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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:

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

This is equivalent to:

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

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

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How to handle a dense set of constraints?

Idea 1: Subsampling Inequalities

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

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

Relax it to:

$$f_n = \sup_{c \in \mathbb{R}} c$$

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

Can we do any better?

Idea 2: Representing Non-negative Functions

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We need a *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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$$g(x) = \sum_{k=1}^{m} g_k(x)^2 = (\langle \varphi(x), A\varphi(x) \rangle.)$$

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 $(h_k)_k$ 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:

$$f = \sigma_0 + \sum_{k=1}^m \sigma_k h_k.$$

The Moment – SoS Hierarchy

Let f a polynomial of degree d_0 . We want to solve:

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

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

Find
$$c, X_k \succeq 0, k = 0, ..., m$$
 such that
$$\forall \alpha \in \mathbb{N}_{d_0}^p, \quad f_{\alpha} - c\mathbf{1}_{\alpha=0} = \sum_{k=0}^m \langle C_{\alpha}^k, X_k \rangle$$

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

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$$\boxed{\forall \alpha \in \mathbb{N}_{2r}^p \setminus \mathbb{N}_{d_0}^p, \quad 0 = \sum_{k=0}^m \langle C_{\alpha}^k, X_k \rangle.}$$

The monomials are indexed by $\mathbb{N}_r^p := \{\alpha \in \mathbb{N}^p : |\alpha| \le r\}$ 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 $K : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ such that $\forall n \geq 1, \forall (x_1, ..., x_n)$, the matrix $(K(x_i, x_i))$ is PSD.

It is associated to a Hilbert space ${\cal H}$ 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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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

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

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 $h_1, ..., h_m \in \mathcal{H}$, 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:

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

No need for a hierarchy!



Non-convex Optimization of Smooth Functions

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

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

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

$$\begin{split} f^* &= \sup_{c \in \mathbb{R}, \mathcal{A} \in \mathbb{S}_+(\mathcal{H})} c \\ \text{s.t. } \forall x, \ f(x) - c &= \langle \varphi(x), \mathcal{A} \varphi(x) \rangle. \end{split}$$

Non-convex Optimization of Smooth Functions

We can now subsample equalities:

$$\begin{split} f_n &= \sup_{c \in \mathbb{R}, \mathcal{A} \in \mathbb{S}_+(\mathcal{H})} c - \lambda \mathsf{Tr}(\mathcal{A}) \\ \text{s.t. } \forall i \in \{1, ..., n\}, \ f(x_i) - c &= \langle \varphi(x_i), \mathcal{A}\varphi(x_i) \rangle. \end{split}$$

Non-convex Optimization of Smooth Functions

We can now *subsample equalities*:

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s.t. $\forall i \in \{1, ..., n\}, \ f(x_i) - c = \langle \varphi(x_i), \mathcal{A}\varphi(x_i) \rangle.$

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

$$f_n = \sup_{c \in \mathbb{R}, B \succeq 0} c - \lambda \mathsf{Tr}(B)$$

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

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

This achieves an almost optimal rate of $O(n^{-(s-3)/p+1/2})$ for $s \ge 3 + p/2$. The lower-bound is $O(n^{-s/p})$.



In short... (see [3])



Subsampling inequalities

Subsampling equalities

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Optimal Control as a Linear Program

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

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

$$\forall t \in [t_0, T], \ \dot{x}(t) = f(t, x(t), u(t)), \quad x(0) = x_0.$$

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 Under convexity assumptions, this is equivalent to finding a maximal subsolution of the Hamilton-Jacobi-Bellman equation [2]:

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

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

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A Simple Baseline: Subsampling Inequalities

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

$$\begin{split} \sup_{\theta \in \mathbb{R}^m} \ \frac{1}{n} \sum_{i=1}^n V_{\theta}(0, x^{(i)}) \\ \forall i \in I, \quad H_{\theta}(t^{(i)}, x^{(i)}, u^{(i)}) \geq 0. \end{split}$$

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 $(w_i)_{1 \le i \le p} \in C^s(\Omega)$:

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

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:

$$\sup_{B\succcurlyeq 0,\theta,\delta} c^\top \theta - \lambda_\theta \|\theta\|_2^2 - \lambda \mathrm{Tr}(B) - \gamma \|\delta\|^2 + \varepsilon \log \det B + C$$
 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:

$$H^*(t, x, u) = (u + F(t)x)^{\top} R(u + F(t)x).$$

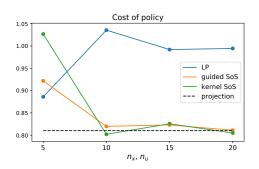
We use:
$$K((t,x,u),(t',x',u')) = \langle u,u' \rangle + \langle x,x' \rangle e^{-|t-t'|}$$
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Again...



Subsampling inequalities

Subsampling equalities



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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