

Séminaire de Mathématiques Appliquées du CERMICS



State-constrained Linear-Quadratic Optimal Control as a Kernel Regression with Hard Shape Constraints

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<https://pcaubin.github.io/>

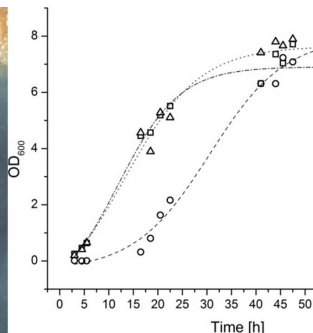
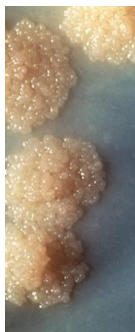
October 2020



École des Ponts
ParisTech

What are shape/state constraints?

Estimation



Side information

↪ compensates small number of samples or excessive noise

Control



Physical constraints

↪ provides feasible trajectories in path-planning

Ubiquitous and both handled as a constrained optimization problem

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1 Shape constraints in RKHSs over non-finite compact sets

2 State-constrained Linear Quadratic Regulator as a kernel regression

Based on

- *Kernel Regression for Vehicle Trajectory Reconstruction under Speed and Inter-vehicular Distance Constraints*, PCAF, Nicolas Petit and Zoltán Szabó, *IFAC World Congress 2020*
- *Hard Shape-Constrained Kernel Machines*, PCAF and Zoltán Szabó, *NeurIPS 2020*, <https://arxiv.org/abs/2005.12636>
- *Linearly-constrained Linear Quadratic Regulator from the viewpoint of kernel methods*, PCAF, June 2020, Accepted with minor revision in *SIAM Journal on Control and Optimization*

Problem statement

Given samples $(x_n, y_n)_{n \in [M]} \in (\mathcal{X} \times \mathbb{R})^M$, a loss $L : (\mathcal{X} \times \mathbb{R} \times \mathbb{R})^M \rightarrow \mathbb{R} \cup \{\infty\}$, a regularizer $\Omega : \mathbb{R}_+ \rightarrow \mathbb{R}$. For $x \in \mathcal{X} \subset \mathbb{R}^d$, $f \in \mathcal{C}^s(\mathcal{X}, \mathbb{R})$, consider

$$\begin{aligned} \bar{f} \in \arg \min_{f \in \mathcal{F}} \mathcal{L}(f) &= L\left((x_n, y_n, f(x_n))_{n \in [M]}\right) + \Omega(\|f\|_{\mathcal{F}}) \\ \text{s.t.} \quad b_i &\leq D_i f(x), \quad \forall x \in \mathcal{K}_i, \forall i \in [\mathcal{I}] = \llbracket 1, \mathcal{I} \rrbracket. \end{aligned}$$

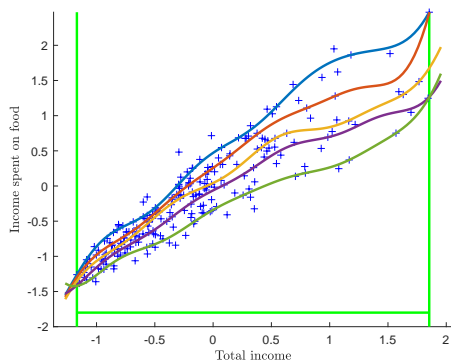
where \mathcal{F} is a Hilbert space of smooth functions from \mathcal{X} to \mathbb{R} , D_i is a differential operator ($D_i = \sum_j \gamma_j \partial^{r_j}$), $b_i \in \mathbb{R}$ is a lower bound, \mathcal{K}_i is compact.

For non-finite \mathcal{K}_i , we have an infinite number of constraints!

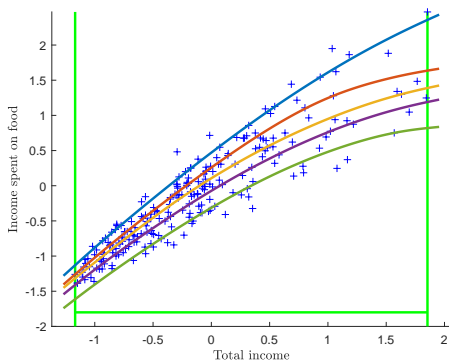
How can we make this optimization problem computationally tractable?

In practice: nonparametric estimation under constraints

In statistics: nonnegative densities, non-crossing quantiles



non-crossing+increasing



non-crossing+increasing+concave

Qualitative priors have a great effect on the shape of solutions!

Glimpse of content of the talk

From dealing with a real-valued problem $f : x \in \mathcal{X} \subset \mathbb{R}^d \rightarrow y \in \mathbb{R}$

$$\begin{aligned} \bar{f} \in \arg \min_{f \in \mathcal{F}} \mathcal{L}(f) &= L\left((x_n, y_n, f(x_n))_{n \in [M]}\right) + \Omega(\|f\|_{\mathcal{F}}) \\ \text{s.t.} \quad b_i &\leq D_i f(x), \quad \forall x \in \mathcal{K}_i, \forall i \in [\mathcal{I}] = \llbracket 1, \mathcal{I} \rrbracket. \end{aligned}$$

ex: least-squares with monotonicity constraint

to a path-planning vector-valued problem $f : t \in [0, T] \rightarrow y \in \mathbb{R}^Q$

Take \mathcal{F} to be a Hilbert space of trajectories (e.g. Sobolev space)

$$\begin{aligned} \min_{f(\cdot) \in \mathcal{F}} g(f(T)) + \|f\|_{\mathcal{F}}^2 \\ \text{s.t.} \quad f(0) &= y_0, \\ c_i(t)^\top f(t) &\leq d_i(t), \quad \forall t \in [0, T], \forall i \in [\mathcal{I}]. \end{aligned}$$

ex: $g(f(T)) = \|y_T - f(T)\|_{\mathbb{R}^Q}^2$

Dealing with an infinite number of constraints: an overview

$$\bar{f} \in \arg \min_{f \in \mathcal{F}} \mathcal{L}(f) \text{ s.t. } "b_i \leq D_i f(x), \forall x \in \mathcal{K}_i, \forall i \in [I]", \mathcal{K}_i \text{ non-finite}$$

Relaxing

- Discretize constraint at “virtual” samples $\{\tilde{x}_{m,i}\}_{m \leq M} \subset \mathcal{K}_i$,
↪ no guarantees out-of-samples [Agrell, 2019, Takeuchi et al., 2006]
- Add constraint-inducing penalty, $\Omega_{\text{cons}}(f) = -\lambda \int_{\mathcal{K}_i} \min(0, D_i f(x) - b_i) dx$
↪ no guarantees, changes the problem objective [Braut et al., 2019]

