15 Sums of squares and moment relaxations

In this section we deal with optimization problems whose feasible sets are sets of polynomials satisfying certain positivity constraints. The decision variables are hence the coefficient vectors of these polynomials. The vector spaces underlying the optimization problems are thus essentially finite-dimensional function spaces.

References on semi-definite relaxations in polynomial optimization are [1, 3].

15.1 Positive polynomials and sums of squares

A real polynomial in n real variables $x_1,\dots,x_n$ is a function $x = (x_1,\dots,x_n)^T \mapsto \sum_{\alpha\in\mathbb{N}^n} c_\alpha x^\alpha$, where the sum is over a finite subset of the discrete set $\mathbb{N}^n$ of multi-indices $\alpha = (\alpha_1,\dots,\alpha_n)$, c_α are real numbers, and $x^\alpha = \prod_{i=1}^n x_i^{\alpha_i}$.

Definition 15.1. The set $P_{d,n}$ of positive polynomials in n variables of degree d is defined as the set of homogeneous polynomials $p : \mathbb{R}^n \to \mathbb{R}$ of degree d such that $p(x) \geq 0$ for all $x \in \mathbb{R}^n$.

Clearly d has to be even in order for $P_{d,n}$ to contain a non-zero element. The set $P_{d,n}$ is a closed convex cone.

In some situations optimization problems contain conic constraints of the form $p(x) \in P_{d,n}$. Here the decision variables are the coefficients of the polynomial p. The variable x is just a dummy variable denoting the argument of the polynomials in question. The constraint is concerning the polynomial p as a whole, without referencing specific values of x.

The constraint $p \in P_{d,n}$ is in general hard to check. A common relaxation of this constraint in polynomial optimization is to replace it by the stronger constraint $x \in \Sigma_{d,n}$.

Definition 15.2. The set $\Sigma_{d,n}$ of sum of squares (SOS) polynomials in n variables of degree d is defined as the set of homogeneous polynomials $p : \mathbb{R}^n \to \mathbb{R}$ of degree d which can be represented as a finite sum $p(x) = \sum_k q_k^2(x)$, where $q_k(x)$ are homogeneous polynomials of degree $d/2$ in n variables.

Clearly

$$\Sigma_{d,n} \subset P_{d,n}.$$

Theorem 15.3. *Let n, d be positive integers, d even. The equality $\Sigma_{d,n} = P_{d,n}$ holds if and only if $\min(d,n) \leq 2$ or if $(d,n) = (4,3)$.*

We shall prove only the cases $d = 2$ and $n = 2$. The case $(d,n) = (4,3)$ is more involved and has been proven by Hilbert in 1888.

$d = 2$. A homogeneous polynomial of degree 2 is a quadratic form, which can be written as $p(x) = x^T Ax$ with A a real symmetric matrix. The polynomial p is in $P_{2,n}$ if and only if the corresponding matrix A is positive semi-definite. This in turn is the case if and only if there exists a matrix $B \in \mathbb{R}^{k\times n}$ such that $A = B^T B$.

On the other hand, $p \in \Sigma_{2,n}$ if and only if $p(x) = \sum_{j=1}^k q_j^2(x)$, where each q_j is a linear homogeneous function, i.e., $q_j(x) = c_j^T x$ for some vector $c_j \in \mathbb{R}^n$. We then get $p(x) = \sum_{j=1}^k (c_j^T x)^2 = x^T \left(\sum_{j=1}^k c_j c_j^T\right) x = x^T C^T C x$, where $C \in \mathbb{R}^{k\times n}$ is a matrix containing the vectors c_j as its rows.

Thus the two conditions are equivalent.

$n = 2$. A homogeneous polynomial of degree n in two variables x, y can be written as $p(x,y) = \sum_{k=0}^d c_k x^k y^{d-k}$. We suppose that the polynomial is not identically zero (in which case it is trivially in both $P_{d,2}$ and $\Sigma_{d,2}$). Then we may suppose, by making a linear change of coordinates if necessary, that $c_d \neq 0$. Let $z_1,\dots,z_d$ be the roots of the polynomial $\sum_{k=0}^d c_k z^k$. Then this polynomial factorizes as $c_d \prod_{k=1}^d (z - z_k)$. Accordingly, we obtain

$$p(x,y) = c_d \prod_{k=1}^d (x - z_k y). \tag{1}$$

Suppose now that $p \in P_{d,2}$. Then $c_d = p(1,0) > 0$ and can be written as a square $c_d = (\sqrt{c_d})^2$. The multiplicity of every real root z_k must be even, otherwise p becomes negative near the root $(x,y) = (z_k, 1)$. The corresponding factors in (1) hence group into squares. For every complex root $z_k = a_k + ib_k$ there exists a complex conjugate root $z_{k'} = \bar{z}_k = a_k - ib_k$, and the corresponding product can be written as

$$(x - z_k y)(x - z_{k'} y) = x^2 - 2a_k xy + (a_k^2 + b_k^2)y^2 = (x - a_k y)^2 + (b_k y)^2.$$

The polynomial (1) is then a sum of squares, which shows $p \in \Sigma_{d,2}$.

