Minimizing Polynomials Over Semialgebraic Sets

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Abstract

This paper concerns a method for finding the minimum of a polynomial on a semialgebraic set, i.e., a set in \( \mathbb{R}^m \) defined by finitely many polynomial equations and inequalities, using the Karush-Kuhn-Tucker (KKT) system and sum of squares (SOS) relaxations. This generalizes results in the recent paper [15], which considers minimizing polynomials on algebraic sets, i.e., sets in \( \mathbb{R}^m \) defined by finitely many polynomial equations. Most of the theorems and conclusions in [15] generalize to semialgebraic sets, even in the case where the semialgebraic set is not compact. We discuss the method in some special cases, namely, when the semialgebraic set is contained in the nonnegative orthant \( \mathbb{R}^n_+ \) or in box constraints \([a, b]^n\). These constraints make the computations more efficient.

Keywords: polynomials, semialgebraic sets, Karush-Kuhn-Tucker (KKT) system, Sum of Squares (SOS).

1. Introduction

In this paper, we consider the optimization problem

\[
\begin{align*}
f^* &= \min f(x) \\
\text{s.t.} & \quad g_i(x) = 0, \quad i = 1, \ldots, s, \\
& \quad h_j(x) \geq 0, \quad j = 1, \ldots, t
\end{align*}
\]

where \( x = [x_1, \ldots, x_n]^T \in \mathbb{R}^n \) and \( f(x), g_i(x), h_j(x) \in \mathbb{R}[x] \) (the ring of real multivariate polynomials in \( x \)). Let \( \mathcal{F} \) be the feasible region, i.e., the subset of \( \mathbb{R}^n \) which satisfies constraints \( \text{(1.2)} - \text{(1.3)} \); \( \mathcal{F} \) is a semialgebraic set. Many optimization problems in practice can be formulated as \( \text{(1.1)} - \text{(1.3)} \). Finding the global optimal solutions to \( \text{(1.1)} - \text{(1.3)} \) is an NP-hard problem, even if \( f(x) \) is quadratic and \( g_i, h_j \) are linear. For instance, the Maximum-Cut problem for graphs is of this form, and it is NP-hard [7].

Recently, the techniques of sum of squares (SOS) relaxations and moment matrix methods have made it possible to find the global optimal solutions to \( \text{(1.1)} - \text{(1.3)} \) by approximating nonnegative polynomials with SOS polynomials, which allows the problem to be implemented as a semidefinite program. For more details about these methods and their applications, see [11, 12, 15, 17, 18]. To prove the convergence of these methods, it is often

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necessary to assume that the feasible region \( \mathcal{F} \) is compact or even finite. In \[22\], it is shown that SOS relaxations can solve \( \text{1.1}-\text{1.3} \) globally in finitely many steps in the case where \( \{ x \in \mathbb{C}^n : g_1(x) = \cdots = g_s(x) = 0 \} \) is finite and the ideal \( \langle g_1(x), \ldots, g_s(x) \rangle \) is radical. If we only assume that \( \{ x \in \mathbb{C}^n : g_1(x) = \cdots = g_s(x) = 0 \} \) is finite, it is shown in \[12\] that the moment matrix method can solve \( \text{1.1}-\text{1.3} \) globally in finitely many steps. Finally, if \( \mathcal{F} \) is compact and the set of polynomials \( \{ g_i, h_i \} \) satisfies an additional assumption (see Theorem \[2.4\]), then arbitrarily close lower bounds for \( f^* \) can be obtained by SOS relaxations or moment matrix methods \[11\]. In this case, the convergence is asymptotic, however little is known about the errors in the bounds.

The above global optimization methods are based on representation theorems from real algebraic geometry for polynomials positive and nonnegative on semialgebraic sets. On the other hand, the traditional local methods in optimization often follow the first order optimality conditions (zero gradient in the unconstrained case or the Karush-Kuhn-Tucker (KKT) system in the constrained case). The underlying idea in \[15\] and the present paper is to combine these two types of methods in order to more efficiently solve \( \text{1.1}-\text{1.3} \) globally. In \[15\], SOS relaxations are applied on the gradient ideal \( \mathcal{I}_{\text{grad}} \) (the ideal generated by all the partial derivatives of \( f(x) \)) in the unconstrained case, and on the KKT ideal \( \mathcal{I}_{\text{KKT}} \) in the constrained case, where only equality constraints are allowed. When \( \mathcal{I}_{\text{grad}} \) or \( \mathcal{I}_{\text{KKT}} \) is radical, which is generically true in practice, the method in \[15\] can solve the optimization \( \text{1.1}-\text{1.3} \) globally; otherwise, arbitrarily close lower bounds of \( f^* \) can be obtained. No assumptions about \( \mathcal{F} \) are made, i.e., it need not be finite or even compact.

The convergence of the method in \[15\] assumes that the constraints are algebraic sets. If there are any inequality constraints, \( \mathcal{F} \) is no longer algebraic but only semialgebraic and the proof in \[15\] does not work. The motivation of this paper is to generalize the method in \[15\] to handle semialgebraic constraints.

The KKT system of problem \( \text{1.1}-\text{1.3} \) is

\[
F \triangleq \nabla f(x) + \sum_{i=1}^s \lambda_i \nabla g_i(x) - \sum_{j=1}^t \nu_j \nabla h_j(x) = 0,
\]

\[
h_j(x) \geq 0, \nu_j h_j(x) = 0, \quad j = 1, \cdots, t,
\]

\[
g_i(x) = 0, \quad i = 1, \cdots, s,
\]

where vectors \( \lambda = [\lambda_1 \cdots \lambda_s]^T \) and \( \nu = [\nu_1 \cdots \nu_t]^T \) are called Lagrange multipliers. See \[16\] for some regularity conditions that make the KKT system hold at local or global minimizers. For an example where the KKT system fails, see Example \[14\] in Section 4.

Note that we do not require \( \nu \geq 0 \) in the above; this makes the SOS relaxations simpler and does not affect the convergence of the method, since omitting the constraint \( \nu \geq 0 \) means simply that there are more feasible points for \( \text{1.1}-\text{1.3} \), including maxima as well as minima. But since we minimize over this larger set, we get the same minima. Minimizing over this larger set makes our problem easier, because it reduces the number of inequality constraints, which as we will see greatly lowers the complexity of our algorithm.

Let \( f_{\text{KKT}} \) be the global minimum of \( f(x) \) over the KKT system defined by \( \text{1.1}-\text{1.3} \). Assume the KKT system holds at the global minimizers. Then we claim that \( f^* = f_{\text{KKT}} \).

