Sum of Squares Programs and Polynomial Inequalities

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1 Introduction

Consider a given system of polynomial equations and inequalities, for instance:

$$\begin{aligned} f_1(x_1, x_2) &:= \quad x_1^2 + x_2^2 - 1 = 0, \\ g_1(x_1, x_2) &:= \quad 3\,x_2 - x_1^3 - 2 \geq 0, \\ g_2(x_1, x_2) &:= \quad x_1 - 8\,x_2^3 \geq 0. \end{aligned} \tag{1}$$

How can one find real solutions (x_1, x_2)? How to *prove* that they do not exist? And if the solution set is nonempty, how to optimize a polynomial function over this set?

Until a few years ago, the default answer to these and similar questions would have been that the possible nonconvexity of the feasible set and/or objective function precludes any kind of analytic global results. Even today, the methods of choice for most practitioners would probably employ mostly local techniques (Newton's and its variations), possibly complemented by a systematic search using deterministic or stochastic exploration of the solution space, interval analysis or branch and bound.

However, very recently there have been renewed hopes for the efficient solution of specific instances of this kind of problems. The main reason is the appearance of methods that combine in a very interesting fashion ideas from *real algebraic geometry* and *convex optimization* [27, 30, 21]. As we will see, these methods are based on the intimate links between sum of squares decompositions for multivariate polynomials and semidefinite programming (SDP).

In this note we outline the essential elements of this new research approach as introduced in [30, 32], and provide pointers to the literature. The centerpieces will be the following two facts about multivariate polynomials and systems of polynomials inequalities:

> Sum of squares decompositions can be computed using semidefinite programming.
>
> The search for infeasibility certificates is a convex problem. For bounded degree, it is an SDP.

In the rest of this note, we define the basic ideas needed to make the assertions above precise, and explain the relationship with earlier techniques. For this, we will introduce sum of squares polynomials and the notion of *sum of squares programs*. We then explain how to use them to provide infeasibility certificates for systems of polynomial inequalities, finally putting it all together via the surprising connections with optimization.

On a related but different note, we mention a growing body of work also aimed at the integration of ideas from algebra and optimization, but centered instead on integer programming and toric ideals; see for instance [7, 42, 3] and the volume [1] as starting points.

2 Sums of squares and SOS programs

Our notation is mostly standard. The *monomial* x^α associated to the n-tuple $\alpha = (\alpha_1, \ldots, \alpha_n)$ has the form $x_1^{\alpha_1} \ldots x_n^{\alpha_n}$, where $\alpha_i \in \mathbb{N}_0$. The *degree* of a monomial x^α is the nonnegative integer $\sum_{i=1}^n \alpha_i$. A *polynomial* is a finite linear combination of monomials $\sum_{\alpha \in S} c_\alpha x^\alpha$, where the coefficients c_α are real. If all the monomials have the same degree d, we will call the polynomial *homogeneous* of degree d. We denote the ring of multivariate polynomials with real coefficients in the indeterminates $\{x_1, \ldots, x_n\}$ as $\mathbb{R}[x]$.

A multivariate polynomial is a *sum of squares* (SOS) if it can be written as a sum of squares of other polynomials, i.e.,

$$p(x) = \sum_i q_i^2(x), \quad q_i(x) \in \mathbb{R}[x].$$

If $p(x)$ is SOS then clearly $p(x) \geq 0$ for all x. In general, SOS decompositions are not unique.

