficient criterion on the coefficients of a polynomial to imply the SONC property as well as the sum of (binomial) squares property and significantly extends previous sums of squares criteria given in [FK11, GM12, Las07]. This extension relies on the fact that the cited results assume the Newton polytope of the polynomial being the scaled standard simplex with degree $2d$, whereas Theorem 7.1.1 is, in particular, valid for *all* H-simplices containing the scaled standard simplex as a special instance.

We now describe the application of Theorem 7.1.1 in global optimization. To provide new lower bounds for polynomials, we prove our second main result.

Theorem 7.1.2. *Let $f \in \mathbb{R}[\mathbf{x}]_{2d}$ be of the Form* (7.1.2) *with constant term $f_0 = \sum_{\alpha \in \Omega(f)} \lambda_0^{(\alpha)} > 0$ and let $r \in \mathbb{R}$. Suppose that for every $\alpha \in \Delta(f)$ there exist $a_{\alpha,1}, \ldots, a_{\alpha,n} \geq 0$ with $a_{\alpha,j} = 0$ if and only if $\lambda_j^{(\alpha)} = 0$ (with $\lambda_j^{(\alpha)}$ in the sense of (7.1.1)) such that the following conditions hold.*

(1) $|f_\alpha| = \prod_{j=1}^n \left(\frac{a_{\alpha,j}}{\lambda_j^{(\alpha)}}\right)^{\lambda_j^{(\alpha)}}$ *for all $\alpha \in \Delta(f)$ with $|\alpha| = 2d$,*

(2) $f_{\alpha(j)} \geq \sum_{\alpha \in \Delta(f)} a_{\alpha,j}$ *for all $1 \leq j \leq n$,*

(3) $f_0 - r \geq \sum_{\alpha \in \Delta^{<2d}(f)} \lambda_0^{(\alpha)} \cdot |f_\alpha|^{\frac{1}{\lambda_0^{(\alpha)}}} \cdot \prod_{j=1}^n \left(\frac{\lambda_j^{(\alpha)}}{a_{\alpha,j}}\right)^{\frac{\lambda_j^{(\alpha)}}{\lambda_0^{(\alpha)}}}$*,*

where $\Delta^{<2d}(f) = \{\alpha \in \Delta(f) : |\alpha| < 2d\}$. Then $f - r - \sum_{\alpha \in \Omega(f) \setminus \Delta(f)} f_\alpha \mathbf{x}^\alpha$ and hence also $f - r$ is a SONC. If, additionally, $\Omega(f) \subseteq \Delta^*$, then $f - r$ is a sum of binomial squares.

Proof. We apply Theorem 7.1.1 to the homogenization of the polynomial $f - r$, which is given by

$$\overline{f - r} \quad = \quad (f_0 - r)x_0^{2d} + \sum_{j=1}^n f_{\alpha(j)} \mathbf{x}^{\alpha(j)} x_0^{2d - |\alpha(j)|} + \sum_{\alpha \in \Omega(f)} f_\alpha \mathbf{x}^\alpha x_0^{2d - |\alpha|}.$$

Then $\overline{f - r}$ is a SONC resp. a sum of binomial squares if only only if $f - r$ is a SONC resp. a sum of binomial squares (see [GM12]). Our sufficient conditions in Theorem 7.1.1 now read as follows.

(1') $|f_\alpha| = \prod_{j=0}^n \left(\frac{a_{\alpha,j}}{\lambda_j^{(\alpha)}}\right)^{\lambda_j^{(\alpha)}} = \left(\frac{a_{\alpha,0}}{\lambda_0^{(\alpha)}}\right)^{\lambda_0^{(\alpha)}} \prod_{j=1}^n \left(\frac{a_{\alpha,j}}{\lambda_j^{(\alpha)}}\right)^{\lambda_j^{(\alpha)}}$ for $\alpha \in \Delta(f)$,

(2') $f_{\alpha(j)} \geq \sum_{\alpha \in \Delta(f)} a_{\alpha,j}$ for all $1 \leq j \leq n$ and $f_0 - r \geq \sum_{\alpha \in \Delta(f)} a_{\alpha,0}$.