Tightening

- Replace \mathcal{F} by algebraic subclass of functions satisfying the constraints
↪ hard to stack constraints, $\Phi(x)^\top A \Phi(x)$, Sum-Of-Squares [Hall, 2018]
- Use only spaces \mathcal{F} s.t. constraints have a “simple” writing, e.g. splines
↪ highly restricted functions classes [Papp and Alizadeh, 2014]
- **Our solution:** discretize \mathcal{K}_i but replace b_i using RKHS geometry

Reproducing kernel Hilbert spaces (RKHS) at a glance (1)

A **RKHS** $(\mathcal{F}_k, \langle \cdot, \cdot \rangle_{\mathcal{F}_k})$ is a Hilbert space of real-valued¹ functions over a set \mathcal{X} if one of the following **equivalent** conditions is satisfied [Aronszajn, 1950]

$$\exists k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \text{ s.t. } k_x(\cdot) = k(x, \cdot) \in \mathcal{F}_k \text{ and } f(x) = \langle f(\cdot), k_x(\cdot) \rangle_{\mathcal{F}_k}$$

the topology of $(\mathcal{F}_k, \langle \cdot, \cdot \rangle_{\mathcal{F}_k})$ is stronger than pointwise convergence
i.e. $\delta_x : f \mapsto f(x)$ is **continuous** for all x for $f \in \mathcal{F}_k$.

$$|f(x) - f_n(x)| = |\langle f - f_n, k_x \rangle_k| \leq \|f - f_n\|_k \|k_x\|_k = \|f - f_n\|_k \sqrt{k(x, x)}$$

$$k \text{ is s.t. } \exists \Phi_k : \mathcal{X} \rightarrow \mathcal{F}_k \text{ s.t. } k(x, y) = \langle \Phi_k(x), \Phi_k(y) \rangle_{\mathcal{F}_k}, \Phi_k(x) = k_x(\cdot)$$

k is s.t. $\mathbf{G} = [k(x_i, x_j)]_{i,j=1}^n \succcurlyeq 0$ and $\mathcal{F}_k := \overline{\text{span}(\{k_x(\cdot)\}_{x \in \mathcal{X}})}$, i.e. the completion for the pre-scalar product $\langle k_x(\cdot), k_y(\cdot) \rangle_{k,0} = k(x, y)$

¹There is a natural extension to vector-valued RKHSs (more on this later).

Reproducing kernel Hilbert spaces (RKHS) at a glance (2)

- There is a one-to-one correspondence between kernels k and RKHSs $(\mathcal{F}_k, \langle \cdot, \cdot \rangle_{\mathcal{F}_k})$. Changing \mathcal{X} or $\langle \cdot, \cdot \rangle_{\mathcal{F}_k}$ changes the kernel k .²
- for $\mathcal{X} \subset \mathbb{R}^d$, Sobolev spaces $\mathcal{H}^s(\mathcal{X})$ satisfying $s > d/2$ are RKHSs. For $\mathcal{X} = \mathbb{R}^d$ their (Matérn) kernels are well known. Classical kernels include

$$k_{\text{Gauss}}(x, y) = \exp\left(-\|x - y\|_{\mathbb{R}^d}^2 / (2\sigma^2)\right) \quad k_{\text{lin}}(x, y) = \langle x, y \rangle_{\mathbb{R}^d}$$

- if $\mathcal{X} \subset \mathbb{R}^d$ is contained in the closure of its interior (e.g. $[0, +\infty[$, for $d = 1$), $k \in \mathcal{C}^{s,s}(\mathcal{X} \times \mathcal{X}, \mathbb{R})$, $D = \sum_j \gamma_j \partial^{r_j}$ a differential operator of order at most s , then $\mathcal{F}_k \subset \mathcal{C}^s(\mathcal{X}, \mathbb{R})$ and reproducing formula for derivatives:

$$D_x k(x, \cdot) \in \mathcal{F}_k \quad ; \quad Df(x) = \langle f(\cdot), D_x k(x, \cdot) \rangle_{\mathcal{F}_k}$$

²It is hard to identify \mathcal{F}_k given k , or k given \mathcal{F}_k (more on this later).

Two essential tools for computations

Representer Theorem (e.g. [Schölkopf et al., 2001])

Let $L : (\mathcal{X} \times \mathbb{R} \times \mathbb{R})^N \rightarrow \mathbb{R} \cup \{\infty\}$, strictly increasing $\Omega : \mathbb{R}_+ \rightarrow \mathbb{R}$, and

$$\bar{f} = \arg \min_{f \in \mathcal{F}_k} L \left((x_n, y_n, f(x_n))_{n \in [N]} \right) + \Omega(\|f\|_k)$$

Then $\exists (a_n)_{n \in [N]} \in \mathbb{R}^N$ s.t. $\bar{f}(\cdot) = \sum_{n \in [N]} a_n k(x_n, \cdot)$

\Leftrightarrow Optimal solutions lie in a finite dimensional subspace of \mathcal{F}_k .

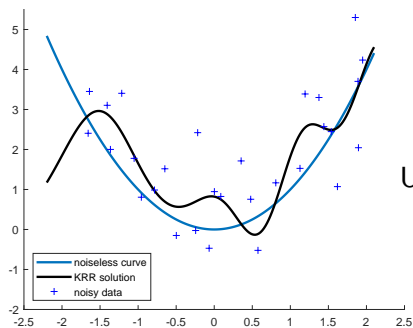
Finite number of evaluations \implies finite number of coefficients

Kernel trick

$$\left\langle \sum_{n \in [N]} a_n k(x_n, \cdot), \sum_{m \in [M]} a'_m k(x'_m, \cdot) \right\rangle_k = \sum_{n \in [N]} \sum_{m \in [M]} a_n a'_m k(x_n, x'_m)$$

\Leftrightarrow On this finite dimensional subspace, no need to know $(\mathcal{F}_k, \langle \cdot, \cdot \rangle_{\mathcal{F}_k})$.

