Sum of Squares: Part 1

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February 2, 2021

Introduction

Reason two basic problems about polynomial inequalities

1. Feasibility of polynomial system.

$$\begin{aligned} p_1(\boldsymbol{x}) &\geq 0 \\ &\vdots \\ p_m(\boldsymbol{x}) &\geq 0 \end{aligned} \tag{1}$$

   Is there an $\boldsymbol{x}$ such that (1) is satisfied?

2. Checking non-negativity: Is $q(\boldsymbol{x}) \geq 0$, $\forall \boldsymbol{x}$ satisfying (1) ?

Justification: Feasibility

Feasibility checking is highly expressive.

- Example: MaxCut.
  - Input: $G = (V, E)$, $|V| = n$.
  - Goal: Find $S \subseteq V$ such that $\left|E(S, \overline{S})\right|$ is maximized.
  - Polynomial Feasibility: For some $\beta \in \mathbb{Z}^+$,

$$\frac{1}{4} \sum_{(i,j) \in E} (\boldsymbol{x}_i - \boldsymbol{x}_j)^2 = \beta \, |E|$$

$$\boldsymbol{x}_i^2 = 1, \qquad \forall 1 \leq i \leq n.$$

  - $n + 1$ degree-2 polynomials. Enumerate over polynomial number of values of β and solve MaxCut.

Other examples: MaxClique, Max 3-SAT, Knapsack. Therefore, polynomial feasibility checking problem is *NP*-Hard.

Goal

- Analyze a relaxation for the feasibility problem, and try to find interesting situations where one can get a poly-time algorithms.

Justification: Non-Negativity

- Checking positivity: Given $f : \{-1,1\}^n \to \mathbb{R}$ with rational coefficients, decide if:
  - $f \geq 0$, $\forall \boldsymbol{x} \in \{-1,1\}^n$, or,
  - find an $\boldsymbol{x} \in \{-1,1\}^n$ such that $f(\boldsymbol{x}) \leq 0$.
- Example MaxCut: Decide if MaxCut $\leq c$.
  - Let $f_G(\boldsymbol{x}) \stackrel{\text{def}}{=} \frac{1}{4}\sum_{(i,j)\in E}(\boldsymbol{x}_i - \boldsymbol{x}_j)^2$.
  - Decide if $c - f_G(\boldsymbol{x}) \geq 0$, $\forall \boldsymbol{x} \in \{-1,1\}^n$.

Certifying Non-Negativity

Given $f : \{-1, 1\}^n \to \mathbb{R}$, find an "efficiently verifiable" certificate of non-negativity.

SoS Certificates

Definition (SoS cert of non-neg (or) SoS proof of non-neg)

A degree-d SoS certificate of non-negativity of $f : \{-1, 1\}^n \to \mathbb{R}$ is a list of polynomials $g_1, \ldots, g_r : \{-1, 1\}^n \to \mathbb{R}$, such such that

- $\deg(g_i) \leq d/2$, and
- $f(\boldsymbol{x}) = \sum_{i \leq r} g_i^2(\boldsymbol{x})$, $\forall \boldsymbol{x} \in \{-1, 1\}^n$.

Efficiently Verifiable (?)

Polynomials $f, g_1, \ldots, g_r$ are represented as a vector of coefficients.

1. How large if r? ($\leq n^d$, see later)
2. How large are coefficients of g_i?

Efficiently Verifiable

Proposition (Efficiently Verifiable)

Suppose $r \leq n^d$, all coefficients of g_i are bounded in magnitude by $2^{\mathrm{poly}(n^d)}$. Then the identity $f = \sum_{i \leq r} g_i^2$ over all $\boldsymbol{x} \in \{-1,1\}^n$ can be checked in poly(n^d) time.

Proof.

