

# Minimum Ellipsoid Bounds for Solutions of Polynomial Systems via Sum of Squares\*

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## Abstract

We study ellipsoid bounds for the solutions  $(x, \mu) \in \mathbb{R}^n \times \mathbb{R}^r$  of polynomial systems of equalities and inequalities. The variable  $\mu$  can be considered as parameters perturbing the solution  $x$ . For example, bounding the zeros of a system of polynomials whose coefficients depend on parameters is a special case of this problem. Our goal is to find minimum ellipsoid bounds just for  $x$ . Using theorems from real algebraic geometry, the ellipsoid bound can be found by solving a particular polynomial optimization problem with sums of squares (SOS) techniques. Some numerical examples are also given.

**Keywords:** polynomial system, perturbation, ellipsoid, real algebraic geometry, sum of squares(SOS), semidefinite programming(SDP).

## 1. Introduction

We propose a method to find guaranteed bounds on the real solutions of a polynomial system of equalities and/or inequalities of the following

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form:

$$\begin{cases} \phi_1(x_1, \dots, x_n; \mu_1, \dots, \mu_r) = 0 \\ \vdots \\ \phi_s(x_1, \dots, x_n; \mu_1, \dots, \mu_r) = 0 \\ \rho_1(x_1, \dots, x_n; \mu_1, \dots, \mu_r) \leq 0 \\ \vdots \\ \rho_t(x_1, \dots, x_n; \mu_1, \dots, \mu_r) \leq 0 \end{cases} \quad (1.1)$$

where  $x = (x_1, \dots, x_n)^T \in \mathbb{R}^n$  and  $\mu = (\mu_1, \dots, \mu_r)^T \in \mathbb{R}^r$ . For each  $1 \leq i \leq s$  and  $1 \leq j \leq t$ ,  $\phi_i$  and  $\rho_j$  are multivariate polynomials in  $(x, \mu) \in \mathbb{R}^{n+r}$ . Throughout this paper, we partition the solution into two parts: the first  $n$  components ( $x$ ) and the last  $r$  components ( $\mu$ ).  $\mu$  can be thought of as parameters perturbing the solution  $x$ . We are only interested in bounding  $x$  for all  $\mu$  determined by (1.1).  $x$  can be also be thought of as the projection of the solution  $(x, \mu) \in \mathbb{R}^{n+r}$  of (1.1) into the subspace  $\mathbb{R}^n$ . We consider only real solutions, since many practical problems concern only real solutions.

Our goal is to bound the projected *solution set* defined as

$$\mathcal{S} = \{x \in \mathbb{R}^n : \exists \mu \in \mathbb{R}^r \text{ s.t. } (x, \mu) \text{ satisfies system (1.1)}\}.$$

For a given  $\mu$ , there may be no real  $x$  satisfying (1.1), or one unique such  $x$ , or several such  $x$ , or infinitely many such  $x$ . So  $\mathcal{S}$  can be quite complicated.

Here is an example (see example 2 in section 6)

$$\begin{aligned} (x_1 - 1)(x_2 - 1)(x_3 - 1) - \mu_1 &= 0 \\ (x_1 + x_2 - 3)(x_2 + x_3 - 3)(x_3 + x_1 - 3) - \mu_2 &= 0 \\ (x_1 + 2x_2 - x_3)(x_2 + 2x_3 - x_1)(x_3 + 2x_1 - x_2) - \mu_3 &= 0 \\ \mu_1^2 - .1^2 \leq 0, \mu_2^2 - .1^2 \leq 0, \mu_3^2 - .1^2 &\leq 0. \end{aligned}$$

As the  $\mu_i$ s get smaller, the solution  $x$  approaches one of the solutions of the 27 3-by-3 linear systems implicitly defined by the first 3 equations when  $\mu_i = 0 (i = 1, 2, 3)$ . This example defines the solution set  $\mathcal{S}$  for  $|\mu_i| \leq .1 (i = 1, 2, 3)$ .

The traditional approach in perturbation analysis of a system of equations is to find the maximum distance of the perturbed solutions to the unperturbed solution, i.e. to find a bounding ball of smallest radius with the unperturbed solution at the center. This approach works well when the solution set is almost a ball and the unperturbed solution lies near the center. Unfortunately, this is often not the case in practice, when the solution set is very elongated. Instead, we seek a bounding ellipsoid of smallest volume (in a sense defined below), which can more effectively bound many elongated sets.

The particular idea for finding minimum ellipsoids was introduced in [3, 4], where the authors try to find the minimum ellipsoids for linear systems whose coefficients are rational functions of perturbing parameters. In this paper, we generalize these results to polynomial systems of equalities and/or inequalities.

The computational complexity of our approach may be described as follows. Let  $D$  be the maximum degree of any polynomial in (1.1). Then for fixed  $D$  our method can provide a guaranteed bounding ellipsoid in polynomial time in the number of variables  $n$  and  $r$ . But to guarantee the *minimum* bounding ellipsoid, the complexity can potentially grow much faster (see Section 5).