First, \( f^* \leq f_{\text{KKT}} \) follows immediately from the fact that all \( x \) in the KKT system are feasible. Now let \( x^* \) be a global minimizer such that \( f(x^*) = f^* \), then by assumption, there exist Lagrange multipliers \( \lambda^* \) and \( \nu^* \geq 0 \) such that \( (x^*, \lambda^*, \nu^*) \) satisfies the above KKT system. Thus \( f^* \geq f_{\text{KKT}} \) and hence they are equal.
Define the KKT ideal $I_{KKT}$ and its varieties as follows:

$$I_{KKT} = \langle F_1, \cdots, F_n, g_1, \cdots, g_s, \nu h_1, \cdots, \nu h_t \rangle,$$

$$V_{KKT} = \{(x, \lambda, \nu) \in \mathbb{C}^n \times \mathbb{C}^s \times \mathbb{C}^t : p(x, \lambda, \nu) = 0, \ \forall p \in I_{KKT} \},$$

$$V_{KKT}^\mathbb{R} = \{(x, \lambda, \nu) \in \mathbb{R}^n \times \mathbb{R}^s \times \mathbb{R}^t : p(x, \lambda, \nu) = 0, \ \forall p \in I_{KKT} \}.$$

Here $F = [F_1, \cdots, F_n]^T$ is defined in [14]. Let

$$\mathcal{H} = \{(x, \lambda, \nu) \in \mathbb{R}^n \times \mathbb{R}^s \times \mathbb{R}^t : h_j(x) \geq 0, \ j = 1, \cdots, t \}.$$

The preorder cone $P_{KKT}$ associated with the KKT system is

$$P_{KKT} = \left\{ \sum_{\theta \in \{0,1\}^t} \sigma_\theta h_1^{\theta_1} h_2^{\theta_2} \cdots h_t^{\theta_t} \mid \sigma_\theta \text{ are SOS} \right\} + I_{KKT}.$$

The linear cone associated with the KKT system is

$$M_{KKT} = \left\{ \sigma_0 + \sum_{j=1}^{t} \sigma_j h_j \mid \sigma_0, \cdots, \sigma_t \text{ are SOS} \right\} + I_{KKT}.$$

Note that $I_{KKT} \subseteq M_{KKT} \subseteq P_{KKT} \subseteq \mathbb{R}[x, \lambda, \nu]$.

In solving SOS programs, we often set an upper bound on the degrees of the involved polynomials. Define the truncated KKT ideal

$$I_{N,KKT} = \left\{ \sum_{k=1}^{n} \phi_k F_k + \sum_{i=1}^{s} \psi_i g_i + \sum_{j=1}^{t} \psi_j \nu_j h_j \mid \deg(\phi_k F_k), \deg(\psi_i g_i), \deg(\psi_j \nu_j h_j) \leq N \right\},$$

and truncated preorder and linear cones

$$P_{N,KKT} = \left\{ \sum_{\theta \in \{0,1\}^t} \sigma_\theta h_1^{\theta_1} h_2^{\theta_2} \cdots h_t^{\theta_t} \mid \deg(\sigma_\theta h_1^{\theta_1} \cdots h_t^{\theta_t}) \leq N \right\} + I_{N,KKT}.$$

$$M_{N,KKT} = \left\{ \sigma_0 + \sum_{j=1}^{t} \sigma_j h_j \mid \sigma_0, \cdots, \sigma_t \text{ are SOS} \right\} + I_{N,KKT}.$$

A sequence $\{p_N^*\}$ of lower bounds of [14], [15] can be obtained by the following SOS relaxations:

$$p_N^* = \max_{\gamma \in \mathbb{R}} \gamma \quad \text{s.t.} \quad f(x) - \gamma \in P_{N,KKT}. \quad (1.7)$$

Since $P_{N,KKT}$ has a summation over $2^t$ terms like $\sigma_\theta h_1^{\theta_1} h_2^{\theta_2} \cdots h_t^{\theta_t}$, it is usually very expensive to solve the SOS program [14], [15] in practice. So in practice, it is natural to replace the truncated preorder cone $P_{N,KKT}$ by truncated linear cone $M_{N,KKT}$, which leads to the SOS relaxations:

$$f_N^* = \max_{\gamma \in \mathbb{R}} \gamma \quad \text{s.t.} \quad f(x) - \gamma \in M_{N,KKT}. \quad (1.9)$$
Thus we have the increasing sequences of lower bounds \( \{f_N^*\}_{N=2}^\infty \) and \( \{p_N^*\}_{N=2}^\infty \) such that 
\( f_N^* \leq p_N^* \leq f^* \).

The following notation is used throughout: We denote by \( \deg(p) \) the degree of a polynomial \( p \). The vector inequality \( u \leq v \) for \( u, v \in \mathbb{R}^n \) is defined component-wise, i.e., \( u_i \leq v_i \) for each \( i \).

\[ [u, v]_n \] denotes the set of all vectors \( w \in \mathbb{R}^n \) such that \( u \leq w \leq v \).

This paper is organized as follows. Section 2 is a review of some fundamental results from algebraic geometry. In Section 3 we discuss the representation of the polynomial \( f(x) \) in the cones \( M_{KKT} \) and \( P_{KKT} \). We analyze the convergence of the lower bounds \( \{p_N^*\} \) and \( \{f_N^*\} \) in Section 4. In Section 5, we consider some special cases of inequality constraints, in particular, the nonnegative orthant \( \mathbb{R}_n^+ \) and the box \([a, b]_n\). Section 6 draws conclusions.

2. Preliminaries

This section will introduce some basic notions from algebraic geometry needed for our discussion. Readers may consult \([1, 2, 4]\) for more details. In this section, all polynomials are in the indeterminate \( x = (x_1, \ldots, x_m) \) for the simplicity of notation. Here \( x \) is not the “\( x \)” in the Introduction, but rather a generic indeterminate. In later sections, \( x \) will be again the “\( x \)” in \([1, 2, 3]\), and all polynomials will be in the variables \((x, \lambda, \nu)\), unless explicitly stated otherwise.

We write \( \mathbb{R}[x] = \mathbb{R}[x_1, \ldots, x_m] \) for the ring of polynomials in indeterminates \( x = (x_1, \ldots, x_m) \) with real coefficients. A polynomial \( p \in \mathbb{R}[x] \) is \( \textit{SOS} \) if it can be written as a sum of squares of polynomials in \( \mathbb{R}[x] \). A subset \( I \) of \( \mathbb{R}[x] \) is an \( \textit{ideal} \) if \( p \cdot q \in I \) for any \( p \in I \) and \( q \in \mathbb{R}[x] \). For \( p_1, \ldots, p_r \in \mathbb{R}[x] \), \( \langle p_1, \ldots, p_r \rangle \) denotes the smallest ideal containing the \( p_i \). Equivalently, \( \langle p_1, \ldots, p_r \rangle \) is the set of all polynomials that are polynomial linear combinations of the \( p_i \).

Every ideal arises in this way:

**Theorem 2.1 (Hilbert Basis Theorem)**

Every ideal \( I \subseteq \mathbb{R}[x] \) has a finite generating set, i.e., \( I = \langle p_1, \ldots, p_r \rangle \) for some \( p_1, \ldots, p_r \in I \).

The \textit{variety} of an ideal \( I \) is the set of all common \textit{complex} zeros of the polynomials in \( I \):

\[
V(I) = \{ X \in \mathbb{C}^m : p(X) = 0 \text{ for all } p \in I \}.
\]

The subset of all real points in \( V(I) \) is the \textit{real variety} of \( I \). It is denoted

\[
V^\mathbb{R}(I) = \{ X \in \mathbb{R}^m : p(X) = 0 \text{ for all } p \in I \}.
\]

If \( I = \langle p_1, \ldots, p_r \rangle \) then \( V(I) = V(p_1, \ldots, p_r) = \{ X \in \mathbb{C}^m : p_1(X) = \cdots = p_r(X) = 0 \} \). An ideal \( I \subseteq \mathbb{R}[x] \) is \textit{zero-dimensional} if its variety \( V(I) \) is a finite set. This condition is much stronger than requiring that the real variety \( V^\mathbb{R}(I) \) be a finite set. For example, \( I = \langle X_1^2 + X_2^2 \rangle \) is not zero-dimensional, however the real variety \( V^\mathbb{R}(I) = \{(0,0)\} \) consists of one point of the curve \( V(I) \).

