Infinite-Dimensional Sums-of-Squares for Optimal Control

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Introduction

• We present a representation of non-negative smooth functions in reproducing kernel Hilbert spaces (RKHS), extending the sum-of-squares (SoS) representation of polynomials.
• We apply such representations to optimal control problems, leading to a sample-based numerical method.
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- We apply such representations to optimal control problems, leading to a sample-based numerical method.

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https://arxiv.org/abs/2110.07396
Contents

1 Sums-of-squares Representations for Non-convex Optimization

2 Application to Optimal Control Problems
Non-convex Optimization as a Linear Program

We are interested in finding the global minimum of a possibly non-convex function:

\[ f^* = \min_{x \in \mathbb{R}^p} f(x). \]

This is equivalent to:

\[ f^* = \sup_{c \in \mathbb{R}} c \quad \text{s.t.} \quad \forall x \in \mathbb{R}^p, \quad f(x) - c \geq 0. \]
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*How to handle a dense set of constraints?*
Idea 1: Subsampling Inequalities

\[ f^* = \sup_{c \in \mathbb{R}} c \text{ s.t. } \forall x \in \mathbb{R}^p, f(x) - c \geq 0. \]

Relax it to:

\[ f_n = \sup_{c \in \mathbb{R}} c \text{ s.t. } \forall i \in \{1, ..., n\}, f(x_i) - c \geq 0, \]

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which is equivalent to... \[ f^* \simeq f_n = \min_i f(x_i). \]

If \( f \) Lipschitz, we need \( O(\varepsilon^{-p}) \) samples to approximate \( f^* \) up to \( \varepsilon \).
If \( f \in C^s(\mathbb{R}^p) \) is smooth, the lower-bound is \( O(\varepsilon^{-p/s}) \) [3].

*Can we do any better?*
Idea 2: Representing Non-negative Functions

\[ f^* = \sup_{c \in \mathbb{R}} c \quad \text{s.t. } \forall x \in \mathbb{R}^p, f(x) - c \geq 0. \]

We need a \textit{practical representation} of non-negative functions.
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We need a *practical representation* of non-negative functions.

Imagine we know how to represent some \( g_k \), e.g., of the form:

\[ g_k(x) = \langle \theta_k, \varphi(x) \rangle. \]

Then we can generate non-negative functions as sum-of-squares:

\[ g(x) = \sum_{k=1}^{m} g_k(x)^2 \]
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Then we can generate non-negative functions as sum-of-squares:
\[ g(x) = \sum_{k=1}^{m} g_k(x)^2 = \langle \varphi(x), A\varphi(x) \rangle. \]

where \( A = \sum_{k=1}^{m} \theta_k \otimes \theta_k \succeq 0 \) has rank less than \( m \).
Polynomial Sum-of-Squares (SoS)

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Theorem (Putinar’s Positivstellensatz (simplified))

Let \((h_k)_k\) a family of polynomials and \(W = \{x \mid \forall k, h_k(x) \geq 0\}\) a semi-algebraic set. Assume that \(\{x \in \mathbb{R}^d \mid h_k(x) \geq 0\}\) is compact for some \(k\). If a polynomial \(f\) is strictly positive on \(W\), then there exists SoS polynomials \((\sigma_k)_{0 \leq k \leq m}\) such that:

\[
f = \sigma_0 + \sum_{k=1}^{m} \sigma_k h_k.
\]
Let $f$ a polynomial of degree $d_0$. We want to solve:

$$f^* = \min_{x \in \mathbb{R}^p} f(x) \text{ s.t. } \forall k \in \{1, \ldots, m\}, \ h_k(x) \geq 0.$$ 

Lasserre’s Hierarchy of semi-definite programs (SDP):

Find $c$, $X_k \succeq 0$, $k = 0, \ldots, m$ such that

$$\forall \alpha \in \mathbb{N}^p_{d_0}, \ f_{\alpha} - c1_{\alpha=0} = \sum_{k=0}^{m} \langle C_{\alpha}^k, X_k \rangle$$

$$\forall \alpha \in \mathbb{N}^p_{2r} \setminus \mathbb{N}^p_{d_0}, \ 0 = \sum_{k=0}^{m} \langle C_{\alpha}^k, X_k \rangle.$$
The Moment – SoS Hierarchy