Example: The *Motzkin polynomial* $p(x, y, z) = x^4y^2 + x^2y^4 + z^6 - 3x^2y^2z^2$ is in $P_{6,3}$ by the arithmetic-geometric inequality, but not in $\Sigma_{6,3}$.

That not every nonnegative polynomial can be represented as a sum of squares of polynomials with lower degree was already known to Hilbert in the 19th century. At the 2nd ICM in 1900 he posed the following question:

Hilberts 17th problem: Can every nonnegative polynomial be represented as a sum of squares of *rational* functions?

The question was positively answered by Artin in the 20s.

Consider a real symmetric $n \times n$ matrix A and the quartic polynomial

$$p(x) = \sum_{i,j=1}^{n} A_{ij} x_i^2 x_j^2$$

on $\mathbb{R}^n$. We have $p \in P_{4,n}$ if and only if the quadratic polynomial $\sum_{i,j=1}^{n} A_{ij} x_i x_j = x^T Ax$ takes nonnegative values for all $x \in \mathbb{R}_+^n$, i.e., if the matrix A is copositive. This is NP-hard to decide, however.

To detect whether a given polynomial is in the cone $P_{2d,n}$ is therefore in general a difficult problem. In contrast to this stands the easy algorithmic accessibility of the cone of sums of squares $\Sigma_{2d,n}$.

Let us devise an algorithm to check whether a given polynomial p is an element of $\Sigma_{2d,n}$. To this end, form the vector $\mathbf{x}$ of *monomials* $\prod_{k=1}^{n} x_k^{\alpha_k}$ of degree d in the variables x_k. The exponents α_k are hence nonnegative integers which sum to d. Let N be the size of the vector $\mathbf{x}$.

Suppose there exists a positive semi-definite matrix $A \in \mathcal{S}_+^N$ such that $p(x) = \mathbf{x}^T A\mathbf{x}$. Factor the matrix A as $A = B^T B$ with $B \in \mathbb{R}^{k\times N}$, and let b_j be the rows of B. Then we obtain

$$p(x) = \mathbf{x}^T B^T B\mathbf{x} = \sum_{j=1}^{k} \langle b_j, \mathbf{x}\rangle^2,$$

and p has been represented as a sum of squares of k polynomials $q_j(x) = \langle b_j, \mathbf{x}\rangle$ of degree d. Thus $p \in \Sigma_{2d,n}$.

On the other hand, suppose that $p \in \Sigma_{2d,n}$. Then there exist k homogeneous polynomials $q_1(x), \dots, q_k(x)$ of degree d such that $p(x) = \sum_{j=1}^{k} q_j^2(x)$. Every polynomial $q_j(x)$ can be written as a scalar product $\langle c_j, \mathbf{x}\rangle$ for some vector $c_j \in \mathbb{R}^N$. Let $C \in \mathbb{R}^{k\times N}$ be the matrix whose rows are the vectors c_j. Then we get

$$p(x) = \sum_{j=1}^{k} \langle c_j, \mathbf{x}\rangle^2 = \mathbf{x}^T C^T C\mathbf{x},$$

and the polynomial p has been written as $\mathbf{x}^T A\mathbf{x}$ with A positive semi-definite.

We obtain the following result.

Lemma 15.4. *A homogeneous polynomial p of degree $2d$ in n variables $x_1, \dots, x_n$ is an element of the cone $\Sigma_{2d,n}$ if and only if there exists a positive semi-definite real symmetric $N \times N$ matrix A such that $p(x) = \mathbf{x}^T A\mathbf{x}$.*

Apart from the conic constraint $A \in \mathcal{S}_+^N$, this imposes a finite number of equality relations on A which are jointly linear in the coefficients of p and the elements of A. The existence of such a matrix A can hence be incorporated as a constraint into a semi-definite program involving the coefficients of the polynomial p.

If we want to check whether a single polynomial p is a sum of squares, it may be not necessary to check the condition in Lemma 15.4 for the full monomial basis vector $\mathbf{x}$. We can often reduce the size of A by using the following object.

Definition 15.5. Let $p = \sum_\alpha c_\alpha x^\alpha$ be a polynomial in n variables. The *Newton polytope* N_p of p is the convex hull of all points $\alpha \in \mathbb{N}^n$ such that $c_\alpha \neq 0$.