Solving (1') for $a_{\alpha,0}$ yields

$$a_{\alpha,0} \quad = \quad \lambda_0^{(\alpha)} \cdot |f_\alpha|^{\frac{1}{\lambda_0^{(\alpha)}}} \cdot \prod_{j=1}^n \left(\frac{\lambda_j^{(\alpha)}}{a_{\alpha,j}}\right)^{\frac{\lambda_j^{(\alpha)}}{\lambda_0^{(\alpha)}}}$$

if $|\alpha| < 2d$. Set $a_{\alpha,0} = 0$ for $|\alpha| = 2d$. Conversely, defining $a_{\alpha,0}$ in this way, for every $\alpha \in \Delta$, one can verify that conditions (1) – (3) imply conditions (1'),(2') as follows: (2') follows immediately from (2) and (3) and definition of $a_{\alpha,0}$. Condition (1') follows from (1) again by homogenization and using definition of $a_{\alpha,0}$. ■

Again, setting $\alpha(j) = 2d$ for $1 \leq j \leq n$, the sum of binomial squares statement recovers [GM12, Theorem 3.1]. Now, we can define

$$f_{gp}^* = \sup \left\{ r \in \mathbb{R} \ : \begin{array}{l} \forall \alpha \in \Delta(f) \ \forall j \in \{1, \ldots, n\} \ \exists a_{\alpha,j} \geq 0 \text{ with} \\ a_{\alpha,j} = 0 \Leftrightarrow \lambda_j^{(\alpha)} = 0 \\ \text{s.t. conditions (1)-(3) of Theorem 7.1.2 hold} \end{array} \right\}.$$

Indeed, f_{gp}^* is naturally connected to SONC certificates of nonnegativity as the following theorem shows.

Theorem 7.1.3. *Let $f \in \mathbb{R}[\mathbf{x}]_{2d}$ be of the Form* (7.1.2). *Then*

$$f_{gp}^* = \sup \left\{ r \in \mathbb{R} \ : \begin{array}{l} \exists g_1, \ldots, g_s \in \mathbb{R}[\mathbf{x}]_{2d} \textit{ with } \mathrm{New}(f) = \mathrm{New}(g_j) \\ \textit{for } 1 \leq j \leq s \textit{ and} \\ f - r - \sum_{\alpha \in \Omega(f) \setminus \Delta(f)} f_\alpha \mathbf{x}^\alpha = \sum_{j=1}^s g_j \textit{ is a SONC} \end{array} \right\}$$

Note in this context again that $\sum_{\alpha \in \Omega(f) \setminus \Delta(f)} f_\alpha \mathbf{x}^\alpha$ is a sum of monomial squares, which is irrelevant for the computation of f_{gp}^* by Theorem 7.1.2.

Proof. By definition of f_{gp}^* and by Theorem 7.1.2, we already know that for every $r \leq f_{gp}^*$ it holds that $f - r - \sum_{\alpha \in \Omega(f) \setminus \Delta(f)} f_\alpha \mathbf{x}^\alpha$ is a SONC. And, by the construction (7.1.3) in the proof of Theorem 7.1.1, we know that every polynomial g_j in the SONC decomposition satisfies $\mathrm{New}(g_j) = \mathrm{New}(f)$.