Example 1 *The polynomial $p(x_1, x_2) = x_1^2 - x_1 x_2^2 + x_2^4 + 1$ is SOS. Among infinite others, it has the decompositions:*

$$\begin{aligned} p(x_1, x_2) &= \frac{3}{4}(x_1 - x_2^2)^2 + \frac{1}{4}(x_1 + x_2^2)^2 + 1 \\ &= \frac{1}{9}(3 - x_2^2)^2 + \frac{2}{3}x_2^2 + \\ &\quad + \frac{1}{288}(9x_1 - 16x_2^2)^2 + \frac{23}{32}x_1^2. \end{aligned}$$

The sum of squares condition is a quite natural sufficient test for polynomial nonnegativity. Its rich mathematical structure has been analyzed in detail in the past, notably by Reznick and his coauthors [6, 38], but until very recently the computational implications have not been fully explored. In the last few years there have been some very interesting new developments surrounding sums of squares, where several independent approaches have produced a wide array of results linking foundational questions in algebra with computational possibilities arising from convex optimization. Most of them employ semidefinite programming (SDP) as the essential computational tool. For completeness, we present in the next paragraph a brief summary of SDP.

Semidefinite programming SDP is a broad generalization of linear programming (LP), to the case of symmetric matrices. Denoting by $\mathcal{S}^n$ the space of $n \times n$ symmetric matrices, the standard SDP primal-dual formulation is:

$$\min_X \; C \bullet X \qquad \text{s.t.} \begin{cases} A_i \bullet X = b_i, & i = 1, \ldots, m \\ X \succeq 0 \end{cases}$$

$$\max_y \; b^T y, \qquad \text{s.t.} \; \textstyle\sum_{i=1}^m A_i y_i \preceq C \tag{2}$$

where $A_i, C, X \in \mathcal{S}^n$ and $b, y \in \mathbb{R}^m$. The matrix inequalities are to be interpreted in the partial order induced by the positive semidefinite cone, i.e., $X \succeq Y$ means that $X - Y$ is a positive semidefinite matrix. Since its appearance almost a decade ago (related ideas, such as eigenvalue optimization, have been around for decades) there has been a true "revolution" in computational methods, supported by an astonishing variety of applications. By now there are several excellent introductions to SDP; among them we mention the well-known work of Vandenberghe and Boyd [44] as a wonderful survey of the basic theory and initial applications, and the handbook [45] for a comprehensive treatment of the many aspects of the subject. Other survey works, covering different complementary aspects are the early work by Alizadeh [2], Goemans [15], as well as the more recent ones due to Todd [43], De Klerk [9] and Laurent and Rendl [25].

From SDP to SOS The main object of interest in semidefinite programming is

> **Quadratic** forms, that are **positive semidefinite**.

When attempting to generalize this construction to homogeneous polynomials of higher degree, an unsurmountable difficulty that appears is the fact that deciding nonnegativity for quartic or higher degree forms is an NP-hard problem. Therefore, a computational tractable replacement for this is the following:

> **Even degree** polynomials, that are **sums of squares**.

Sum of squares programs can then be defined as optimization problems over affine families of polynomials, subject to SOS contraints. Like SDPs, there are several possible equivalent descriptions. We choose below a free variables formulation, to highlight the analogy with the standard SDP dual form discussed above.

Definition 1 *A sum of squares program has the form*

$$\begin{array}{ll} \max_y & b_1 y_1 + \cdots + b_m y_m \\ s.t. & P_i(x, y) \text{ are SOS}, \quad i = 1, \ldots, p \end{array}$$

where $P_i(x, y) := C_i(x) + A_{i1}(x) y_1 + \cdots + A_{im}(x) y_m$, and the C_i, A_{ij} are given polynomials in the variables x_i.

SOS programs are very useful, since they directly operate with polynomials as their basic objects, thus providing a quite natural modelling formulation for many problems. Among others, examples for this are the search for Lyapunov functions for nonlinear systems [30, 28], probability inequalities [4], as well as the relaxations in [30, 21] discussed below.

Interestingly enough, despite their apparently greater generality, sum of squares programs are in fact *equivalent* to SDPs. On the one hand, by choosing the polynomials $C_i(x), A_{ij}(x)$ to be quadratic forms, we recover standard SDP. On the other hand, as we will see in the next section, it is possible to exactly embed every SOS program into a larger SDP. Nevertheless, the rich algebraic structure of SOS programs will allow us a much deeper understanding of their special properties, as well as enable customized, more efficient algorithms for their solution [26].