We have the following result.

Lemma 15.6. *Let $p(x) = \sum_k q_k(x)^2$ be a sum of squares of polynomials q_k. Then $N_p = \bigcup_k (2N_{q_k})$. In particular, $N_{q_k} \subset \frac{1}{2}N_p$ for all k.*

Proof. For a given polynomial q, we shall first investigate the relation between the Newton polytopes N_q, N_{q^2}. We claim that $N_{q^2} = 2N_q = N_q + N_q$.

Indeed, if $q(x) = \sum_\alpha c_\alpha x^\alpha$, then

$$q^2(x) = \sum_{\beta,\gamma} c_\beta c_\gamma x^{\beta+\gamma}. \tag{2}$$

Since $c_\beta c_\gamma \neq 0$ if and only if $c_\beta \neq 0$ and $c_\gamma \neq 0$, the points generating N_{q^2} are obtained as sums of pairs of points generating N_q. This proves that $N_{q^2} \subset 2N_q$. Let us now show the converse inclusion. It suffices to prove that the extreme points of $2N_q$ are in N_{q^2}. Clearly the extreme points of $2N_q$ are of the form 2α, where α is an extreme point of N_q. The point 2α cannot be written as a sum $2\alpha = \beta + \gamma$ for *distinct* points $\beta, \gamma \in N_q$, otherwise we would have $\alpha = \frac{\beta+\gamma}{2}$, contradicting the extremality of α in N_q. Thus the coefficient in q^2 at $c_{2\alpha}$ in (2) equals c_α^2, because only the values $\beta = \alpha$, $\gamma = \alpha$ sum to 2α. It follows that $2\alpha \in N_{q^2}$.

Clearly we have that $N_p \subset \bigcup_k N_{q_k^2} = \bigcup_k (2N_{q_k})$. Let us show the converse inclusion.

It suffices to show that the extreme points of $\bigcup_k (2N_{q_k})$ are in N_p. Any such extreme point α cannot be non-extreme in $2N_{q_k}$ for any k, otherwise it can be represented as a non-trivial convex combination of points from $2N_{q_k}$ and hence from $\bigcup_k (2N_{q_k})$. Thus α is extreme in every $2N_{q_k}$ in which it is contained. But then the coefficient at x^α in q_k^2 is zero if $\alpha \notin 2N_{q_k}$ and it is positive if $\alpha \in 2N_{q_k}$. Hence the coefficient at x^α in p is also positive, and $\alpha \in N_p$. □

This leads to the following result.

Corollary 15.7. *Let p be a polynomial and N_p its Newton polytope. If p is a sum of squares of polynomials, then the extreme points of N_p must be even. Equivalently, the extreme points of $\frac{1}{2}N_p$ are integer.* □

Example: We want to check whether $p(x,y) = \sum_{j=0}^{2d} c_j x^j y^{2d-j} \in \Sigma_{2d,2}$. Let us form the vector $\mathbf{x} = (x^d, x^{d-1}y, \dots, y^d)^T$ of length $N = d+1$. We shall index the elements of $\mathbf{x}$ as well as the elements of $N \times N$ matrices from 0 to d for convenience. Then we have $\mathbf{x}^T A \mathbf{x} = \sum_{j=0}^d A_{ij}\mathbf{x}_i\mathbf{x}_j = \sum_{i,j=0}^n A_{ij} x^{(d-i)+(d-j)} y^{i+j} = \sum_{k=0}^{2d} x^{2d-k} y^k \sum_{i,j:i+j=k} A_{ij}$. The condition $p(x) = \mathbf{x}^T A \mathbf{x}$ can then be written as

$$\sum_{i,j:i+j=k} A_{ij} = c_k, \qquad \forall\ k = 0, \dots, 2d. \tag{3}$$

In other words, the sums of the elements of A on the skew-diagonals have to equal the coefficients of the polynomial p. We get the following result.

