

A brief introduction to sums of squares

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ABSTRACT. We give a brief overview and history of nonnegative polynomials and sums of squares. This chapter also provides a guide to how the subsequent chapters connect to this central theory.

This chapter is an informal introduction to the theory of nonnegative polynomials and sums of squares. We assume that the reader is familiar with linear algebra, and especially with positive semidefinite symmetric matrices. For more details on these we recommend [6, Appendix A] and [3, Section II.12]. The study of nonnegativity and its relation with sums of squares is a classical topic in real algebraic geometry, starting with the work of Hilbert, who classified the cases in terms of degree and number of variables where nonnegative polynomials are always sums of squares of polynomials (Theorem 3.2). Generalizations of this theorem are the subject of Mauricio Velasco’s chapter. Hilbert’s 17th problem asked whether any globally nonnegative polynomial is a sum of squares of rational functions. Artin’s positive solution of Hilbert’s 17th problem in the 1920’s, using the Artin-Schreier theory of real closed fields left a lasting imprint on the subject.

The study of the subject changed substantially in the early 2000’s when it was realized by Lasserre and Parrilo, following earlier work by N.Z. Shor and Choi, Lam and Reznick, that one can use semidefinite programming to efficiently search for sums of squares certificates of nonnegativity in practice [9, 14, 19, 25]. The resulting hierarchies (called Lasserre, moment or sums of squares hierarchies) were motivated by theorems of Schmüdgen and Putinar on representations of nonnegative polynomials as sums of squares on compact semialgebraic sets (see Section 5). The sum of squares method has many applications in engineering, robotics and computer science. For more details see Georgina Hall’s chapter.

1. Two guiding questions

How can we decide if a function, for instance a polynomial in one variable, takes only nonnegative values? Consider for example, $p(x) = 5x^4 - 4x^3 - x^2 + 2x + 2$. It is not immediately clear, although quite elementary to show, that $p(x)$ is globally nonnegative. However, if we write $p(x)$ as a sum of squares of polynomials:

$$p(x) = (x^2 + 1)^2 + (2x^2 - x - 1)^2,$$

then its nonnegativity is readily apparent.

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This simple example immediately poses two important questions:

- (1) Are representations of nonnegative polynomials as sums of squares always possible?
- (2) If a polynomial is a sum of squares, then how can we find a sum of squares decomposition?

We address the second question first.

2. Finding sum of squares decompositions

Consider a single square $(1 - 3x + 2x^2)^2$. We introduce two vectors, the vector of coefficients $v = (1, -3, 2)^T$ and the vector of monomials $\mathbf{x} = (1, x, x^2)^T$. We can write $1 - 3x + 2x^2$ as $v^T \mathbf{x}$ and therefore

$$(1 - 3x + 2x^2)^2 = (\mathbf{x}^T v)(v^T \mathbf{x}) = \mathbf{x}^T (vv^T) \mathbf{x}.$$

Observe that vv^T is a rank 1 positive semidefinite matrix, and any rank 1 positive semidefinite matrix has the form vv^T for some real vector v . By applying this procedure to all squares in a sum of squares, we see that any sum of squares $p(x)$ can be written as

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

where A is a positive semidefinite matrix. The converse can be established using the following exercise:

EXERCISE 2.1. Show that any positive semidefinite matrix A can be written as a sum of rank A many positive semidefinite matrices of rank one.

Aside on positive semidefinite matrices: Positive semidefinite matrices form a *convex cone* in the vector space of real symmetric matrices, which we denote by $\mathcal{S}_+^n$. We use notation $A \succeq 0$ to indicate that a symmetric matrix A is positive semidefinite. A good reference for the geometry of $\mathcal{S}_+^n$ is given in [3, Section II.12]. A slice of this cone with an affine subspace is called a *spectrahedron*. An interesting spectrahedron, directly related to univariate sums of squares is the *Hankel spectrahedron*, which consists of all positive-semidefinite Hankel matrices (matrices that are constant on anti-diagonals), with $(1, 1)$ entry equal to 1. For instance the 3×3 Hankel spectrahedron has the form:

$$H_3 = \left\{ (x, y, z, w) : \begin{pmatrix} 1 & x & y \\ x & y & z \\ y & z & w \end{pmatrix} \succeq 0 \right\}.$$

