Global Optimization of Polynomials Using Generalized Critical Values and Sums of Squares [*]

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ABSTRACT

Let $\bar{X} = [X_1, \ldots, X_n]$ and $f \in \mathbb{R}[\bar{X}]$. We consider the problem of computing the global infimum of f when f is bounded below. For $\mathbf{A} \in \mathrm{GL}_n(\mathbb{C})$, we denote by $f^{\mathbf{A}}$ the polynomial $f(\mathbf{A}\bar{X})$. Fix a number $M \in \mathbb{R}$ greater than $\inf_{x \in \mathbb{R}^n} f(x)$. We prove that there exists a Zariski-closed subset $\mathscr{A} \subsetneq \mathrm{GL}_n(\mathbb{C})$ such that for all $\mathbf{A} \in \mathrm{GL}_n(\mathbb{Q}) \setminus \mathscr{A}$, we have $f^{\mathbf{A}} \geq 0$ on $\mathbb{R}^n$ if and only if for all $\epsilon > 0$, there exist sums of squares of polynomials s and t in $\mathbb{R}[\bar{X}]$ and polynomials $\phi_i \in \mathbb{R}[\bar{X}]$ such that $f^{\mathbf{A}} + \epsilon = s + t\left(M - f^{\mathbf{A}}\right) + \sum_{1 \leq i \leq n-1} \phi_i \frac{\partial f^{\mathbf{A}}}{\partial X_i}$. Hence we can formulate the original optimization problems as semidefinite programs which can be solved efficiently in Matlab. Some numerical experiments are given. We also discuss how to exploit the sparsity of SDP problems to overcome the ill-conditionedness of SDP problems when the infimum is not attained.

Keywords

Global optimization, polynomials, generalized critical values, sum of squares, semidefinite programing, moment matrix.

Categories and Subject Descriptors

G.1.6 [**Numerical Analysis**]: Optimization; I.1.2 [**Symbolic and Algebraic Manipulation**]: Algorithms: algebraic algorithms; F.2.2 [**Analysis of Algorithms and Problem Complexity**]: Non numerical algorithms and problems: geometrical problems and computation

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General Terms

Theory, algorithms.

1. INTRODUCTION

We consider the global optimization problem

$$f^* := \inf\{f(x) \mid x \in \mathbb{R}^n\} \in \mathbb{R} \cup \{-\infty\} \qquad (1)$$

where $f \in \mathbb{R}[\bar{X}] := \mathbb{R}[X_1, \ldots, X_n]$. The problem is equivalent to compute

$$f^* = \sup\{a \in \mathbb{R} \mid f - a \geq 0 \text{ on } \mathbb{R}^n\} \in \mathbb{R} \cup \{-\infty\}.$$

It is well known that this optimization problem is NP-hard even when $\deg(f) \geq 4$ and is even [13]. There are many approaches to approximate f^*. For example, we can get a lower bound by solving the sum of squares (SOS) problem:

$$
\begin{aligned}
f^{\mathrm{sos}} &= \sup\{a \in \mathbb{R} \mid f - a \text{ is a sum of squares in } \mathbb{R}[\bar{X}]\} \\
&\in \mathbb{R} \cup \{-\infty\}.
\end{aligned}
$$

The SOS problem can be solved efficiently by algorithms in GloptiPoly [4], SOSTOOLS [15], YALMIP [12], SeDuMi [22] and SparsePOP [24]. An overview about SOS and nonnegative polynomials is given in [17]. However, it is pointed out in [1] that for fixed degree $d \geq 4$, the volume of the set of sums of squares of polynomials in the set of nonnegative polynomials tends to 0 when the number of variable increases.

In recent years, a lot of work has been done in proving existence of SOS certificates which can be exploited for optimization, e.g., the "Big ball" method proposed by Lasserre [10] and "Gradient perturbation" method proposed by Jibetean and Laurent [6]. These two methods solve the problem by perturbing the coefficients of the input polynomials. However, small perturbations of coefficients might generate numerical instability and lead to SDPs which are hard to solve. The "Gradient variety" method by Nie, Demmel and Sturmfels [14] is an approach without perturbation. For a polynomial $f \in \mathbb{R}[\bar{X}]$, its *gradient variety* is defined as

$$V(\nabla f) := \{x \in \mathbb{C}^n \mid \nabla f(x) = 0\}$$

and its *gradient ideal* is the ideal generated by all partial derivatives of f:

$$\langle \nabla f \rangle := \left\langle \frac{\partial f}{\partial X_1}, \frac{\partial f}{\partial X_2}, \cdots, \frac{\partial f}{\partial X_n} \right\rangle \subseteq \mathbb{R}[\bar{X}].$$

It is shown in [14] that if the polynomial $f \in \mathbb{R}[\bar{X}]$ is nonnegative on $V(\nabla f)$ and $\langle \nabla f \rangle$ is radical then f is an SOS modulo its gradient ideal. If the gradient ideal is not necessarily radical, the conclusion still holds for polynomials positive on their gradient variety. However, if f does not attain the infimum, the method outlined in [14] may provide a wrong answer. For example, consider $f := (1 - xy)^2 + y^2$. The infimum of f is $f^* = 0$, but $V(\nabla f) = \{(0,0)\}$ and $f(0,0) = 1$. This is due to the fact that any sequence (x_n, y_n) such that $f(x_n, y_n) \to 0$ when $n \to \infty$ satisfies $||(x_n, y_n)|| \to \infty$ (here and throughout the paper we use the l^2-norm). Roughly speaking the infimum is not reached at finite distance but "at infinity". Such phenomena are related to the presence of *asymptotic* critical values, which is a notion introduced in [9].

Recently, there are some progress in dealing with these hard problems for which polynomials do not attain a minimum on $\mathbb{R}^n$. Let us outline Schweighofer's approach [21]. We recall some notations firstly.

DEFINITION 1.1. *For any polynomial $f \in \mathbb{R}[\bar{X}]$ and subset $S \in \mathbb{R}^n$, the set $R_\infty(f, S)$ of asymptotic values of f on S consists of all $y \in \mathbb{R}$ for which there exists a sequence $(x_k)_{k \in \mathbb{N}}$ of points $x_k \in S$ such that $\lim_{k \to \infty} ||x_k|| = \infty$ and $\lim_{k \to \infty} f(x_k) = y$.*

DEFINITION 1.2. *The preordering generated by polynomials $g_1, g_2, \ldots, g_m \in \mathbb{R}[\bar{X}]$ is denoted by $T(g_1, g_2, \ldots, g_m)$:*

$$T(g_1, g_2, \ldots, g_m) := \left\{ \begin{array}{c} \sum_{\delta \in \{0,1\}^m} s_\delta g_1^{\delta_1} g_2^{\delta_2} \ldots g_m^{\delta_m} \mid s_\delta \\ \text{is a sum of squares in } \mathbb{R}[\bar{X}] \end{array} \right\}.$$

THEOREM 1.3. *([21, Theorem 9]). Let $f, g_1, g_2, \ldots, g_m \in \mathbb{R}[\bar{X}]$ and set*

$$S := \{x \in \mathbb{R}^n \mid g_1(x) \geq 0, \ g_2(x) \geq 0, \ \ldots, \ g_m(x) \geq 0\}. \quad (2)$$

Suppose that

  (i) f is bounded on S;

  (ii) $R_\infty(f, S)$ is a finite subset of $]0, +\infty[$;

  (iii) $f > 0$ on S;

Then $f \in T(g_1, g_2, \ldots, g_m)$.

The idea in [21] is to replace the real part $V(\nabla f) \bigcap \mathbb{R}^n$ of the gradient variety by several larger semialgebraic sets on which the partial derivatives do not necessarily vanish but get very small far away from the origin. For these sets two things must hold at the same time:

- There exist suitable SOS certificates for nonnegative polynomials on the set.