- Given g_i, can compute g_i^2, and $\sum_{i \leq r} g_i^2$ in polynomial time.
- Check if $(f - \sum_{i \leq r} g_i^2)(\boldsymbol{x}) = 0$, $\forall \boldsymbol{x} \in \{-1,1\}^n$.
- Using the fact that coefficient vector representation is unique, just check if $f - \sum_{i \leq r} g_i^2 = \mathbf{0}$

□

Fact (Unique Representation)

$\forall f : \{-1,1\}^n \to \mathbb{R}$, there exists a unique representation of f: The multi-linear representation of f

$$f = \sum_{S \subseteq [n]} \hat{f}(S) \prod_{i \in S} \boldsymbol{x}_i \,.$$

(this representation is its Fourier transform)

$\implies$ coefficient vector representation is unique.
(multilinear representation exists because $\boldsymbol{x}_i^2 = 1$)

Are non-negative functions always certifiable?

Proposition (Certifiablity of non-negative functions)

Let $f : \{-1, 1\}^n \to \mathbb{R}$ be non-negative over $\{-1, 1\}^n$. Then, there exists a $\deg(2n)$*-SoS certificate of non-negativity.*

Proof.

- Consider $g : \{-1, 1\}^n \to \mathbb{R}$, and $g(\boldsymbol{x}) = \sqrt{f(\boldsymbol{x})}$.
- Every function on $\{-1, 1\}^n$ is a polynomial of deg $\leq n$.
- $f = g^2 \implies \deg(2n)$-SoS Certificate.

$\square$

Tensor Notation

- Suppose vector $\boldsymbol{v} \in \mathbb{R}^n$.
- $\boldsymbol{v}^{\otimes 2} \in \mathbb{R}^{n^2}$, where $\boldsymbol{v}(i, j) = \boldsymbol{v}_i \boldsymbol{v}_j$.
- $\boldsymbol{v}^{\otimes k} \in \mathbb{R}^{n^k}$.

Proving Efficient Verifiability

Theorem (PSD Matrices and SoS Certificates)

$f : \{-1,1\}^n \to \mathbb{R}$ has a $\deg(d)$-SoS certificate of non-negativity iff there exists a matrix A such that $A \succcurlyeq 0$, and

$$f(\boldsymbol{x}) = \left\langle (1,\boldsymbol{x})^{\otimes \frac{d}{2}}, A \cdot (1,\boldsymbol{x})^{\otimes \frac{d}{2}} \right\rangle .$$

- Parsing Notation:
  - $(1,\boldsymbol{x}) \in \mathbb{R}^{(n+1)}$.
  - $(1,\boldsymbol{x})^{\otimes \frac{d}{2}}$: populate in a vector all possible monomials in the variable $\boldsymbol{x}$ of degree at most $d/2$.
  - $A \in \mathbb{R}^{(n+1)^{d/2} \times (n+1)^{d/2}}$.

Proof

- If Part:

$$\begin{aligned} f(\boldsymbol{x}) &= \left\langle (1,\boldsymbol{x})^{\otimes\frac{d}{2}}, A\cdot(1,\boldsymbol{x})^{\otimes\frac{d}{2}} \right\rangle \\ &= \left\langle (1,\boldsymbol{x})^{\otimes\frac{d}{2}}, (B^\top B)\cdot(1,\boldsymbol{x})^{\otimes\frac{d}{2}} \right\rangle \\ &= \left\langle B\cdot(1,\boldsymbol{x})^{\otimes\frac{d}{2}}, B\cdot(1,\boldsymbol{x})^{\otimes\frac{d}{2}} \right\rangle \\ &= \left\| B\cdot(1,\boldsymbol{x})^{\otimes\frac{d}{2}} \right\|^2 . \end{aligned} \tag{2}$$

  - Let $g_i(\boldsymbol{x}) = \left\langle e_i, B\cdot(1,\boldsymbol{x})^{\otimes\frac{d}{2}} \right\rangle$, i.e., i-th entry of the vector.
  - B is a matrix of constants, applied to monomials of degree at most $d/2$, therefore, $deg(g_i) \leq d/2$.
  - Therefore,

$$f(\boldsymbol{x}) = \sum_{i=1}^{(n+1)^{\otimes d/2}} g_i^2(\boldsymbol{x}) .$$

Proof Cont...