Lemma 15.8. *A polynomial $p(x,y) = \sum_{j=0}^{2d} c_j x^j y^{2d-j}$ is nonnegative if and only if there exists a positive semi-definite matrix $A \in \mathcal{S}_+^{d+1}$ such that (3) holds.*

Example: We want to check whether the polynomial

$$p(x,y,z) = c_{400}x^4 + c_{310}x^3y + \dots + c_{013}yz^3 + c_{004}z^4$$

is in $\Sigma_{4,3}$. Let us form the vector $\mathbf{x} = (x^2, y^2, z^2, yz, xz, xy)^T$ of length $N = 6$. Then we have

$$\begin{aligned}\mathbf{x}^T A \mathbf{x} = {} & A_{11}x^4 + A_{22}y^4 + A_{33}z^4 + (2A_{12} + A_{66})x^2y^2 + (2A_{13} + A_{55})x^2z^2 + (2A_{23} + A_{44})y^2z^2 + (2A_{14} + 2A_{56})x^2yz \\ & + (2A_{25} + 2A_{46})xy^2z + (2A_{36} + 2A_{45})xyz^2 + 2A_{15}x^3z + 2A_{16}x^3y + 2A_{24}y^3z + 2A_{26}xy^3 + 2A_{34}yz^3 + 2A_{35}xz^3.\end{aligned}$$

The condition $p(x) = \mathbf{x}^T A \mathbf{x}$ can then be written as

$$\begin{aligned} A_{11} &= c_{400}, \\ A_{22} &= c_{040}, \\ A_{33} &= c_{004}, \\ 2A_{12} + A_{66} &= c_{220}, \\ &\vdots \\ 2A_{34} &= c_{013}, \\ 2A_{35} &= c_{103}. \end{aligned}$$

The existence of a positive semi-definite matrix $A \in \mathcal{S}_+^6$ satisfying these linear equations is then equivalent to the inclusion $p \in \Sigma_{4,3}$ and hitherto to the nonnegativity of the polynomial $p(x, y, z)$.

Example: Let us again consider the copositive cone $\mathcal{C}^n$ of all quadratic forms $A \in \mathcal{S}^n$ which are nonnegative on the nonnegative orthant. We have seen above that $A \in \mathcal{C}^n$ if and only if $p_A(x) = \sum_{i,j=1}^n A_{ij} x_i^2 x_j^2 \in P_{4,n}$. Therefore the set

$$\mathcal{K}_0 = \{A \in \mathcal{S}^n \,|\, p_A \in \Sigma_{4,n}\}$$

is an *inner approximation* of the cone $\mathcal{C}^n$. Let us compute this approximation.

Form the vector $\mathbf{x} = (x_1^2, \dots, x_n^2, x_1x_2, x_1x_3, \dots, x_{n-1}x_n)^T \in \mathbb{R}^N$ with $N = \frac{n(n+1)}{2}$. We then have $A \in \mathcal{K}_0$ if and only if there exists a matrix $\mathbf{A} \in \mathcal{S}_+^N$ such that $p_A(x) = \mathbf{x}^T \mathbf{A} \mathbf{x}$. Let us subdivide $\mathbf{A}$ into 4 blocks, according to the subdivision of $\mathbf{x}$ into a subvector $\mathbf{x}^1$ of length n and a subvector $\mathbf{x}^2$ of length $\frac{n(n-1)}{2}$. Then the coefficients at the monomials x_i^4 and $x_i^2 x_j^2$ in the polynomial $\mathbf{x}^T \mathbf{A} \mathbf{x}$ depend only on the elements of the block $\mathbf{A}^{11}$ and the diagonal elements of the block $\mathbf{A}^{22}$. We can therefore assume that all other elements of the matrix $\mathbf{A}$ are zero, and this matrix is of the form

$$\mathbf{A} = \operatorname{diag}(B, c_{12}, c_{13}, \dots, c_{n-1,n})$$

for some matrix $B \in \mathcal{S}_+^n$ and some nonnegative scalars c_{ij}, $1 \le i < j \le n$. We get

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \sum_{i,j=1}^n B_{ij} x_i^2 x_j^2 + \sum_{i<j} c_{ij} x_i^2 x_j^2.$$

Comparing coefficients with $p_A(x) = \sum_{i,j=1}^n A_{ij} x_i^2 x_j^2$ we obtain that the matrix A is in $\mathcal{K}_0$ if and only if there exist $B \in \mathcal{S}_+^n$ and $c_{ij} \ge 0$, $1 \le i < j \le n$, such that $\operatorname{diag} A = \operatorname{diag} B$ and $A_{ij} = B_{ij} + c_{ij}$ for all $i < j$. Thus $\mathcal{K}_0 = \mathcal{S}_+^n + \mathcal{N}^n$, where $\mathcal{N}^n$ is the cone of element-wise nonnegative matrices with zero diagonal (it is easily seen that this last condition can be dropped).