We can think of H_3 as a slice of the cone of 3×3 cones of positive semidefinite matrices with a 4-dimensional affine linear subspace given by:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + x \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + y \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} + z \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + w \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

A matrix is positive semidefinite if and only if all of its principal minors are non-negative. Therefore the spectrahedron H_3 can be defined by algebraic inequalities, by requiring all principal minors of the above matrix to be nonnegative. For the relation of Hankel spectrahedra to the problem of moments we refer the reader to [24]. Cynthia Vinzant's chapter will explain much more about the geometry of $\mathcal{S}_+^n$ and spectrahedra.

We note that Exercise [2.1](#) says, equivalently, that rank 1 positive semidefinite matrices are precisely *the extreme rays* of $\mathcal{S}_+^n$. Another interesting consequence of our observations is that the minimal number of squares needed to write $p(x)$ as a sum of squares is precisely the minimal rank of any matrix A such that $p(x) = \mathbf{x}^T A \mathbf{x}$. For more information see [\[10\]](#). The logic above can be easily applied to the multivariate setting:

REMARK 2.2 (Multivariate Polynomials). For polynomials in several variables we can form a vector $\mathbf{x}$ of multivariate monomials up to a certain degree d . For instance, if we want to check that a bivariate polynomial of degree 4 is a sum of squares, the corresponding vector $\mathbf{x}$ is $(1, x, y, x^2, xy, y^2)$. Via the same reasoning, a bivariate polynomial $p(x, y)$ of degree 4 is a sum of squares if and only if there exists a positive semidefinite matrix A such that $p(x, y) = \mathbf{x}^T A \mathbf{x}$. Furthermore, the choice of the monomial basis is not canonical, and a different basis of the vector space of multivariate polynomials of degree at most d may be used to build the vector $\mathbf{x}$.

2.1. Sums of squares and semidefinite programming: Testing whether a given polynomial $p(x)$ is a sum of squares can be done efficiently on a computer using semidefinite programming [\[6, Chapter 3\]](#). We demonstrate this procedure by an example that is small enough to do by hand.

EXAMPLE 2.3. Let $p(x) = 5x^4 - 4x^3 - x^2 + 2x + 2$. By the above, $p(x)$ is a sum of squares if and only if there exists a positive semidefinite matrix A such that

$$p(x) = \mathbf{x}^T A \mathbf{x}, \quad A = \begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{01} & a_{11} & a_{12} \\ a_{02} & a_{12} & a_{22} \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} 1 \\ x \\ x^2 \end{pmatrix}.$$

A positive semidefinite matrix A such that $p(x) = \mathbf{x}^T A \mathbf{x}$ is called a *Gram matrix* of A . By multiplying $\mathbf{x}^T A \mathbf{x}$ out and comparing coefficients we get equations

$$a_{00} = 2, \quad 2a_{01} = 2, \quad 2a_{02} + a_{11} = -1, \quad 2a_{12} = -4, \quad a_{22} = 5.$$

The matrix A therefore has the form:

$$A = \begin{pmatrix} 2 & 1 & a_{02} \\ 1 & -1 - 2a_{02} & -2 \\ a_{02} & -2 & 5 \end{pmatrix}.$$

The choices of a_{02} that make A positive semidefinite describe the *Gram Spectrahedron* of $p(x)$ [\[10\]](#). By considering the determinant of A one can check that A is positive semidefinite for $\frac{1}{4}(1 - \sqrt{185}) \leq a_{02} \leq -1$ and the choices of $a_{02} = -1$ and $a_{02} = \frac{1}{4}(1 - \sqrt{185})$ will lead to rank 2 matrices, i.e. ways of writing $p(x)$ as a sum of two squares. The decomposition from Section [1](#) has $a_{02} = -1$, and consequently, $a_{11} = 1$.