- Only if Part: Suppose f has a degree-d SoS certificate.

$$f = \sum_{i \le r} g_i^2\,, \text{ and } \underbrace{g_i(\boldsymbol{x})}_{\deg \le d/2} = \left\langle \boldsymbol{v}_i, (1, \boldsymbol{x})^{\otimes \frac{d}{2}} \right\rangle .$$

$$\begin{aligned} f(\boldsymbol{x}) &= \sum_{i \le r} \left\langle \boldsymbol{v}_i, (1, \boldsymbol{x})^{\otimes \frac{d}{2}} \right\rangle^2 \\ &= \left\langle (1, \boldsymbol{x})^{\otimes \frac{d}{2}}, \underbrace{\left(\sum_{i \le r} \boldsymbol{v}_i \boldsymbol{v}_i^\top \right)}_{\succcurlyeq 0} \cdot (1, \boldsymbol{x})^{\otimes \frac{d}{2}} \right\rangle . \end{aligned}$$

$\square$

Efficient Verifiability

Corollary (Bound on r)

If $f : \{-1,1\}^n \to \mathbb{R}$ has a degree-d SoS certificate, then it has a certificate with $r \leq (n+1)^{d/2}$.

Proof.

Follows from (2):

$$f(\boldsymbol{x}) = \left\| B \cdot (1, \boldsymbol{x})^{\otimes \frac{d}{2}} \right\|^2 .$$

$\square$

Efficient Verifiability

Lemma (Bit-complexity of SoS proofs)

Suppose f has a degree-d SoS certificate over $\{-1, 1\}^n$. Then, we can find a degree-d SoS certificate for $f + \varepsilon$ in time $\mathrm{poly}(n^d, \log 1/\varepsilon)$.

- $\{-1, 1\}^n$ is important, and doesn't necessarily hold for other domains.

Proof

Since we are given f, we know that it can be efficiently represented. Therefore, we try to bound the entries of A in terms of f.

- $f(\boldsymbol{x}) = \left\langle (1, \boldsymbol{x})^{\otimes \frac{d}{2}}, A \cdot (1, \boldsymbol{x})^{\otimes \frac{d}{2}} \right\rangle$, for some A.
- $f = \sum_u \hat{f}_u \boldsymbol{x}_u$, where $\boldsymbol{x}_u = \prod_{i \in u} \boldsymbol{x}_i$.
- Expanding the inner product, we see $\hat{f}_u = \sum_{S,T} A_{S,T}$, such that $\mathrm{odd}(S + T) = u$, and $|S|, |T| \leq d/2$.

$$\hat{f}_\emptyset = \sum_S A_{S,S} = \mathrm{tr}(A) = \sum_i \underbrace{\lambda_i(A)}_{\geq 0} .$$

$$\|A\|_F^2 = \sum_{S,T} A_{S,T}^2 = \sum_i \lambda_i^2(A) \leq \hat{f}_\phi^2 .$$

We do not know if entries of A are rational, therefore, above proof doesn't suffice. We now try to find an A.

Connection between SDP and SoS: Find A

Proof Cont...

Recall

$$f(\boldsymbol{x}) = \Bigg\langle \underbrace{(1,\boldsymbol{x})^{\otimes \frac{d}{2}}, A \cdot (1,\boldsymbol{x})^{\otimes \frac{d}{2}}}_{\stackrel{\text{def}}{=} g_A(\boldsymbol{x})} \Bigg\rangle \,,$$

Then, we form the following constraints:

1. $A \succcurlyeq 0$.
2. $\mathrm{mult}\,(g_A(\boldsymbol{x})) = \mathrm{mult}\,(f(\boldsymbol{x}))$.

Therefore, we get the following SDP feasibility problem:

$$\forall u \subseteq [n] : \hat{f}_u = \sum_{\mathrm{odd}(S+T)=u} A_{S,T}; \qquad \Big((n+1)^d \text{constraints}\Big)$$

$$A \succcurlyeq 0\,.$$

It is unknown if we can decide the feasibility of this system.
Therefore, we try to solve it approximately.