Throughout this paper, we will use the following notation. All variables are real.  $X^T$  is the transpose of a matrix  $X$ .  $I_n$  is the standard  $n$ -by- $n$  identity matrix.  $S_+^n(S_{++}^n)$  denotes the set of all the  $n$ -by- $n$  symmetric positive semidefinite (definite) matrices.  $A \succeq 0$  ( $A \succ 0$ ) means that the matrix  $A$  is positive semidefinite (definite). The polynomial inequality  $f \succeq_{sos} g$  means that  $f - g$  can be written as a sum of squares of polynomials, which will be discussed in Section 3.

This paper is organized as follows. Section 2 introduces ellipsoid bounds for the solution of (1.1). Section 3 introduces “sum of squares” polynomials and their connection with semidefinite programming (SDP). Section 4 introduces results we need from real algebraic geometry. In section 5, we discuss how to find the ellipsoid bound by solving a particular SDP. Section 6 will show two numerical examples.

## 2. Ellipsoid bounds for Polynomial Systems

In this section, we formulate the ellipsoid bound for the projected solution set  $\mathcal{S}$ . This idea of finding an ellipsoid bound is from [3, 4], where the authors consider the special case where each polynomial  $\phi_i(x; \mu)$  is affine in  $x$  and rational in  $\mu$ , and the  $\rho_j = \rho_j(\mu)$  are quadratic in  $\mu$ .

An ellipsoid in  $\mathbb{R}^n$  may be defined as

$$\mathcal{E}(P, z) = \{x \in \mathbb{R}^n : (x - z)^T P^{-1} (x - z) < 1\} \quad (2.1)$$

where  $P \in S_{++}^n$  is the *shape matrix*, and  $z \in \mathbb{R}^n$  is the center of the ellipsoid. By taking a Schur complement, the ellipsoid can also be defined as

$$\mathcal{E}(P, z) = \left\{ x \in \mathbb{R}^n : \begin{bmatrix} P & x - z \\ (x - z)^T & 1 \end{bmatrix} \succ 0 \right\}. \quad (2.2)$$

For example, the ellipsoid in the 2D plane given by

$$\frac{(x_1 - z_1)^2}{a^2} + \frac{(x_2 - z_2)^2}{b^2} < 1$$

has the shape matrix  $P = \begin{bmatrix} a^2 & 0 \\ 0 & b^2 \end{bmatrix}$ .

How do we measure the “size” of an ellipsoid? The “best” measure would appear to be its volume, which is proportional to  $\sqrt{\det P}$ . However, we will instead choose  $\text{trace}(P)$  to measure the size, for two reasons: 1)  $\text{trace}(P)$  is an affine function, whereas  $\sqrt{\det P}$  is not, which makes the optimization problem tractable. 2)  $\text{trace}(P)$  is zero if and only if all the axes are zero, but  $\sqrt{\det P}$  is zero if any one axis is zero.

Now we can formulate the minimum ellipsoid problem as the following optimization:

$$\inf_{P \in S_{++}^n, z \in \mathbb{R}^n} \text{trace}(P) \quad (2.3)$$

$$s.t. \quad \left. \begin{array}{l} (x - z)^T P^{-1} (x - z) < 1 \\ \text{for all } (x, \mu) \text{ satisfying} \\ \phi_i(x, \mu) = 0, \rho_j(x, \mu) \leq 0 \end{array} \right\}. \quad (2.4)$$

What we will do in the following sections is to replace the constraint (2.4) by certain matrix inequalities that can be solved by SDP.

### 3. Polynomials that are sums of squares

In this section, we briefly introduce sum of squares polynomials, and their connection with SDP; see [10, 8] for more details. For notational convenience we assume throughout this section that all polynomials are in  $x \in \mathbb{R}^n$ , i.e.  $x$  is not necessarily a solution of (1.1).

First, every polynomial  $p(x)$  can be written as  $v^T A v$  for some symmetric matrix  $A$ , where  $v$  is the vector of monomials

$$v = [1, x_1, \dots, x_n, x_1^2, x_1 x_2, \dots]^T.$$

Since the entries in vector  $v$  depends on each other, the matrix  $A$  is not unique. It can be shown [10] that all possible  $A$ s satisfying  $p = v^T A v$  form an affine set

$$\mathcal{A} = \left\{ A_0 + \sum_i \alpha_i A_i : \alpha_i \in \mathbb{R} \right\}$$

where  $A_0, A_1, \dots$  are constant symmetric matrices.

For example, consider the following polynomial from [10]

$$F(x, y) = 2x^4 + 2x^3y - x^2y^2 + 5y^4.$$

After some algebra, we can show that

$$F(x, y) = \begin{bmatrix} x^2 \\ y^2 \\ xy \end{bmatrix}^T \begin{bmatrix} 2 & -\alpha & 1 \\ -\alpha & 5 & 0 \\ 1 & 0 & 2\alpha - 1 \end{bmatrix} \begin{bmatrix} x^2 \\ y^2 \\ xy \end{bmatrix},$$

where  $\alpha$  is arbitrary.