Diananda proved the following result in 1962:

Theorem 15.9. *The equality $\mathcal{C}^n = \mathcal{S}_+^n + \mathcal{N}^n$ holds if and only if $n \le 4$.*

We can strengthen the inner approximation $\mathcal{K}_0$ by defining the following hierarchy of cones, parameterized by an integer $r \ge 0$.

$$\mathcal{K}_r = \left\{ A \in \mathcal{S}^n \,|\, \left(\sum_{j=1}^n x_j^2 \right)^r \cdot p_A(x) \in \Sigma_{4+2r,n} \right\}.$$

We have the following result:

Theorem 15.10. *Let $A \in \operatorname{int} \mathcal{C}^n$. Then there exists an $r \ge 0$ such that $A \in \mathcal{K}_{r'}$ for all $r' \ge r$.*

The approximations of $\mathcal{C}^n$ by $\mathcal{K}_r$ are increasingly tight, but become also more complex.

15.2 Sums of squares relaxations for polynomial optimization problems

Let us now consider how the approximation of the cone $P_{d,n}$ of nonnegative polynomials by the cone $\Sigma_{d,n}$ of sums of squares polynomials allows to approximate difficult optimization problems with polynomial data by easily solvable semi-definite programs.

Definition 15.11. A set $K \subset \mathbb{R}^n$ is called *basic semi-algebraic* if it is of the form

$$K = \{x \mid f_i(x) = 0,\ g_j(x) \leq 0\} \tag{4}$$

for some polynomials $f_i, g_j : \mathbb{R}^n \to \mathbb{R}$.

A set $K \subset \mathbb{R}^n$ is called *semi-algebraic* if it is a union of a finite number of basic semi-algebraic sets.

Our general optimization problem will be to find the minimum of a polynomial on a semi-algebraic set K:

$$\min_{x \in K} f_0(x).$$

Minimizing over a union $K = \bigcup_j K_j$ of sets is equivalent to minimizing over each set K_j and taking the minimum of the results. Therefore we may assume without loss of generality that K is already a basic semi-algebraic set given by (4).

In order to reformulate the problem we introduce the cone $P_{d,K}$ of polynomials of degree not exceeding d which are nonnegative on the basic semi-algebraic set K. This is a finite-dimensional closed convex cone. Then we may write above problem as

$$\max \tau : \quad f_0(x) - \tau \in P_{d,K},$$

where d is not smaller than the degree of f_0.

The cone $P_{d,K}$ is in general difficult to describe. We replace it by the cone $\Sigma_{d,K}$ consisting of all polynomials $p(x)$ of degree not exceeding d which can be represented as a sum

$$p(x) = \sigma_0(x) + \sum_i p_i(x) f_i(x) - \sum_j \sigma_j(x) g_j(x), \tag{5}$$

where $p_i(x)$ are arbitrary polynomials and $\sigma_0(x), \sigma_j(x)$ are sums of squares of polynomials. Clearly every polynomial in $\Sigma_{d,K}$ is nonnegative on K and hence in $P_{d,K}$, because every term in the above sum is nonnegative on K. Moreover, the above decomposition yields equality relations which are jointly linear in the coefficients of p and the unknown polynomials σ_0, p_i, σ_j. Therefore the inclusion $p \in \Sigma_{d,K}$ can be expressed by a finite number of semi-definite conic and linear equality constraints. The cone $\Sigma_{d,K}$ is hence a semi-definite representable inner approximation of $P_{d,K}$, and the approximating problem

$$\max \tau : \quad f_0(x) - \tau \in \Sigma_{d,K}$$

is a semi-definite program.

We may use more complicated representations of p to define the cone $\Sigma_{d,K}$ by including terms containing products of polynomials g_j defining the inequality constraints. For example, we may define $\Sigma_{d,K}$ by the set of all polynomials which are representable as a sum

$$p(x) = \sigma_0(x) + \sum_i p_i(x) f_i(x) - \sum_j \sigma_j(x) g_j(x) + \sum_{i,j} \sigma_{i,j}(x) g_i(x) g_j(x),$$

where $\sigma_{i,j}$ are also SOS polynomials. We may include also higher order products of the polynomials g_j as basis functions.

We have the following result.

Theorem 15.12 (Putinar 1993)**.** *Let K be compact and let p be strictly positive on K. Then there exists d such that $p \in \Sigma_{d,K}$.*

This result has the following consequence.