- The infimum of f on $\mathbb{R}^n$ and on the set coincide.

DEFINITION 1.4. *For a polynomial $f \in \mathbb{R}[\bar{X}]$, we call*

$$S(\nabla f) := \{x \in \mathbb{R}^n \mid 1 - ||\nabla f(x)||^2 ||x||^2 \geq 0\}$$

the principal gradient tentacle of f.

THEOREM 1.5. *([21, Theorem 25]) Let $f \in \mathbb{R}[\bar{X}]$ be bounded below. Furthermore, suppose that f has only isolated singularities at infinity (which is always true in the case $n = 2$) or the principal gradient tentacle $S(\nabla f)$ is compact, then the following conditions are equivalent:*

  (i) $f \geq 0$ on $\mathbb{R}^n$;

  (ii) $f \geq 0$ on $S(\nabla f)$;

  (iii) For every $\epsilon > 0$, there are sums of squares of polynomials s and t in $\mathbb{R}[\bar{X}]$, such that

$$f + \epsilon = s + t \left(1 - ||\nabla f(\bar{X})||^2 ||\bar{X}||^2\right).$$

For fixed $k \in \mathbb{N}$, let us define

$$f_k^* := \sup \left\{a \in \mathbb{R} \mid f - a = s + t \left(1 - ||\nabla f(x)||^2 ||x||^2\right)\right\}.$$

where s, t are sums of squares of polynomials and the degree of t is at most $2k$. If the assumptions in the above theorem are satisfied, then $\{f_k^*\}_{k \in \mathbb{N}}$ converges monotonically to f^* (see [21, Theorem 30]). The shortage of this method is that it is not clear that these technical assumptions are necessary or not. To avoid it, the author proposed a collection of higher gradient tentacles ([21, Definition 41]) defined by the polynomial inequalities

$$1 - ||\nabla f(x)||^{2N}(1 + ||x||)^{N+1} \geq 0, \ N \in \mathbb{N}.$$

Then for sufficiently large N, for all $f \in \mathbb{R}[\bar{X}]$ bounded below we have an SOS representation theorem ([21, Theorem 46]). However, the corresponding SDP relaxations get very large for large N and one has to deal for each N with a sequence of SDPs. To avoid this disadvantage, another approach using *truncated tangency variety* is proposed in [3]. Their results are mainly based on Theorem 1.3. For nonconstant polynomial function $f \in \mathbb{R}[\bar{X}]$, they define

$$g_{ij}(\bar{X}) := X_j \frac{\partial f}{\partial X_i} - X_i \frac{\partial f}{\partial X_j}, \ 1 \leq i < j \leq n.$$

For a fixed real number $M \in f(\mathbb{R}^n)$, the *truncated tangency variety* of f is defined to be

$$\Gamma_M(f) := \{x \in \mathbb{R}^n \mid M - f(x) \geq 0, \ g_{i,j}(x) = 0, 1 \leq i, j \leq n\}.$$

Then based on Theorem 1.3, the following result is proved.

THEOREM 1.6. *[3, Theorem 3.1] Let $f \in \mathbb{R}[\bar{X}]$ and M be a fixed real number. Then the following conditions are equivalent:*

  (i) $f \geq 0$ on $\mathbb{R}^n$;

  (ii) $f \geq 0$ on $\Gamma_M(f)$;

  (iii) For every $\epsilon > 0$, there are sums of squares of polynomials s and t in $\mathbb{R}[\bar{X}]$ and polynomials $\phi_{ij} \in \mathbb{R}[\bar{X}], 1 \leq i < j \leq n$, such that

$$f + \epsilon = s + t(M - f) + \sum_{1 \leq i < j \leq n} \phi_{ij} g_{ij}.$$

Fix $k \in \mathbb{N}$ and let

$$f_k^* := \sup \left\{a \in \mathbb{R} \mid f - a = s + t(M - f) + \sum_{1 \leq i < j \leq n} \phi_{ij} g_{ij}\right\}.$$

where s, t, ϕ_{ij} are polynomials of degree at most $2k$ and s, t are sums of squares of polynomials in $\mathbb{R}[\bar{X}]$, then the sequence $\{f_k^*\}_{k \in \mathbb{N}}$ converges monotonically increasing to f^* ([3, Theorem 3.2]). This approach does not require the assumptions of [21, Theorem 25]. However, the number of

equality constraints in $\Gamma_M(f)$ is $\frac{n(n-1)}{2}$ which is very large as n increases.

In this paper, based on Theorem 1.3 and the computation of *generalized critical values* of a polynomial mapping in [18, 19], we present a method to solve optimization problem (1) without requiring f attains the infimum on $\mathbb{R}^n$. Our method does not require assumptions as in [21] and use the simpler variety which only contains $n - 1$ equality constraints.

Although approaches in [21] and [3] can handle polynomials which do not attain a minimum on $\mathbb{R}^n$, numerical problems occur when one solves the SDPs obtained from SOS relaxations, see [3, 6, 21]. The numerical problems are mainly caused by the unboundness of the moments. It happens often when one deals with this kind of polynomial optimization problem using SOS relaxations without exploiting the sparsity structure. We propose some strategies to avoid ill-conditionedness of moment matrices.

The paper is organized as follows. In section 2 we present some notations and preliminaries used in our method. The main result and its proof are given in section 3. In section 4, some numerical experiments are given. In section 5, we focus on two polynomials which do not attain the infimum and try to solve the numerical problems. We draw some conclusions in section 6.

2. PRELIMINARIES AND NOTATIONS

DEFINITION 2.1. *[9] A complex (resp. real) number $c \in \mathbb{C}$ (resp. $c \in \mathbb{R}$) is a critical value of the mapping $\widetilde{f}_{\mathbb{C}} : x \in \mathbb{C}^n \to f(x)$ (resp. $\widetilde{f}_{\mathbb{R}} : x \in \mathbb{R}^n \to f(x)$) if and only if there exists $z \in \mathbb{C}^n$ (resp. $z \in \mathbb{R}^n$) such that $f(z) = c$ and $\frac{\partial f}{\partial X_1} = \cdots = \frac{\partial f}{\partial X_n} = 0$.*
A complex (resp. real) number $c \in \mathbb{C}$ (resp. $c \in \mathbb{R}$) is an asymptotic critical value of the mapping $\widetilde{f}_{\mathbb{C}}$ (resp. $\widetilde{f}_{\mathbb{R}}$) if there exists a sequence of points $(z_l)_{l \in \mathbb{N}} \subset \mathbb{C}^n$ (resp. $(z_l)_{l \in \mathbb{N}} \subset \mathbb{R}^n$) such that:

(i) $f(z_l)$ tends to c when l tends to ∞.

(ii) $||z_l||$ tends to $+\infty$ when l tends to ∞.

(iii) $||X_i(z_l)|| \cdot ||\frac{\partial f}{\partial X_j}(z_l)||$ tends to 0 when l tends to ∞ for all $(i, j) \in \{1, \ldots, n\}^2$.

We denote by $K_0(f)$ the set of critical values of f, by $K_\infty(f)$ the set of asymptotic critical values of f, and by $K(f)$ the set of generalized critical values which is the union of $K_0(f)$ and $K_\infty(f)$.

DEFINITION 2.2. *A map $\phi : V \to W$ of topological spaces is said to be proper at $w \in W$ if there exists a neighborhood B of w such that $\phi^{-1}(\overline{B})$ is compact (where $\overline{B}$ denotes the closure of B).*

Recall that for $\mathbf{A} \in \mathrm{GL}_n(\mathbb{C})$ and $f \in \mathbb{R}[\bar{X}]$, $f^{\mathbf{A}}$ the polynomial $f(\mathbf{A}\,\bar{X})$.