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Lasserre’s Hierarchy of semi-definite programs (SDP):

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$$\forall \alpha \in \mathbb{N}^p_{d_0}, \quad f_\alpha - c1_{\alpha=0} = \sum_{k=0}^m \langle C^k_\alpha, X_k \rangle$$

$$\forall \alpha \in \mathbb{N}^p_{2r} \setminus \mathbb{N}^p_{d_0}, \quad 0 = \sum_{k=0}^m \langle C^k_\alpha, X_k \rangle.$$ 

The monomials are indexed by $\mathbb{N}^p_r := \{ \alpha \in \mathbb{N}^p : |\alpha| \leq r \}$ which has size $s_r(d) = \binom{p+r}{r}$. This is exponential in the dimension $p$. 
SoS Functions in Reproducing Kernel Hilbert Spaces

A positive-definite kernel on $\mathbb{R}^p$ is a function $K : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}$ such that $\forall n \geq 1, \forall (x_1, ..., x_n)$, the matrix $(K(x_i, x_j))$ is PSD.

It is associated to a Hilbert space $\mathcal{H}$ such that:

- $\forall x \in \mathbb{R}^p, \varphi(x) := K(x, \cdot) \in \mathcal{H}$;
- $\forall f \in \mathcal{H}, x \in \mathbb{R}^p, \langle f, \varphi(x) \rangle = f(x)$. 

Using the reproducing property, a sum-of-squares of functions in $\mathcal{H}$:

$\forall x \in \mathbb{R}^p, g(x) = \sum_{k=1}^{m} h_k(x)^2$ is such that $\forall x \in \mathbb{R}^d, g(x) = \langle \varphi(x), A \varphi(x) \rangle$, where $A \in \mathbb{S}^+ (\mathcal{H})$ is a PSD operator, possibly infinite-dimensional.
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where $A \in \mathbb{S}_+(\mathcal{H})$ is a PSD operator, possibly infinite-dimensional.
SoS Representation of Smooth Functions [4]

We consider as our RKHS $\mathcal{H}$ the Sobolev space $W_2^s(\mathbb{R}^p)$, with $s \geq p/2 + 3$, of $s$-smooth functions.

**Theorem (informal)**

*If $f \in \mathcal{H}$ has a unique isolated global minimum at $x^*$ s.t. $\frac{\partial^2 f}{\partial x^2} \big|_{x^*} \succ 0$, then there exists $h_1, \ldots, h_m \in \mathcal{H}$, with $m \leq p + 1$ such that:*

$$\forall x, \quad f(x) - f^* = \sum_{k=1}^{m} h_k(x)^2.$$ 

Hence $f - f^*$ is a SoS of (smooth) functions in $\mathcal{H}$, and:

$$\exists A \in \mathbb{S}_+(\mathcal{H}) \text{ s.t. } \forall x, \quad f(x) - f^* = \langle \varphi(x), A\varphi(x) \rangle.$$ 

*No need for a hierarchy!* 

Non-convex Optimization of Smooth Functions

\[ f^* = \sup_{c \in \mathbb{R}} c \]

\text{s.t. } \forall x \in \mathbb{R}^p, f(x) - c \geq 0.

Using the Theorem, if \( f \) is smooth, this is equivalent to:

\[ f^* = \sup_{c \in \mathbb{R}, A \in S_+(\mathcal{H})} c \]

\text{s.t. } \forall x, f(x) - c = \langle \varphi(x), A \varphi(x) \rangle.
Non-convex Optimization of Smooth Functions

We can now *subsample equalities*:

\[
    f_n = \sup_{c \in \mathbb{R}, A \in S_+(\mathcal{H})} c - \lambda \text{Tr}(A)
\]

\[
    \text{s.t. } \forall i \in \{1, \ldots, n\}, \quad f(x_i) - c = \langle \varphi(x_i), A\varphi(x_i) \rangle.
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We can now \textit{subsample equalities}:

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    f_n = \sup_{c \in \mathbb{R}, A \in \mathbb{S}_+(H)} c - \lambda \text{Tr}(A)
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Using the reproducing property, this is equivalent to the SDP:

\[
    f_n = \sup_{c \in \mathbb{R}, B \succeq 0} c - \lambda \text{Tr}(B)
\]

\[\text{s.t. } \forall i \in \{1, \ldots, n\}, \ f(x_i) - c = \Phi_i^\top B \Phi_i,\]

where the $\Phi_i \in \mathbb{R}^n$ are vectors computed from the kernel matrix.