Theorem 15.13 (Lasserre 2001)**.** *Let K be compact. Then the sequence of SOS relaxations described above is asymptotically exact, i.e., the optimal value of the relaxations tends to the optimal value of the original problem as $d \to +\infty$.*

Example: We wish to solve the problem

$$\min x + y : \quad x \geq 0,\ x^2 + y^2 = 1. \tag{6}$$

The set $K = \{(x, y) \mid x \geq 0,\ x^2 + y^2 = 1\}$ is a semi-circle and is already basic semi-algebraic. Choose $d = 3$. We approximate the set $P_{3,K}$ of cubic polynomials which are nonnegative on the semi-circle by the set $\Sigma_{3,K}$ of polynomials which are expressible in the form

$$p(x, y) = \sigma_0(x, y) + l(x, y)(x^2 + y^2 - 1) + \sigma_1(x, y)x,$$

where σ_0, σ_1 are sums of squares polynomials of degree 2 and l is a linear polynomial. Let us introduce the vector of monomials $\mathbf{x} = (x, y, 1)^T$ of degree not exceeding 1. Then $p \in \Sigma_{3,K}$ if and only if p can be written as

$$\begin{aligned} p(x, y) =& \mathbf{x}^T A^0 \mathbf{x} + \mathbf{l}^T \mathbf{x} \cdot (x^2 + y^2 - 1) + (\mathbf{x}^T A^1 \mathbf{x}) \cdot x \\ =& (A^1_{11} + l_x)x^3 + (2A^1_{12} + l_y)x^2 y + (A^0_{11} + 2A^1_{13} + l_1)x^2 + (A^1_{22} + l_x)xy^2 + (2A^0_{12} + 2A^1_{23})xy \\ &+ (2A^0_{13} + A^1_{33} - l_x)x + l_y y^3 + (A^0_{22} + l_1)y^2 + (2A^0_{23} - l_y)y + A^0_{33} - l_1, \end{aligned}$$

where $\mathbf{l} = (l_x, l_y, l_1)^T \in \mathbb{R}^3$ and $A^0, A^1 \in \mathcal{S}^3_+$.

Hence the semi-definite program approximating the original problem can be written as

$$\max_{A^0, A^1 \in \mathcal{S}^3_+} \tau : \quad A^1_{11} + l_x = 2A^1_{12} + l_y = A^0_{11} + 2A^1_{13} + l_1 = A^1_{22} + l_x = 2A^0_{12} + 2A^1_{23} = l_y = A^0_{22} + l_1 = 0,$$

$$2A^0_{13} + A^1_{33} - l_x = 2A^0_{23} - l_y = 1,\ A^0_{33} - l_1 = -\tau.$$

Using the linear equalities to eliminate variables this leads to the equivalent SDP

$$\max -(A^0_{33} + A^0_{11} + 2A^1_{13}) : \quad \begin{pmatrix} A^0_{11} & A^0_{12} & A^0_{13} \\ A^0_{12} & A^0_{11} + 2A^1_{13} & \frac{1}{2} \\ A^0_{13} & \frac{1}{2} & A^0_{33} \end{pmatrix} \succeq 0, \quad \begin{pmatrix} A^1_{11} & 0 & A^1_{13} \\ 0 & A^1_{11} & -A^0_{12} \\ A^1_{13} & -A^0_{12} & 1 - A^1_{11} - 2A^0_{13} \end{pmatrix} \succeq 0.$$

Its solution yields the optimal value -1.

The size of the monomial bases and hence the matrices appearing in the SDPs relaxing polynomial optimization problems quickly grows with the degree d of the relaxation. Several simplifications have been proposed which lower the complexity at the cost of a worsening the approximation. The main idea is to replace a semi-definiteness constraint $A \succeq 0$ by stronger, but simpler sufficient conditions.

Diagonally dominant sums of squares (DSOS) use the criterion of diagonal dominance

$$A_{ii} \geq \sum_{j \neq i} |A_{ij}| \quad \forall\, j.$$

This condition consists of linear inequalities and hence leads to a linear program.

Scaled diagonally dominant sums of squares (SDSOS) use the condition that there exists a positive definite diagonal matrix such that the scaled matrix DAD is diagonally dominant. It can be shown that this condition is equivalent to the decomposability of A into a sum of positive semi-definite matrices with non-zero elements occurring only in a 2×2 principal submatrix for each of the summands. Since positive semi-definiteness of a 2×2 matrix is described by a conic quadratic inequality, this approximation boils down to an SOCP.

15.3 Moment relaxations

Let μ be a nonnegative measure on $\mathbb{R}^n$ with support $\operatorname{supp}\mu$. The set of nonnegative measures with support in some set $K \subset \mathbb{R}^n$ forms a convex cone. If K consists of more than a finite number of points, then this cone has infinite dimension. The extremal measures in this cone are given by the multiples of the δ-functions $\mu(x) = \delta(x - \hat{x})$, where $\hat{x} \in K$. The measure $\delta(x - \hat{x})$ has support $\{\hat{x}\}$ and evaluates on functions as

$$\int_{\mathbb{R}^n} f(x)\delta(x - \hat{x})\, dx = f(\hat{x}).$$

Let $\mathbb{R}^n$ be indexed by the coordinates $x_1, \ldots, x_n$.