LEMMA 2.3. *([18], Lemma 1) For all $\mathbf{A} \in GL_n(\mathbb{Q})$, we have $K_0(f) = K_0(f^{\mathbf{A}})$ and $K_\infty(f) = K_\infty(f^{\mathbf{A}})$.*

THEOREM 2.4. *([18, Theorem 3.6]) There exists a Zariski-closed subset $\mathscr{A} \subsetneq GL_n(\mathbb{C})$ such that for all $\mathbf{A} \in GL_n(\mathbb{Q}) \setminus \mathscr{A}$, the set of real asymptotic critical values of $x \to f(x)$ is contained in the set of non-properness of the projection on T restricted to the Zariski-closure of the semi-algebraic set defined by $f^{\mathbf{A}} - T = \frac{\partial f^{\mathbf{A}}}{\partial X_1} = \cdots = \frac{\partial f^{\mathbf{A}}}{\partial X_{n-1}} = 0, \ \frac{\partial f^{\mathbf{A}}}{\partial X_n} \neq 0$.*

In [18], the above theorem is stated in the complex case and proved for this case. It relies on properness properties of some critical loci. Since these properness properties can be transfered to the real part of these critical loci, its proof can be transposed mutatis mutandis to the real case.

REMARK 2.5. *([19], Remark 1) Note also that the curve defined as the Zariski-closure of the complex solution set of $f^{\mathbf{A}} - T = \frac{\partial f^{\mathbf{A}}}{\partial X_1} = \cdots = \frac{\partial f^{\mathbf{A}}}{\partial X_{n-1}} = 0, \ \frac{\partial f^{\mathbf{A}}}{\partial X_n} \neq 0$ has a degree bounded by $(d - 1)^{(n-1)}$, where d is the total degree of f. Thus the set of the non-properness of the projection on T restricted to this curve has a degree bounded by $(d-1)^{(n-1)}$.*

REMARK 2.6. *In [18], a criterion for choosing $\mathbf{A}$ is given. It is sufficient that the restriction of the projection $(x_1, \ldots, x_n, t) \to (x_{n-i+2}, \ldots, x_n, t)$ to the Zariski-closure of the constructible set $f^{\mathbf{A}} - T = \frac{\partial f^{\mathbf{A}}}{\partial X_1} = \cdots = \frac{\partial f^{\mathbf{A}}}{\partial X_{n-i}} = 0, \ \frac{\partial f^{\mathbf{A}}}{\partial X_{n-i+1}} \neq 0$ is proper. An algorithm, based on Gröbner bases or triangular sets computations, that computes sets of non-properness is given in [20].*

THEOREM 2.7. *([19, Theorem 5]) Let $f \in \mathbb{R}[X_1, \ldots, X_n]$ and $\varepsilon = \{e_1, \ldots, e_l\}$ (with $e_1 < \cdots < e_l$) be the set of real generalized critical values of the mapping $x \in \mathbb{R}^n \to f(x)$. Then $\inf_{x \in \mathbb{R}^n} f(x) > -\infty$ if and only if there exists $1 \leq i_0 \leq l$ such that $\inf_{x \in \mathbb{R}^n} f(x) = e_{i_0}$.*

REMARK 2.8. *Combined with Lemma 2.3, the above theorem leads to $f^* = \inf_{x \in \mathbb{R}^n} f^{\mathbf{A}}(x)$.*

3. MAIN RESULTS

For $\mathbf{A} \in \mathrm{GL}_n(\mathbb{Q})$, we denote by $W_1^{\mathbf{A}}$ the constructible set defined by

$$\left\{ \frac{\partial f^{\mathbf{A}}}{\partial X_1} = \cdots = \frac{\partial f^{\mathbf{A}}}{\partial X_{n-1}} = 0, \frac{\partial f^{\mathbf{A}}}{\partial X_n} \neq 0 \right\},$$

and by $W_0^{\mathbf{A}}$ the algebraic variety defined by

$$\left\{ \frac{\partial f^{\mathbf{A}}}{\partial X_1} = \cdots = \frac{\partial f^{\mathbf{A}}}{\partial X_{n-1}} = \frac{\partial f^{\mathbf{A}}}{\partial X_n} = 0 \right\}.$$

We set $W^{\mathbf{A}} := W_1^{\mathbf{A}} \cup W_0^{\mathbf{A}}$, which is the algebraic variety defined by

$$\left\{ \frac{\partial f^{\mathbf{A}}}{\partial X_1} = \cdots = \frac{\partial f^{\mathbf{A}}}{\partial X_{n-1}} = 0 \right\}.$$

LEMMA 3.1. *If $\inf_{x \in \mathbb{R}} f(x) > -\infty$, then there exists a Zariski-closed subset $\mathscr{A} \subsetneq GL_n(\mathbb{C})$ such that for all $\mathbf{A} \in GL_n(\mathbb{Q}) \setminus \mathscr{A}$,*

$$f^* = \inf\{f(x) \mid x \in \mathbb{R}^n\} = \inf\{f^{\mathbf{A}}(x) \mid x \in W^{\mathbf{A}} \cap \mathbb{R}^n\}.$$

Moreover $R_\infty(f^{\mathbf{A}}, W^{\mathbf{A}})$ is a finite set.

Proof. We start by proving that $f^* = \inf\{f^{\mathbf{A}}(x) \mid x \in W^{\mathbf{A}}\}$. Remark first that $f^* \leq \inf\{f^{\mathbf{A}}(x) \mid x \in W^{\mathbf{A}} \cap \mathbb{R}^n\}$.

- Suppose first that the infimum f^* is reached over $\mathbb{R}^n$. Then, it is reached at a critical point $x \in W_0^{\mathbf{A}}$. Since $W_0^{\mathbf{A}} \subset W^{\mathbf{A}}$, $f^* = \inf\{f^{\mathbf{A}}(x) \mid x \in W^{\mathbf{A}} \cap \mathbb{R}^n\}$.

- Suppose now that the infimum f^* is not reached over $\mathbb{R}^n$. Then, by Theorems 2.4 and 2.7, f^* belongs to the

set of non-properness of the restriction of the projection $(x, t) \to t$ to the Zariski-closure of the set defined by

$$f^{\mathbf{A}} - T = \frac{\partial f}{\partial X_1} = \cdots = \frac{\partial f}{\partial X_{n-1}} = 0, \ \frac{\partial f}{\partial X_n} \neq 0.$$

This implies that for all $\varepsilon > 0$, there exists $(x, t) \in \mathbb{R}^n \times \mathbb{R}$ such that $x \in W_1^{\mathbf{A}} \cap \mathbb{R}^n$ and $f^* \leq t \leq f^* + \varepsilon$. This implies that $f^* \geq \inf\{f^{\mathbf{A}}(x) \mid x \in W^{\mathbf{A}} \cap \mathbb{R}^n\}$. We conclude that $f^* = \inf\{f^{\mathbf{A}}(x) \mid x \in W^{\mathbf{A}} \cap \mathbb{R}^n\}$ since we previously proved that $f^* \leq \inf\{f^{\mathbf{A}}(x) \mid x \in W^{\mathbf{A}} \cap \mathbb{R}^n\}$