Example: 1D monotonic kernel ridge regression (KRR)

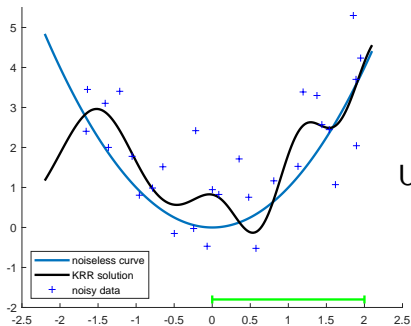


$$\min_{f \in \mathcal{F}_k} \frac{1}{N} \sum_{n=1}^N |y_n - f(x_n)|^2 + \lambda \|f\|_{\mathcal{F}_k}^2$$

Applying the representer theorem

$$\text{Unconstrained KRR } \bar{f} = \sum_{n=1}^N \alpha_n k_{x_n},$$
$$\alpha = (\mathbf{G} + N\lambda \cdot \text{Id})^{-1} \mathbf{y}$$

Example: 1D monotonic kernel ridge regression (KRR)



$$\min_{f \in \mathcal{F}_k} \frac{1}{N} \sum_{n=1}^N |y_n - f(x_n)|^2 + \lambda \|f\|_{\mathcal{F}_k}^2$$

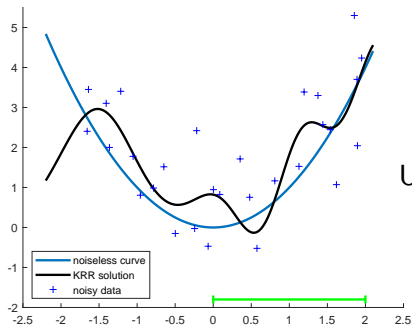
$$\text{s.t. } 0 \leq f'(x), \forall x \in [0, 2]$$

$$\text{Unconstrained KRR } \bar{f} = \sum_{n=1}^N \alpha_n k_{x_n},$$
$$\alpha = (\mathbf{G} + N\lambda \cdot \text{Id})^{-1} \mathbf{y}$$

here is not monotonic on $[0, 2]$!

Infinite number of evaluations \Rightarrow no representer theorem!
How to modify the problem to ensure constraint satisfaction?

Example: 1D monotonic kernel ridge regression (KRR)



$$\min_{f \in \mathcal{F}_k} \frac{1}{N} \sum_{n=1}^N |y_n - f(x_n)|^2 + \lambda \|f\|_{\mathcal{F}_k}^2$$

$$\text{s.t. } \eta_m \|f\|_k \leq f'(\tilde{x}_m), \forall m \in [M]$$

$$\text{Unconstrained KRR } \bar{f} = \sum_{n=1}^N \alpha_n k_{x_n},$$
$$\alpha = (\mathbf{G} + N\lambda \cdot \text{Id})^{-1} \mathbf{y}$$

vs

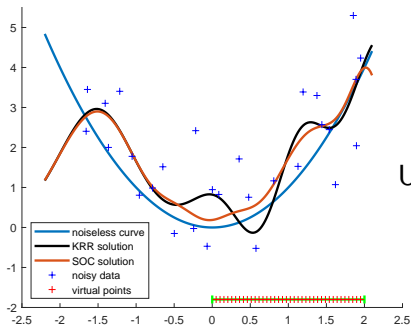
Second-Order Cone
(SOC) constrained KRR

Second-Order Cone constraints: $\{f \mid \|Af + b\|_k \leq c^\top f + d\}$

SOC comes from adding a buffer, $\eta_m > 0$, to a discretization, $\{\tilde{x}_m\}_{m \in [M]}$

$$\text{LP} \subset \text{QP} \subset \text{SOCP} \subset \text{SDP}$$

Example: 1D monotonic kernel ridge regression (KRR)



$$\min_{f \in \mathcal{F}_k} \frac{1}{N} \sum_{n=1}^N |y_n - f(x_n)|^2 + \lambda \|f\|_{\mathcal{F}_k}^2$$

$$\text{s.t. } \eta_m \|f\|_k \leq f'(\tilde{x}_m), \forall m \in [M]$$

$$\text{Unconstrained KRR } \bar{f} = \sum_{n=1}^N \alpha_n k_{x_n},$$

$$\alpha = (\mathbf{G} + N\lambda \cdot \text{Id})^{-1} \mathbf{y}$$

vs

Second-Order Cone
(SOC) constrained KRR

Second-Order Cone constraints: $\{f \mid \|Af + b\|_k \leq c^\top f + d\}$

SOC comes from adding a buffer, $\eta_m > 0$, to a discretization, $\{\tilde{x}_m\}_{m \in [M]}$

$$"b \leq Df(x), \forall x \in \mathcal{K}" \Leftarrow "b + \eta_m \|f(\cdot)\| \leq Df(\tilde{x}_m), \forall m \in [M]"$$

This choice is related to continuity moduli.

Deriving SOC constraints through continuity moduli

Take $\delta \geq 0$ and x s.t. $\|x - \tilde{x}_m\| \leq \delta$

$$\begin{aligned} |Df(x) - Df(\tilde{x}_m)| &= |\langle f(\cdot), D_x k(x, \cdot) - D_x k(\tilde{x}_m, \cdot) \rangle_k| \\ &\leq \|f(\cdot)\|_k \underbrace{\sup_{\{x \mid \|x - \tilde{x}_m\| \leq \delta\}} \|D_x k(x, \cdot) - D_x k(\tilde{x}_m, \cdot)\|_k}_{\eta_m(\delta)} \end{aligned}$$

$$\omega_m(Df, \delta) := \sup_{\{x \mid \|x - \tilde{x}_m\| \leq \delta\}} |Df(x) - Df(\tilde{x}_m)| \leq \eta_m(\delta) \|f(\cdot)\|_k$$

For a covering $\mathcal{K} = \bigcup_{m \in [M]} \mathbb{B}_X(\tilde{x}_m, \delta_m)$

$$"b \leq Df(x), \forall x \in \mathcal{K}" \Leftrightarrow "b + \omega_m(Df, \delta) \leq Df(\tilde{x}_m), \forall m \in [M]"$$