One can ask whether given a multivariate sum of squares $p(x)$ with rational coefficients there always exists a Gram matrix A filled with rational numbers such that $p(x) = \mathbf{x}^T A \mathbf{x}$? In general, the answer is “no” as shown by Scheiderer in [\[22\]](#). We now discuss semidefinite programming in general.

2.2. A primer on semidefinite programming. Semidefinite programming is a generalization of linear programming where we also allow positive semidefiniteness constraints. More precisely, a general semidefinite program has the form:

$$\begin{aligned} & \underset{X}{\text{minimize}} && \langle C, X \rangle \\ & \text{subject to} && \langle A_i, X \rangle = b_i \quad i = 1, \dots, m, \\ & && X \succeq 0. \end{aligned}$$

The inner product is the trace inner product $\langle A, B \rangle = \text{tr } AB$. We note that if X is restricted to being a diagonal matrix then the above semidefinite program becomes a linear program, since positive-semidefiniteness constraint only ensures that the diagonal entries are nonnegative.

Semidefinite programs can be efficiently solved using interior point methods [4]. However, these methods will struggle when the matrix size grows large, and this becomes quite relevant for sums of squares methods, as seen in the remark below.

REMARK 2.4. Observe that the size of the Gram matrix A is given by the number of relevant monomials (or more precisely the dimension of the vector space from which squares come). If we want to check whether an n -variate polynomial of degree $2d$ is a sum of squares, then $\mathbf{x}$ should be the vector of all monomials in n variables of degree at most d , and therefore the size of A is $\binom{n+d}{d} \times \binom{n+d}{d}$. As the number of variables and the degree grows the size of A increases rapidly, and this is perhaps the greatest practical limitation of the sum of squares method, as matrices may soon become too large to be effectively handled by SDP solvers.

2.3. Lifted representations. We can define a map Φ which sends a symmetric matrix A to the polynomial $\mathbf{x}^T A \mathbf{x}$. Another way of interpreting and generalizing Example 2.3 is that the map Φ projects the cone S_+^n to sums of squares, or equivalently, it provides a *lifted SDP representation* of the cone of sums of squares. For instance, Example 2.3 shows that a univariate polynomial $a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4$ of degree 4 is a sum of squares if and only if there exists a positive semidefinite matrix

$$\begin{pmatrix} a_0 & \frac{1}{2}a_1 & b \\ \frac{1}{2}a_1 & c & \frac{1}{2}a_3 \\ b & \frac{1}{2}a_3 & a_4 \end{pmatrix} \succeq 0,$$

where $2b + c = a_2$. Therefore the cone of univariate sums of squares of degree 4 is a projection of the cone S_+^3 of 3×3 positive semidefinite matrices.

One can study, in general, which sets can be written as projections of “simple sets”, for instance spectrahedra. Such lifted representations allow to us to lift an optimization problem from a complicated set to the simple set upstairs, where optimization can be done efficiently. See Hamza Fawzi’s chapter for more on lifted representations.

3. Nonnegative polynomials and sums of squares

We now discuss in detail the comparison between nonnegative polynomials and sums of squares. The story begins in 1885 at the Ph.D. defense of Hermann Minkowski, where David Hilbert was one of the examiners. During his defense Minkowski claimed that there exist nonnegative polynomials that are not sums of squares, although he did not provide an example or a proof. Three years later

Hilbert published a seminal paper [12] classifying all cases in terms of number of variables n and degree $2d$ for which all n -variate nonnegative polynomials of degree at most $2d$ are sums of squares.

We use $P_{n,\leq 2d}$ and $\Sigma_{n,\leq 2d}$ to respectively denote the sets of n -variate nonnegative polynomials and sum of squares of degree at most $2d$. We note that both form convex cones in the vector space $\mathbb{R}[x]_{n,\leq 2d}$ of n -variate polynomials of degree at most $2d$, and $\dim \mathbb{R}[x]_{n,\leq 2d} = \binom{n+2d}{2d}$.

EXERCISE 3.1. Show that $P_{n,\leq 2d}$ and $\Sigma_{n,\leq 2d}$ are closed full-dimensional convex cones with no lines in $\mathbb{R}[x]_{n,\leq 2d}$. For a hint see [6] Exercise 4.17].