We prove now that $R_\infty(f^{\mathbf{A}}, W^{\mathbf{A}})$ is finite. Remark that $R_\infty(f^{\mathbf{A}}, W^{\mathbf{A}}) = R_\infty(f^{\mathbf{A}}, W_0^{\mathbf{A}}) \cup R_\infty(f^{\mathbf{A}}, W_1^{\mathbf{A}})$. The set

$$R_\infty(f^{\mathbf{A}}, W_0^{\mathbf{A}}) \subset \{f^{\mathbf{A}} \mid x \in W_0^{\mathbf{A}}\} = K_0(f^{\mathbf{A}})$$

is finite. Moreover, by Definition 1.1 and 2.2, $R_\infty(f^{\mathbf{A}}, W_1^{\mathbf{A}})$ is a subset of the non-properness set of the mapping $\widetilde{f}$ restricted to $W_1^{\mathbf{A}}$, which by Remark 2.5 is a finite set. Hence $R_\infty(f^{\mathbf{A}}, W^{\mathbf{A}})$ is a finite set. $\qquad \square$

Fix a real number $M \in f(\mathbb{R}^n)$ and for all $\mathbf{A} \in \mathrm{GL}_n(\mathbb{Q})$, consider the following semi-algebraic set

$$W_M^{\mathbf{A}} = \left\{ x \in \mathbb{R}^n \mid M - f^{\mathbf{A}}(x) \geq 0, \frac{\partial f^{\mathbf{A}}}{\partial X_i} = 0, 1 \leq i \leq n-1 \right\}.$$

LEMMA 3.2. *There exists a Zariski-closed subset $\mathscr{A} \subsetneq GL_n(\mathbb{C})$ such that for all $\mathbf{A} \in GL_n(\mathbb{Q}) \setminus \mathscr{A}$, if*

$$\inf\{f^{\mathbf{A}}(x) \mid x \in W_M^{\mathbf{A}}\} > 0,$$

then $f^{\mathbf{A}}$ can be written as a sum

$$f^{\mathbf{A}} = s + t\left(M - f^{\mathbf{A}}\right) + \sum_{1 \leq i \leq n-1} \phi_i \frac{\partial f^{\mathbf{A}}}{\partial X_i}, \qquad (3)$$

where $\phi_i \in \mathbb{R}[\bar{X}]$ for $1 \leq i \leq n-1$, and s, t are sums of squares in $\mathbb{R}[\bar{X}]$.

Proof. By Lemma 3.1, $f^{\mathbf{A}}$ is bounded, positive on $W_M^{\mathbf{A}}$. By Lemma 3.1, $R_\infty(f^{\mathbf{A}}, W_M^{\mathbf{A}})$ is a finite set. Then, Theorem 1.3 implies that $f^{\mathbf{A}}$ can be written as a sum (3). $\qquad \square$

THEOREM 3.3. *Let $f \in \mathbb{R}[\bar{X}]$ be bounded below, and $M \in f(\mathbb{R}^n)$. There exists a Zariski-closed subset $\mathscr{A} \subsetneq GL_n(\mathbb{C})$ such that for all $\mathbf{A} \in GL_n(\mathbb{Q}) \setminus \mathscr{A}$, the following conditions are equivalent:*

(i) *$f^{\mathbf{A}} \geq 0$ on $\mathbb{R}^n$;*

(ii) *$f^{\mathbf{A}} \geq 0$ on $W_M^{\mathbf{A}}$;*

(iii) *For every $\epsilon > 0$, there are sums of squares of polynomials s and t in $\mathbb{R}[\bar{X}]$ and polynomials $\phi_i \in \mathbb{R}[\bar{X}], 1 \leq i \leq n-1$, such that*

$$f^{\mathbf{A}} + \epsilon = s + t\left(M - f^{\mathbf{A}}\right) + \sum_{1 \leq i \leq n-1} \phi_i \frac{\partial f^{\mathbf{A}}}{\partial X_i}.$$

Proof. By Lemma 3.2 and Theorem 1.3. $\qquad \square$

DEFINITION 3.4. *For all polynomials $f \in \mathbb{R}[\bar{X}]$, denote by d the total degree of f. Then for all $k \in \mathbb{N}$, we define*

$f_k^* \in \mathbb{R} \cup \{\pm\infty\}$ *as the supremum over all $a \in \mathbb{R}$ such that $f^{\mathbf{A}} - a$ can be written as a sum*

$$f^{\mathbf{A}} - a = s + t\left(M - f^{\mathbf{A}}\right) + \sum_{1 \leq i \leq n-1} \phi_i \frac{\partial f^{\mathbf{A}}}{\partial X_i} \qquad (4)$$

where $t, \phi_i, 1 \leq i \leq n-1$ are polynomials of degree at most $2k$, for $k \in \mathbb{N}$ and s, t are sums of squares of polynomials in $\mathbb{R}[\bar{X}]$.

THEOREM 3.5. *Let $f \in \mathbb{R}[\bar{X}]$ be bounded below. Then there exists a Zariski-closed subset $\mathscr{A} \subsetneq GL_n(\mathbb{C})$ such that for all $\mathbf{A} \in GL_n(\mathbb{Q}) \setminus \mathscr{A}$, the sequence $\{f_k^*\}, k \in \mathbb{N}$ converges monotonically increasing to the infimum $(f^{\mathbf{A}})^*$ which equals to f^* by Lemma 2.8.*

4. NUMERICAL RESULTS

Examples below are cited from [3, 6, 10, 14, 21]. We use Matlab package SOSTOOLS [15] to compute optimal values f_k^* by relaxations of order k over

$$W_M^{\mathbf{A}} = \left\{ x \in \mathbb{R}^n \mid M - f^{\mathbf{A}}(x) \geq 0, \frac{\partial f^{\mathbf{A}}}{\partial X_i} = 0, 1 \leq i \leq n-1 \right\}.$$

In the following test, we set $\mathbf{A} := I_{n \times n}$ be an identity matrix, and without loss of generality, we let $M := f^{\mathbf{A}}(0) = f(0)$. The set $W_M^{\mathbf{A}}$ is very simple and the results we get are very similar to or better than the given results in literatures [3, 6, 10, 14, 21].

EXAMPLE 4.1. *Let us consider the polynomial*

$$f(x, \ y) := (xy - 1)^2 + (x - 1)^2.$$

Obviously, $f^* = f^{sos} = 0$ which can be reached at $(1, 1)$. The computed optimal values are $f_0^* \approx 0.34839 \cdot 10^{-8}$, $f_1^* \approx 0.21183 \cdot 10^{-8}$ and $f_2^* \approx 0.69594 \cdot 10^{-8}$.

EXAMPLE 4.2. *Let us consider the Motzkin polynomial*

$$f(x, \ y) := x^2 y^4 + x^4 y^2 - 3x^2 y^2 + 1.$$

It is well known that $f^* = 0$ but $f^{sos} = -\infty$. The computed optimal values are $f_0^* \approx -6138.2$, $f_1^* \approx -0.52508$, $f_2^* \approx -0.19588$ and $f_3^* \approx 0.37327 \cdot 10^{-8}$.

EXAMPLE 4.3. *Let us consider the Berg polynomial*

$$f(x, \ y) := x^2 y^2 (x^2 + y^2 - 1).$$

We know that $f^* = -1/27 \approx -0.037037037$. But $f^{sos} = -\infty$. Our computed optimal values are $f_0^* \approx -563.01$, $f_1^* \approx -0.056591$, $f_2^* \approx -0.047805$ and $f_3^* \approx -0.037037$.

EXAMPLE 4.4. *Let*

$$f(x, \ y) := (x^2 + 1)^2 + (y^2 + 1)^2 - 2(x + y + 1)^2.$$

Since f is a bivariate polynomial of degree 4, $f - f^*$ must be a sum of squares. By computation, we obtain f_0^*, f_1^*, f_2^* all approximately equal to -11.458.