Definition 15.14. Let $\alpha = (\alpha_1, \dots, \alpha_n)$ be a vector of nonnegative integers. The *moment* m_α of the measure μ is the value of the integral

$$m_\alpha(\mu) = \int_{\mathbb{R}^n} x_1^{\alpha_1} \cdot x_2^{\alpha_2} \cdot \dots \cdot x_n^{\alpha_n} \mu(x)\, dx = \int_{\mathbb{R}^n} x^\alpha \mu(x)\, dx.$$

Here and in the sequel we shall use the notation x^α for the product $\prod_{i=1}^n x_i^{\alpha_i}$.

A given moment m_α is a linear functional on the cone of measures. Not all moments may exist for a given measure, because the integral may diverge. For the δ-function $\mu(x) = \delta(x - \hat{x})$ all moments exist, however, and are given by $m_\alpha(\mu) = \hat{x}^\alpha$.

Since we work only with finite-dimensional objects, we shall fix a degree d and consider only moments m_α for which $|\alpha| = \sum_{i=1}^n \alpha_i$ does not exceed d. The set of such index vectors α has finite cardinality N and gives rise to an N-dimensional *moment vector* $m(\mu) = (m_\alpha(\mu))_{\alpha:|\alpha|\le d}$.

The *moment cone* $M_d \subset \mathbb{R}^N$ is then the set of all vectors which can be produced as moment vectors of some nonnegative measure μ. For subsets $K \subset \mathbb{R}^n$, we shall also consider the cones $M_{d,K} \subset \mathbb{R}^N$ consisting of moment vectors of nonnegative measures μ with support in K. The moment cones can be seen as finite-dimensional projections of the infinite-dimensional cone of nonnegative measures.

The moment cones of the real line and the unit circle in the complex plane can be represented as linear sections of the corresponding positive semi-definite matrix cones. This means that they are spectrahedral cones.

Theorem 15.15. *A vector $m = (m_0, \dots, m_{2d})$ is in the moment cone of $\mathbb{R}$ if and only if the Hankel matrix*

$$H_{2d}(m) = \begin{pmatrix} m_0 & m_1 & \cdots & m_d \\ m_1 & m_2 & \cdots & m_{d+1} \\ \vdots & \vdots & \vdots & \vdots \\ m_d & \cdots & m_{2d-1} & m_{2d} \end{pmatrix}$$

is positive semi-definite.

Theorem 15.16. *A vector $m = (m_{-d}, \dots, m_d)$ is in the moment cone of $\mathbb{T}$ if and only if the Toeplitz matrix*

$$T_d(m) = \begin{pmatrix} m_0 & m_1 & \ddots & m_d \\ m_{-1} & m_0 & \ddots & m_{d-1} \\ \ddots & \ddots & \ddots & \ddots \\ m_{-d} & \ddots & m_{-1} & m_0 \end{pmatrix}$$

is positive semi-definite.

Similar descriptions by block-Hankel and block-Toeplitz matrices hold for matrix-valued positive semi-definite measures on the line and the circle.

The moment cones $M_{d,K}$ are in general difficult to describe. We shall consider necessary conditions which a moment vector $m(\mu)$ of a nonnegative measure has to satisfy. The set of vectors satisfying these conditions will then yield an *outer* approximation of the moment cone.

Let $\mathbf{x} = (1, x_1, \dots, x_n, x_1^2, x_1x_2, \dots, x_n^{[d/2]})^T$ be the vector of monomials x^α for $|\alpha|$ not exceeding the integer part of $\frac{d}{2}$. Then all entries in the rank 1 matrix $\mathbf{x}\mathbf{x}^T$ will be monomials of degree not exceeding d. Consider the matrix-valued integral

$$\int_{\mathbb{R}^n} \mathbf{x}\mathbf{x}^T \mu(x)\, dx.$$

This is a positive semi-definite matrix whose entries are elements of the moment vector $m(\mu)$. We therefore obtain a semi-definite conic constraint on the moment vector, namely that the above matrix should be in the cone of positive semi-definite matrices.

Let now $K = \{x \in \mathbb{R}^n \,|\, f_i(x) = 0,\ g_j(x) \le 0\}$ be a basic semi-algebraic set, and let μ be a nonnegative measure with support in K.

Let d_i be the degree of the polynomial f_i. Then for every polynomial p of degree not exceeding $d - d_i$ we have

$$\int_{\mathbb{R}^n} p(x) f_i(x) \mu(x)\, dx = 0.$$

On the other hand, the left-hand side is a linear combination of elements of the moment vector $m(\mu)$. This yields a linear equality relation on the moment vector $m(\mu)$. A maximal linearly independent set of such equalities can be obtained if $p(x)$ runs through all monomials x^β with $|\beta| \le d - d_i$.