We now state Hilbert's 1888 theorem:

THEOREM 3.2. $P_{n,\leq 2d} = \Sigma_{n,\leq 2d}$ only in the following three cases:

- (1) $n = 1$, the case of univariate polynomials
- (2) $2d = 2$, the case of quadratic polynomials
- (3) $n = 2$, $2d = 4$, the exceptional case of ternary quartics.

In all other cases there exist nonnegative polynomials that are not sums of squares.

It should be noted that Hilbert did not provide an explicit nonnegative polynomial that is not a sum of squares of polynomials. The first explicit example appeared only much later and is due to Motzkin [16] (See Exercise 3.5). The main difficulty of constructing an example is certifying that a given polynomial is globally nonnegative without relying on a sums of squares decomposition. Motzkin's idea was to guarantee nonnegativity via classical inequalities! The Motzkin polynomial

$$M(x, y) = x^2y^4 + x^4y^2 + 1 - 3x^2y^2$$

is nonnegative by applying the Arithmetic Mean/Geometric Mean inequality, and an argument detailed in the exercises below shows that it is not a sum of squares.

EXERCISE 3.3. The *Newton Polytope* N_p of a polynomial p is the convex hull of the vectors of monomial exponents that occur in p . For example, the Newton Polytope of $x^2 + y + 1$ is the convex hull of vectors $(2, 0)$, $(0, 1)$ and $(0, 0)$. Show that if a polynomial $p = \sum_i q_i^2$ is a sum of squares, then the Newton Polytope of each q_i is contained in $\frac{1}{2}N_p$. Hint: It helps to consider the convex hull of the Newton polytopes of q_i 's.

EXERCISE 3.4. Define homogenization $\tilde{p}$ of a polynomial $p(x_1, \dots, x_n)$ of degree d by introducing a new variable x_0 and multiplying all monomials in p by a power of x_0 , so that all monomials have degree d . More formally:

$$\tilde{p} = x_0^d \cdot p\left(\frac{x_1}{x_0}, \dots, \frac{x_n}{x_0}\right).$$

Show that p is nonnegative if and only if $\tilde{p}$ is, and the same is also true for sums of squares.

In view of the above exercise, questions about global nonnegativity and sums of squares are often studied for homogeneous polynomials, which are also called forms.

EXERCISE 3.5. Use Exercise 3.3 to show that the Motzkin polynomial is not a sum of squares. Also show that the homogeneous polynomial $S(x, y, z) = x^4y^2 + y^4z^2 + z^4x^2 - 3x^2y^2z^2$, constructed by Choi and Lam, is nonnegative but not a sum of squares.

Since then many other examples of nonnegative polynomials that are not sums of squares have appeared, particularly in the work of Choi, Lam and Reznick (see [21] for a nice overview).

After proving his 1888 Theorem, Hilbert showed in 1893 that any nonnegative bivariate polynomial is a sum of squares of rational functions. At first, writing

$$f = \sum \left(\frac{p_i}{q_i} \right)^2$$

may seem quite limiting, however observe that if we bring all of the rational functions to a common denominator r then we are writing

$$f \cdot r^2 = \sum s_i^2,$$

i.e. we hope to find a square multiplier r^2 , such that $f \cdot r^2$ is a sum of squares of polynomials. This is clearly a generalization of writing f as a sum of squares of polynomials, where we take r to be the constant polynomial 1. In fact we can even allow sum of squares multipliers, instead of just a single square:

EXERCISE 3.6. Show that f is a sum of squares of rational functions if and only if there exists a sum of squares polynomial h such that $f \cdot h$ is a sum of squares of polynomials.

Hilbert's 17th problem asked to prove that a nonnegative polynomial in any number of variables is a sum of squares of rational functions. Artin's original proof, which relied on the newly established Artin-Schreier theory of real closed fields, was purely existential. In particular, it did not provide any bounds on the degree of the multiplier h [8]. Searching for multiplier h of fixed degree such that $f \cdot h$ is a sum of squares can also be formulated as a semidefinite program, so it is important for computations to understand in what degree rational certificates exist.