**Definition 3.1** A polynomial  $p(x)$  is a sum of squares (SOS) polynomial if it can be expressed as a finite sum of squares of other polynomials, i.e.,  $p(x) = \sum_{i=1}^{\ell} p_i^2(x)$ .

One good property of SOS polynomials is that they are closely related to SDP. If a polynomial  $p(x) = \sum_i p_i^2(x)$ , then we can find a particular  $A$  satisfying  $0 \preceq A \in \mathcal{A}$ . In fact, we can write  $p_i(x) = v^T a_i$  for some constant vector  $a_i$ , then  $p(x) = v^T (\sum_i a_i a_i^T) v$ , and so  $A = \sum_i a_i a_i^T \succeq 0$  is such a choice. Conversely, if we can find some  $A$  satisfying  $0 \preceq A \in \mathcal{A}$ , then the spectral decomposition of  $A = \sum_i \lambda_i^2 q_i q_i^T$  provides the  $a_i = \lambda_i q_i$  defining the  $p_i(x) = v^T a_i$  in the SOS expression. Since  $\mathcal{A}$  is affine, we can determine whether  $\mathcal{A}$  contains an  $A \succeq 0$  by solving an SDP, as described in the following theorem:

**Theorem 3.2 (Parrilo, [10])** A polynomial is SOS if and only if we can find some  $A \in \mathcal{A}$  such that  $A$  is positive semidefinite. This can be confirmed by solving an SDP feasibility problem.

The computational complexity of this problem will depend on the size of the corresponding SDP: a polynomial  $p(x)$  of degree  $d$  and  $n$  variables can be represented as  $v^T A v$ , where  $v$  is the monomial vector up to degree  $d/2$ . The number of coefficients of  $p(x)$  is at most  $\binom{n+d}{d}$ , and the dimension of matrix  $A$  is  $\binom{n+d/2}{d/2}$ . We return to the complexity issue in Section 5.

## 4. Some theorems in real algebraic geometry

This section will introduce some results about positive semidefinite (PSD) polynomials, the positivstellensatz, and other theorems about infeasibility of semi-algebraic sets (the subsets in Euclidean space that can be described by polynomial equalities and/or inequalities). For a more detailed introduction to real algebra, see [1].

In this section, to comply with the traditional notation in multivariate polynomial algebra, we will denote by  $x \in \mathbb{R}^n$  the variable of a multivariate polynomial, not the solution to (1.1), unless explicitly stated otherwise.

**Definition 4.1** A polynomial  $p(x)$  is said to be positive semidefinite (PSD) if  $p(x) \geq 0, \forall x \in \mathbb{R}^n$ .

PSD polynomials appear frequently in practice. Unfortunately, testing whether a polynomial is PSD or not is an NP-hard problem if the polynomial has degree at least four [7]. Therefore (unless  $P=NP$ ) any algorithm guaranteed to test the nonnegativity of a polynomial in every possible case will run too slowly when the number of variables is large

[8]. However, one obvious sufficient condition for a polynomial to be PSD is that it be SOS.

As we saw in section 3, testing whether a polynomial is SOS is tractable, i.e. can be done in polynomial time. Thus, unless  $P=NP$ , some PSD polynomials are not SOS. Indeed, this is consistent with the solution to Hilbert's 17<sup>th</sup> problem; see [12] for a good introduction. Now let  $P_{n,d}$  denote the set of PSD polynomials of degree  $d$  in  $n$  variables, and let  $\Sigma_{n,d}$  denote the set of polynomials of degree  $d$  in  $n$  variables which are SOS. Clearly  $\Sigma_{n,d} \subseteq P_{n,d}$ , but the equality may not hold. Hilbert (1888, [2, 12]) showed that  $\Sigma_{n,d} = P_{n,d}$  if and only if  $(n, d) \in \{(1, \geq 1), (\geq 1, 2), (2, 4)\}$ . However, the first explicit polynomial that is PSD but not SOS appeared in 1967 [11, 12], which is the famous Motzkin polynomial  $M(x_1, x_2, x_3) = x_1^4 x_2^2 + x_1^2 x_2^4 + x_3^6 - 3x_1^2 x_2^2 x_3^2$ . The nonnegativity of  $M(x_1, x_2, x_3)$  is obtained immediately from the arithmetic-geometric mean inequality. The proof that  $M(x_1, x_2, x_3)$  is not SOS can be found in [12].