Deriving SOC constraints through continuity moduli

Take $\delta \geq 0$ and x s.t. $\|x - \tilde{x}_m\| \leq \delta$

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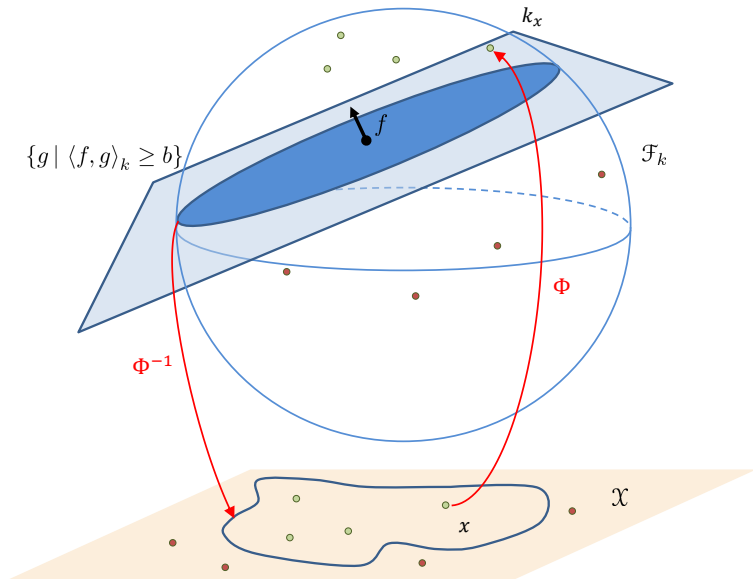
$$\omega_m(Df, \delta) := \sup_{\{x \mid \|x - \tilde{x}_m\| \leq \delta\}} |Df(x) - Df(\tilde{x}_m)| \leq \eta_m(\delta) \|f(\cdot)\|_k$$

For a covering $\mathcal{K} \subset \bigcup_{m \in [M]} \mathbb{B}_x(\tilde{x}_m, \delta_m)$

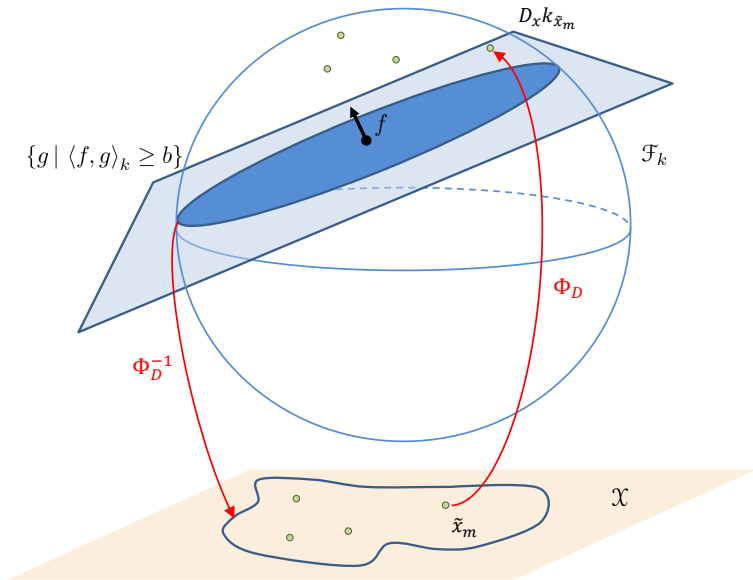
$$\begin{aligned} "b \leq Df(x), \forall x \in \mathcal{K}" &\Leftarrow "b + \omega_m(Df, \delta) \leq Df(\tilde{x}_m), \forall m \in [M]" \\ &\Leftarrow "b + \eta_m \|f(\cdot)\| \leq Df(\tilde{x}_m), \forall m \in [M]" \end{aligned}$$

Since the kernel is smooth, $\delta \rightarrow 0$ gives $\eta_m(\delta) \rightarrow 0$.

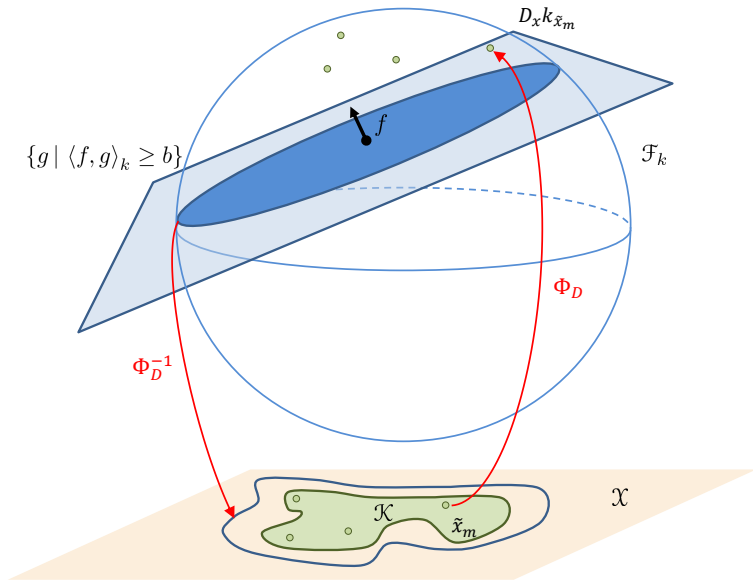
There is also a geometrical interpretation for this choice of η_m .



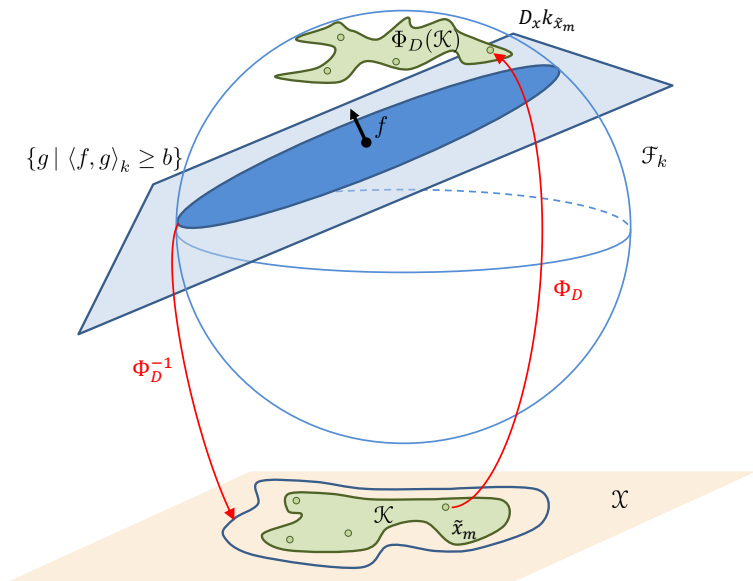
Support Vector Machine (SVM) is about separating red and green points by blue hyperplane.