Hence, assume that there exist nonnegative circuit polynomials $g_1, \ldots, g_s \in \mathbb{R}[\mathbf{x}]_{2d}$ with $\mathrm{New}(g_j) = \mathrm{New}(f)$ for every j satisfying

$$f - r - \sum_{\alpha \in \Omega(f) \setminus \Delta(f)} f_\alpha \mathbf{x}^\alpha = \sum_{j=1}^s g_j.$$

W.l.o.g., we can assume that every $\alpha \in \Delta(f)$ is contained in the support of a unique g_j – otherwise we can replace some $g_i + g_j$ by g_j'. By Theorem 6.2.6, every g_j satisfies $g_j = \lambda_0^{\alpha(g_j)} + \sum_{i=1}^n g_{j,i} \mathbf{x}^{\alpha(i)} + c_j \mathbf{x}^{\alpha(g_j)}$ with $\lambda_0^{\alpha(g_j)} \in \mathbb{R}_{>0}, g_{i,j} \in \mathbb{R}_{>0}$ for all $1 \leq i \leq n$, $\alpha(g_j) \in \Delta(f)$ and $|c_j| \leq \prod_{i=1}^n (g_{j,i}/\lambda_i^{(\alpha(g_j))})^{\lambda_i^{(\alpha(g_j))}}$. Hence, we have

$$\begin{aligned} f - r - \sum_{\alpha \in \Omega(f) \setminus \Delta(f)} f_\alpha \mathbf{x}^\alpha &= \sum_{j=1}^s g_j \\ &= \sum_{j=1}^s \lambda_0^{(\alpha(g_j))} + \sum_{i=1}^n \left(\sum_{j=1}^s g_{j,i} \right) \mathbf{x}^{\alpha(i)} + \sum_{j=1}^s c_j \mathbf{x}^{\alpha(g_j)} \end{aligned}$$

satisfying conditions (1') and (2') in the proof of Theorem 7.1.2 and hence also conditions (1) – (3) of Theorem 7.1.2. ∎

In the beginning of this chapter, we denoted that the observation of Ghasemi and Marshall was a trade-off between fast solvability of the corresponding geometric programs in comparison with semidefinite programs and the fact that $f_{gp}^* \leq f_{sos}^*$. Here, we conclude the surprising fact that geometric programs do not have this lack in case of polynomials with simplex Newton polytope satisfying the conditions of Theorem 6.3.5. Quite the contrary, the bound f_{gp}^* will be at least as good as the bound f_{sos}^*. Note that the special instance $\#\Omega(f) = 1$ and $\mathrm{New}(f)$ being the standard simplex with edge length $2d$ was already observed by Ghasemi and Marshall (see [GM12, Corollary 3.4]).

Corollary 7.1.4. *Let f be a polynomial of the Form* (7.1.2) *with* $\mathrm{New}(f) = \mathrm{conv}\{0, \alpha(1), \ldots, \alpha(n)\}$ *being a simplex, all $\alpha(j) \in (2\mathbb{N})^n$, and such that $\Omega(f) \subseteq (\mathrm{int}(\Delta) \cap \mathbb{N}^n)$. Suppose that there exists a vector $v \in (\mathbb{R}^*)^n$ such that $f_\alpha v^\alpha < 0$ for all $\alpha \in \Omega(f)$. Then the following statements hold.*

1. $f_{sos}^* \leq f_{gp}^* = f^*$,
2. *if $\Delta(f) \subset \Delta^*$, then $f_{sos}^* \geq f_{gp}^*$ and hence $f_{gp}^* = f_{sos}^* = f^*$,*

Proof. The statement follows immediately from Theorems 6.3.5 and 7.1.3. ∎

If $\Delta(f) \subset \Delta^*$, then it always holds that $f_{gp}^* \leq f_{sos}^*$, since the SONC property coincides with the property of being a sum of binomial squares, regardless of the existence of a vector $v \in (\mathbb{R}^*)^n$ such that $f_\alpha v^\alpha < 0$ for all $\alpha \in \Omega(f)$. However, note that the condition $\Omega(f) \subseteq (\mathrm{int}(\Delta) \cap \mathbb{N}^n)$ is essential as the following example shows.