Given polynomials  $q_1, \dots, q_m \in \mathbb{R}[x_1, \dots, x_n]$ , let  $P(q_1, \dots, q_m)$  denote the *preorder cone* generated by the  $q_i$ 's, i.e.,

$$P(q_1, \dots, q_m) = \left\{ \sum_{I \subset \{1, 2, \dots, m\}} \sigma_I(x) \prod_{j \in I} q_j(x) \mid \sigma_I \text{ SOS} \right\}.$$

Define the *basic closed semi-algebraic set* generated by the  $q_i$ 's as

$$S(q_1, \dots, q_m) = \{x \in \mathbb{R}^n : q_i(x) \geq 0, \text{ for all } 1 \leq i \leq m\}.$$

**Theorem 4.2 (Stengle, [14])** *Let  $(f_i)_{i=1, \dots, s}$ ,  $(h_k)_{k=1, \dots, t}$  be a set of polynomials in  $\mathbb{R}[x_1, \dots, x_n]$ . Then the following two properties are equivalent:*

1. *The following set is empty*

$$\left\{ x \in \mathbb{R}^n \mid \begin{array}{l} f_i(x) = 0, i = 1, \dots, s \\ h_k(x) \geq 0, k = 1, \dots, t \end{array} \right\}; \quad (4.1)$$

2. *There exist polynomials  $\lambda_i$  and  $\sigma_K$  such that*

$$\sum_{i=1}^s \lambda_i f_i + \sum_{K \subset \{1, 2, \dots, t\}} \sigma_K \prod_{k \in K} h_k + 1 = 0.$$

This theorem is the so-called *positivstellensatz* in real algebraic geometry. It is a powerful tool to testify the infeasibility of a polynomial system of equalities and inequalities.

However, the *positivstellensatz* involves cross products among different  $h_k$ 's, which makes the computation more expensive. To avoid this expense, we will introduce other theorems which do not involve the

cross products of  $h_k$ 's, i.e., just the linear part of preorder cone. The following assumption and theorem are due to Jacobi [5] and Putinar [11], and used by Lasserre [6].

**Assumption 4.3** *Let  $h_1, \dots, h_\ell \in \mathbb{R}[x_1, \dots, x_n]$  be polynomials such that  $S(h_1, \dots, h_\ell)$  is compact. Assume that there exists a polynomial  $u(x) \in \mathbb{R}[x_1, \dots, x_n]$  such that  $S(u)$  is compact and*

$$u(x) = u_0(x) + \sum_{i=1}^{\ell} u_i(x)h_i(x)$$

where  $u_0, u_1, \dots, u_\ell$  are all SOS, i.e.,  $u(x)$  is just the linear part of the preorder cone  $P(h_1, \dots, h_\ell)$ .

In fact, Assumption 4.3 is often satisfied [6]. For example, if there is one polynomial  $h_j(x)$  such that  $S(h_j)$  is compact, or if all  $h_i$ 's are linear, then Assumption 4.3 is satisfied. Another way to ensure Assumption 4.3 is true is to add one more inequality  $h_{\ell+1} = a^2 - \|x\|_2^2$  for sufficiently large  $a$ .

**Theorem 4.4 ([5, 11])** *Let  $h_1, \dots, h_\ell \in \mathbb{R}[x_1, \dots, x_n]$  be a set of polynomials satisfying Assumption 4.3. Then every polynomial  $p(x)$ , strictly positive on  $S(h_1, \dots, h_\ell)$ , can be represented as*

$$p(x) = p_0(x) + \sum_{i=1}^{\ell} p_i(x)h_i(x)$$

where  $p_0, p_1, \dots, p_\ell$  are all SOS.

If Assumption 4.3 is not satisfied, we have another theorem, due to Schmüdgen, which is a simplified version of the positivstellensatz.

**Theorem 4.5 ([13])** *Let  $h_1, \dots, h_\ell \in \mathbb{R}[x_1, \dots, x_n]$  be polynomials such that  $S(h_1, \dots, h_\ell)$  is compact. Then every polynomial  $p(x)$ , strictly positive on  $S(h_1, \dots, h_\ell)$ , must belong to  $P(h_1, \dots, h_\ell)$ , i.e.,*

$$p(x) = \sum_{K \subset \{1, 2, \dots, \ell\}} p_K(x) \prod_{i \in K} h_i(x)$$

for some SOS polynomials  $p_K (K \subset \{1, 2, \dots, \ell\})$ .

In the rest of this section,  $x$  and  $\mu$  will again denote the solutions to polynomial system (1.1). All polynomials are in  $(x, \mu)$  unless explicitly stated otherwise.

Now return to the constraint (2.4). It holds if and only if

$$1 - (x - z)^T P^{-1} (x - z) > 0 \text{ for all } \left\{ x \in \mathbb{R}^n \mid \begin{array}{l} \phi_i(x, \mu) = 0, i = 1, \dots, s \\ \rho_j(x, \mu) \leq 0, j = 1, \dots, t \end{array} \right\}.$$

Replacing one equality with two inequalities with opposite directions, we can see that (1.1) is the same as

$$\left\{ \begin{array}{l} \phi_1(x_1, \dots, x_n; \mu_1, \dots, \mu_r) \geq 0 \\ \vdots \\ \phi_s(x_1, \dots, x_n; \mu_1, \dots, \mu_r) \geq 0 \\ - \phi_1(x_1, \dots, x_n; \mu_1, \dots, \mu_r) \geq 0 \\ \vdots \\ - \phi_s(x_1, \dots, x_n; \mu_1, \dots, \mu_r) \geq 0 \\ - \rho_1(x_1, \dots, x_n; \mu_1, \dots, \mu_r) \geq 0 \\ \vdots \\ - \rho_t(x_1, \dots, x_n; \mu_1, \dots, \mu_r) \geq 0 \end{array} \right. \quad (4.2)$$