This achieves an \textit{almost optimal rate} of $O(n^{-(s-3)/p+1/2})$ for $s \geq 3 + p/2$. The lower-bound is $O(n^{-s/p})$. 
In short… (see [3])

Subsampling inequalities

Subsampling equalities
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1 Sums-of-squares Representations for Non-convex Optimization

2 Application to Optimal Control Problems
Optimal Control as a Linear Program

- The optimal control problem is to find $V^*$ such that:

$$V^*(t_0, x_0) = \inf_{u(\cdot)} \int_{t_0}^{T} L(t, x(t), u(t)) dt + M(x(T))$$

$$\forall t \in [t_0, T], \quad \dot{x}(t) = f(t, x(t), u(t)), \quad x(0) = x_0.$$
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Under convexity assumptions, this is equivalent to finding a maximal subsolution of the Hamilton-Jacobi-Bellman equation [2]:

$$\sup_{V \in C^1([0, T] \times \mathcal{X})} \int V(0, x_0) d\mu_0(x_0)$$

$$\forall (t, x, u), \quad \frac{\partial V}{\partial t}(t, x) + L(t, x, u) + \nabla V(t, x)^\top f(t, x, u) \geq 0$$

$$\forall x, \quad V(T, x) \leq M(x).$$
Optimal Control as a Linear Program

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\forall (t, x, u), \left( \frac{\partial V}{\partial t} (t, x) + L(t, x, u) + \nabla V(t, x)^\top f(t, x, u) \right) \geq 0
\]

\[
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\]
A Simple Baseline: Subsampling Inequalities

Using a linear parameterization of $V$, and simply subsampling inequalities leads to an LP:

$$\sup_{\theta \in \mathbb{R}^m} \frac{1}{n} \sum_{i=1}^{n} V_{\theta}(0, x^{(i)})$$

$$\forall i \in I, \quad H_{\theta}(t^{(i)}, x^{(i)}, u^{(i)}) \geq 0.$$  

This is already a non-trivial numerical method.

*Can we do any better?*
SoS Representation of the Hamiltonian

**Theorem (informal)**

Assume that:
- $f$ is control-affine: $f(t, x, u) = g(t, x) + B(t, x)u$;
- $L$ is strongly convex in $u$;
- $L$, $B$ and $V^*$ are sufficiently smooth;

Then $H^*$ is a SoS of $p$ smooth functions $(w_j)_{1 \leq j \leq p} \in C^s(\Omega)$:

$$\forall (t, x, u) \in \Omega, \quad H^*(t, x, u) = \sum_{j=1}^{p} w_j(t, x, u)^2.$$

**Limit:** in general $V^*$ is not even $C^1$. A possible workaround is to add noise to the dynamics to smoothen $V^*$. 
Adding regularization terms, we get the following SDP:

\[
\sup_{B \succeq 0, \theta, \delta} c^\top \theta - \lambda \theta \|\theta\|_2^2 - \lambda \text{Tr}(B) - \gamma \|\delta\|^2 + \varepsilon \log \det B + C
\]

such that \( \forall i \in \{1, \ldots, n\}, b_i + a_i^\top \theta = (\Phi_i)^\top B \Phi_i + \delta_i. \)

The dual is solved with damped Newton’s method, an algorithm with cost \( O(n^3) \) in time and \( O(n^2) \) in space for each iteration.
Numerical Example

We solve a linear quadratic regulator. We know that:

\[ H^*(t, x, u) = (u + F(t)x)^\top R(u + F(t)x). \]

We use:

\[ K((t, x, u), (t', x', u')) = \langle u, u' \rangle + \langle x, x' \rangle e^{-|t-t'|}. \]
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Again...

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Conclusion

- We have presented an **extension** of the SoS framework in RKHS.
- It leads to **sample-based** numerical methods involving SDPs.
- There are **many potential applications**, e.g., to optimal transport, sampling, modelling of probability distributions...
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