Example 7.1.5 ([GM12])**.** *Let*

$$f = 2 + x^6 + y^6 + z^6 + x^2yz^2 - x^4 - y^4 - z^4 - yz^3 - xy^2.$$

Here, $\Omega(f)$ contains boundary points of the simplex

$$\mathrm{New}(f) = \mathrm{conv}\{(0,0,0)^T, (6,0,0)^T, (0,6,0)^T, (0,0,6)^T\}$$

and there exists $v \in \mathbb{R}^3 \backslash \{0\}$ at which all non-vertex monomials have a negative sign (e.g., $v = (1,-1,-1)$). One can check (e.g., with the method described in the next section) that $f_{gp}^* = f_{sos}^* \approx -1.6728 < f^* = 0.667$

7.2 Geometric Programming

In this section we prove that the number f_{gp}^* can be obtained by a geometric program, which we introduce first.

Definition 7.2.1. *A function $f : \mathbb{R}_{>0}^n \to \mathbb{R}$ of the form $f(\mathbf{x}) = cx_1^{a_1} \cdots x_n^{a_n}$ with $c > 0, a_i \in \mathbb{R}$ and $\mathbf{x} = (x_1, \ldots, x_n)$ is called a monomial. A sum of monomial functions $\sum_{i=0}^k c_i x_1^{a_{1i}} \cdots x_n^{a_{ni}}$ with $c_i > 0$ is called a posynomial function.*

A *geometric program* has the following form.

$$\inf\{f_0(\mathbf{x}) \ : \ x \in \mathbb{R}^n\} \quad \text{such that} \tag{7.2.1}$$
$$f_i(\mathbf{x}) \leq 1 \ \text{ for all } \ 1 \leq i \leq m \quad \text{and} \quad g_j(\mathbf{x}) = 1 \ \text{ for all } \ 1 \leq j \leq p,$$

where $f_0, \ldots, f_m$ are posynomials and $g_1, \ldots, g_p$ are monomial functions.

Geometric programs can be solved with an interior point method. In [NN94] the authors prove worst-case polynomial-time complexity of these programs. For an introduction and practical ability of geometric programs, see, e.g., [BKVH07, BV04]. Based on our main results Theorem 7.1.1 and 7.1.2, we can draw the following corollary.

Corollary 7.2.2. *Let $f \in \mathbb{R}[\mathbf{x}]$ be a non-constant polynomial of degree $2d$ with $f_0 = \sum_{\alpha \in \Omega(f)} \lambda_0^{(\alpha)}$ and $f_{\alpha(j)} > 0$ for $1 \leq j \leq n$. Then $f_{gp}^* = f_0 - m^*$, where m^* is given by the following geometric program.*

$$\inf \left\{ \sum_{\alpha \in \Delta^{<2d}(f)} \lambda_0^{(\alpha)} \cdot |f_\alpha|^{\frac{1}{\lambda_0^{(\alpha)}}} \cdot \prod_{j=1}^{n} \left(\frac{\lambda_j^{(\alpha)}}{a_{\alpha,j}} \right)^{\frac{\lambda_j^{(\alpha)}}{\lambda_0^{(\alpha)}}} \ : \ \begin{array}{l} (a_{\alpha,1}, \ldots, a_{\alpha,n}) \in \mathbb{R}_{\geq 0}^n \\ \textit{for all } \alpha \in \Delta^{<2d}(f) \end{array} \right\}$$

$$\textit{s.t.} \sum_{\alpha \in \Delta(f)} \left(\frac{a_{\alpha,j}}{f_{\alpha(j)}} \right) \leq 1 \ \ \textit{for all} \ \ 1 \leq j \leq n \ \ \textit{and}$$

$$1/|f_\alpha| \cdot \prod_{j=1}^{n} \left(\frac{a_{\alpha,j}}{\lambda_j^{(\alpha)}} \right)^{\lambda_j^{(\alpha)}} = 1 \ \ \textit{for all} \ \ \alpha \in \Delta(f) \ \ \textit{with} \ \ |\alpha| = 2d.$$