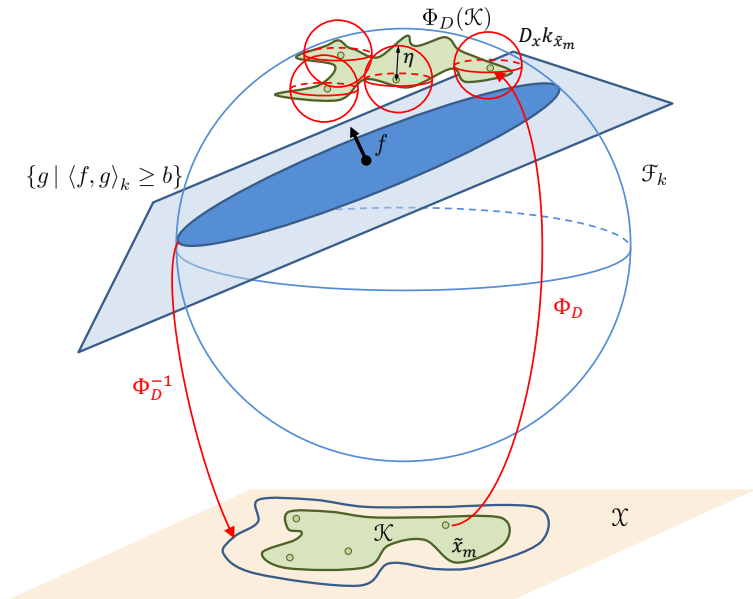
Using the nonlinear embedding $\Phi_D : x \mapsto D_x k(x, \cdot)$, the idea is the same. Consider only the green points, it looks like one-class SVM.



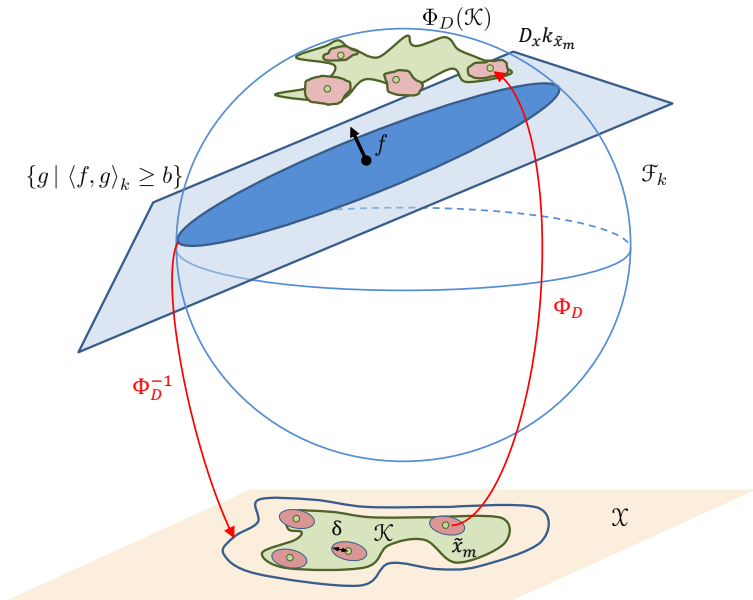
The green points are now samples of a compact set \mathcal{K} .



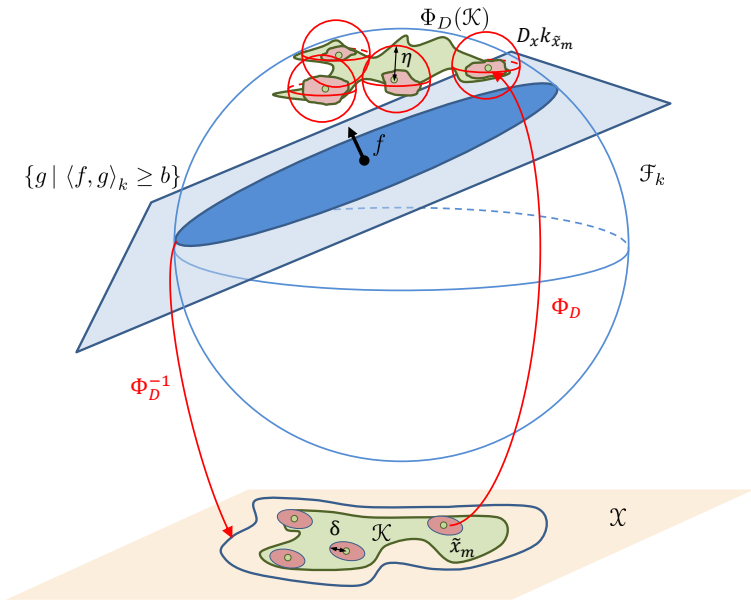
The image $\Phi_D(\mathcal{K})$ looks ugly...



The image $\Phi_D(\mathcal{K})$ looks ugly, can we cover it by balls? How to choose η ?



First cover $\mathcal{K} \subset \bigcup \{\tilde{x}_m + \delta \mathbb{B}\}$, and then look at the images $\Phi_D(\{\tilde{x}_m + \delta \mathbb{B}\})$



Cover the $\Phi_D(\{\tilde{x}_m + \delta\mathbb{B}\})$ with tiny balls! This is how SOC was defined.

Main theorem

$$(f_\eta, b_\eta) \in \arg \min_{f \in \mathcal{F}_k, b \in \mathcal{B}} \mathcal{L}(f) = L\left(b, (x_n, y_n, f(x_n))_{n \in [M]}\right) + \Omega(\|f\|_k)$$

s.t. $b_i + \eta_{i,m} \|f(\cdot)\|_k \leq D_i f(\tilde{x}_{m,i}), \quad \forall m \in [M_i], \forall i \in [I].$

where \mathcal{B} is a closed convex constraint set over $(b_i)_{i \in [I]}$. If $\Omega(\cdot)$ is strictly increasing, then

Theoretical guarantees [Aubin-Frankowski and Szabó, 2020]

- i) The finite number of SOC constraints is **tighter** than the infinite number of affine constraints.
- ii) **Representer theorem** (optimal solutions have a finite expression)
$$f_\eta = \sum_{i \in [I], m \in [M_i]} \tilde{a}_{i,m} D_{i,x} k(\tilde{x}_{i,m}, \cdot) + \sum_{n \in [M]} a_n k(x_n, \cdot)$$
- iii) If \mathcal{L} is μ -strongly convex, we have **bounds**: computable/theoretical^a

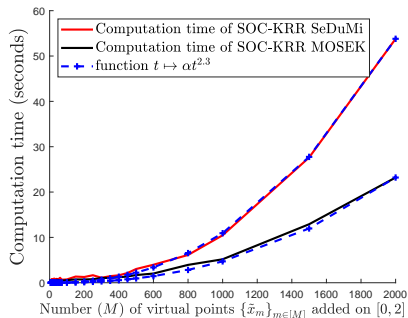
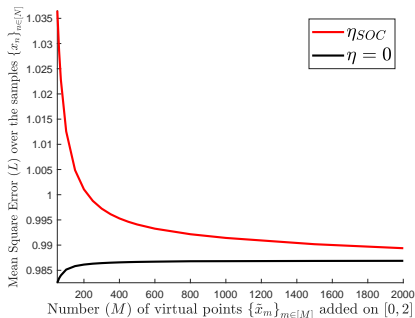
$$\|f_\eta - \bar{f}\|_k \leq \min \left(\sqrt{\frac{2(\mathcal{L}(f_\eta) - \mathcal{L}(f_{\eta=0}))}{\mu}}, \sqrt{\frac{L_{\bar{f}} \|\eta\|_\infty}{\mu}} \right)$$

^aAssuming $\mathcal{B} = \mathbb{R}^I$ for the *a priori* bound to hold.