A variety \( V \subseteq \mathbb{C}^m \) is \textit{irreducible} if there do not exist two proper subvarieties \( V_1, V_2 \subseteq V \) such that \( V = V_1 \cup V_2 \). The reader should note that in this paper, “irreducible” means that the set of \textit{complex} zeros cannot be written as a proper union of subvarieties defined by \textit{real} polynomials. Given a variety \( V \subseteq \mathbb{C}^m \), the set of all polynomials that vanish on \( V \) is an ideal

\[
I(V) = \{ p \in \mathbb{R}[x] : p(u) = 0 \text{ for all } u \in V \}.
\]

Given any ideal \( I \) of \( \mathbb{R}[x] \), its \textit{radical} is the ideal

\[
\sqrt{I} = \{ q \in \mathbb{R}[x] : q^\ell \in I \text{ for some } \ell \in \mathbb{N} \}.
\]

Note that \( I \subseteq \sqrt{I} \). We say that \( I \) is a \textit{radical ideal} if \( \sqrt{I} = I \). Clearly, the ideal \( I(V) \) defined by a variety \( V \) is a radical ideal. The following theorems offer a converse to this observation:
Theorem 2.2 (Hilbert’s Weak Nullstellensatz)
If I is an ideal in \( \mathbb{R}[x] \) such that \( V(I) = \emptyset \) then \( 1 \in I \).

Theorem 2.3 (Hilbert’s Strong Nullstellensatz)
If I is an ideal in \( \mathbb{R}[x] \) then \( I(V(I)) = \sqrt{I} \).

Remark. Theorems 2.2 and 2.3 are normally stated for ideals in \( \mathbb{C}[x] \). However, keeping in mind that \( V(I) \) lies in \( \mathbb{C}^m \), they hold as stated.

In real algebraic geometry, we are also interested in subsets of \( \mathbb{R}^m \) of the form

\[
S = \{ X \in \mathbb{R}^m : p_1(X) = \cdots = p_r(X) = 0, q_1(X) \geq 0, \ldots, q_t(X) \geq 0 \},
\]

where \( p_i, q_j \in \mathbb{R}[x] \). Such \( S \) is called a basic closed semialgebraic set. Given \( S \) as above, the preorder and linear cones associated with \( S \) are defined as

\[
P(S) = \left\{ \sum_{\theta \in \{0,1\}^t} \sigma_\theta(X) q_1^{\theta_1}(X) \cdots q_t^{\theta_t}(X) \bigg| \sigma_0, \ldots, \sigma_\ell \text{ are SOS} \right\} + \langle p_1, \ldots, p_r \rangle
\]

\[
M(S) = \left\{ \sigma_0(X) + \sum_{j=1}^r q_j(X)\sigma_j(X) \bigg| \sigma_0, \sigma_1, \ldots, \sigma_\ell \text{ are SOS} \right\} + \langle p_1, \ldots, p_r \rangle.
\]

A linear cone or preorder \( M \) is archimedean if there exists \( \rho(x) \in M \) such that the set \( \{ X \in \mathbb{R}^m : \rho(X) \geq 0 \} \) is compact, equivalently, if there exists \( N \in \mathbb{N} \) such that \( N - \sum_{i=1}^m x_i^2 \in M \). Note that if \( M(S) \) or \( P(S) \) is archimedean, then \( S \) is compact.

Theorem 2.4 (Putinar, 25)
Suppose \( M(S) \) is archimedean, then every polynomial \( p(x) \) which is positive on \( S \) belongs to \( M(S) \).

Remark. There are examples of compact \( S \) for which \( M(S) \) is not archimedean and the conclusion of Putinar’s Theorem does not hold. In the case of the preorder \( P(S) \), it is a deep theorem of Schm" udgen [24] that if \( S \) is compact then \( P(S) \) is archimedean and any polynomial which is positive on \( S \) is in \( P(S) \). For this reason, the SOS relaxations \( f_N^r \) always converge to the minimum if \( S \) is compact, however, the relaxations \( f_N^r \) may not converge to the minimum. On the other hand, it is sometimes the case in practice that we know or can compute some \( N \in \mathbb{N} \) such that our semialgebraic set \( S \) is contained in the sphere \( \{ N - \sum_{i=1}^m x_i^2 \geq 0 \} \). In this case, we can simply add one additional constraint, namely \( N - \sum_{i=1}^m x_i^2 \geq 0 \), and force \( M(S) \) to be archimedean.

The sets \( P(S) \) and \( M(S) \) contain the ideal \( J = \langle p_1, \ldots, p_r \rangle \). If \( J \) is radical and \( V(J) \) is finite, we have the following theorem:

Theorem 2.5 (Parrilo, 22)
Let \( S \) and \( J \) be defined as in the above. Suppose \( J \) is a zero-dimensional radical ideal in \( \mathbb{R}[x] \). Then a polynomial \( w(x) \in \mathbb{R}[x] \) is nonnegative on \( S \) if and only if \( w(x) \in M(S) \).

For a semialgebraic set, there is a well-known generalization of the Hilbert’s Weak Nullstellensatz, see e.g. [3, 4.2.13].

Theorem 2.6
Suppose \( S \) and \( P(S) \) are defined as above, then \( S = \emptyset \) if and only if \( -1 \in P(S) \).

We need the following lemma from [15]:
Lemma 2.7 (Lemma 3.2, [15]) Let \( V_1, \ldots, V_r \) be pairwise disjoint varieties of \( \mathbb{C}^m \). Then there exist polynomials \( p_1, \ldots, p_r \in \mathbb{C}[X] \) such that \( p_i(V_j) = \delta_{ij} \), where \( \delta_{ij} \) is the Kronecker delta function.

Furthermore, if each \( V_i \) is conjugate symmetric, i.e., a point \( z \in \mathbb{C}^m \) belongs to \( V_i \) if and only if its complex conjugate \( \bar{z} \in V_i \), then the polynomials \( p_i \) can be chosen such that \( p_i \in \mathbb{R}[X] \), since we can replace \( p_i(x) \) by \( (p_i(X) + \bar{p}_i(X))/2 \), where \( \bar{p}_i(X) \) is obtained from \( p_i(X) \) by conjugating its coefficients.

3. Representations in \( P_{KKT} \) and \( M_{KKT} \)

In [15], it is shown that if a polynomial \( f(x) \in \mathbb{R}[x] \) is globally nonnegative and its gradient ideal is radical, then \( f(x) \) has a representation as a sum of squares modulo the gradient ideal. In this section we generalize this result to real polynomials which are nonnegative on the semialgebraic set \( V_{KKT} \): We will show that such polynomials have a representation in \( P_{KKT} \) modulo the ideal \( I_{KKT} \), if the later is radical. Furthermore, in some cases we can replace the preorder cone \( P_{KKT} \) by the linear cone \( M_{KKT} \).

Throughout this section we fix a polynomial \( f(x) \in \mathbb{R}[x] \) along with an optimization of the form (1.1)-(1.3) and the corresponding ideal \( I_{KKT} \), variety \( V_{KKT} \), the preorder cone \( P_{KKT} \) and the linear cone \( M_{KKT} \).