Proof. We have $f_{gp}^* = f_0 - m^*$ by definition of f_{gp}^*. Since

$$\sum_{\alpha \in \Delta^{<2d}(f)} \lambda_0^{(\alpha)} \cdot |f_\alpha|^{\frac{1}{\lambda_0^{(\alpha)}}} \cdot \prod_{j=1}^{n} \left(\frac{\lambda_j^{(\alpha)}}{a_{\alpha,j}} \right)^{\frac{\lambda_j^{(\alpha)}}{\lambda_0^{(\alpha)}}} \quad \text{and} \quad \sum_{\alpha \in \Delta(f)} \left(\frac{a_{\alpha,j}}{f_{\alpha(j)}} \right) \quad \text{for all} \ \ 1 \leq j \leq n$$

are posynomials in the variables $a_{\alpha,j}$ and for all $\alpha \in \Delta(f)$ with $|\alpha| = 2d$

$$1/|f_\alpha| \cdot \prod_{j=1}^{n} \left(\frac{a_{\alpha,j}}{\lambda_j^{(\alpha)}} \right)^{\lambda_j^{(\alpha)}}$$

is a monomial in the variables $a_{\alpha,j}$, m^* is indeed the output of a geometric program. ∎

Corollary 7.2.3. *Let $\{(a_{\alpha,1}, \ldots, a_{\alpha,n}) \ : \ \alpha \in \Delta(f)^{<2d}\}$ be the global minimizer of a geometric program as in Corollary 7.2.2. If $\Delta(f) = \Delta(f)^{<2d}$, then we have $\sum_{\alpha \in \Delta(f)} a_{\alpha,j} = f_{\alpha(j)}$ for every $1 \leq j \leq n$.*

Proof. Follows immediately from Theorem 7.1.3 and Corollary 7.2.2. ∎

7.3 Examples

We demonstrate our method and reflect our results by various examples. All geometric programs are solved via the MATLAB solver GPPOSY[1].

1. First, consider the polynomial $f = \frac{1}{4} + x^8 + x^2y^6 + 4x^3y^3$. The geometric program proposed in [GM12] is infeasible, since the pure power y^8 is missing in the polynomial to make the Newton polytope a standard simplex of edge length 8. However, New(f) is an H-simplex and we can use our results to compute f_{gp}^*. Here, we have $\Delta = \{\alpha\} = \{(3,3)\}$. Hence, we introduce the variables $a_{\alpha,j}$ for $j \in \{1,2\}$. Therefore, by Corollary 7.2.2, we have to solve the following geometric program.
$$\inf \left\{ \frac{1}{4} \cdot 4^4 \cdot \left(\frac{1}{4}\right)^{\frac{4}{4}} \cdot \left(\frac{1}{2}\right)^{\frac{4}{2}} \cdot a_{\alpha,1}^{-1} a_{\alpha,2}^{-2} \ : \ a_{\alpha,1}, a_{\alpha,2} \leq 1 \right\}.$$
The optimal solution is given by $a_{\alpha,1} = a_{\alpha,2} = 1$ (as expected due to Corollary 7.2.3) yielding $m^* = 4$ and hence $f_{gp}^* = \frac{1}{4} - 4 = -3.75 = f_{sos}^* = f^*$ by Corollary 7.1.4.