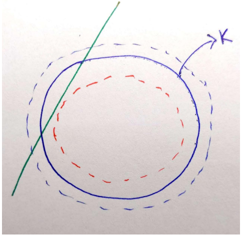
Tools for Approximately Solving SDP

Definition (Weak Separation Oracle)

Let $K \subseteq \mathbb{R}^N$ be a convex set. Weak Separation Oracle:

- Input: Rational vector $\boldsymbol{x} \in \mathbb{R}^N$, and $\varepsilon > 0$.
- Output: Either
  - Correctly asserts that $\boldsymbol{x} \in K + \mathcal{B}(0, \varepsilon)$, or,
  - Returns an "almost separating hyperplane", i.e., returns $\boldsymbol{y} \neq \boldsymbol{0} \in \mathbb{R}^N$, such that

$$\langle \boldsymbol{y}, \boldsymbol{x} \rangle > \langle \boldsymbol{y}, \boldsymbol{z} \rangle - \varepsilon \|\boldsymbol{y}\|_2, \forall \boldsymbol{z} \in K.$$



Tools for Approximately Solving SDP

Theorem (Grötschel, Lovász, Schrijver '81)

Let K be a closed, convex, and bounded set. Suppose there exists $R > r > 0$, such that $\mathcal{B}(\boldsymbol{p}, r) \subseteq K \subseteq \mathcal{B}(\mathbf{0}, R)$. Assume that we have a poly-time weak-separation oracle for K. Then given any rational vector $\boldsymbol{v} \in \mathbb{R}^N$, we can compute a rational vector $\boldsymbol{x} \in \mathbb{R}^N$ such that

1. $\boldsymbol{x} \in K$.
2. $\langle \boldsymbol{v}, \boldsymbol{x} \rangle \geq \langle \boldsymbol{v}, \boldsymbol{z} \rangle - \varepsilon, \forall \boldsymbol{z} \in K$.

Running time: $\operatorname{poly}(\log R/r + \log 1/\varepsilon + N)$.

- Interpreting theorem: If I have a convex set K with non-empty interior, with a weak separation oracle, then I can approximately maximize $\boldsymbol{v}^\top \boldsymbol{x}$ over K.

Proof Cont...

Applying this to our problem. We define the following:

$$S = \left\{ A \,\middle|\, A \succcurlyeq 0, \langle C_i, A \rangle = b_i, \forall i, \|A\|_F^2 \leq \hat{f}_\emptyset^2 \right\} .$$

We note that S is convex, bounded, closed. Now,

$$\mathcal{B}(\boldsymbol{p}, r) \not\subseteq S \, .$$

Therefore, relax the equality constraints. And find a point in S',

$$S' = \left\{ A \,\middle|\, A \succcurlyeq 0, \langle C_i, A \rangle = [b_i - \varepsilon, b_i + \varepsilon], \forall i, \|A\|_F^2 \leq \hat{f}_\emptyset^2 \right\} .$$

Now, $\mathcal{B}(\boldsymbol{p}, r) \subseteq S'$ because for any point $A \in S$, then $A + \delta I \in S'$ for δ small enough.

Applying the Theorem

Proof Cont...

- We can find some f' such that f' has a degree-d SoS certificate and $\left|\hat{f}_u - \hat{f}'_u\right| \leq \varepsilon$.
- Note: $f(\boldsymbol{x}) = f'(\boldsymbol{x}) + (f - f')(\boldsymbol{x})$.
- Small coefficient: $\sum_{|u| \leq d} \left|\hat{f}_u - \hat{f}'_u\right| \leq \varepsilon(n+1)^d$.
- Let $L = \sum_{|u| \leq d} \left|\hat{f}_u - \hat{f}'_u\right|$.
- Then, $L + f - f'$ has a degree d-SoS certificate.
- Then, it implies, $L + f$ has a degree-d SoS certificate, i.e., $\varepsilon(n+1)^d + f$ has a degree-d SoS certificate.
- $\varepsilon = \mathcal{O}\left(n^{-d}\right)$ finishes the proof.