From Theorem 2.5 we immediately obtain the following representation theorem:

**Theorem 3.1** Assume \( I_{KKT} \) is zero-dimensional and radical. If \( f(x) \) is nonnegative on \( V_{KKT}^* \cap H \), then \( f(x) \) belongs to \( M_{KKT} \).

Using a proof similar to that of Theorem 3.1 in [15], we can remove the restrictive hypothesis that \( I_{KKT} \) be zero-dimensional, however to obtain the most general result we must replace the linear cone \( M_{KKT} \) by the preorder cone \( P_{KKT} \).

**Theorem 3.2** Assume \( I_{KKT} \) is radical. If \( f(x) \) is nonnegative on \( V_{KKT}^* \cap H \), then \( f(x) \) belongs to \( P_{KKT} \).

We need a generalization of a lemma from [15]:

**Lemma 3.3** Let \( W \) be an irreducible component of \( V_{KKT} \). Then \( f(x) \) is constant on \( W \).

**Proof.** We first note that

\[
F(x) = f(x) + \sum_{i=1}^s \lambda_i g_i(x) + \sum_{j=1}^t \nu_j h_j(x)
\]

is equal to \( f(x) \) on \( V_{KKT} \), and the right hand side has zero gradient on \( V_{KKT} \). With this in mind, the proof of [15, 3.3] generalizes easily to this case. \( \square \)

**Proof of Theorem 3.2.** Decompose \( V_{KKT} \) into its irreducible components, then by Lemma 3.3 \( f(x) \) is constant on each of them. Let \( W_0 \) be the union of all the components whose intersection with \( H \) is empty, and group together the components on which \( f(x) \) attains the same value, say \( W_1, \ldots, W_r \). Suppose \( f(x) = \alpha_i \geq 0 \) on \( W_i \).

We have \( V_{KKT} = W_0 \cup W_1 \cup \cdots \cup W_r \), and \( W_i \) are pairwise disjoint. Note that by our definition of irreducible, each \( W_i \) is conjugate symmetric. By Lemma 2.7 there exist polynomials \( p_0, p_1, \cdots, p_r \in \mathbb{R}[x, \lambda, \nu] \) such that \( p_i(W_j) = \delta_{ij} \), where \( \delta_{ij} \) is the Kronecker delta function.
By assumption, \( W_0 \cap \mathcal{H} = \emptyset \) and so, by Theorem 2.6, there are SOS polynomials \( v_{\theta} \ (\theta \in \{0, 1\}^t) \) such that

\[
-1 \equiv \sum_{\theta \in \{0, 1\}^t} v_{\theta} h_{1}^{\theta_1} \cdots h_{t}^{\theta_t} \overset{\text{def}}{=} v_0 \mod I(W_0).
\]

We have \( f = (f + \frac{1}{2})^2 - (f^2 + (\frac{1}{2})^2) = f_1 + v_0 f_2 \) for the SOS polynomials \( f_1 = (f + \frac{1}{2})^2, f_2 = f^2 + (\frac{1}{2})^2 \).

Then

\[
f \equiv f_1 + v_0 f_2 \equiv \sum_{\theta \in \{0, 1\}^t} u_{\theta} h_{1}^{\theta_1} \cdots h_{t}^{\theta_t} \overset{\text{def}}{=} q_0 \mod I(W_0)
\]

for some SOS polynomials \( u_{\theta} \ (\theta \in \{0, 1\}^t) \). Recall that \( f(x) = \alpha_i \), a constant, on each \( W_i (1 \leq i \leq r) \). Set \( q_i(x) = \sqrt{\alpha_i} \), then \( f(x) = q_i(x)^2 \) on \( I(W_i) \).

Now let \( q = q_0(p_0)^2 + \sum_{i=1}^r (q_i p_i)^2 \). Then \( f - q \) vanishes on \( \mathcal{V}_{KKT} \) and hence \( f - q \in I_{KKT} \) since \( I_{KKT} \) is radical. It follows that \( f \in P_{KKT} \). \( \square \)

Remark. The assumption that \( I_{KKT} \) is radical is needed in Theorem 3.4 as shown by Example 3.4 in [14]. However, when \( I_{KKT} \) is not radical, the conclusion also holds if \( f(x) \) is strictly positive on \( \mathcal{V}_{KKT}^* \).

**Theorem 3.4** If \( f(x) \) is strictly positive on \( \mathcal{V}_{KKT}^* \) \( \cap \mathcal{H} \) then \( f(x) \) belongs to \( P_{KKT} \).

*Proof.* As in the proof of Theorem 2.6, we decompose \( \mathcal{V}_{KKT} \) into subvarieties \( W_0, W_1, \ldots, W_r \) such that \( W_0 \cap \mathcal{H} = \emptyset \), and for \( i = 1, \ldots, r \), \( W_i \cap \mathcal{H} \neq \emptyset \) and \( f \) is constant on \( W_i \). Since each \( W_i, i > 0 \) contains at least one real point and \( f(x) > 0 \) on \( \mathcal{V}_{KKT}^* \), each \( \alpha_i > 0 \). The \( W_i \) were chosen so that each \( \alpha_i \) is distinct, hence the \( W_i \)'s are pairwise disjoint.

Consider the primary decomposition \( I_{KKT} = \bigcap_{i=0}^r J_i \) corresponding to our decomposition of \( \mathcal{V}_{KKT} \), i.e., \( V(J_i) = W_i \) for \( i = 0, 1, \ldots, r \). Since \( W_i \cap W_j = \emptyset \), we have \( J_i + J_j = \mathbb{R}[x, \alpha, \nu] \) by Theorem 2.6. The Chinese Remainder Theorem, see e.g. [14] 2.13], implies that there is an isomorphism

\[
\rho: \mathbb{R}[x, \alpha, \nu]/I_{KKT} \rightarrow \mathbb{R}[x, \alpha, \nu]/J_0 \times \mathbb{R}[x, \alpha, \nu]/J_1 \times \cdots \times \mathbb{R}[x, \alpha, \nu]/J_r.
\]

For any \( p \in \mathbb{R}[x, \alpha, \nu] \), let \( [p] \) and \( \rho([p]) \), denote the equivalence classes of \( p \in \mathbb{R}[x, \alpha, \nu]/I_{KKT} \) and \( \mathbb{R}[x, \alpha, \nu]/J_i \), respectively.

Recall that that \( V(J_0) \cap \mathcal{H} = \emptyset \), hence by Theorem 2.6 there exist SOS polynomials \( u_{\theta} \ (\theta \in \{0, 1\}^t) \) such that

\[
-1 \equiv \sum_{\theta \in \{0, 1\}^t} u_{\theta} \rho([h_1^{\theta_1}])_0 \cdots \rho([h_t^{\theta_t}])_0 \overset{\text{def}}{=} u_0 \mod J_0.
\]

As in the proof of Theorem 2.6, we write \( f = f_1 - f_2 \) for SOS polynomials \( f_1, f_2 \) and then we have

\[
f \equiv f_1 + u_0 f_2 \equiv \sum_{\theta \in \{0, 1\}^t} u_{\theta} \rho([h_1^{\theta_1}])_0 \cdots \rho([h_t^{\theta_t}])_0 \overset{\text{def}}{=} q_0 \mod J_0
\]

for some SOS polynomials \( v_{\theta} \ (\theta \in \{0, 1\}^t) \). Thus the preimage \( \rho^{-1}((q_0, 0, \ldots, 0)) \in P_{KKT} \).