2. Let $f = \frac{187}{208} + x^{80} + y^{78} - 8x^5y^3$. Again, the geometric program proposed in [GM12] is infeasible. But New(f) is an H-simplex and with $\lambda_1^{(5,3)} = 1/16$ and $\lambda_2^{(5,3)} = 1/26$ our corresponding geometric program is given by
$$\inf \left\{ \frac{187}{208} \cdot 8^{\frac{208}{187}} \cdot \left(\frac{1}{16}\right)^{\frac{13}{187}} \cdot \left(\frac{1}{26}\right)^{\frac{8}{187}} \cdot a_{\alpha,1}^{-\frac{13}{187}} \cdot a_{\alpha,2}^{-\frac{8}{187}} \ : \ a_{\alpha,1}, a_{\alpha,2} \leq 1 \right\}.$$
Using the software GLOPTIPOLY (see [HLJL09]), $f^* \approx -5.6179$ was computed in 4327, 2 seconds, i.e., approximately **1.2 hours**. However, using the above geometric program, we get a global minimizer $a_{\alpha,1} = a_{\alpha,2} = 1$ (again, as we would expect due to Corollary 7.2.3) and the optimal solution $m^* = \frac{187}{208} \cdot \left(\frac{8^{208}}{16^{13} \cdot 26^8}\right)^{\frac{1}{187}}$ and hence $f^* = \lambda_0 - m^* = \frac{187}{208} \cdot \left(1 - \left(\frac{8^{208}}{16^{13} \cdot 26^8}\right)^{\frac{1}{187}}\right) \approx -5.6179$ in **0.5 seconds**.

3. Let now $f = \frac{17}{20} + 3x^8y^4 + 2x^6y^8 - 10x^3y^3 + x^5y^4$. Again, the geometric program in [GM12] cannot be used but the geometric program in Corollary 7.2.2 with $\Delta = \{\overline{\alpha}, \alpha\} = \{(3,3),(5,4)\}$ now reads as follows:
$$\inf \left\{ \frac{9 \cdot 2^{\frac{1}{3}} \cdot 5^{\frac{2}{3}}}{1250} \cdot a_{\alpha,1}^{-\frac{4}{3}} \cdot a_{\alpha,2}^{-1} + \frac{11 \cdot 10^{\frac{3}{11}} \cdot 3^{\frac{9}{11}} \cdot 20^{\frac{8}{11}}}{40} \cdot a_{\overline{\alpha},1}{}^{-\frac{3}{11}} a_{\overline{\alpha},2}{}^{-\frac{6}{11}} \right\}$$
$$\text{such that } \frac{a_{\alpha,1} + a_{\overline{\alpha},1}}{3} \leq 1 \text{ and } \frac{a_{\alpha,2} + a_{\overline{\alpha},2}}{2} \leq 1.$$

[1]The Matlab version used was R2011a, running on a desktop computer with Intel(R) Core(TM)2 @ 2.33 GHz and 2 GB of RAM.

Here, the variables $a_{\alpha,j}$ come from $\alpha = (5,4)$ and $a_{\overline{\alpha},j}$ come from $\overline{\alpha} = (3,3)$. Again, we use the MATLAB solver GPPOSY to solve this geometric program with the following code:

```
>> A0=[-4/3,-1,0,0;0,0,-3/11,-6/11]
>> A1=[1,0,0,0;0,0,1,0]
>> A2=[0,1,0,0;0,0,0,1]
>> A=[A0;A1;A2]
>> coeff1 = 9/1250*2^(1/3)*5^(2/3)
>> coeff2 = 11/40*10^(3/11)*3^(9/11)*20^(8/11))
>> b0=[coeff1;coeff2]
>> b1=[1/3;1/3]
>> b2=[1/2;1/2]
>> b=[b0;b1;b2]
>> szs=[size(A0,1);size(A1,1);size(A2,1)]
>> [x,status,lambda,nu]=gpposy(A,b,szs)
```

The optimal solution is given by

$$(a_{\alpha,1}, a_{\alpha,2}, a_{\overline{\alpha},1}, a_{\overline{\alpha},2}) \;=\; (0.5910, 0.1685, 2.4090, 1.8315)$$

(Corollary 7.2.3 holds again) yielding $m^* \approx -6.644$ and hence

$$f^*_{gp} = \frac{17}{20} - 6.644 \approx -5.794.$$

By Corollary 7.1.4, we have $f^*_{gp} = f^*_{sos} = f^* \approx -5.794$.

4. The Motzkin polynomial $f = \frac{1}{3} + \frac{1}{3}x^4y^2 + \frac{1}{3}x^2y^4 - x^2y^2$ satisfies $f^*_{gp} = f^* = 0$ by Corollary 7.1.4. However, $f^*_{sos} = -\infty$.