**Theorem 4.6** Suppose the set of polynomials  $\{\pm\phi_1, \dots, \pm\phi_s, \rho_1, \dots, \rho_t\}$  satisfies Assumption 4.3. Then if constraint (2.4) holds, there exist polynomials  $\lambda_i = \lambda_i(x, \mu)$ ,  $\sigma_j = \sigma_j(x, \mu)$  such that

$$1 - (x - z)^T P^{-1}(x - z) + \sum_{i=1}^s \lambda_i \phi_i - \sum_{j=1}^t \sigma_j \rho_j \succeq_{\text{sos}} 0$$

$$\sigma_1, \dots, \sigma_t \succeq_{\text{sos}} 0.$$

*Proof* Let  $p = 1 - (x - z)^T P^{-1}(x - z)$  and  $\{\pm\phi_1, \dots, \pm\phi_s, -\rho_1, \dots, -\rho_t\}$  be the polynomials defining the semi-algebraic set in Theorem 4.4. Notice that  $p(x)$  is strictly positive on  $S(\pm\phi_1, \dots, \pm\phi_s, -\rho_1, \dots, -\rho_t)$ . Then by Theorem 4.4, there exist SOS polynomials  $\varphi$ ,  $\tau_i$ ,  $\nu_i$  ( $i = 1, \dots, s$ ), and  $\sigma_j$  ( $j = 1, \dots, t$ ) such that

$$1 - (x - z)^T P^{-1}(x - z) = \varphi + \sum_{i=1}^s (\tau_i - \nu_i) \phi_i + \sum_{j=1}^t \sigma_j \rho_j.$$

Let  $\lambda_i = \nu_i - \tau_i$ . Then we get the result in the theorem.  $\square$

*Remark:* (i) By Theorem 4.2, the SOS inequalities in Theorem 4.6 are also sufficient, in the sense that we can get only a weak instead of strict inequality in (2.4). But this does not affect much in the optimization. (ii) However, if  $\{\pm\phi_1, \dots, \pm\phi_s, -\rho_1, \dots, -\rho_t\}$  does not satisfy Assumption 4.3, but  $S(\pm\phi_1, \dots, \pm\phi_s, -\rho_1, \dots, -\rho_t)$  is compact, we can use Schmüdgen's theorem 4.5 to get another similar equivalent formulation of constraint (2.4), by adding those items involving cross products.

We can also get a certificate of feasibility for (2.4) via the posi-



tivstellensatz. Notice that (2.4) is valid if and only the following set

$$\left\{ \begin{array}{ll} (x-z)^T P^{-1}(x-z) - 1 & \geq 0 \\ \phi_1(x_1, \dots, x_n; \mu_1, \dots, \mu_r) & = 0 \\ \vdots & \\ \phi_s(x_1, \dots, x_n; \mu_1, \dots, \mu_r) & = 0 \\ - \rho_1(x_1, \dots, x_n; \mu_1, \dots, \mu_r) & \geq 0 \\ \vdots & \\ - \rho_t(x_1, \dots, x_n; \mu_1, \dots, \mu_r) & \geq 0 \end{array} \right.$$

is empty. By Theorem 4.2, we obtain that

**Theorem 4.7** *The constraint (2.4) holds if and only if there exist polynomials  $\gamma = \gamma(x, \mu) \neq 0$ ,  $\lambda_i = \lambda_i(x, \mu)$ ,  $\sigma_I = \sigma_I(x, \mu)$  such that*

$$\begin{aligned} ((x-z)^T P^{-1}(x-z) - 1)\gamma + \sum_{i=1}^s \lambda_i \phi_i - \sum_{I \subset \{1, \dots, t\}} \sigma_I \prod_{j \in I} \rho_j + 1 &= 0 \\ \gamma \succeq_{\text{sos}} 0, \sigma_I \succeq_{\text{sos}} 0, \forall I \subset \{1, \dots, t\}. \end{aligned}$$

*Proof* Verify directly by Theorem 4.2.  $\square$

*Remark:* i) In Theorems 4.6 and 4.7, the polynomials  $\lambda_i$ ,  $\sigma_j$  and others may depend on  $P$  and  $z$ . ii) The degree bounds and structures of  $\lambda_i$  and  $\sigma_j$  are not clear yet, as far as the authors know. There are some exponential degree bounds [15]. The bound may be as high as  $O(\frac{1}{\epsilon})$  where  $\epsilon$  is the minimum value of  $1 - (x-z)^T P^{-1}(x-z)$  over the solution set. iii) For arbitrary fixed degrees, any ellipsoid satisfying Theorem 4.6 or 4.7 is an upper bound for the *solution set*  $\mathcal{S}$ . iv) However, as the readers will see in the next section, the found ellipsoids will converge the minimum one when the degrees of  $\lambda_i$  and  $\sigma_j$  go to infinity.