$\square$

$L + f - f'$ has a degree d-SoS certificate

Proof.

Claim

Let $f = \sum_{|S|\le d} \hat{f}_S \boldsymbol{x}_S$. Then $(1 - \boldsymbol{x}_S)$ and $(1 + \boldsymbol{x}_S)$ has a degree-d SoS certificate.

- $f = \sum_S \left|\hat{f}_S\right| \left(\mathrm{sign}(\hat{f}_S)\boldsymbol{x}_S\right)$.
- By claim: $\sum_S \left|\hat{f}_S\right| \left(1 + \mathrm{sign}(\hat{f}_S)\boldsymbol{x}_S\right)$ has a degree-d SoS certificate.

$$\begin{aligned}\sum_S \left|\hat{f}_S\right| \left(1 + \mathrm{sign}(\hat{f}_S)\boldsymbol{x}_S\right) &= \sum_S \left|\hat{f}_S\right| + \sum_S \left|\hat{f}_S\right| \mathrm{sign}(\hat{f}_S)\boldsymbol{x}_S \\ &= \sum_S \left|\hat{f}_S\right| + f\,.\end{aligned}$$

$\square$

Proof of Claim

Proof.

- Let $|S| \leq d$.
- $S = T_1 \cup T_2$, $|T_1| \leq |T_2| \leq d/2$.
- Then $\boldsymbol{x}_s = \boldsymbol{x}_{T_1} \cdot \boldsymbol{x}_{T_2}$.

$$\begin{aligned}
(\boldsymbol{x}_{T_1} - \boldsymbol{x}_{T_2})^2 &= \boldsymbol{x}_{T_1}^2 + \boldsymbol{x}_{T_2}^2 - 2\boldsymbol{x}_{T_1}\boldsymbol{x}_{T_2} \\
&= 2 - 2\boldsymbol{x}_{T_1}\boldsymbol{x}_{T_2} \\
\therefore (1 - \boldsymbol{x}_S) &= \frac{1}{2}(\boldsymbol{x}_{T_1} - \boldsymbol{x}_{T_2})^2 \,.
\end{aligned}$$

- Similarly for $(1 + \boldsymbol{x}_S)$.

$\square$

Halfway Through

What if Degree-d SoS Certificate Doesn't Exist for f?

In that case

1. $\exists\ \boldsymbol{x}$, such that $f(\boldsymbol{x}) < 0$, or,
2. If $d \leq 2n$, then f may be non-negative and yet a degree-d SoS certificate doesn't exist.

- Ideally, if f does not have a degree-d SoS certificate, we would like the "algorithm" to output an $\boldsymbol{x}$ such that $f(\boldsymbol{x}) < 0$.
- However, that may not always be possible.
- To achieve that ideal aim, we construct an object called *Pseudo-distribution*.

Towards Constructing Pseudo-distribution

Fact

The set $SoS_d \subseteq \mathbb{R}^{2^n}$, where

$$SoS_d \stackrel{\text{def}}{=} \{f \mid f \text{ has a degree-}d\text{ SoS certificate}\} ,$$

is a closed, convex cone.

Theorem (Hyperplane Separation Theorem)

Suppose $K \subseteq \mathbb{R}^N$ is a convex set. Let $\boldsymbol{v} \notin K$. Then there exists a hyperplane $\mathcal{H} = \{\boldsymbol{x} | \langle \boldsymbol{u}, \boldsymbol{x} \rangle \geq 0\}$, such that $K \subseteq \mathcal{H}$, and $\boldsymbol{v} \notin \mathcal{H}$.