5. Let $f = \frac{5}{12} + \frac{5}{24}x^6 + \frac{5}{24}x^2y^4 + \frac{5}{24}x^2y^2 - \frac{5}{8}xy$. Then one can check that

$$f^*_{gp} \approx -0.41 < f^*_{sos} = f^* \approx 0.196.$$

7.4 Conclusion and Outlook

We have proposed a new geometric program for producing lower bounds for polynomials that extends the existing one in [GM12]. This extension sheds light on the crucial structure of the Newton polytope of polynomials. In particular, our results serve as a next step in optimization of polynomials with simplex Newton polytopes and connect this problem to

1. the SONC nonnegativity certificates, and

2. the construction of simplices with an interesting lattice point structure, namely, what we have called H-simplices in this thesis.

We proved that f_{gp}^* and f_{sos}^* are not comparable, which cannot be observed in the precursor works about geometric programming. Interestingly, for very rich classes there is a win-win situation in the sense that $f_{sos}^* \leq f_{gp}^* = f^*$ though f_{gp}^* can be computed much faster than f_{sos}^*. It would be interesting to classify more classes for which the bounds are comparable. Hence, an analysis of the gap $f_{sos}^* - f_{gp}^*$ is an interesting task having major impact on computational complexity of solving polynomial optimization problems. Equivalently, looking from a convex geometric viewpoint, it would be interesting to analyze the gap between the cone of sums of squares and the cone of sums of binomial squares as well as the gap between the cone of sums of squares and the cone of sums of nonnegative circuit polynomials.

Chapter 8

Open Problems

In the following we present some open problems that arose during the preparation of this thesis and that are more general than the open problems formulated at the end of the chapters.

Boundary Structure

The boundary structure of the cones $P_{n,2d}$ and $\Sigma_{n,2d}$ is very important to understand the difference between these two cones. In spite of the progress made, many interesting questions/problems remain widely open. In particular, the following ones can be considered as an interesting future work.

1. The study of the algebraic boundary of $P_{n,2d}$ and $\Sigma_{n,2d}$ as well as of their dual cones. This has been established in [BHO$^+$12] for $(n, 2d) \in \{(3,6),(4,4)\}$ but remains open in all other cases.

2. A description of the extreme rays of $P_{n,2d}$ and $\Sigma_{n,2d}$ as well as of their dual cones. This also has been established for special instances ([Ble12a, Ble12b]) but is widely open in all other cases.

3. Closely related to the question of the extreme rays of these cones is the problem of determining the maximum number of zeros a nonnegative polynomial (resp. a sum of squares polynomial) can have (see Theorem 2.6.8 for partial results). This would have a major impact on the study of the boundary structure of $P_{n,2d}$ and $\Sigma_{n,2d}$.

Symmetric Polynomials

In Chapter 5 we considered the problem of deciding nonnegativity of symmetric polynomials and added to some earlier results. Considering previous results on symmetric polynomials ([BR12, CLR87]), the difference between $P_{n,2d}$ and $\Sigma_{n,2d}$ is conjectured to be much more delicate than in the general case. Therefore, the following questions are very interesting for possible future directions of research.

1. What is the quantitative relationship between nonnegative symmetric polynomials and symmetric sums of squares polynomials?

2. Is it possible to derive explicit semialgebraic descriptions for rich classes of nonnegative symmetric polynomials and sums of squares?

Sparse Polynomials

In Chapter 6 we studied sparse polynomials with simplex Newton polytope supported on a circuit and completely characterized nonnegative polynomials and sums of squares. Furthermore, we extended this approach partially to arbitrary Newton polytopes. We consider the following questions/problems to be very interesting in this setting.