Now on each \( W_i, 1 \leq i \leq r \), \( f(x) = \alpha_i > 0 \), and hence \( (f(x)/\alpha_i - 1)^{1/2} \) vanishes on \( W_i \). Then by Theorem 2.6 there is \( \ell \in \mathbb{N} \) such that \( (f(x)/\alpha_i - 1)^{\ell} \in J_i \). From the binomial theorem, it follows that

\[
(1 + (f(x)/\alpha_i - 1))^{1/2} \equiv \frac{1}{2} \sum_{k=1}^{\ell-1} \binom{\ell-1}{k} (f(x)/\alpha_i - 1)^k \overset{\text{def}}{=} q_0 / \sqrt{\alpha_i} \mod J_i.
\]
Thus \((\rho(f))_i = q_i^2\) is SOS in \(\mathbb{R}[x, \lambda, \nu]/J_i\), and hence \(\rho^{-1}(q_i^2e_i+1)\) is SOS in \(\mathbb{R}[x, \lambda, \nu]/I_{KKT}\), where \(e_i+1\) is the \((i+1)\)-st standard unit vector in \(\mathbb{R}^{r+1}\).

Finally, we see that \(\rho([f]) = (q_0, q_1^2, \cdots, q_r^2)\). The preimage of the latter is
\[
\rho^{-1}([q_0, q_1^2, \cdots, q_r^2]) = \rho^{-1}(q_0e_1) + \sum_{i=1}^r \rho^{-1}(q_i^2e_i+1),
\]
which implies that \(f \in P_{KKT}\). □

**Remark.** The conclusions in Theorem 3.2 and Theorem 3.4 cannot be strengthened to show that \(f(x) \in M_{KKT}\). The following is a counterexample.

**Example 3.5** Consider the optimization
\[
\begin{align*}
\min & \quad f(x) = (x_3 - x_1^2x_2)^2 - 1 + \epsilon \\
\text{s.t.} & \quad h_1(x) = 1 - x_1^2 \geq 0 \\
& \quad h_2(x) = x_2 \geq 0 \\
& \quad h_3(x) = x_3 - x_2 - 1 \geq 0
\end{align*}
\]
where \(0 < \epsilon < 1\). From the constraints, we can easily observe that the global minimum \(f^* = \epsilon > 0\) which is attained at \(x^* = (0, 0, 1)\). Its KKT ideal
\[
I_{KKT} = \left\{ 2x_1x_2(x_3 - x_1^2x_2) - \nu_1x_1, 2x_1^2(x_3 - x_1^2x_2) + \nu_2 - \nu_3, \\
2(x_3 - x_1^2x_2) - \nu_3, \nu_1(1 - x_1^2), \nu_2x_2, \nu_3(x_3 - x_2 - 1) \right\}
\]
is radical (verified in Macaulay 2 [2]). However, we cannot find SOS polynomials \(\sigma_0, \sigma_1, \sigma_2, \sigma_3\) and general polynomials \(\phi_1, \phi_2, \phi_3\) such that
\[
f(x) = \sigma_0 + \sigma_1h_1 + \sigma_2h_2 + \sigma_3h_3 + \phi_1(\partial f/\partial x_1) - \nu_1x_2) + \phi_2(\partial f/\partial x_2) - \nu_2 - \nu_3
\]
Suppose to the contrary that they exist. Plugging \(\nu = (0, 0)\) in the above identity yields
\[
0 = 1 - \epsilon + \sigma_0 + \sigma_1(1 - x_1^2) + \sigma_2x_2 + \sigma_3(x_3 - x_2 - 1) + \phi(x_3 - x_1^2x_2)
\]
where \(\phi = -4x_1\phi_1 - x_1^2\phi_2 + 2\phi_3 - (x_3 - x_1^2x_2)\). Now substitute \(x_3 = x_1^2x_2\) in the above, yielding
\[
\sigma_3((1 - x_1^2)x_2 + 1) = 1 - \epsilon + \sigma_0 + \sigma_1(1 - x_1^2) + \sigma_2x_2.
\]
Here \(\sigma_0, \sigma_1, \sigma_2, \sigma_3\) are now considered as SOS polynomials in \((x_1, x_2)\). Since \(1 - \epsilon > 0\), \(\sigma_3\) cannot be the zero polynomial. If \(\sigma_3 = \sigma_3(x_1)\) is independent of \(x_2\), we can derive a contradiction using an argument identical to the argument in the proof of [20, Thm. 2]. Thus \(2m = \deg_2\sigma_3(x_1, x_2) \geq 2\) and \(2d = \deg_1\sigma_3(x_1, x_2) \geq 0\). On the left hand side, the leading term is of the form \(A \cdot x_1^{2d+2}x_2^{m+1}\) with coefficient \(A < 0\). Since the degree in \(x_2\) on the left hand side is odd, the leading term on the right hand side must come from \(\sigma_3(x_1, x_2)x_2\), and is of the form like \(B \cdot x_1^{2d}x_2^{m+1}\) with \(B > 0\). This is a contradiction. Therefore we can conclude that \(f(x) \notin M_{KKT}\).

**4. Convergence of the Lower Bounds**

In this section, we will show that the lower bounds \(\{p_n^\epsilon\}\) obtained from (1.7)-(1.8) converge to \(f^*\) in (1.1)-(1.8). The conclusions in Section 4 of [13] can generalized, based on Theorem 3.2 and Theorem 3.4 in the preceding section. However, we need an extra assumption to ensure the convergence of \(\{f_n^\epsilon\}\).
Theorem 4.1 Assume $f^*$ is finite and the global optimizers $x^*$ of (1.1)-(1.3) satisfy the KKT system (1.4)-(1.6). Then $\lim_{N \to \infty} p_N^* = f^*$. Furthermore, if $I_{KKT}$ is radical, then there exists some $N \in \mathbb{N}$ such that $p_N^* = f^*$, i.e., the SOS relaxations (1.4)-(1.8) converge in finitely many steps.

Proof. The sequence $\{p_N^*\}$ is monotonically increasing, and $p_N^* \leq f^*$ for all $N \in \mathbb{N}$, since $f^*$ is attained by $f(x)$ in the KKT system (1.4)-(1.6) by assumption and the constraint (1.10) implies that $\gamma \leq f^*$. Now for arbitrary $\epsilon > 0$, let $\gamma_\epsilon = f^* - \epsilon$ and replace $f(x)$ by $f(x) - \gamma_\epsilon$ in (1.1)-(1.3). The KKT system remains unchanged, and $f(x) - \gamma_\epsilon$ is strictly positive on $V_{KKT}^\epsilon$. By Theorem 3.4, $f(x) - \gamma_\epsilon \in P_{KKT}$. Since $f(x) - \gamma_\epsilon$ is fixed, there must exist some integer $N_1$ such that $f(x) - \gamma_\epsilon \in P_{N_1,KKT}$. Hence $f^* - \epsilon \leq p_{N_1}^* \leq f^*$. Therefore we have that $\lim_{N \to \infty} p_N^* = f^*$.

