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## 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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The preprint is available on arxiv:
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)
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This is equivalent to:

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\begin{aligned}
& \qquad f^{*}=\sup _{c \in \mathbb{R}} c \\
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How to handle a dense set of constraints?

## Idea 1: Subsampling Inequalities

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Relax it to:

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& \qquad f_{n}=\sup _{c \in \mathbb{R}} c \\
& \text { s.t. } \forall i \in\{1, \ldots, n\}, f\left(x_{i}\right)-c \geq 0,
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which is equivalent to... $f^{*} \simeq f_{n}=\min _{i} f\left(x_{i}\right)$.
If $f$ Lipschitz, we need $O\left(\varepsilon^{-p}\right)$ samples to approximate $f^{*}$ up to $\varepsilon$. If $f \in \mathcal{C}^{s}\left(\mathbb{R}^{p}\right)$ is smooth, the lower-bound is $O\left(\varepsilon^{-p / s}\right)$ [3].

Can we do any better?

## Idea 2: Representing Non-negative Functions

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Imagine we know how to represent some $g_{k}$, e.g., of the form:

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g_{k}(x)=\left\langle\theta_{k}, \varphi(x)\right\rangle .
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Then we can generate non-negative functions as sum-of-squares:

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g(x)=\sum_{k=1}^{m} g_{k}(x)^{2}
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$$
g(x)=\sum_{k=1}^{m} g_{k}(x)^{2}=\langle\varphi(x), A \varphi(x)\rangle .
$$

where $A=\sum_{k=1}^{m} \theta_{k} \otimes \theta_{k} \succeq 0$ has rank less than $m$.

## Polynomial Sum-of-Squares (SoS)

In dimension 1, all non-negative polynomials are SoS.
This is not true in larger dimensions.
Powerful theorems describe cases of tight SoS representations [1].

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## Theorem (Putinar's Positivstellensatz (simplified))

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

$$
f=\sigma_{0}+\sum_{k=1}^{m} \sigma_{k} h_{k}
$$

## The Moment - SoS Hierarchy

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

$$
\begin{aligned}
& \forall \alpha \in \mathbb{N}_{d_{0}}^{p}, \quad f_{\alpha}-c \mathbf{1}_{\alpha=0}=\sum_{k=0}^{m}\left\langle C_{\alpha}^{k}, X_{k}\right\rangle \\
& \forall \alpha \in \mathbb{N}_{2 r}^{p} \backslash \mathbb{N}_{d_{0}}^{p}, \quad 0=\sum_{k=0}^{m}\left\langle C_{\alpha}^{k}, X_{k}\right\rangle
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\end{aligned}
$$

The monomials are indexed by $\mathbb{N}_{r}^{p}:=\left\{\alpha \in \mathbb{N}^{p}:|\alpha| \leq r\right\}$ 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 $\forall n \geq 1, \forall\left(x_{1}, \ldots, x_{n}\right)$, the matrix $\left(K\left(x_{i}, x_{j}\right)\right)$ is PSD.

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

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


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

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

$$
\forall x \in \mathbb{R}^{p}, \quad g(x)=\sum_{k=1}^{m} h_{k}(x)^{2}
$$

is such that

$$
\forall x \in \mathbb{R}^{d}, \quad g(x)=\langle\varphi(x), \mathcal{A} \varphi(x)\rangle
$$

where $\mathcal{A} \in \mathbb{S}_{+}(\mathcal{H})$ is a PSD operator, possibly infinite-dimensional.

## SoS Representation of Smooth Functions [4]

We consider as our RKHS $\mathcal{H}$ the Sobolev space $W_{2}^{s}\left(\mathbb{R}^{p}\right)$, 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. $\left.\frac{\partial^{2} f}{\partial x^{2}}\right|_{x^{*}} \succ 0$, 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:

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

No need for a hierarchy!