Discussion

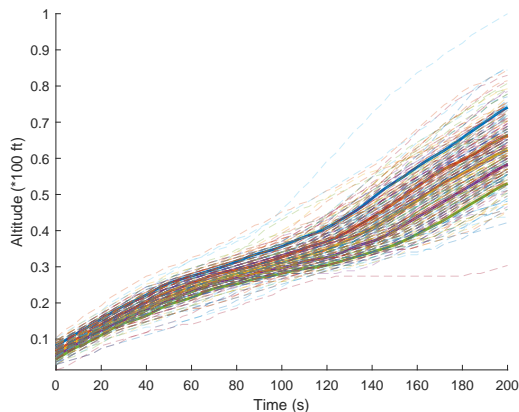
- (i) This theorem holds for given samples $(x_n, y_n)_{n \in [M]}$ (optimization rather than statistical properties - no asymptotics)
- (ii) The representer theorem provides an equivalent finite-dimensional problem of size $N + M$ with SOC constraints $\sim \mathcal{O}((N + M)^3)$
- (iii) Better bound \equiv smaller $\eta \equiv$ smaller $\delta \equiv$ larger $M \equiv$ costly in time
- (iv) The virtual points can be chosen among the samples (*recycling*)

KRR example



Joint quantile regression (JQR): airplane data

Airplane trajectories at takeoff have **increasing altitude**.



JQR with monotonic constraint over $[x_{\min}, x_{\max}]$:

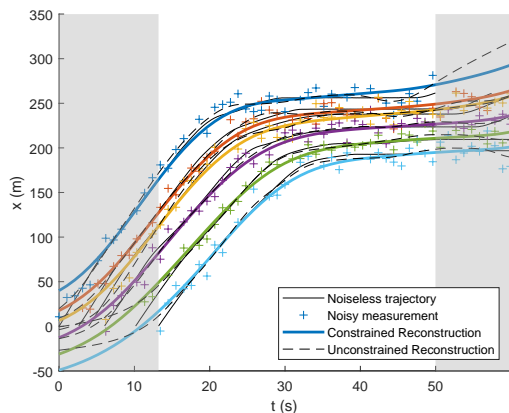
Increasing quantiles
should be
non-crossing

Data provided by ENAC
(flights Paris→Toulouse)
[Nicol, 2013]

Two shape constraints jointly handled with 15k samples.
Works with higher dimensions too!

Kernel ridge regression (KRR): trajectory reconstruction

Very noisy GPS data: six non-overtaking cars in a traffic jam



KRR with monotonic constraint over $[t_{\min}, t_{\max}]$:

Forward trajectories also maintain security distance

Data from IFSTTAR (MOCOpo Project) [Buisson et al., 2016]

(In *Kernel Regression for Vehicle Trajectory Reconstruction under Speed and Inter-vehicular Distance Constraints*, PCAF and Nicolas Petit and Zoltán Szabó IFAC World Congress 2020)

Teaser slide

This approach works as well for

- Other compact coverings than balls, iterative covering
- SDP constraints (e.g. convexity for $d \geq 2$): $0 \preceq \mathbf{Hess}(f)(x)$
- Vector-valued functions $f : \mathcal{X} \rightarrow \mathbb{R}^Q$
- Other applications: finance, control theory,...

Control: Take \mathcal{F}_k to be a Hilbert space of trajectories $[0, T] \rightarrow \mathbb{R}^Q$

$$\begin{aligned} \min_{x(\cdot) \in \mathcal{F}_k} \quad & g(x(T)) + \|x(\cdot)\|_k^2 \\ \text{s.t.} \quad & x(0) = x_0, \\ & c_i(t)^\top x(t) \leq d_i(t), \quad \forall t \in [0, T], \forall i \in [\mathcal{I}]. \end{aligned}$$

Partial conclusion/Take-home message

We have seen how to tighten an **infinite number of affine constraints over a compact set** into **finitely many SOC constraints** in RKHSs

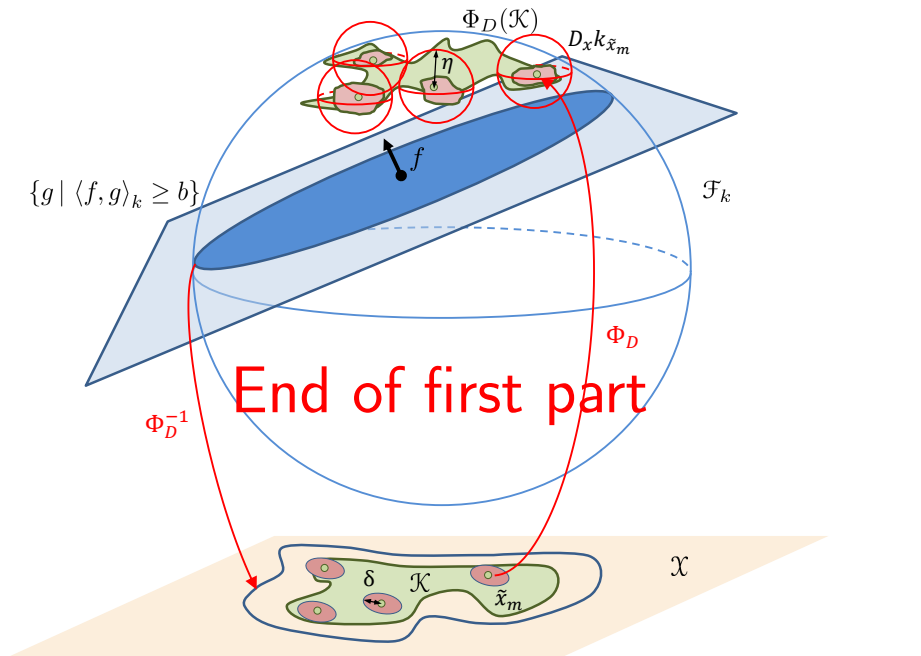
↪ we have a representer theorem!