Let now d_j be the degree of the polynomial g_j and let $q(x)$ be a polynomial which is nonnegative on K. Then we obtain

$$\int_{\mathbb{R}^n} q(x) g_j(x) \mu(x)\, dx \le 0.$$

This leads in a similar way to a linear inequality relation on $m(\mu)$.

We may also form the vector $\mathbf{x}'$ of all monomials with degree not exceeding the integer part of $\frac{d-d_j}{2}$ and consider the matrix-valued integral

$$-\int_{\mathbb{R}^n} \mathbf{x}'(\mathbf{x}')^T g_j(x) \mu(x)\, dx.$$

This integral evaluates to a positive semi-definite matrix and every of its entries is a linear combination of elements of $m(\mu)$. This yields a semi-definite conic constraint on $m(\mu)$.

Let us now consider the problem

$$\min_{x \in K} f_0(x), \tag{7}$$

where $f_0 = \sum_\alpha c_\alpha x^\alpha$ is a polynomial of degree not exceeding some integer d, and K is a basic semi-algebraic set as above. We can rewrite this problem equivalently as

$$\min_{\mu \ge 0 : \operatorname{supp} \mu \subset K} \int_{\mathbb{R}^n} f_0(x) \mu(x)\, dx : \quad \int_{\mathbb{R}^n} \mu(x)\, dx = 1.$$

Here the minimization is performed over all probability measures with support in K.

The equality condition on μ can, however, be written as $m_0(\mu) = 1$, and the integral in the cost function evaluates to the linear combination $\sum_\alpha c_\alpha m_\alpha(\mu)$ of elements of the moment vector $m(\mu)$. The problem thus becomes

$$\min_{m \in M_{d,K}} \sum_\alpha c_\alpha m_\alpha : \quad m_0 = 1.$$

Replacing the difficult condition $m \in M_{d,K}$ by a set of semi-definite and linear constraints like those constructed above then yields a semi-definite approximation of the problem.

The moment relaxations are dual to the SOS relaxations considered in the previous section.

Example: Let us again consider problem (6). Set $d = 3$, then the moment vector is 10-dimensional. We obtain the SDP

$$\min m_{10} + m_{01} : \quad \begin{pmatrix} m_{00} & m_{10} & m_{01} \\ m_{10} & m_{20} & m_{11} \\ m_{01} & m_{11} & m_{02} \end{pmatrix} \succeq 0,\ m_{20} + m_{02} - m_{00} = m_{30} + m_{12} - m_{10} = m_{21} + m_{03} - m_{01} = 0,$$

$$\begin{pmatrix} m_{10} & m_{20} & m_{11} \\ m_{20} & m_{30} & m_{21} \\ m_{11} & m_{21} & m_{12} \end{pmatrix} \succeq 0,\ m_{00} = 1.$$

Its solution also yields the optimal value -1.

15.4 SOS relaxations yielding upper bounds

The idea to obtain upper bounds for polynomial minimization problems is based on the use of sums of squares to get *sufficient* conditions for a measure to be nonnegative [2].

Let again K be a basic semi-algebraic set, and let μ be a *fixed* nonnegative measure with support equal to K. If now $h \in \Sigma_{d,K}$ is a SOS representable polynomial which is nonnegative on K, then $\mu_h(x) = \mu(x) \cdot h(x)$ also defines a nonnegative measure on K. The moments of this measure are given by linear combinations of the moments of μ, with the coefficients in these combinations defined by the coefficients of the polynomial h.

We may then approximate the original polynomial minimization problem (7) by the semi-definite program

$$\min_{h \in \Sigma_{d,K}} \int_K h(x) \cdot f_0(x) \cdot \mu(x)\, dx : \quad \int_K h(x) \cdot \mu(x)\, dx = 1.$$

Here the inclusion $h \in \Sigma_{d,K}$ is described by semi-definite constraints, and the cost function depends linearly on the coefficients of the design variable h.

Since $h \in \Sigma_{d,K}$ is a sufficient condition for the measure μ_h to be nonnegative, the minimization is essentially performed over an inner approximation of the cone of nonnegative measures. Hence the relaxation yields upper bounds on the optimal value of the problem.

The relaxations get increasingly tighter with increasing degree d of the allowed SOS representable polynomials. For compact sets K the relaxation hierarchy is asymptotically exact, i.e., the upper bounds tend to the optimal value if the degree grows to infinity. However, they are never exact unless the objective function is constant.

The technique is conditioned on the availability of a nonnegative measure μ with support equal to K such that the moments of μ are easily computable or explicitly known.

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