## Non-convex Optimization of Smooth Functions

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& f^{*}=\sup _{c \in \mathbb{R}} c \\
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$$

Using the Theorem, if $f$ is smooth, this is equivalent to:

$$
\begin{gathered}
f^{*}=\sup _{c \in \mathbb{R}, \mathcal{A} \in \mathbb{S}_{+}(\mathcal{H})} c \\
\text { s.t. } \forall x, f(x)-c=\langle\varphi(x), \mathcal{A} \varphi(x)\rangle
\end{gathered}
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## Non-convex Optimization of Smooth Functions

We can now subsample equalities:

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\begin{gathered}
f_{n}=\sup _{c \in \mathbb{R}, \mathcal{A} \in \mathbb{S}_{+}(\mathcal{H})} c-\lambda \operatorname{Tr}(\mathcal{A}) \\
\text { s.t. } \forall i \in\{1, \ldots, n\}, f\left(x_{i}\right)-c=\left\langle\varphi\left(x_{i}\right), \mathcal{A} \varphi\left(x_{i}\right)\right\rangle .
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\end{aligned}
$$

Using the reproducing property, this is equivalent to the SDP:

$$
\begin{aligned}
& \qquad f_{n}=\sup _{c \in \mathbb{R}, B \succeq 0} c-\lambda \operatorname{Tr}(B) \\
& \text { s.t. } \forall i \in\{1, \ldots, n\}, f\left(x_{i}\right)-c=\Phi_{i}^{\top} B \Phi_{i},
\end{aligned}
$$

where the $\Phi_{i} \in \mathbb{R}^{n}$ are vectors computed from the kernel matrix.
This achieves an almost optimal rate of $O\left(n^{-(s-3) / p+1 / 2}\right)$ for $s \geq 3+p / 2$. The lower-bound is $O\left(n^{-s / p}\right)$.

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## Optimal Control as a Linear Program

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

$$
\begin{aligned}
& V^{*}\left(t_{0}, x_{0}\right)=\inf _{u(\cdot)} \int_{t_{0}}^{T} L(t, x(t), u(t)) \mathrm{d} t+M(x(T)) \\
& \forall t \in\left[t_{0}, T\right], \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]:

$$
\begin{gathered}
\sup _{V \in C^{1}([0, T] \times \mathcal{X})} \int V\left(0, x_{0}\right) \mathrm{d} \mu_{0}\left(x_{0}\right) \\
\forall(t, x, u), \frac{\partial V}{\partial t}(t, x)+L(t, x, u)+\nabla V(t, x)^{\top} f(t, x, u) \geq 0 \\
\forall x, V(T, x) \leq M(x) .
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$$

## A Simple Baseline: Subsampling Inequalities

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

$$
\begin{aligned}
& \sup _{\theta \in \mathbb{R}^{m}} \frac{1}{n} \sum_{i=1}^{n} V_{\theta}\left(0, x^{(i)}\right) \\
& \forall i \in I, \quad H_{\theta}\left(t^{(i)}, x^{(i)}, u^{(i)}\right) \geq 0
\end{aligned}
$$

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 $\left(w_{j}\right)_{1 \leq j \leq p} \in C^{s}(\Omega)$ :

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

Limit: in general $V^{*}$ is not even $C^{1}$. A possible workaround is to add noise to the dynamics to smoothen $V^{*}$.

## A Practical Algorithm for Smooth Optimal Control

- Adding regularization terms, we get the following SDP:

$$
\sup _{B \succcurlyeq 0, \theta, \delta} c^{\top} \theta-\lambda_{\theta}\|\theta\|_{2}^{2}-\lambda \operatorname{Tr}(B)-\gamma\|\delta\|^{2}+\varepsilon \log \operatorname{det} B+C
$$

such that $\forall i \in\{1, \ldots, n\}, b_{i}+a_{i}^{\top} \theta=\left(\Phi_{i}\right)^{\top} B \Phi_{i}+\delta_{i}$.

- The dual is solved with damped Newton's method, an algorithm with cost $O\left(n^{3}\right)$ in time and $O\left(n^{2}\right)$ 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: $K\left((t, x, u),\left(t^{\prime}, x^{\prime}, u^{\prime}\right)\right)=\left\langle u, u^{\prime}\right\rangle+\left\langle x, x^{\prime}\right\rangle e^{-\left|t-t^{\prime}\right|}$.

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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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