Now assume that $I_{KKT}$ is radical. Replace $f(x)$ by $f(x) - f^*$ in (1.1)-(1.3). The KKT system still remains the same, and $f(x) - f^*$ is now nonnegative on $V_{KKT}^\epsilon$. By Theorem 3.2, $f(x) - f^* \in P_{KKT}$. So there exists some integer $N_2$ such that $f(x) - f^* \in P_{N_2,KKT}$, and hence $P_{N_2} \geq f^*$. Then $p_{N_2}^* \leq f^*$ for all $N$ implies that $p_{N_2}^* = f^*$. □

Remarks. (1) In Lasserre’s method [11], a sequence of lower bounds that converge to $f^*$ asymptotically can be obtained when the feasible region $F$ is compact; but those lower bounds usually do not converge in finitely many steps. However, from Theorem 4.1, we see that when $I_{KKT}$ is radical then the lower bounds $\{p_N^*\}$ converge in finitely many steps, even if $F$ is not compact. This implies that the lower bounds $\{p_N^*\}$ may have better convergence even in the case where $F$ is compact.

(2) The assumption in Theorem 4.1 cannot be removed, which is illustrated by the following example.

Example 4.2 Consider the optimization: min $x$ s.t. $x^3 \geq 0$. Obviously $f^* = 0$ and the global minimizer $x^* = 0$. However, the KKT system

$$1 - \nu \cdot 3x^2 = 0, \quad \nu \cdot x^3 = 0, \quad x^3 \geq 0, \quad \nu \geq 0$$

is not satisfied, since $V_{KKT} = \emptyset$. Actually we can see that the lower bounds $\{f_N^*\}$ given by (1.1)- (1.4) tend to infinity. By Theorem 2.3, $V_{KKT} = \emptyset$ implies that $1 \in P_{KKT}$, i.e.,

$$(1 + 3\nu x^2)(1 - 3\nu x^2) + 9\nu^2 x \cdot \nu x^3 = 1.$$ 

In the SOS relaxation (1.2)-(1.4), for arbitrarily large $\gamma$, $x - \gamma \in P_{KKT}$, since

$$x - \gamma = (x - \gamma)(1 + 3\nu x^2)(1 - 3\nu x^2) + 9\nu^2 x(x - \gamma) \cdot \nu x^3 \in P_{KKT}.$$ 

Thus $p_N^* = \infty$. In this example, the conclusion in Theorem 4.1 does not hold.

The convergence of lower bounds $\{f_N^*\}$ cannot be guaranteed, as we see in Example 4.2. In that example, replace the objective by the perfect square $(x_3 - x_1^2 x_2)^2$. Then $f^* = 1$, but we do not have $\lim_{N \to \infty} f_N^* = 1$. From the arguments there, we can see that $f(x) - (1 - \epsilon) \notin M_{KKT}$ for all $0 < \epsilon < 1$, which implies that $f_N^* \leq 0$. But $f_N^* \geq 0$ is obvious since $(x_3 - x_1^2 x_2)^2$ is a perfect square. Therefore $\lim_{N \to \infty} f_N^* = 0 < 1 = f^*$, i.e., the lower bounds $\{f_N^*\}$ obtained from (1.9)-(1.10) may not converge.

On the other hand, the situation is often not that bad in practice. In the examples in the rest of this paper, it always happens that $\lim_{N \to \infty} p_N^* = \lim_{N \to \infty} f_N^* = f^*$. If we further assume that $M_{KKT}$ is archimedean then it must hold that $\lim_{N \to \infty} p_N^* = \lim_{N \to \infty} f_N^* = f^*$ from Theorem 2.4.
The SOS relaxation (1.9)-(1.10) can be solved using software SOSTOOLS [21]. The dual problem of (1.9)-(1.10) is to minimize a linear functional over some linear moment matrix inequalities. It can also be obtained by applying moment matrix methods to minimize $f(x)$ over the semialgebraic set defined by KKT system (1.4)-(1.6). The dual problem can be solved using software Gloptipoly [14]. Actually, the formulations of SOS relaxations and moment matrix methods are dual to each other, see [11, 12]. The SOS relaxations (1.9)-(1.10) not only give the lower bounds $f_N^*$, but also the information about global minimizers $x^*$ and their Lagrange multipliers $(\lambda^*, \nu^*)$. Gloptipoly can extract the minimizer if the moment matrix satisfies some rank condition. Gloptipoly does not need the moment matrix to be rank one. The tricks to extract global minimizers in Section 5.2 in [15] can be applied here directly to find $(x^*, \lambda^*, \nu^*)$, so omit further discussion. For more details about how extracting minimizers from SOS relaxations or moment matrix methods, see [9].

**Example 4.3 (Exercise 2.18, [10])** Consider the global optimization:

$$\min \ (-4x_1^2 + x_2^2)(3x_1 + 4x_2 - 12)$$

s.t. $3x_1 - 4x_2 \leq 12$, $2x_1 - x_2 \leq 0$, $-2x_1 - x_2 \geq 0$.

The global minimum $f^* = -18.6182$ and the minimizer $x^* = (-24/55, 128/55) \approx (-0.4364, 2.3273)$. The lower bound obtained from (1.9)-(1.10) is $f_4^* = -18.6182$. The extracted minimizer $\hat{x} = (-0.4364, 2.3273)$.

**Example 4.4** Consider the Quadratically Constrained Quadratic Program (QCQP):

$$\min \ -\frac{4}{3}x_1^2 + \frac{2}{3}x_2^2 - 2x_1x_2$$

s.t. $x_2^2 - x_1^2 \geq 0$, $-x_1x_2 \geq 0$.

The global minimum $f^* = 0$ and minimizer $x^* = (0, 0)$. The feasible region $\mathcal{F}$ defined by the constraints is non-compact. The lower bound returned by (1.9)-(1.10) is $f_4^* = -2.6 \times 10^{-15}$ (Note: this computation was done in double precision floating point, with round off error bounded by $2^{-53} \sim 10^{-16}$). The extracted minimizer is $\hat{x} = (6.1 \times 10^{-16}, -9.0 \times 10^{-17})$ and the Lagrange multiplier is $\hat{\nu} = (0.3884, 0.3909)$.

## 5. Optimization over Some Special Semialgebraic Sets

In problem (1.9)-(1.10), the polynomials are in $(x, \lambda, \nu) \in \mathbb{R}^{n+s+t}$ which means that when there are many constraints, the problem is very expensive to solve. If $u(x, \lambda, \nu)$ is a polynomial of degree $d$, it can have $\binom{n+s+t+d}{d}$ coefficients; this will be huge for large $s$, $t$, or $d$. Frequently, if the polynomials $g_i(x)$ and $h_j(x)$ are of some special form, then the KKT system (1.4)-(1.6) can be simplified and hence the SOS relaxations (1.9)-(1.10) will be easier to solve. In this section we look at the case where $\{x \in \mathbb{R}^n : h_1(x), \ldots, h_t(x) \geq 0\}$ is the nonnegative orthant $\mathbb{R}_+^n$ or the box $[a, b]_n$ and show how these type of problems can be simplified.
5.1. Minimizing Over the Nonnegative Orthant \( \mathbb{R}_+^n \)