## 5. Finding the ellipsoids

In this section, we will show how to solve the problem (2.3)-(2.4) by formulating it as an optimization with SOS polynomials. Denote by  $R_N[x, \mu]$  all the real polynomials in  $(x, \mu)$  with degrees less than or equal to  $N$ .

By Theorem 4.6-4.7 and the remarks afterwards, the problem (2.3)-(2.4) can be relaxed as

$$\begin{aligned} \hat{E}_N : \quad & \min_{\substack{P \in S_{++}^n, z \in \mathbb{R}^n \\ \lambda_i, \sigma_j \in R_N[x, \mu]}} \text{trace}(P) \quad \text{subject to} \\ & 1 - (x-z)^T P^{-1}(x-z) + \sum_{i=1}^s \lambda_i(x, \mu) \phi_i - \sum_{j=1}^t \sigma_j(x, \mu) \rho_j \succeq_{\text{sos}} 0 \\ & \sigma_1, \dots, \sigma_t \succeq_{\text{sos}} 0 \end{aligned}$$

which can be rewritten as

$$\begin{aligned}
& \min_{\substack{P \in S_{++}^n, z \in \mathbb{R}^n \\ \lambda_i, \sigma_j \in R_N[x, \mu]}} \text{trace}(P) \\
& s.t. \quad 1 - \begin{bmatrix} x \\ 1 \end{bmatrix}^T \begin{bmatrix} I & -z \end{bmatrix}^T P^{-1} \begin{bmatrix} I & -z \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix} + \\
& \quad \sum_{i=1}^s \lambda_i(x, \mu) \phi_i - \sum_{j=1}^t \sigma_j(x, \mu) \rho_j \succeq_{sos} 0 \\
& \quad \sigma_1, \dots, \sigma_t \succeq_{sos} 0.
\end{aligned}$$

Now by introducing a new matrix variable  $Q$ , this becomes

$$\begin{aligned}
& \min_{\substack{Q, P \in S_{++}^n, z \in \mathbb{R}^n \\ \lambda_i, \sigma_j \in R_N[x, \mu]}} \text{trace}(P) \quad \text{subject to} \\
& 1 - \begin{bmatrix} x \\ 1 \end{bmatrix}^T Q \begin{bmatrix} x \\ 1 \end{bmatrix} + \sum_{i=1}^s \lambda_i(x, \mu) \phi_i - \sum_{j=1}^t \sigma_j(x, \mu) \rho_j \succeq_{sos} 0 \\
& \begin{bmatrix} I & -z \end{bmatrix}^T P^{-1} \begin{bmatrix} I & -z \end{bmatrix} \preceq Q \\
& \sigma_1, \dots, \sigma_t \succeq_{sos} 0.
\end{aligned}$$

Taking a Schur complement, this is equivalent to

$$E_N : p_N^* = \min_{\substack{Q, P \in S_{++}^n, z \in \mathbb{R}^n \\ \lambda_i, \sigma_j \in R_N[x, \mu]}} \text{trace}(P) \quad \text{subject to} \quad (5.1)$$

$$1 - \begin{bmatrix} x \\ 1 \end{bmatrix}^T Q \begin{bmatrix} x \\ 1 \end{bmatrix} + \sum_{i=1}^s \lambda_i(x, \mu) \phi_i - \sum_{j=1}^t \sigma_j(x, \mu) \rho_j \succeq_{sos} 0 \quad (5.2)$$

$$\begin{bmatrix} P & (I \ -z) \\ (I \ -z)^T & Q \end{bmatrix} \succeq 0 \quad (5.3)$$

$$\sigma_1, \dots, \sigma_t \succeq_{sos} 0. \quad (5.4)$$

The objective function is an affine function of  $P$ , and the constraints are either linear matrix inequality (LMIs) or SOS inequalities, which are also essentially LMIs ([10]). Therefore it can be solved by a standard SDP routine.

Now we consider the complexity of problem  $E_N$ . Let  $D$  be the maximum degree of polynomials defining system (1.1). From the discussion at the end of Section 3, we can see that the LMI corresponding to (5.2) has size  $\binom{n+r+(N+D)/2}{(N+D)/2}$ , LMI (5.3) has size  $2n+1$ , and LMIs corresponding to (5.4) have size  $\binom{n+r+N/2}{N/2}$ . Therefore, the total cost for solving problem (5.1)-(5.4) via SDP is  $O(M^{3+1/2})$ , where

$M = \binom{n+r+(N+D)/2}{(N+D)/2}$ . When  $D$  and  $N$  are fixed, this is a polynomial function of  $n$  and  $r$ .

As we pointed out in the remark after Theorem 4.7, for any fixed degree  $N$ , the ellipsoid  $\mathcal{E}_N$  found in  $E_N$  is a bound for the solution set  $\mathcal{S}$ . When the degree  $N$  is higher, the ellipsoid bound by solving  $E_N$  is tighter. The convergence of  $\mathcal{E}_N$  is described as follows.