EXAMPLE 4.5. *Consider the polynomial of three variables:*

$$f(x, \ y, \ z) := (x + x^2 y + x^4 yz)^2.$$

As mentioned in [21], this polynomial has non-isolated singularities at infinity. It is clear that $f^* = 0$. Our computed optimal values are: $f_0^* \approx -0.36282 \cdot 10^{-8}$, $f_1^* \approx -0.12725 \cdot 10^{-7}$, $f_2^* \approx -0.1346 \cdot 10^{-7}$ and $f_3^* \approx -0.62199 \cdot 10^{-8}$.

EXAMPLE 4.6. *Let us consider the homogenous Motzkin polynomial of three real variables:*

$$f(x,\ y,\ z) := x^2 y^2 (x^2 + y^2 - 3z^2) + z^6.$$

It is known that $f^* = 0$ *but* $f^{sos} = -\infty$. *By computation, we get optimal values:* $f_0^* \approx -0.27651$, $f_1^* \approx -.15039 \cdot 10^{-2}$, $f_2^* \approx -0.31073 \cdot 10^{-3}$, $f_3^* \approx -0.10552 \cdot 10^{-3}$, $f_4^* \approx -0.66181 \cdot 10^{-4}$, $f_5^* \approx -0.3114 \cdot 10^{-4}$ *and* $f_6^* \approx -0.29321 \cdot 10^{-4}$.

EXAMPLE 4.7. *Consider the polynomial from* [11]

$$f := \sum_{i=1}^{5} \prod_{j \neq i} (X_i - X_j) \in \mathbb{R}[X_1, X_2, X_3, X_4, X_5].$$

It is shown in [11] *that* $f^* = 0$ *but* $f^{sos} = -\infty$. *In* [21], *the results computed using gradient tentacles are* $f_0^* \approx -0.2367$, $f_1^* \approx -0.0999$ *and* $f_2^* \approx -0.0224$. *Using truncated tangency variety in* [3], *we get* $f_0^* \approx -1.9213$, $f_1^* \approx -0.060899$ *and* $f_2^* \approx -0.012281$. *The optimal values we computed are better:* $f_0^* \approx -4.4532$, $f_1^* \approx -0.59884 \cdot 10^{-8}$, $f_2^* \approx -0.7685 \cdot 10^{-7}$. *The number of equality constraints in* [3] *is 10 while we only add 4 equality constrains.*

EXAMPLE 4.8. *Let us consider the following example of Robinson* [17].

$$R(x, y, 1) := x^6 + y^6 + 1 - (x^4 y^2 + x^2 y^4 + x^4 + x^2 + y^4 + y^2) + 3x^2 y^2.$$

It is proved that $f^* = 0$ *but* $f^{sos} = -\infty$. *Our computed lower bounds are:* $f_0^* \approx -0.9334$, $f_1^* \approx -0.23419$, $f_2^* \approx -0.70394 \times 10^{-2}$ *and* $f_3^* \approx 0.65325 \times 10^{-9}$.

5. UNATTAINABLE INFIMUM VALUE

EXAMPLE 5.1. *Consider the polynomial*

$$f(x, y) := (1 - xy)^2 + y^2.$$

The polynomial f *does not attain its infimum* $f^* = 0$ *on* $\mathbb{R}^2$. *Since* f *is a sum of squares, we have* $f^{sos} = 0$ *and therefore* $f_k^* = 0$ *for all* $k \in \mathbb{N}$. *However, as shown in* [3, 6, 21], *there are always numerical problems. For example, the results given in* [3] *are* $f^{sos} \approx 1.5142 \cdot 10^{-12}$, $f_0^* \approx -0.12641 \cdot 10^{-3}$, $f_1^* \approx 0.12732 \cdot 10^{-1}$, $f_2^* \approx 0.49626 \cdot 10^{-1}$.

For polynomials which do not attain their infimum values, we investigate the numerical problem involved in solving the SOS relaxation:

$$\sup \left\{ a \mid f - a = m_d(\bar{X})^T \cdot W \cdot m_d(\bar{X}),\ W \succeq 0, W^T = W \right\}, \tag{5}$$

where $m_d(\bar{X})$ is a vector of monomials of degree less than or equal to d, W is also called the Gram matrix.

SDPTools is a package for solving SDPs in Maple [2]. It includes an SDP solver which implements the classical primal-dual potential reduction algorithm [23]. This algorithm requires initial strictly feasible primal and dual points. Usually, it is difficult to find a strictly feasible point for (5). According to the Big-M method, after introducing two big positive numbers M_1 and M_2, we convert (5) to the following

# iter.	prec.	gap	lower bound r	M_1	M_2
50	75	.74021e-17	.46519e-1	10^3	10^3
50	75	.12299e-11	.47335e-2	10^3	10^5
50	75	.68693e-12	.47335e-2	10^5	10^5
50	75	.38601e-10	.47424e-3	10^3	10^7
70	75	.76145e-18	.47424e-3	10^7	10^7
50	75	.43114e-10	.47433e-4	10^3	10^9
70	75	.33233e-12	.47433e-4	10^9	10^9
75	90	.86189e-10	.47426e-5	10^3	10^{11}

Table 1: Lower bounds with $m_d(\bar{X}) = [1, x, y, x^2, xy, y^2]^T$

form:

$$\left. \begin{array}{ll} \sup\limits_{\widehat{r} \in \mathbb{R}, \widehat{W}} & \widehat{r} - M_2 z \\[2mm] s.t. & f(\bar{X}) - \widehat{r} + z(m_d(\bar{X})^T \cdot m_d(\bar{X})) \\[1mm] & \quad = m_d(\bar{X})^T \cdot \widehat{W} \cdot m_d(\bar{X}), \\[1mm] & \widehat{W} \succeq 0, \quad \widehat{W}^T = \widehat{W}, \quad z \geq 0, \\[1mm] & \mathbf{Tr}(\widehat{W}) \leq M_1. \end{array} \right\} \tag{6}$$

The dual form of (6) is

$$\left. \begin{array}{ll} \inf\limits_{y_\alpha, t \in \mathbb{R}} & \sum\limits_\alpha f_\alpha y_\alpha + M_1 t \\[2mm] s.t. & \text{Moment}_d(y) + tI \succeq 0, \quad t \geq 0 \\[1mm] & \mathbf{Tr}(\text{Moment}_d(y)) \leq M_2. \end{array} \right\} \tag{7}$$

Assuming the primal and dual problems are both bounded, suppose M_1 and M_2 are chosen larger than the upper bounds on the traces of the Gram matrix and the moment matrix respectively, then this entails no loss of generality. In practice, these upper bounds are not known, and we can only guess some appropriate values for M_1, M_2 from the given polynomials. If we can not get the right results, we will increase M_1, M_2 and solve the SDPs again.

In Table 1, we choose $m_d(\bar{X}) := [1, x, y, x^2, xy, y^2]^T$ and solve (6) and (7) for different M_1 and M_2.