In this subsection, suppose the inequality constraints (1.3) are the standard constraints for the nonnegative orthant \( \mathbb{R}_+^n := \{ x \in \mathbb{R}^n : x_1 \geq 0, \cdots, x_n \geq 0 \} \). The constraints are of the form

\[
g_1(x) = \cdots = g_s(x) = 0, \quad x \in \mathbb{R}_+^n.
\]

Then the KKT system (1.4)-(1.6) becomes

\[
\nabla f(x) + \sum_{i=1}^s \lambda_i \nabla g_i(x) - \nu = 0,
\]

\[
g_1(x) = \cdots = g_s(x) = 0,
\]

\[
x_k \nu_k = 0, \quad k = 1, \cdots, n,
\]

\[
x \in \mathbb{R}_+^n, \quad \nu \in \mathbb{R}^n.
\]

In this KKT system, the variable \( \nu \) can be solved for explicitly. By eliminating \( \nu \), the above system simplifies to

\[
x_k \left( \frac{\partial f}{\partial x_k} + \sum_{i=1}^s \lambda_i \frac{\partial g_i}{\partial x_k} \right) = 0, \quad k = 1, \cdots, n \tag{5.1}
\]

\[
g_1(x) = \cdots = g_s(x) = 0. \tag{5.2}
\]

We define cones \( M_{KKT}^{\mathbb{R}^n} \) and \( M_{N,KKT}^{\mathbb{R}^n} \) similar to the definition of \( M_{KKT} \) and \( M_{N,KKT} \) (see Section 1), define associated to the above simplified system. Note that \( M_{KKT}^{\mathbb{R}^n}, M_{KKT}^{\mathbb{R}^n} \subseteq \mathbb{R}[x, \lambda] \) and the Lagrange multiplier \( \nu \) does not appear. Similar to (1.9)-(1.10), a sequence \( \{ \hat{f}_N \} \) of lower bounds of (1.1)-(1.3) can be obtained by the following SOS relaxations:

\[
\hat{f}_N = \max_{\gamma \in \mathbb{R}} \gamma \tag{5.3}
\]

s.t. \( f(x) - \gamma \in M_{N,KKT}^{\mathbb{R}^n} \). \tag{5.4}

Now the indeterminates in the above SOS program are \((x, \lambda)\) instead of \((x, \lambda, \nu)\). Thus a polynomial \( u(x, \lambda) \) of degree \( d \) has at most \( \frac{(n+s+t+d)(n+s+t+d)}{d} \) coefficients, which is much smaller than \( \frac{(n+s+t+d)(n+s+t+d)}{d} \) when \( t \) is large. This makes solving (5.3)-(5.4) much less expensive.

Since \( \nu = (\nu_1, \cdots, \nu_t) \) are eliminated by direct substitutions, systems (1.4)-(1.6) and (5.1)-(5.4) are equivalent. Thus we see that \( f(x) - \gamma \in M_{N_1,KKT} \) if and only if \( f(x) - \gamma \in M_{N_2,KKT}^{\mathbb{R}^n} \), for some integers \( N_1 \) and \( N_2 \). Therefore the lower bounds \( \{ \hat{f}_N \} \) have the same property of convergence as \( \{ f_N \} \) obtained from (1.9)-(1.10).

If, in addition, the equality constraints (1.2) are hyperplanes, i.e., the constraints are the standard simplex:

\[
Ax = b, \quad x \geq 0
\]

where \( A \in \mathbb{R}^{s \times n}, b \in \mathbb{R}^s \), then the KKT system (1.4)-(1.6) can be reduced to

\[
x_k \left( \frac{\partial f}{\partial x_k} + a_k^T \lambda \right) = 0, \quad k = 1, \cdots, n
\]

\[
Ax = b, \quad x \geq 0
\]
where \( a_k \in \mathbb{R}^n \) is the \( k \)-th column of matrix \( A \).

Furthermore, if \( Ax = b \) consists of a single equation \( a^T x = b \neq 0 \), then \( \lambda = \frac{-e^T \nabla f(x)}{b} \) and the KKT system has the simpler form

\[
x_k \left( \frac{\partial f}{\partial x_k} - \alpha_k \frac{e^T \nabla f(x)}{b} \right) = 0, \quad k = 1, \ldots, n
\]

where \( \alpha = [\alpha_1, \ldots, \alpha_n]^T \).

Based on the above two simplified KKT systems, SOS relaxations similar to (5.3)-(5.4) can be obtained immediately, improving the computational efficiency.

**Example 5.1 (Test Problem 2.9, [6])** Consider the Maximum Clique Problem for \( n = 5 \):  

\[
\min \quad - \left( \sum_{i=1}^{4} x_i(x_{i+1} + x_1x_5 + x_1x_4) \right)
\]

s.t. \( x_1 + x_2 + x_3 + x_4 + x_5 = 1 \)

\( x_1, x_2, x_3, x_4, x_5 \geq 0 \).

The global minimum \( f^* = -1/3 \) and minimizers \( x^* \) are \((1/3, 1/3, 0, 0, 1/3), (1/3, 0, 0, 1/3, 1/3), (0, 1/3, 1/3, 0, 1/3), \) and \((0, 0, 1/3, 1/3, 1/3)\). The lower bound obtained from (5.3)-(5.4) is \( \bar{f}^*_4 = -0.3333333378814 \). The difference \( f^* - \bar{f}^*_4 \approx 4.5 \times 10^{-10} \).

**Example 5.2 (Exercise 1.20, [10])** Consider the optimization:

\[
\min \quad \sum_{i=1}^{n-1} x_i^2 x_{i+1} + x_n x_1
\]

s.t. \( \sum_{i=1}^{n} x_i = 1, \quad x \geq 0 \).

The global minimum \( f^* = 0 \) and the minimizers are the vertices of the simplex defined by the constraints. The lower bound obtained from (5.3)-(5.4) is \( \bar{f}^*_4 = -4.0 \times 10^{-8} \).

**Example 5.3** \( f(x) = x^T H x \) and the constraints are \( 0 \leq x \leq e \), where \( x \in \mathbb{R}^5 \) and \( e = [1, 1, 1, 1, 1]^T \), and

\[
H = \begin{bmatrix}
1 & -1 & 1 & 1 & -1 \\
-1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 \\
1 & 1 & 1 & 1 & 1 \\
-1 & 1 & 1 & -1 & 1
\end{bmatrix}
\]

is a co-positive matrix (CPL [7]), i.e., \( f(x) \geq 0 \ \forall x \geq 0 \). If each \( x_i \) is replaced by \( x_i^2 \), then the resulting quartic polynomial is nonnegative, but not SOS. Consider the Quadratic Program (QP):

\[
\min \quad x^T H x
\]

s.t. \( x_1, x_2, x_3, x_4, x_5 \geq 0 \).

The lower bound obtained from (5.3)-(5.4) is \( \bar{f}^*_4 = -3.35 \times 10^{-9} \). Actually, we have the following decomposition

\[
x^T H x = 0 + \sum_{i=1}^{5} 2 \cdot (x_i \cdot h_i^T x)
\]

in (5.3)-(5.4). Here \( h_i \) is the \( i \)-th column of matrix \( H \).
5.2. Minimizing Over the Box

In this subsection, we consider the case that (1.3) are given by box constraints, i.e., \( x \in [a, b]^n \) where \( a = [a_1, \cdots, a_n]^T \) and \( b = [b_1, \cdots, b_n]^T \). Here we assume that \( a < b \). In this case, the feasible region \( F \) is compact, and Lasserre’s method [11] can be applied here. However, as remarked after Theorem 4.1, if \( I_{KKT} \) is radical then our method will converge after finitely many steps. Usually Lasserre’s method has only asymptotic convergence.