Towards Constructing Pseudo-distribution

Suppose $p \notin \mathrm{SoS}_d$. Then, there exists μ such that p is on one side of the hyperplane (defined by μ) and SoS_d on the other side, i.e.,

$$\sum_{\boldsymbol{x}\in\{-1,1\}^n} \mu(\boldsymbol{x}) \cdot p(\boldsymbol{x}) < 0,$$

$$\sum_{\boldsymbol{x}\in\{-1,1\}^n} \mu(\boldsymbol{x}) \cdot f(\boldsymbol{x}) \geq 0, \qquad \forall f \in \mathrm{SoS}_d$$

$$\sum_{\boldsymbol{x}\in\{-1,1\}^n} \mu(\boldsymbol{x}) = 1, \qquad \text{(by scaling)}\,.$$

- Hypothetical: Suppose $\mu \geq 0$, then it describes a probability distribution over $\{-1,1\}^n$.
- Therefore, there exists a distribution such that for $p \notin \mathrm{SoS}_d$

$$\mathop{\mathbb{E}}_{\mu} p < 0,$$

$$\mathop{\mathbb{E}}_{\mu} f \geq 0, \qquad \forall f \in \mathrm{SoS}_d.$$

Pseudo-distribution

- Notation: Pseudo-expectation (when μ is not non-negative)

$$\tilde{\mathbb{E}}_{\mu} f = \sum_{x \in \{-1,1\}^n} \mu(\boldsymbol{x}) \cdot f(\boldsymbol{x}) \,.$$

Definition (Pseudo-distribution)

A degree-d pseudo-distribution over $\{-1,1\}^n$ is a function $\mu : \{-1,1\}^n \to \mathbb{R}$ such that $\tilde{\mathbb{E}}_{\mu}$ satisfies:

1. $\tilde{\mathbb{E}}_{\mu} \mathbf{1} = \mathbf{1}$.
2. $\forall f : \deg(f) \leq \frac{d}{2}$, $\tilde{\mathbb{E}}_{\mu} f^2 \geq 0$.

Fact

Every degree $\geq 2n$ pseudo-distribution μ is an actual probability distribution.

Proof Sketch.

- Define indicator polynomial $f_{\boldsymbol{y}} : \{-1, 1\}^n \to \mathbb{R}$, such that $f_{\boldsymbol{y}}(\boldsymbol{y}) = 1$, and $f_{\boldsymbol{y}}(\boldsymbol{x}) = 0$, $\forall \boldsymbol{x} \neq \boldsymbol{y}$. Moreover, $\deg(f) \leq n$.
- By definition $\tilde{\mathbb{E}}_\mu f_{\boldsymbol{y}}^2 \geq 0$.
- Construct the distribution $\mathrm{prob}(\boldsymbol{y}) \stackrel{\text{def}}{=} \tilde{\mathbb{E}}_\mu f_{\boldsymbol{y}}^2$. And this distribution is the pseudo-distribution μ.

□

Specifying Pseudo-distributions

Pseudo-distributions can be specified as a vector $\mu' \in \mathbb{R}^{n^d}$.

Claim

For all degree-d pseudo-distributions, there exists a degree-d multi-linear polynomial $\mu' : \{-1, 1\}^n \to \mathbb{R}$, *such that* $\tilde{\mathbb{E}}_\mu p = \tilde{\mathbb{E}}_{\mu'} p$ *for all* p *such that* $\deg(p) \leq d$.

Proof Sketch.

Write μ and p in multilinear form.

$$\mu(\boldsymbol{x}) = \sum_{S \subseteq [n]} \hat{\mu}_S \boldsymbol{x}_S$$

$$p(\boldsymbol{x}) = \sum_{S \subseteq [n], |S| \leq d} \hat{p}_S \boldsymbol{x}_S \, .$$

$\tilde{\mathbb{E}}_\mu p = \langle \mu, p \rangle = \langle \mu', p \rangle$, where μ' is a degree $\leq d$ part of μ. $\square$

- Notation- Pseudo-moments: $\tilde{\mathbb{E}}\mu(1, \boldsymbol{x})^{\otimes d}$.

  (Expectation of a vector) expectations of degree $\leq d$ monomials.