Furthermore, as illustrated in later sections, there are numerous questions related to some foundational issues in nonconvex optimization that have simple and natural formulations as SOS programs.

SOS programs as SDPs Sum of squares programs can be written as SDPs. The reason is the following theorem:

Theorem 1 *A polynomial $p(x)$ is SOS if and only if $p(x) = z^T Q z$, where z is a vector of monomials in the x_i variables, $Q \in \mathcal{S}^N$ and $Q \succeq 0$.*

In other words, every SOS polynomial can be written as a quadratic form in a set of monomials of cardinality N, with the corresponding matrix being positive semidefinite. The vector of monomials z (and therefore N) in general depends on the degree and sparsity pattern of $p(x)$. If $p(x)$ has n variables and total degree $2d$, then z can always be chosen as a subset of the set of monomials of degree less than or equal to d, of cardinality $N = \binom{n+d}{d}$.

Example 2 *Consider again the polynomial from Example 1. It has the representation*

$$p(x_1, x_2) = \frac{1}{6}\begin{bmatrix} 1 \\ x_2 \\ x_2^2 \\ x_1 \end{bmatrix}^T \begin{bmatrix} 6 & 0 & -2 & 0 \\ 0 & 4 & 0 & 0 \\ -2 & 0 & 6 & -3 \\ 0 & 0 & -3 & 6 \end{bmatrix} \begin{bmatrix} 1 \\ x_2 \\ x_2^2 \\ x_1 \end{bmatrix},$$

and the matrix in the expression above is positive semidefinite.

In the representation $f(x) = z^T Q z$, for the right- and left-hand sides to be identical, all the coefficients of the corresponding polynomials should be equal. Since Q is simultaneously constrained by linear equations and a positive semidefiniteness condition, the problem can be easily seen to be directly equivalent to an SDP feasibility problem in the standard primal form (2).

Given a SOS program, we can use the theorem above to construct an equivalent SDP. The conversion step is fully algorithmic, and has been implemented, for instance, in the SOSTOOLS [36] software package. Therefore, we can in principle directly apply all the available numerical methods for SDP to solve SOS programs.

SOS and convexity The connection between sum of squares decompositions and convexity can be traced back to the work of N. Z. Shor [39]. In this 1987 paper, he essentially outlined the links between Hilbert's 17th problem and a class of convex bounds for unconstrained polynomial optimization problems. Unfortunately, the approach went mostly unnoticed for several years, probably due to the lack of the convenient framework of SDP.

3 Algebra and optimization

A central theme throughout convex optimization is the idea of *infeasibility certificates* (for instance, in LP via Farkas' lemma), or equivalently, *theorems of the alternative*. As we will see, the key link relating algebra and optimization in this approach is the fact that infeasibility can *always* be certified by a particular algebraic identity, whose solution is found via convex optimization.

We explain some of the concrete results in Theorem 5, after a brief introduction to two algebraic concepts, and a comparison with three well-known infeasibility certificates.

Ideals and cones For later reference, we define here two important algebraic objects: the *ideal* and the *cone* associated with a set of polynomials:

Definition 2 *Given a set of multivariate polynomials $\{f_1, \ldots, f_m\}$, let*

$$\mathbf{ideal}(f_1, \ldots, f_m) := \{f \mid f = \sum_{i=1}^m t_i f_i, \quad t_i \in \mathbb{R}[x]\}.$$

Definition 3 *Given a set of multivariate polynomials $\{g_1, \ldots, g_m\}$, let*

$$\mathbf{cone}(g_1, \ldots, g_m) := \{g \mid g = s_0 + \sum_{\{i\}} s_i g_i + \\ + \sum_{\{i,j\}} s_{ij} g_i g_j + \sum_{\{i,j,k\}} s_{ijk} g_i g_j g_k + \cdots\},$$

where each term in the sum is a squarefree product of the polynomials g_i, with a coefficient $s_\alpha \in \mathbb{R}[x]$ that is a sums of squares. The sum is finite, with a total of $2^m - 1$ terms, corresponding to the nonempty subsets of $\{g_1, \ldots, g_m\}$.