The first column is the number of iterations and the second column is the number of digits we used in Maple. The third column is the gap of the primal and dual SDPs at the solutions. It is clear that the corresponding SDPs can be solved quite accurately with enough number of iterations. However, the lower bounds we get are not so good. If we choose larger M_2, the lower bound becomes better. As mentioned earlier, the number M_2 is chosen as the upper bound on the trace of the moment matrix at the optimizers. So it implies that the trace of the corresponding moment matrix may be unbounded. Let us consider the primal and dual SDPs obtained from SOS relaxation of (1):

$$\mathbb{P} \mapsto \begin{cases} \inf\limits_{y_\alpha \in \mathbb{R}} & \sum\limits_\alpha f_\alpha y_\alpha \\[2mm] s.t. & \text{Moment}_d(y) \succeq 0. \end{cases} \tag{8}$$

$$\mathbb{P}^* \mapsto \begin{cases} \sup\limits_{r \in \mathbb{R}} & r \\[2mm] s.t. & f(\bar{X}) - r = m_d(\bar{X})^T \cdot W \cdot m_d(\bar{X}), \\[1mm] & W \succeq 0, \quad W^T = W. \end{cases} \tag{9}$$

For Example 5.1, f is a sum of squares, so $\mathbb{P}^*$ has a feasible solution. By proposition 3.1 in [10], $\mathbb{P}^*$ is solvable and $\inf \mathbb{P} =$

$\max \mathbb{P}^* = 0$. We show that for $m_d(\bar{X}) = [1, x, y, x^2, xy, y^2]^T$, $\mathbb{P}$ does not attain the minimum. To the contrast, if y^* is a minimizer of the SDP problem $\mathbb{P}$, then we have

$$1 - 2y_{1,1} + y_{2,2} + y_{0,2} = 0, \tag{10}$$

and

$$\text{Moment}_2(y) = \begin{bmatrix} 1 & y_{1,0} & y_{0,1} & y_{2,0} & y_{1,1} & y_{0,2} \\ y_{1,0} & y_{2,0} & y_{1,1} & y_{3,0} & y_{2,1} & y_{1,2} \\ y_{0,1} & y_{1,1} & y_{0,2} & y_{2,1} & y_{1,2} & y_{0,3} \\ y_{2,0} & y_{3,0} & y_{2,1} & y_{4,0} & y_{3,1} & y_{2,2} \\ y_{1,1} & y_{2,1} & y_{1,2} & y_{3,1} & y_{2,2} & y_{1,3} \\ y_{0,2} & y_{1,2} & y_{0,3} & y_{2,2} & y_{1,3} & y_{0,4} \end{bmatrix} \succeq 0.$$

Since $\text{Moment}_2(y)$ is a positive semidefinite matrix, we have $y_{0,2} \geq 0$ and $|2y_{1,1}| \leq (1 + y_{2,2})$. Combining with (10), we must have $y_{0,2} = 0$ and

$$2y_{1,1} = 1 + y_{2,2}. \tag{11}$$

Because $\text{Moment}_2(y)$ is positive semidefinite, from $y_{0,2} = 0$, we can derive $y_{1,1} = 0$. Therefore, by (11), we have $y_{2,2} = -1$. It is a contradiction.

Let us show that the dual problem of (9) is not bounded if we choose $m_d(\bar{X}) = [1, x, y, x^2, xy, y^2]^T$. The infimum of $f(x, y)$ can only be reached at "infinity": $p^* = (x^*, y^*) \in \{\mathbb{R} \cup \pm\infty\}^2$. The vector

$$[x^*, y^*, x^{*2}, x^*y^*, y^{*2}, x^{*3}, x^{*2}y^*, x^*y^{*2},$$
$$y^{*3}, x^{*4}, x^{*3}y^*, x^{*2}y^{*2}, x^*y^{*3}, y^{*4}]$$

is a minimizer of (8) at "infinity". Since $x^*y^* \to 1$ and $y^* \to 0$, when $\|(x^*, y^*)\|$ goes to ∞, any moment $y_{i,j}$ with $i > j$ tends to ∞. So the trace of the moment matrix tends to ∞.

If we increase the bound M_2, we can get better results as shown in Table 1. For example, by setting $M_1 = 10^3$, $M_2 = 10^{11}$, we get $f^* = 0.4743306 \times 10^{-5}$. However this method converges very slowly at the beginning and needs large amount of computations.

THEOREM 5.2. *[16] For a polynomial $p(x) = \sum_\alpha p_\alpha x^\alpha$, we define $C(p)$ as the convex hull of $\sup(p) = \{\alpha | p_\alpha \neq 0\}$, then we have $C(p^2) = 2C(p)$; for any positive semidefinite polynomials f and g, $C(f) \subseteq C(f + g)$; if $f = \sum_j g_j^2$ then $C(g_j) \subseteq \frac{1}{2}C(f)$.*

For the polynomial f in Example 5.1, $C(f)$ is the convex hull of the points $(0,0), (1,1), (0,2), (2,2)$; see Figure 1. According to Theorem 5.2, the SOS decomposition of f contains only monomials whose supports are $(0,0), (0,1), (1,1)$. Hence, if we choose a sparse monomial vector $m_d(\bar{X}) = [1, y, xy]^T$, for $M_1 = 1000$ and $M_2 = 1000$, from Table 2, we can see a very accurate optimal value is obtained. This is due to the fact that the trace of the moment matrix at the optimizer (x^*, y^*) now is $1 + y^{*2} + x^{*2}y^{*2}$, which is bounded when x^*y^* goes to 1 and y^* goes to 0. That is the main reason that we get very different results in Table 1 and 2. We can also verify the above results by using `solvesos` in YALMIP[12]; see Table 3.

In the following, in order to remove the monomials which cause the ill-conditionedness of the moment matrix, we also try to exploit the sparsity structure when we compute optimal values f_k^* by SOS relaxations of order k over $W_M^{\mathbf{A}}$.
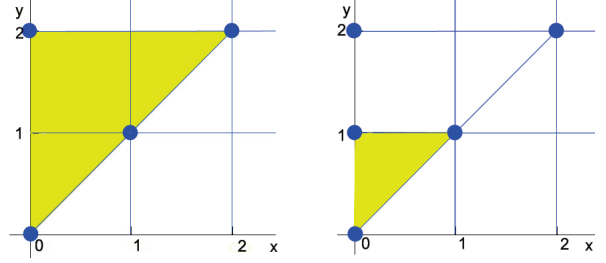

Figure 1: Newton polytope for the polynomial f (left), and the possible monomials in its SOS decomposition (right).

# iter.	prec.	gap	lower bound r	M_1	M_2
50	75	.97565e-27	-.38456e-28	10^3	10^3

Table 2: The lower bounds using $m_d(\bar{X}) = [1, y, xy]^T$

Let $A = I_{2\times2}$, $m_{d_1}(\bar{X}) = m_{d_2}(\bar{X}) := [1, x, y, x^2, xy, y^2]$, and symmetric semidefinite positive matrices W, V satisfying

$$f + \epsilon = m_{d_1}(\bar{X})^T \cdot W \cdot m_{d_1}(\bar{X})$$
$$+ m_{d_2}(\bar{X})^T \cdot V \cdot m_{d_2}(\bar{X}) \cdot (M - f) + \phi \frac{\partial f}{\partial x}.$$

Hence

$$f + \epsilon \equiv m_{d_1}(\bar{X})^T \cdot W \cdot m_{d_1}(\bar{X}) \tag{12}$$
$$+ m_{d_2}(\bar{X})^T \cdot V \cdot m_{d_2}(\bar{X}) \cdot (M - f) \bmod J,$$

where $J = \langle \frac{\partial f}{\partial x} \rangle$.