To this day, our understanding of both upper and lower degree bounds is quite poor. For the best current upper bound see [15] and for the lower bounds see [5]. For the special case of nonnegative polynomials on curves see [7]. While philosophically, Artin's solution to Hilbert's 17th problem provides a quite satisfactory answer on the power of sums of squares to explain nonnegativity, computationally much remains unknown. As we are about to see, in applications we usually just use sums of squares of polynomials, as rational sums of squares often lead to numerical problems in solving semidefinite programs.

4. Sums of squares and optimization

We briefly discuss the relevance of sums of squares in optimization. We begin with a crucial observation, that being able to optimize, i.e. minimize or maximize, polynomials efficiently is equivalent to algorithmically understanding nonnegative polynomials. Consider the problem of finding the global infimum of a polynomial $p(x)$:

$$\lambda = \inf_{x \in \mathbb{R}^n} p(x).$$

Then λ is the best lower bound for p , or equivalently, λ is the largest value that we can subtract so that $p(x) - \lambda$ is nonnegative. Therefore, if we can efficiently test whether a polynomial is nonnegative, then we can do optimization.

Unfortunately, the cone of nonnegative polynomials is quite complicated, and testing nonnegativity of a polynomial is already an NP-complete problem when

the degree is 4. However, we can replace nonnegative polynomials, with “obviously nonnegative” polynomials, i.e. sums of squares! What we can compute, in practice, is instead λ^* , which is the largest value, such that $p(x) - \lambda^*$ is a sum of squares. It is clear that λ^* is a lower bound for the true infimum λ , and furthermore, very importantly, the fact that $p(x) - \lambda^*$ is nonnegative comes with a *sum of squares certificate*.

In applications, we often have problems with additional constraints, but the idea behind sum of squares approach is the same: we “relax” the intractable set of nonnegative polynomials with the tractable set of “obviously nonnegative” polynomials, which we construct using sums of squares. More details are given in the next section. This simple idea has had a profound impact in engineering and theoretical computer science, see [1, 2, 13] for some examples. For applications of sums of squares method in optimization see Georgina Hall’s chapter and for applications in computer science see Ankur Moitra’s chapter.

5. Adding constraints

Suppose that instead of global nonnegativity we want to understand polynomials nonnegative on an algebraic set X in $\mathbb{R}^n$ defined by equations $g_1(x) = \cdots = g_k(x) = 0$. Such an algebraic set is also called a *variety*. Since all polynomials g_i are identically zero on X , we have a larger class of “obviously nonnegative” polynomials on X , namely sums of squares and also multiples of g_i , which we can multiply and add together. This leads to an interesting phenomenon of degree cancellation, which we illustrate by an example:

EXAMPLE 5.1. Let $X = \{0, 1\} \subset \mathbb{R}$ be given by $g(x) = x(1 - x) = 0$. We want to certify that the function x is nonnegative on X . This is not possible using sums of squares only, since the degree of x is one. However we can write:

$$x = x^2 + x(1 - x),$$

so x is “obviously nonnegative” on X .

By considering sums of squares on varieties it is possible to generalize Hilbert’s 1888 theorem, and find more cases of equality between nonnegative polynomials and sums of squares, even without degree cancellation. See Mauricio Velasco’s chapter for more details.

This brings us to a very important theorem, which has been crucial for the development of applications of sums of squares in optimization. If we are allowed to use degree cancellation, then is it true that any polynomial p nonnegative on a compact variety X is “obviously nonnegative”? This is false in general (see Exercise 5.5 below), but it is true for strictly positive p .

THEOREM 5.2 (Schmüdgen, [23]). *Let $X \subset \mathbb{R}^n$ be a compact real variety defined by equations $g_1(x) = \cdots = g_k(x) = 0$ and let f be a polynomial strictly positive on X . Then f is “obviously nonnegative” on X , i.e. there exist polynomials $h_1, \dots, h_k$ and a sum of squares σ such that*

$$f = \sigma + g_1 h_1 + \cdots + g_k h_k.$$

Due to the central role that Schmüdgen’s theorem plays in applications in optimization, we will discuss its statement and applications in detail.