These algebraic objects will be used for deriving *valid inequalities*, which are logical consequences of the given constraints. Notice that by construction, every polynomial in $\mathbf{ideal}(f_i)$ vanishes in the solution set of $f_i(x) = 0$. Similarly, every element of $\mathbf{cone}(g_i)$ is clearly nonnegative on the feasible set of $g_i(x) \geq 0$.

The notions of *ideal* and *cone* as used above are standard in real algebraic geometry; see for instance [5]. In particular, the cones are also referred to as a *preorders*. Notice that as geometric objects, ideals are affine sets, and cones are closed under convex combinations and nonnegative scalings (i.e., they are actually cones in the convex geometry sense). These convexity properties, coupled with the relationships between SDP and SOS, will be key for our developments in the next section.

Infeasibility certificates If a system of equations does not have solutions, how do we *prove* this fact? A very useful concept is that of *certificates*, which are formal algebraic identities that provide irrefutable evidence of the inexistence of solutions.

We briefly illustrate some well-known examples below. The first two deal with linear systems and polynomial equations over the complex numbers, respectively.

Theorem 2 (Range/kernel)

$$
\begin{array}{c}
Ax = b \quad \textit{is infeasible} \\
\Updownarrow \\
\exists\, \mu \;\; s.t. \;\; A^T\mu = 0, \; b^T\mu = -1.
\end{array}
$$

Theorem 3 (Hilbert's Nullstellensatz) *Let $f_i(z), \ldots, f_m(z)$ be polynomials in complex variables $z_1, \ldots, z_n$. Then,*

$$
\begin{array}{c}
f_i(z) = 0 \quad (i = 1, \ldots, m) \quad \textit{is infeasible in } \mathbb{C}^n \\
\Updownarrow \\
-1 \in \mathbf{ideal}(f_1, \ldots, f_m).
\end{array}
$$

Each of these theorems has an "easy" direction. For instance, for the first case, given the multipliers μ the infeasibility is obvious, since

$$
Ax = b \quad \Rightarrow \quad \mu^T A x = \mu^T b \quad \Rightarrow \quad 0 = -1,
$$

which is clearly a contradiction.

The two theorems above deal only with the case of *equations*. The inclusion of inequalities in the problem formulation poses additional algebraic challenges, because we need to work on an *ordered* field. In other words, we need to take into account special properties of the *reals*, and not just the complex numbers.

For the case of *linear* inequalities, LP duality provides the following characterization:

Theorem 4 (Farkas lemma)

$$
\begin{array}{c}
\left\{ \begin{array}{rcl} Ax + b & = & 0 \\ Cx + d & \geq & 0 \end{array} \right. \quad \textit{is infeasible} \\
\Updownarrow \\
\exists\, \lambda \geq 0, \, \mu \;\; s.t. \; \left\{ \begin{array}{rcl} A^T\mu + C^T\lambda & = & 0 \\ b^T\mu + d^T\lambda & = & -1. \end{array} \right.
\end{array}
$$

Although not widely known in the optimization community until recently, it turns out that similar certificates do exist for *arbitrary* systems of polynomial equations and inequalities over the reals. The result essentially appears in this form in [5], and is due to Stengle [40].