1. Let $f \in \mathbb{R}[\mathbf{x}]_{2d}$ be such that $\mathrm{supp}(f) = \mathrm{vert}(\mathrm{New}(f)) \cup \{y\}$ with $y \in \mathrm{int}(\mathrm{New}(f))$. We characterized nonnegativity in the case of $\mathrm{New}(f)$ being a simplex. It would be very interesting to explicitly characterize the nonnegativity region of f in the non-simplex case.

2. Similar as in the simplex case, is it possible to determine a global minimizer for such polynomials explicitly? We suspect that this can be established via clever triangulations of $\mathrm{New}(f)$ and using results from the simplex case.

3. In Theorem 6.4.1 we established a very interesting connection between sums of squares polynomials supported on circuits and properties from toric geometry as well as from lattice polytopes. Is it possible to gain more insight to this connection for more general polynomials?

4. In Chapter 6 we introduced the convex cone of sums of nonnegative circuit polynomials, which plays a major role in polynomial optimization via geometric programming. It would be interesting to analyze convex geometric properties of this cone, such as, e.g., the structure of the extreme rays and of the faces as well as intersections with the cones of nonnegative polynomials and sums of squares.

Convex Polynomials

When restricting to homogeneous polynomials, a very interesting convex cone is given by the cone of convex forms, since it is contained in the cone of nonnegative forms. But still, the cone of convex forms seems to be mysterious, as almost nothing is known about structures that characterize/prevent convexity of polynomials. Many polynomial optimization problems can be solved more efficiently with additional convexity structure in the problems. However, deciding convexity is NP-hard in general ([AOPT13]). Therefore, it is very interesting to understand the cone of convex forms in more detail. Specifically, we consider the following questions/problems to be very delicate.

1. There are many sums of squares forms that are not convex ([Rez11]). However, there are also many convex forms that are not sums of squares ([Ble09]). As for now, it is still an open problem to provide an explicit convex form that is not a sum of squares.

2. What can be said about the (algebraic) boundary structure of the cone of convex forms?

3. Which structures prevent polynomials from being convex? In Theorem 6.5.4 we proved that sparsity should be among these structures.

4. Which matrix polynomials are valid Hessian matrices? In our opinion, this is a key problem in analyzing the cone of convex forms in more detail.

In [Tim03] Timofte proves that a symmetric polynomial $p \in \mathbb{R}[\mathbf{x}]_d$ is nonnegative if and only if p is nonnegative at all points $\mathbf{x} \in \mathbb{R}^n$ with at most $\lfloor \frac{d}{2} \rfloor$ distinct components. We conjecture that an analagous version holds for convexity of symmetric polynomials. More precisely, we provide the following conjecture.

Conjecture 8.0.1. *Let $p \in \mathbb{R}[\mathbf{x}]_d$ be a symmetric polynomial and let $H_p(\mathbf{x})$ be the Hessian of p.*

1. *There exists a function $f : \mathbb{N} \to \mathbb{N}$ such that the following does hold: p is convex if and only if $H_p(\mathbf{x})$ is positive semidefinite at all points $\mathbf{x} \in \mathbb{R}^n$ with at most $f(d)$ distinct components. Note that f is independent of n.*

2. *Every convex symmetric nonnegative polynomial is a sum of squares.*

3. *Every convex symmetric form is a sum of squares.*

Note that we have to distinguish between forms and polynomials in this case, since convexity is not preserved under homogenization.

Some More General Open Problems

In polynomial optimization, one is interested in the quality of sums of squares relaxations. This is equivalent to understand the quantitative relationship between $P_{n,2d}$ and $\Sigma_{n,2d}$. The asymptotic result in [Ble06] based on the volume ratio of a compact section of $P_{n,2d}$ and $\Sigma_{n,2d}$ is very poor in small dimensions. Hence, the following questions are very important both theoretically and practically.

1. What is the precise quantitative relationship between $P_{n,2d}$ and $\Sigma_{n,2d}$ in small dimensions?

2. Is it possible to provide better bounds for the volume ratio of a compact section of $P_{n,2d}$ and $\Sigma_{n,2d}$ than in [Ble06]?

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