- tightening intractable constraints is the only way to have guarantees
- but tightening is “harder” to perform (here computationally)

Covering schemes suffer from the curse of dimensionality!

$$\mathcal{X} \subset \mathbb{R}^d, d \gg 1$$

But the control problem is only defined over $\mathcal{X} = [0, T]$ ($d = 1$)!



Linearly-constrained Linear Quadratic Regulator (LQR)

Problem of time-varying linear quadratic optimal control with finite horizon and affine inequality state constraints

$$\begin{aligned} \min_{x(\cdot), u(\cdot)} \quad & g(x(T)) + \int_0^T [x(t)^\top Q(t)x(t) + u(t)^\top R(t)u(t)] dt \\ \text{s.t.} \quad & x(0) = x_0, \\ & x'(t) = A(t)x(t) + B(t)u(t), \text{ a.e. in } [0, T], \\ & c_i(t)^\top x(t) \leq d_i(t), \forall t \in [0, T], \forall i \in \llbracket 1, P \rrbracket, \end{aligned}$$

with state $x(t) \in \mathbb{R}^N$, control $u(t) \in \mathbb{R}^M$, $A(\cdot) \in L^1(0, T)$, $B(\cdot) \in L^2(0, T)$, $Q(t) \succcurlyeq 0$ and $R(t) \succcurlyeq \text{rId}_M$

Linearly-constrained Linear Quadratic Regulator (LQR)

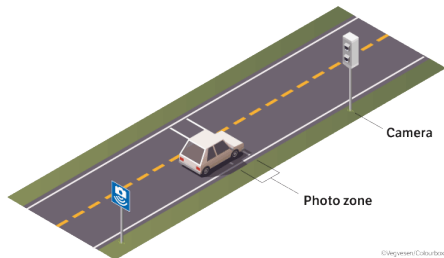
Problem of time-varying linear quadratic optimal control with finite horizon and affine inequality state constraints with $Q \equiv 0$ and $R \equiv \text{Id}_M$

$$\begin{aligned} \min_{x(\cdot), u(\cdot)} \quad & g(x(T)) + \int_0^T \|u(t)\|_{\mathbb{R}^M}^2 dt \\ \text{s.t.} \quad & x(0) = x_0, \\ & x'(t) = A(t)x(t) + B(t)u(t), \text{ a.e. in } [0, T], \\ & c_i(t)^\top x(t) \leq d_i(t), \forall t \in [0, T], \forall i \in \{1, \dots, P\}, \end{aligned}$$

with state $x(t) \in \mathbb{R}^N$, control $u(t) \in \mathbb{R}^M$, $A(\cdot) \in L^1(0, T)$, $B(\cdot) \in L^2(0, T)$, $x(\cdot) : [0, T] \rightarrow \mathbb{R}^N$ absolutely continuous and $u(\cdot) \in L^2(0, T)$.

Why are state constraints difficult to study?

- **Theoretical obstacle:** Pontryagin's Maximum Principle involves not only an adjoint vector $p(t)$ but also measures/BV functions $\psi(t)$ supported at times where the constraints are saturated. You cannot just backpropagate the Hamiltonian system from the transversality condition.
- **Numerical obstacle:** Time discretization of constraints may fail e.g.



Speed cameras in traffic control

In between two cameras, drivers always break the speed limit.

Objective: Turn the state-constrained LQR into “KRR”

We have a vector space \mathcal{S} of trajectories $x(\cdot) : [0, T] \rightarrow \mathbb{R}^N$

$$\mathcal{S} := \{x(\cdot) \mid \exists u(\cdot) \in L^2(0, T) \text{ s.t. } x'(t) = A(t)x(t) + B(t)u(t) \text{ a.e. } \}$$

The space of trajectories \mathcal{S} depends on $T, A(\cdot), B(\cdot)$.

LQR (Linear Quadratic Regulator)

$$\min_{\substack{x(\cdot) \in \mathcal{S} \\ u(\cdot) \in L^2(0, T)}} g(x(T)) + \|u(\cdot)\|_{L^2(0, T)}^2$$

$$\begin{aligned} x(0) &= x_0 \\ c_i(t)^\top x(t) &\leq d_i(t), t \in [0, T], i \leq P \end{aligned}$$

“KRR” (Kernel Ridge Regression)

$$\min_{x(\cdot) \in \mathcal{S}} g(x(T)) + \lambda \|x(\cdot)\|_{\mathcal{S}}^2$$

$$\begin{aligned} x(0) &= x_0 \\ c_i(t)^\top x(t) &\leq d_i(t), t \in [0, T], i \leq P \end{aligned}$$

Is \mathcal{S} a RKHS? For which inner product?

Vector-valued reproducing kernel Hilbert space (vRKHS)

Definition (vRKHS)

Let \mathcal{T} be a non-empty set. A Hilbert space $(\mathcal{F}_K, \langle \cdot, \cdot \rangle_K)$ of \mathbb{R}^N -vector-valued functions defined on \mathcal{T} is a vRKHS if there exists a matrix-valued kernel $K : \mathcal{T} \times \mathcal{T} \rightarrow \mathbb{R}^{N \times N}$ such that the **reproducing property** holds:

$$K(\cdot, t)p \in \mathcal{F}_K, \quad p^\top f(t) = \langle f, K(\cdot, t)p \rangle_K, \quad \text{for } t \in \mathcal{T}, p \in \mathbb{R}^N, f \in \mathcal{F}_K$$

Necessarily, K has a Hermitian symmetry: $K(s, t) = K(t, s)^\top$

There is also a one-to-one correspondence between K and $(\mathcal{F}_K, \langle \cdot, \cdot \rangle_K)$ [Micheli and Glaunès, 2014], so changing \mathcal{T} or $\langle \cdot, \cdot \rangle_K$ changes K .