Theorem 5 (Positivstellensatz)

$$
\begin{array}{c}
\left\{ \begin{array}{rcll} f_i(x) & = & 0, & (i = 1, \ldots, m) \\ g_i(x) & \geq & 0, & (i = 1, \ldots, p) \end{array} \right. \quad \textit{is infeasible in } \mathbb{R}^n \\
\Updownarrow \\
\exists\, F(x), G(x) \in \mathbb{R}[x] \;\; s.t. \; \left\{ \begin{array}{l} F(x) + G(x) = -1 \\ F(x) \in \mathbf{ideal}(f_1, \ldots, f_m) \\ G(x) \in \mathbf{cone}(g_1, \ldots, g_p). \end{array} \right.
\end{array}
$$

The theorem states that for every infeasible system of polynomial equations and inequalities, there exists a simple algebraic identity that directly certifies the inexistence of real solutions. By construction, the evaluation of the polynomial $F(x) + G(x)$ at any feasible point should produce a nonnegative number. However, since this expression is identically equal to the polynomial -1, we arrive at a contradiction. Remarkably, the Positivstellensatz holds under *no assumptions* whatsoever on the polynomials.

The use of the German word "Positivstellensatz" is standard in the field, and parallels the classical "Nullstellensatz" (roughly, "theorem of the zeros") obtained by Hilbert in 1901 and mentioned above.

In the worst case, the degree of the infeasibility certificates $F(x), G(x)$ could be high (of course, this is to be expected, due to the NP-hardness of the original question). In fact, there are a few explicit counterexamples where large degree refutations are necessary [16]. Nevertheless, for many problems of practical interest, it is often the case that it is possible to prove infeasibility using relatively low-degree certificates. There is significant numerical evidence that this is the case, as indicated by the large number of practical applications where SDP relaxations based on these techniques have provided solutions of very high quality.

Degree \ Field	Complex	Real
Linear	*Range/Kernel* Linear Algebra	*Farkas Lemma* Linear Programming
Polynomial	*Nullstellensatz* Bounded degree: Linear Algebra Groebner bases	*Positivstellensatz* Bounded degree: SDP

Table 1: Infeasibility certificates and associated computational techniques.

Of course, we are concerned with the effective computation of these certificates. For the cases of Theorems 2–4, the corresponding refutations can be obtained using either linear algebra, linear programming, or Groebner bases techniques (see [8] for a superb introduction to Groebner bases).

For the Positivstellensatz, we notice that the cones and ideals as defined above are always *convex sets* in the space of polynomials. A key consequence is that the conditions in Theorem 5 for a certificate to exist are therefore *convex*, regardless of any convexity property of the original problem. Even more, the same property holds if we consider only bounded-degree sections, i.e., the intersection with the set of polynomials of degree less than or equal to a given number D. In this case, the conditions in the P-satz have *exactly* the form of a SOS program! Of course, as discussed earlier, this implies that we can find bounded-degree certificates, by solving semidefinite programs. In Table 1 we present a summary of the infeasibility certificates discussed, and the associated computational techniques.

Example 3 *Consider again the system (1). We will show that it has no solutions $(x_1, x_2) \in \mathbb{R}^2$. By the P-satz, the system is infeasible if and only if there exist polynomials $t_1, s_0, s_1, s_2, s_{12} \in \mathbb{R}[x_1, x_2]$ that satisfy*

$$\underbrace{f_1 \cdot t_1}_{\mathbf{ideal}(f_1)} + \underbrace{s_0 + s_1 \cdot g_1 + s_2 \cdot g_2 + s_{12} \cdot g_1 \cdot g_2}_{\mathbf{cone}(g_1, g_2)} \equiv -1, \tag{3}$$

where s_0, s_1, s_2 and s_{12} are SOS.