If we do not exploit the sparsity structure, the associated moment matrix is a diagonal matrix $\begin{bmatrix} P & 0 \\ 0 & Q \end{bmatrix}$, where

$$P = \begin{bmatrix} y_{0,0} & y_{1,0} & y_{0,1} & y_{2,0} & y_{1,1} & y_{0,2} \\ y_{1,0} & y_{2,0} & y_{1,1} & y_{3,0} & y_{2,1} & y_{1,2} \\ y_{0,1} & y_{1,1} & y_{0,2} & y_{2,1} & y_{1,2} & y_{0,3} \\ y_{2,0} & y_{3,0} & y_{2,1} & y_{4,0} & y_{3,1} & y_{2,2} \\ y_{1,1} & y_{2,1} & y_{1,2} & y_{3,1} & y_{2,2} & y_{1,3} \\ y_{0,2} & y_{1,2} & y_{0,3} & y_{2,2} & y_{1,3} & y_{0,4} \end{bmatrix}$$

and $Q =$

$$\begin{bmatrix} 4y_{0,2} - y_{2,4} + 2y_{1,3} - y_{0,4} & 4y_{1,1} - y_{3,3} - y_{1,3} + 2y_{2,2} \\ -y_{0,5} + 4y_{0,3} + 2y_{1,4} - y_{2,5} & 4y_{1,2} - y_{3,4} - y_{1,4} + 2y_{2,3} \\ 4y_{1,2} - y_{3,4} - y_{1,4} + 2y_{2,3} & 4y_{2,1} + 2y_{3,2} - y_{2,3} - y_{4,3} \\ -y_{0,6} + 4y_{0,4} + 2y_{1,5} - y_{2,6} & 2y_{2,4} + 4y_{1,3} - y_{3,5} - y_{1,5} \\ 2y_{2,4} + 4y_{1,3} - y_{3,5} - y_{1,5} & -y_{4,4} - y_{2,4} + 2y_{3,3} + 4y_{2,2} \\ -y_{4,4} - y_{2,4} + 2y_{3,3} + 4y_{2,2} & 4y_{3,1} + 2y_{4,2} - y_{3,3} - y_{5,3} \end{bmatrix}$$

$$\begin{bmatrix} 2y_{3,1} + 4y_{2,0} - y_{4,2} - y_{2,2} & 2y_{1,1} + 4y_{0,0} - y_{0,2} - y_{2,2} \\ 4y_{2,1} + 2y_{3,2} - y_{2,3} - y_{4,3} & 2y_{1,2} + 4y_{0,1} - y_{0,3} - y_{2,3} \\ 4y_{3,0} - y_{3,2} - y_{5,2} + 2y_{4,1} & 2y_{2,1} - y_{1,2} + 4y_{1,0} - y_{3,2} \\ -y_{4,4} - y_{2,4} + 2y_{3,3} + 4y_{2,2} & 4y_{0,2} - y_{2,4} + 2y_{1,3} - y_{0,4} \\ 4y_{3,1} + 2y_{4,2} - y_{3,3} - y_{5,3} & 4y_{1,1} - y_{3,3} - y_{1,3} + 2y_{2,2} \\ 4y_{4,0} - y_{4,2} + 2y_{5,1} - y_{6,2} & 2y_{3,1} + 4y_{2,0} - y_{4,2} - y_{2,2} \end{bmatrix}$$

$m_d(\bar{X})$	lower bounds r
$[1, y, xy]^T$	.14853e-11
$[1, x, y, xy]^T$	.414452e-4
$[1, x, y, x^2, xy, y^2]^T$	.15952e-2

Table 3: The lower bounds using `solvesos` in Matlab

$$\left.\begin{array}{ll} 2y_{1,2}+4y_{0,1}-y_{0,3}-y_{2,3} & 2y_{2,1}-y_{1,2}+4y_{1,0}-y_{3,2} \\ 4y_{0,2}-y_{2,4}+2y_{1,3}-y_{0,4} & 4y_{1,1}-y_{3,3}-y_{1,3}+2y_{2,2} \\ 4y_{1,1}-y_{3,3}-y_{1,3}+2y_{2,2} & 2y_{3,1}+4y_{2,0}-y_{4,2}-y_{2,2} \\ -y_{0,5}+4y_{0,3}+2y_{1,4}-y_{2,5} & 4y_{1,2}-y_{3,4}-y_{1,4}+2y_{2,3} \\ 4y_{1,2}-y_{3,4}-y_{1,4}+2y_{2,3} & 4y_{2,1}+2y_{3,2}-y_{2,3}-y_{4,3} \\ 4y_{2,1}+2y_{3,2}-y_{2,3}-y_{4,3} & 4y_{3,0}-y_{3,2}-y_{5,2}+2y_{4,1} \end{array}\right]$$

We can see that the moment matrix has lots of terms $y_{i,j}$ for $i > j$ which tend to infinity when we get close to the optimizer.

In the following we will try to remove these terms. At first, we compute the normal form of (12) modulo the ideal J, and then compare the coefficients of $x^i y^j$ of both sides to obtain the monomial vectors $m_{d_1}(\bar{X})$ and $m_{d_2}(\bar{X})$ which exploit the sparsity structure.

- The normal form of two sides of (12) modulo the ideal J
  $-xy + 1 + y^2 + \epsilon = w_{1,1} - v_{1,1} + v_{1,1}M$
  $+ (w_{2,1} + w_{1,2} - v_{2,1} + v_{2,1}M - v_{1,2} + v_{1,2}M)x$
  $+ (w_{3,5} + w_{5,3} - v_{3,4} - v_{2,1} + v_{2,6}M + w_{6,2}$
  $- v_{1,2} + v_{3,5}M + w_{2,6} - v_{2,5} + v_{1,3}M - v_{4,3}$
  $- v_{5,2} + w_{3,1} + w_{1,3} + v_{3,1}M + v_{5,3}M + v_{6,2}M)y$
  $+ (w_{1,4} + w_{4,1} - v_{4,1} + v_{4,1}M - v_{2,2} + v_{2,2}M - v_{1,4}$
  $+ w_{2,2} + v_{1,4}M)x^2 + (v_{3,2}M + v_{6,4}M + w_{5,5} + w_{4,6}$
  $+ v_{2,3}M + v_{5,5}M + w_{2,3} - v_{2,2} + w_{1,5} + w_{3,2}$
  $+ v_{4,6}M - v_{1,4} + w_{6,4} + v_{5,1}M - v_{5,4} + v_{1,1}$
  $+ v_{5,1} + v_{1,5}M - v_{4,5} - v_{4,1})xy + (v_{3,3}M + v_{6,1}M$
  $- v_{2,3} + w_{6,5} - v_{5,5} - v_{4,6} + v_{6,1} + w_{1,6} - v_{1,1}$
  $+ w_{3,3} - v_{3,2} - v_{1,5} + v_{1,6}M - v_{5,1} - v_{6,4} + v_{6,5}M$
  $+ v_{5,6}M + w_{5,6})y^2 + (w_{4,2} - v_{2,4} + v_{4,2}M - v_{4,2}$
  $+ v_{2,4}M + w_{2,4})x^3 + (-v_{2,4} + w_{4,3} + v_{5,2}M + v_{1,2}$
  $+ v_{3,4}M + w_{3,4} + v_{2,1} + v_{4,3}M + w_{2,5} - v_{4,2} + v_{2,5}M$
  $+ w_{5,2})x^2y + (w_{3,6} + w_{6,3} - v_{3,5} - v_{2,6} - v_{3,1}$
  $+ v_{6,3}M - v_{6,2} - v_{5,3} - v_{1,3} + v_{3,6}M)y^3$
  $+ (-v_{4,4} + v_{4,4}M + w_{4,4})x^4$
  $+ (w_{5,4} + v_{2,2} + v_{1,4} + v_{4,1} + v_{4,5}M + v_{5,4}M$
  $+ w_{4,5} - v_{4,4})x^3y + (-v_{6,5} - v_{6,1} - v_{5,6} - v_{3,3}$
  $+ v_{6,6}M - v_{1,6} + w_{6,6})y^4 + (v_{4,2} + v_{2,4})x^4y$
  $+ (-v_{6,3} - v_{3,6})y^5 - v_{6,6}y^6 + v_{4,4}x^5y$.