Now the KKT system (1.4)-(1.6) has the form

\[
\nabla f(x) + \sum_{i=1}^{s} \lambda_i \nabla g_i(x) - \nu + \mu = 0,
\]

\[
g_i(x) = \cdots = g_s(x) = 0,
\]

\[
(x_k - a_k)(b_k - x_k) = 0, \quad k = 1, \cdots, n,
\]

\[
x - a \geq 0, \quad b - x \geq 0,
\]

where \( \nu_i(\mu, \lambda_i) \) is the \( i \)-th component of Lagrange multipliers \( \nu(\mu, \lambda) \) respectively. One good property of this KKT system is that the vectors \( \nu \) and \( \mu \) can be solved for explicitly. Eliminating \( \nu \) and \( \mu \), we obtain

\[
\frac{\partial f}{\partial x_k} + \sum_{i=1}^{s} \lambda_i \frac{\partial g_i}{\partial x_k}(x_k - a_k)(b_k - x_k) = 0, \quad k = 1, \cdots, n,
\]

\[
g_1(x) = \cdots = g_s(x) = 0, \quad x - a \geq 0, \quad b - x \geq 0.
\]

Like the definition of \( M^{[n]}_{KKT} \) and \( M^{[n]}_{N,KKT} \) (see the preceding subsection), define the cones \( M^{[a,b]}_{KKT} \) and \( M^{[a,b]}_{N,KKT} \) associated with the above simplified KKT system, where \( M^{[a,b]}_{KKT} \), \( M^{[a,b]}_{N,KKT} \subset \mathbb{R}[x, \lambda] \). Similar to (5.3)-(5.6), a sequence of lower bounds \( \{\tilde{f}_N^s\} \) of (1.4)-(1.6) can be obtained by the following SOS relaxations:

\[
\tilde{f}_N^s = \max_{\gamma \in \mathbb{R}} \gamma \quad \text{s.t.} \quad f(x) - \gamma \in M^{[a,b]}_{N,KKT}.
\]

(5.5)

Now a polynomial \( u(x, \lambda) \) of degree \( d \) in \( M^{[a,b]}_{N,KKT} \) has at most \( \binom{n+d}{d} \) coefficients, which is much smaller than \( \binom{n+2d}{d} \), the number of coefficients of one polynomial of degree \( d \) in \( M^{[a,b]}_{N,KKT} \). So (5.5)-(5.6) can be solved much more efficiently. Similarly as \( \{\tilde{f}_N^s\} \), the lower bounds \( \{\tilde{f}_N^s\} \) have the same properties of convergence as \( \{f_N^s\} \).

Consider the special case that \( f(x) = \frac{1}{4} x^T H x + g^T x \) is a quadratic function and there are no equality constraints. Here \( g \in \mathbb{R}^n \) and \( H = H^T \in \mathbb{R}^{n \times n} \) is symmetric. The above KKT system can be further reduced to

\[
(h_k^T x + g_k)(x_k - a_k)(b_k - x_k) = 0, \quad k = 1, \cdots, n,
\]

\[
x - a \geq 0, \quad b - x \geq 0.
\]

Here \( h_k(g_k) \) is the \( k \)-th row (component) of arrays \( H(g) \). Finding the global minimum of a general nonconvex quadratic function over a box is an NP-hard problem. The relaxations (5.5)-(5.6) provides a new approach for such nonconvex quadratic programming.
Example 5.4 (Test Problem 4.7, [6]) Consider the optimization:

\[
\begin{align*}
\min & \quad -12x_1 - 7x_2 + x_2^2 \\
\text{s.t.} & \quad -2x_1^4 + 2 - x_2 = 0 \\
& \quad 0 \leq x_1 \leq 2, \quad 0 \leq x_2 \leq 3.
\end{align*}
\]

The best known objective value is \(-16.73889\). The lower bound obtained from (5.5)-(5.6) is \(\tilde{f}_6^* = -16.73889\). So \(f^* = \tilde{f}_6^*\). The extracted minimizer \(\tilde{x} = (0.7175, 1.4698)\) and Lagrange multiplier \(\tilde{\lambda} = -4.0605\).

Example 5.5 (Test Problem 2.1, [6]) Consider the optimization:

\[
\begin{align*}
\min & \quad 42x_1 + 44x_2 + 45x_3 + 47x_4 + 47.5x_5 - 50 \sum_{i=1}^{5} x_i^2 \\
\text{s.t.} & \quad 20x_1 + 12x_2 + 11x_3 + 7x_4 + 4x_5 \leq 40 \\
& \quad 0 \leq x_1, x_2, x_3, x_4, x_5 \leq 1.
\end{align*}
\]

The global minimum \(f^* = -17\) and the minimizer \(x^* = (1, 1, 0, 1, 0)\). The lower bound obtained from (5.5)-(5.6) is \(\tilde{f}_6^* = 17.00\). The extracted minimizer \(\tilde{x} = (1.00, 1.00, 0.00, 1.00, 0.00)\) and Lagrange multiplier \(\tilde{\nu} = 0.1799\).

Example 5.6 (Exercise 2.22, [10]) Consider the Maximum Independent Set Problem

\[
\begin{align*}
\min & \quad -\sum_{i=1}^{n} x_i + \sum_{(i,j) \in E} x_i x_j \\
\text{s.t.} & \quad 0 \leq x_i \leq 1, \quad i = 1, \ldots, n.
\end{align*}
\]

The negative of the global minimum \(-f^*\) equals the cardinality of the maximum independent vertex set of \(G = (V, E)\). Let \(G\) be a pentagon with two diagonals which do not intersect in the interior. Now \(n = 5\) and \(f^* = -2\). The lower bound obtained from (5.5)-(5.6) is \(\tilde{f}_5^* = -2.00\).

Example 5.7 (Exercise 1.32, [10]) Consider the optimization:

\[
\begin{align*}
\min & \quad \prod_{i=1}^{n} x_i - \sum_{i=1}^{n} x_i \\
\text{s.t.} & \quad 0 \leq a \leq x_1, \ldots, x_n \leq b.
\end{align*}
\]

The global minimum \(f^* = a^n - na\) when \(a \geq 1\). For \(n = 4, a = 2, b = 3\), the lower bound obtained from (5.5)-(5.6) is \(\tilde{f}_6^* = 8.00\). The extracted minimizer is \(\tilde{x} = (2.00, 2.00, 2.00, 2.00)\).

6. Conclusions

This paper generalizes most of the theorems in [15] from optimizations constrained by algebraic sets to optimizations constrained by semialgebraic sets, under the assumption that the global minimizers satisfy the KKT system. The special structures of the KKT system are exploited to accelerate the algorithm when the constraints include the nonnegative orthant \(\mathbb{R}_+^n\) or the standard box \([a, b]^n\).

In general, the SOS relaxations (1.9)-(1.10) are very hard to solve when there are many constraints, which introduces many Lagrange multipliers. So the structures of (1.9)-(1.10) should be exploited to improve the efficiency of the method. Section 5 discusses the specifications with the nonnegative orthant \(\mathbb{R}_+^n\) and the standard box \([a, b]^n\).

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