**Theorem 5.1** *Suppose Assumption 4.3 is satisfied for polynomial system (4.2). Then the trace  $p_N^*$  of the ellipsoid  $\mathcal{E}_N$  found in  $E_N$  converges to trace  $p^*$  of the minimum ellipsoid containing the solution set  $\mathcal{S}$  when the degree  $N$  tends to infinity.*

*Proof* Let  $\mathcal{E}^* = \{x \in \mathbb{R}^n : (x - z^*)^T (P^*)^{-1} (x - z^*) \leq 1\}$  be the minimum ellipsoid containing the solution set  $\mathcal{S}$ , with  $\text{trace}(P^*) = p^*$ . Then for arbitrary  $\epsilon > 0$ , the polynomial  $1 - (x - z^*)^T (P^* + \epsilon I_n)^{-1} (x - z^*)$  is strictly positive on the set of  $(x, \mu)$  defined by (4.2). By Theorem 4.4, there exist some general polynomials  $\lambda_i(x, \mu)$  ( $i = 1, \dots, s$ ) and SOS polynomials  $\sigma_j(x, \mu)$  ( $j = 1, \dots, t$ ) such that

$$1 - (x - z^*)^T (P^* + \epsilon I_n)^{-1} (x - z^*) + \sum_{i=1}^s \lambda_i \phi_i - \sum_{j=1}^t \sigma_j \rho_j \succeq_{\text{sos}} 0.$$

As we showed in this section, problems  $\hat{E}_N$  and  $E_N$  are equivalent formulations. So they have the same optimal objective values. When  $N$  is large enough, then in  $\hat{E}_N$  we find one feasible solution with objective value  $p^* + n\epsilon$ . Thus it must be true that  $p_N^* \leq p^* + n\epsilon$ . Here  $n$  is the dimension of  $x$ , which is a constant. Since  $\mathcal{E}^*$  is minimum, it holds that  $p_N^* \geq p^*$ . Therefore we have that  $\lim_{N \rightarrow \infty} p_N^* = p^*$ .  $\square$

### 5.1. Alternative formulation

We can obtain another formulation like (5.1)-(5.4) starting from Theorem 4.7 instead of Theorem 4.6. The new optimization is

$$\begin{aligned} & \min_{\substack{Q, P \in S^n, z \in \mathbb{R}^n \\ \lambda_i, \sigma_j \in R_N[x, \mu]}} \text{trace}(P) \\ s.t. \quad & (1 - \begin{bmatrix} x \\ 1 \end{bmatrix}^T Q \begin{bmatrix} x \\ 1 \end{bmatrix}) \gamma + \sum_{i=1}^s \lambda_i(x, \mu) \phi_i \\ & \quad - \sum_{I \subset \{1, \dots, t\}} \sigma_I \prod_{j \in I} \rho_j \succeq_{\text{sos}} 0 \\ & \sigma_I \succeq_{\text{sos}} 0, \forall I \subset \{1, \dots, t\} \\ & \begin{bmatrix} P & (I - z) \\ (I - z)^T & Q \end{bmatrix} \succeq 0 \end{aligned}$$

Here the SOS polynomial  $\gamma$  must be specified before hand to preserve the convexity of the problem. In practice, we usually choose  $\gamma = 1$  and the subsets  $I \subset \{1, \dots, t\}$  with cardinality  $|I| = 1$ . As the readers may see, formulation (5.1)-(5.4) is a special case of this one (with  $\gamma = 1$ ). One might expect that this new formulation would give us better ellipsoid bounds. However, as the authors discovered in practice, choosing other  $\gamma$  (like  $x_1^2 + x_2^2 + \dots$ ) or choosing subsets  $I \subset \{1, \dots, t\}$  with  $|I| > 1$  does not help much in general, and on the other hand it could increase the complexity greatly and cause numerical convergence difficulties in SOSTOOLS.

## 6. Numerical examples

In this section, we will illustrate how the algorithm works for two examples. All of them are solved via SOSTOOLS [9].

**Example 1.** Consider the following polynomial system of two equations and two inequalities.

$$\begin{aligned} (1 + \mu_1^2)x^2 + \mu_2xy + (1 - \mu_2^2)y^2 + (\mu_1 + \mu_2)x + (\mu_1 - \mu_2)y - 1 &= 0 \\ (1 - \mu_1^2)x^2 + \mu_1xy + (1 + \mu_2^2)y^2 + (\mu_1 - \mu_2)x + (\mu_1 + \mu_2)y - 1 &= 0 \\ \epsilon^2 - \mu_1^2 \geq 0, \epsilon^2 - \mu_2^2 &\geq 0 \end{aligned}$$

where  $\epsilon = 0.1$ . Formulate the optimization (5.1)-(5.4) for this polynomial system, and then solve it by SOSTOOLS. In this problem,  $n = 2, r = 2, D = 4$ . We choose  $N = 2$  since any nonconstant SOS polynomials have degree at least 2. The resulting 2D-ellipsoid is at the top of Figure 1. The asterisks are the solutions  $(x, y)$  when  $(\mu_1, \mu_2)$  are chosen randomly according to the two inequalities. As you can see, the found ellipsoid is much larger than the set of real solutions. This is because the solution set is not connected. However, if we want more information about one branch, we can add one more inequality of the form  $(x - a)^2 + (y - b)^2 \leq r^2$ , where  $a, b, r$  are chosen according to the user's interests for the solution region, and then solve the optimization problem again. The role of this new inequality is that it can help to find the ellipsoid bound for just one solution component, and it also assures that Assumption 4.3 is satisfied. The middle and bottom pictures are obtained by adding two such different polynomials respectively, leading to much tighter bounds.