A SOS relaxation is obtained by looking for solutions where all the terms in the left-hand side have degree less than or equal to D. For each fixed integer $D > 0$ this can be tested by semidefinite programming. For instance, for $D = 4$ we find the certificate

$$t_1 = -3x_1^2 + x_1 - 3x_2^2 + 6x_2 - 2,$$

$$s_1 = 3, \qquad s_2 = 1, \qquad s_{12} = 0,$$

$$\begin{aligned} s_0 &= 3x_1^4 + 2x_1^3 + 6x_1^2x_2^2 - 6x_1^2x_2 - x_1^2 - x_1x_2^2 + \\ &\qquad + 3x_2^4 + 2x_2^3 - x_2^2 - 3x_2 + 3 \\ &= \frac{1}{2} z^T \begin{bmatrix} 6 & -3 & -3 & 0 & 0 & -3 \\ -3 & 4 & 2 & 0 & 1 & 1 \\ -3 & 2 & 6 & -2 & 0 & -3 \\ 0 & 0 & -2 & 4 & -7 & 2 \\ 0 & 1 & 0 & -7 & 18 & 0 \\ -3 & 1 & -3 & 2 & 0 & 6 \end{bmatrix} z, \end{aligned}$$

where

$$z = \begin{bmatrix} 1 & x_2 & x_2^2 & x_1 & x_1x_2 & x_1^2 \end{bmatrix}^T.$$

The resulting identity (3) thus certifies the inconsistency of the system $\{f_1 = 0,\ g_1 \ge 0,\ g_2 \ge 0\}$.

As outlined in the preceding paragraphs, there is a direct connection going from general polynomial optimization problems to SDP, via P-satz infeasibility certificates. Pictorially, we have the following:

$$\begin{array}{c} \text{Polynomial systems} \\ \Downarrow \\ \text{P-satz certificates} \\ \Downarrow \\ \text{SOS programs} \\ \Downarrow \\ \text{SDP} \end{array}$$

Even though we have discussed only feasibility problems, there are obvious straightforward connections with optimization. By considering the emptiness of the sublevel sets of the objective function, sequences of converging bounds indexed by certificate degree can be directly constructed.

4 Further developments and applications

We have covered only the core elements of the SOS/SDP approach. Much more is known, and even more still remains to be discovered, both in the theoretical and computational ends. Some specific issues are discussed below.

Exploiting structure and numerical computation To what extent can the inherent structure in SOS programs be exploited for efficient computations? Given the algebraic origins of the formulation, it is perhaps not surprising to find that several intrinsic properties of the input polynomials can be profitably used [29]. In this direction, symmetry reduction techniques have been employed by Gatermann and Parrilo in [14] to provide novel representations for symmetric polynomials. Kojima, Kim and Waki [20] have recently presented some results for sparse polynomials. Parrilo [31] and Laurent [23] have analyzed the further simplifications that occur when the inequality constraints define a zero-dimensional ideal.

Other relaxations Lasserre [21, 22] has independently introduced a scheme for polynomial optimization dual to the one described here, but relying on Putinar's representation theorem for positive polynomials rather than the P-satz. There are very interesting relationship between SOS-based methods and earlier relaxation and approximation schemes, such as Lovász-Schrijver and Sherali-Adams. Laurent [24] analyzes this in the specific case of 0-1 programming.

Implementations The software SOSTOOLS [36] is a free, third-party MATLAB[1] toolbox for formulating and solving general sum of squares programs. The related sofware Gloptipoly [17] is oriented toward global optimization problems. In their current version, both use the SDP solver SeDuMi [41] for numerical computations.

Approximation properties There are several important open questions regarding the provable quality of the approximations. In this direction, De Klerk and Pasechnik [11] have established some approximations guarantees of a SOS-based scheme for the approximation of the stability number of a graph. Recently, De Klerk, Laurent and Parrilo [10] have shown that a related procedure based on a result by Pólya provides a polynomial-time approximation scheme (PTAS) for polynomial optimization over simplices.

Applications There are many exciting applications of the ideas described here. The descriptions that follow are necessarily brief; our main objective here is to provide the reader with some good starting points to this growing literature.

In systems and control theory, the techniques have provided some of the best available analysis and design methods, in areas such as nonlinear stability and robustness analysis [30, 28, 35], state feedback control [19], fixed-order controllers [18], nonlinear synthesis [37], and model validation [34]. Also, there have been interesting recent applications in geometric theorem proving [33] and quantum information theory [12, 13].

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