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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

Non-convex Optimization as a Linear Program

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

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

This is equivalent to:

$$\begin{aligned} f^\star = &\sup_{c \in \mathbb{R}} c \\ \text{s.t. } &\forall x \in \mathbb{R}^p, \; f(x) - c \geq 0. \end{aligned}$$

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How to handle a dense set of constraints?

Idea 1: Subsampling Inequalities

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

Relax it to:

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

which is equivalent to...

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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 ε.
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

$$
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f^{\star} &= \sup_{c \in \mathbb{R}} \ c \\
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We need a *practical representation* of non-negative functions.

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

$$g_k(x) = \langle \alpha_k, \varphi(x) \rangle.$$

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

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

where $A = \sum_{k=1}^{m} \alpha_k \alpha_k^\top \succeq 0$ 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:

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

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

$$\boxed{\begin{array}{l} \text{Find } c,\ X_k \succeq 0,\ k = 0, \ldots, m \text{ such that} \\ \qquad \forall \alpha \in \mathbb{N}^p_{d_0}, \quad f_\alpha - c\mathbf{1}_{\alpha=0} = \displaystyle\sum_{k=0}^{m} \langle C^k_\alpha, X_k \rangle \\ \forall \alpha \in \mathbb{N}^p_{2r} \setminus \mathbb{N}^p_{d_0}, \quad 0 = \displaystyle\sum_{k=0}^{m} \langle C^k_\alpha, X_k \rangle. \end{array}}$$

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

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 $K : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ such that $\forall n \geq 1, \forall (x_1, \dots, x_n)$, the matrix $(K(x_i, x_j))$ is PSD.

It is associated to a Hilbert space H such that:

$\forall x \in \mathbb{R}^p$, $\varphi(x) := K(x, \cdot) \in H$;

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

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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 $\mathcal{H}$:

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

is such that

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

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

Theorem (informal)

If $f \in H$ has a unique **isolated** *global minimum at x_* s.t. $\frac{\partial^2 f}{\partial x^2}(x_*) \succ 0$, then there exists $h_1, \ldots, h_m \in H$, 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 H, and:

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

No need for a hierarchy!

Non-convex Optimization of Smooth Functions

$$\begin{aligned} f_* &= \sup_{c \in \mathbb{R}} \; c \\ \text{s.t. } & \forall x \in \mathbb{R}^p, \; \boxed{f(x) - c \geq 0.} \end{aligned}$$

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

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

Non-convex Optimization of Smooth Functions

We can now *subsample equalities*:

$$f_n = \sup_{c \in \mathbb{R},\, A \in \mathbb{S}_+(H)} c - \mathrm{Tr}(A)$$

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

Non-convex Optimization of Smooth Functions

We can now *subsample equalities*:

$$f_n = \sup_{c \in \mathbb{R},\, A \in S_+(H)} c - \mathrm{Tr}(A)$$

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

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

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

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

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

This achieves an *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])

Contents

Optimal Control as a Linear Program

The optimal control problem is to find V such that:

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

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

Optimal Control as a Linear Program

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

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

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

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

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

$$\forall x, \ V(T, x) \leq M(x).$$

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$$\forall x, \ V(T, x) \le M(x).$$

A Simple Baseline: Subsampling Inequalities

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

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

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

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-a ne**: $\quad f(t;x;u) = g(t;x) + B(t;x)u$;
- L *is strongly convex in* u;
- L, B *and* V *are* **su ciently smooth**;

Then H *is a SoS of* p *smooth functions* $(w_j)_{1 \; j \; p}$ 2 $C^s(\Omega)$:

$$8(t;x;u)\ 2\ \Omega; \quad H\ (t;x;u) = \sum_{j=1}^{p} w_j(t;x;u)^2:$$

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:

$$\sup_{B \succcurlyeq 0;\ ;} \quad c^{>} \qquad k\ k_2^2 \qquad \mathrm{Tr}(B) \qquad k\ k^2 + "\log\det B + C$$

$$\text{such that} \quad 8i\ 2\ f1; : : : ; ng;\ b_i + a_i^{>} \quad = (\Phi_i)^{>} B \Phi_i + \ {}_i :$$

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...

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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