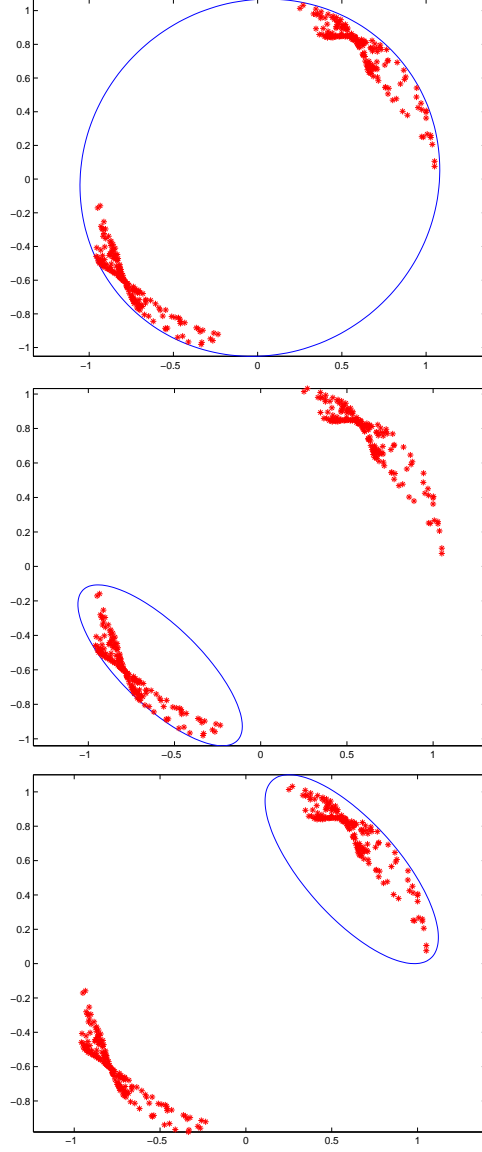


Figure 1: The top one is ellipsoid for the original system without adding any inequalities; the middle picture is obtained by adding inequality  $(x + 0.6)^2 + (y + 0.6)^2 \leq 0.6^2$ ; the bottom picture is obtained by adding inequality  $(x - 0.9)^2 + (y - 0.8)^2 \leq 0.8^2$ .

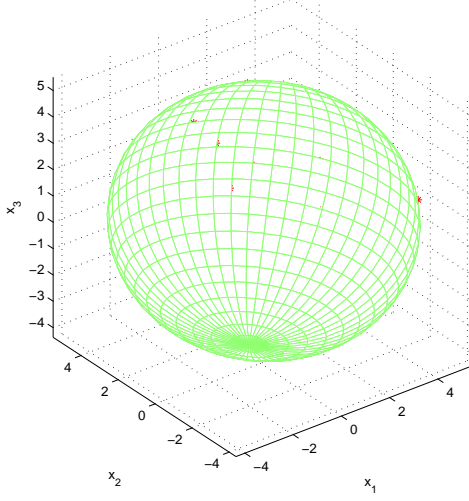


Figure 2: This is the ellipsoid found for Example 2.

**Example 2.** Consider the 3D problem introduced in Section 1:

$$\begin{aligned}
 (x_1 - 1)(x_2 - 1)(x_3 - 1) - \mu_1 &= 0 \\
 (x_1 + x_2 - 3)(x_2 + x_3 - 3)(x_3 + x_1 - 3) - \mu_2 &= 0 \\
 (x_1 + 2x_2 - x - 3)(x_2 + 2x_3 - x_1)(x_3 + 2x_1 - x_2) - \mu_3 &= 0 \\
 \mu_1^2 - .1^2 \leq 0, \mu_2^2 - .1^2 \leq 0, \mu_3^2 - .1^2 &\leq 0.
 \end{aligned}$$

In this example,  $n = 3, r = 3, D = 3$ . We also choose  $N = 2$  as in Example 1. The found 3D ellipsoid is in figure 2. We randomly chose  $(\mu_1, \mu_2, \mu_3)$  satisfying the inequality constraints, solve the equations for  $(x_1, x_2, x_3)$  using Matlab symbolic toolbox, and also plot all these solutions  $(x_1, x_2, x_3)$  as asterisks in figure 2. As we can be see, most asterisks that stand for solutions are contained inside the ellipsoid and a few are near the boundary. The back side of the ellipsoid, which is not shown, also has a number of asterisks appearing at its surface. This means that ellipsoid cannot be made any smaller while containing all the solutions. Adding constraint inequalities to focus on a particular solution component would lead to much smaller ellipsoids as in Example 1.

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