- The coefficients of y^6 and x^5y are $-v_{6,6}$ and $v_{4,4}$ respectively. Therefore $v_{4,4} = v_{6,6} = 0$. The matrix V is positive semidefinite, we have $v_{4,i} = v_{i,4} = v_{6,i} = v_{i,6} = 0$ for $1 \leq i \leq 6$.

- The coefficient of x^4 is $-v_{4,4} + v_{4,4}M + w_{4,4}$, we have $w_{4,4} = 0$. Since W is also positive semidefinite, we have $w_{i,4} = w_{4,i} = 0$ for $1 \leq i \leq 6$. From the coefficients of x^3y and x^2, we can obtain that $v_{2,2} = w_{2,2} = 0$ and $v_{2,i} = v_{i,2} = w_{2,i} = w_{i,2} = 0$ for $1 \leq i \leq 6$.

- After eliminating all zero terms obtained above, we have
  $-xy + 1 + y^2 + \epsilon = w_{1,1} - v_{1,1} + v_{1,1}M$
  $+ (w_{3,5} + w_{5,3} + v_{3,5}M + v_{1,3}M + w_{3,1}$
  $+ w_{1,3} + v_{3,1}M + v_{5,3}M)y + (w_{5,5} + v_{5,5}M$
  $+ w_{1,5} + v_{5,1}M + v_{1,1} + w_{5,1} + v_{1,5}M)xy$
  $+ (v_{3,3}M + w_{6,5} - v_{5,5} + w_{6,1} + w_{1,6} - v_{1,1}$
  $+ w_{3,3} - v_{1,5} - v_{5,1} + w_{5,6})y^2$
  $+ (w_{3,6} + w_{6,3} - v_{3,5} - v_{3,1} - v_{5,3}$
  $- v_{1,3})y^3 + (-v_{3,3} + w_{6,6})y^4$.

- Deleting all zero rows and columns, one gets the simplified Gram matrices
  $$W = \left[\begin{array}{cccc} w_{1,1} & w_{1,3} & w_{1,5} & w_{1,6} \\ w_{3,1} & w_{3,3} & w_{3,5} & w_{3,6} \\ w_{5,1} & w_{5,3} & w_{5,5} & w_{5,6} \\ w_{6,1} & w_{6,3} & w_{6,5} & w_{6,6} \end{array}\right],$$
  $$V = \left[\begin{array}{ccc} v_{1,1} & v_{1,3} & v_{1,5} \\ v_{3,1} & v_{3,3} & v_{3,5} \\ v_{5,1} & v_{5,3} & v_{5,5} \end{array}\right]$$

corresponding to $m_{d_1}(\bar{X}) = [1, y, xy, y^2]$ and $m_{d_2}(\bar{X}) = [1, y, xy]$ respectively.

- The moment matrices corresponding to $m_{d_1}(\bar{X})$ and $m_{d_2}(\bar{X})$ are
  $$\left[\begin{array}{cccc} y_{0,0} & y_{0,1} & y_{1,1} & y_{0,2} \\ y_{0,1} & y_{0,2} & y_{1,2} & y_{0,3} \\ y_{1,1} & y_{1,2} & y_{2,2} & y_{1,3} \\ y_{0,2} & y_{0,3} & y_{1,3} & y_{0,4} \end{array}\right],$$
  $$\left[\begin{array}{ccc} 4y_{0,0}+y_{1,1}-y_{0,2} & 5y_{0,1}-y_{0,3} & 5y_{1,1}-y_{0,2} \\ 5y_{0,1}-y_{0,3} & 5y_{0,2}-y_{0,4} & 5y_{0,1}-y_{0,3} \\ 5y_{1,1}-y_{0,2} & 5y_{0,1}-y_{0,3} & 5y_{1,1}-y_{0,2} \end{array}\right].$$

  We can see that these moment matrices only consist of terms $y_{i,j}$ for $i \leq j$ which will go to 1 $(i = j)$ or 0 $(i < j)$ when xy goes to 1 and y goes to 0. Therefore the elements of the moment matrices which may cause the ill-conditionedness are removed.

For $k = 2, M = 5, A = I_{2 \times 2}, M_1 = 1000, M_2 = 1000$, the matrices W and V computed by our SDP solver in Maple for Digits = 60 are
$$W = \left[\begin{array}{cccc} 0.50804 & 0.0 & 0.0 & -0.50804 \\ 0.0 & 0.33126 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.13374 & 0.0 \\ -0.50804 & 0 & 0.0 & 0.50804 \end{array}\right],$$
$$V = \left[\begin{array}{ccc} 0.12298 & 0.0 & -0.12298 \\ 0.0 & 0.13374 & 0.0 \\ -0.12298 & 0.0 & 0.12298 \end{array}\right].$$

The associated moment matrices are
$$\left[\begin{array}{cccc} 1 & 0.0 & 0.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 \\ 1.0 & 0.0 & 0.0 & 1.0 \end{array}\right], \left[\begin{array}{ccc} 5.0 & 0.0 & 5.0 \\ 0.0 & 0.0 & 0.0 \\ 5.0 & 0.0 & 5.0 \end{array}\right].$$

The lower bound we get is $f_2^* \approx 4.029500408 \times 10^{-24}$. Moreover, by SDPTools in Maple [2], we can obtain the certified lower bound

$f_2^{**} = -4.029341206383157355520229568612510632 \times 10^{-24}$

by writing $f - f_2^{**}$ as an exact rational SOS over $W_M^{\mathbf{A}}$ [7, 8].

EXAMPLE 5.3. *Consider the following polynomial*

$$f(x,y) = 2y^4(x+y)^4 + y^2(x+y)^2 + 2y(x+y) + y^2.$$

As mentioned in [3], we have $f^* = -\frac{5}{8}$ and f does not attain its infimum. It is also observed in [3] that there are obviously numerical problems since the output of their algorithm are $f_0^* = -0.614, f_1^* = -0.57314, f_2^* = -0.57259$, and $f_3^* = -0.54373$.

In fact, we have $f^* = f^{\text{sos}} = -\frac{5}{8}$ since

$$\begin{aligned} f + \frac{5}{8} &= \frac{(2y^2+2xy+1)^2(2y^2+2xy-1)^2}{8} \\ &+ \frac{(2y^2+2xy+1)^2}{2} + y^2. \end{aligned}$$

If we take $x_n = -(\frac{1}{n} + \frac{n}{2})$, $y_n = \frac{1}{n} - \frac{1}{n^3}$, it can be verified that $-\frac{5}{8}$ is a generalized critical value of f. For $k = 4$, if we do not exploit the sparsity structure, and choose

$$m_{d_1}(\bar{X}) = m_{d_2}(\bar{X}) := [1, x, y, x^2, xy, y^2, x^3, x^2y, xy^2,$$
$$y^3, x^4, x^3y, x^2y^2, xy^3, x^4]^T,$$

then numerical problems will appear.

By exploiting the sparsity structure of the SOS problem, we get

$$m_{d_1}(\bar{X}) = m_{d_2}(\bar{X}) := [1, y, y^2, xy, y^3, xy^2, y^4, xy^3, x^2y^2]^T,$$

the terms which cause ill-conditionedness of the moment matrix are removed. The lower bound computed by our SDP solver in Maple is $f_4^* = -0.625000000000073993$. It is very close to the true infimum -0.625.

6. CONCLUSIONS

We use important properties in the computation of generalized critical values of a polynomial mapping [18, 19] and Theorem 1.3 to given a method to solve optimization (1). We do not require that f attains the infimum in $\mathbb{R}^n$ and use a much simpler variety in the SOS representation. We try to investigate and fix the numerical problems involved in computing the infimum of polynomials in Example 5.1 and 5.3. The strategies we propose here are just a first try. We hope to present a more general method to overcome these numerical problems in future.

Acknowledgments

7. REFERENCES

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