Degree Truncation: To make Schmüdgen’s Theorem useful for computations we search for certificates of bounded degree. This means given a degree bound d we search for $h_1, \dots, h_k$ and a sum of squares σ such that

$$\deg g_i h_i \leq d \quad \text{for } 1 \leq i \leq k \quad \text{and} \quad \deg \sigma \leq d.$$

This can still be formulated as a semidefinite programming problem, and is referred to in the literature as *Lasserre* or *Lasserre-Parrilo* or *sums of squares* or *moment relaxation* (technically moment relaxation refers to the dual semidefinite problem).

EXAMPLE 5.3. Let X be the set $\{-1, 0, 1\} \subset \mathbb{R}$ given by the equation $g(x) = x(x^2 - 1)$, and let $p(x) = 2 + x$. It is clear that p is nonnegative on X . If we choose two as a bound for the degree of an “obviously nonnegative” representation, then p cannot have a certificate, since we cannot use any multiples of g , and p is not a sum of squares, since it is not globally nonnegative. We leave it as an exercise to show that we can show that p is obviously nonnegative with degree bound 4.

Low Degree Certificates: The size of the semidefinite program that needs to be solved depends on the degree truncation d . Usually, the size of underlying matrices grows quickly with d (cf. Remark 2.4). Therefore, for practical consideration and from point of view of computational complexity, understanding of *low-degree certificates* is paramount. See Ankur Moitra’s chapter for the theoretical computer science perspective.

Semialgebraic sets: We stated Schmüdgen’s Positivstellensatz only for varieties, but it also holds for semialgebraic sets given by inequalities $g_i \geq 0$ (such sets are called basic closed semialgebraic sets). In this case products of g_i are obviously nonnegative, as are sums of squares. An “obviously nonnegative” polynomial on X has the form

$$\sum_j \sigma_j \Pi_{a_i \in \{0,1\}} g_i^{a_i},$$

where σ_j are sums of squares. By Schmüdgen’s theorem any strictly positive polynomial on X is “obviously nonnegative”. Under a mild technical assumption Putinar’s Positivstellensatz [20] guarantees that we do not need to consider products with more than one g_i in them, and we can take “obviously nonnegative” polynomials of the form:

$$\sigma_0 + \sum_j \sigma_j g_j.$$

Compactness is necessary: Schmüdgen’s theorem may fail if the variety X is not compact. For instance consider the case of global nonnegativity, when we have no constraints and the variety X is $\mathbb{R}^n$. The following Exercise is useful:

EXERCISE 5.4. Show that if a polynomial p of degree $2d$ is a sum of squares, then the degree $2d$ part of p , i.e. the sum of all monomials of degree exactly $2d$ with the coefficients from p , is also a sum of squares. Hint: Use Exercise 3.3

Consider again the Motzkin form $M(x, y, z) = x^2 y^4 + x^4 y^2 + z^6 - 3x^2 y^2 z^2$ (or any homogeneous polynomial that is not a sum of squares). It is now easy to show that $M(x, y, z) + 1$ is strictly positive on $\mathbb{R}^n$ but is not “obviously nonnegative”, since $M(x, y, z)$ is not a sum of squares.

Strict positivity is necessary: If f is only nonnegative on X and is not strictly positive, then it may fail to be “obviously nonnegative”. The following example is taken (with minimal modification) from [11]. Let $X \subset \mathbb{R}^2$ be the curve defined by the equation $g(x) = x^4 - x^3 + y^2 = 0$. Then X is a compact subset of $\mathbb{R}^2$ with a singularity at the origin.

EXERCISE 5.5. Show that the function $f(x) = x$ is nonnegative on X , but f is not “obviously nonnegative”.

There has been extensive work on additional conditions under which nonnegative polynomials are guaranteed to be “obviously nonnegative” [17][18]. This is sometimes referred to as “finite convergence” of the sum of squares hierarchy.

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