Representer theorem in vRKHSs

Theorem (Representer theorem with SOC constraints)

Let $(\mathcal{F}_K, \langle \cdot, \cdot \rangle_K)$ be a vRKHS defined on a set \mathcal{T} . For a “loss” $L : \mathbb{R}^{N_0} \rightarrow \mathbb{R} \cup \{+\infty\}$, strictly increasing “regularizer” $\Omega : \mathbb{R}_+ \rightarrow \mathbb{R}$, and constraints $d_i : \mathbb{R}^{N_i} \rightarrow \mathbb{R}$, consider the optimization problem

$$\begin{aligned} \bar{f} \in \arg \min_{f \in \mathcal{F}_K} & \quad L\left(c_{0,1}^\top f(t_{0,1}), \dots, c_{0,N_0}^\top f(t_{0,N_0})\right) + \Omega(\|f\|_K) \\ \text{s.t.} & \quad \lambda_i \|f\|_K \leq d_i(c_{i,1}^\top f(t_{i,1}), \dots, c_{i,N_i}^\top f(t_{i,N_i})), \forall i \in \llbracket 1, P \rrbracket. \end{aligned}$$

Then there exists $\{p_{i,m}\}_{m \in \llbracket 1, N_i \rrbracket} \subset \mathbb{R}^N$ and $\alpha_{i,m} \in \mathbb{R}$ such that

$$\bar{f} = \sum_{i=0}^P \sum_{m=1}^{N_i} K(\cdot, t_{i,m}) p_{i,m} \text{ with } p_{i,m} = \alpha_{i,m} c_{i,m}.$$

Application to linear control systems with quadratic cost

$\mathcal{S} := \{x(\cdot) \in W^{1,1} \mid \exists u(\cdot) \in L^2(0, T) \text{ s.t. } x'(t) = A(t)x(t) + B(t)u(t) \text{ a.e.}\}$

Given $x(\cdot) \in \mathcal{S}$, for the pseudoinverse $B(t)^\ominus$ of $B(t)$, set

$$u(t) := B(t)^\ominus [x'(t) - A(t)x(t)] \text{ a.e. in } [0, T].$$

$$\langle x_1(\cdot), x_2(\cdot) \rangle_K := x_1(0)^\top x_2(0) + \int_0^T u_1(t)^\top u_2(t) dt$$

Lemma

$(\mathcal{S}, \langle \cdot, \cdot \rangle_K)$ is a *vRKHS* with uniformly continuous $K(\cdot, \cdot)$.

$\|\cdot\|_K$ is a Sobolev-like norm split into two semi-norms

$$\|x(\cdot)\|_K^2 = \underbrace{\|x(0)\|^2}_{\|x(\cdot)\|_{K_0}^2} + \underbrace{\int_0^T \|B(t)^\ominus (x'(t) - A(t)x(t))\|^2 dt}_{\|x(\cdot)\|_{K_1}^2}.$$

Splitting \mathcal{S} into subspaces and identifying their kernels

$$\begin{aligned}\mathcal{S}_0 &:= \{x(\cdot) \mid x'(t) = A(t)x(t), \text{ a.e. in } [0, T]\} & \|x(\cdot)\|_{K_0}^2 &= \|x(0)\|^2 \\ \mathcal{S}_u &:= \{x(\cdot) \mid x(\cdot) \in \mathcal{S} \text{ and } x(0) = 0\} & \|x(\cdot)\|_{K_1}^2 &= \|u(\cdot)\|_{L^2(0, T)}^2.\end{aligned}$$

As $\mathcal{S} = \mathcal{S}_0 \oplus \mathcal{S}_u$, $K = K_0 + K_1$.

Splitting \mathcal{S} into subspaces and identifying their kernels

$$\begin{aligned}\mathcal{S}_0 &:= \{x(\cdot) \mid x'(t) = A(t)x(t), \text{ a.e. in } [0, T]\} & \|x(\cdot)\|_{K_0}^2 &= \|x(0)\|^2 \\ \mathcal{S}_u &:= \{x(\cdot) \mid x(\cdot) \in \mathcal{S} \text{ and } x(0) = 0\} & \|x(\cdot)\|_{K_1}^2 &= \|u(\cdot)\|_{L^2(0, T)}^2.\end{aligned}$$

As $\mathcal{S} = \mathcal{S}_0 \oplus \mathcal{S}_u$, $K = K_0 + K_1$. Since $\dim(\mathcal{S}_0) = N$, for $\Phi_A(t, s) \in \mathbb{R}^{N, N}$ the state-transition matrix $s \rightarrow t$ of $x'(\tau) = A(\tau)x(\tau)$

$$K_0(s, t) = \Phi_A(s, 0)\Phi_A(t, 0)^\top$$

Only using the reproducing property and that for $x(\cdot) \in \mathcal{S}$,

$$x(t) = \Phi_A(t, 0)x(0) + \int_0^t \Phi_A(t, \tau)B(\tau)u(\tau)d\tau. \quad (1)$$

For fixed t , define control matrix $U_t(s) := \begin{cases} B(s)^\top \Phi_A(t, s)^\top & \forall s \leq t, \\ 0 & \forall s > t. \end{cases}$

$\partial_1 K_1(s, t) = A(s)K_1(s, t) + B(s)U_t(s)$ a.e. in $[0, T]$ with $K_1(0, t) = 0$.

$$K_1(s, t) = \int_0^{\min(s, t)} \Phi_A(s, \tau)B(\tau)B(\tau)^\top \Phi_A(t, \tau)^\top d\tau.$$

Examples: controllability Gramian/transversality condition

Steer a point from $(0, 0)$ to (T, x_T) , with e.g. $g(x(T)) = \|x_T - x(T)\|_N^2$

Exact planning ($x(T) = x_T$)

$$\min_{\substack{x(\cdot) \in \mathcal{S} \\ x(0)=0}} \chi_{x_T}(x(T)) + \frac{1}{2} \|u(\cdot)\|_{L^2(0,T)}^2$$

Relaxed planning ($g \in \mathcal{C}^1$ convex)

$$\min_{\substack{x(\cdot) \in \mathcal{S} \\ x(0)=0}} g(x(T)) + \frac{1}{2} \|u(\cdot)\|_{L^2(0,T)}^2$$

As, $x(0) = 0$, applying the representer theorem: $\exists p_T, \bar{x}(\cdot) = K_1(\cdot, T)p_T$

Controllability Gramian

$$K_1(T, T) = \int_0^T \Phi_A(T, \tau) B(\tau) B(\tau)^\top \Phi_A(T, \tau)^\top d\tau$$

$$\bar{x}(T) = x_T \Leftrightarrow x_T \in \text{Im}(K_1(T, T))$$

Transversality Condition

$$\begin{aligned} 0 &= \nabla \left(p \mapsto g(K_1(T, T)p) + \frac{1}{2} p^\top K_1(T, T)p \right) (p_T) \\ &= K_1(T, T)(\nabla g(K_1(T, T)p_T) + p_T). \end{aligned}$$

$$\text{Take } p_T = -\nabla g(\bar{x}(T))$$

From affine state constraints to SOC constraints

Take (t_m, δ_m) such that $[0, T] \subset \cup_{m \in \llbracket 1, N_P \rrbracket} [t_m - \delta_m, t_m + \delta_m]$, take

$$\eta_i(\delta_m, t_m) := \sup_{t \in [t_m - \delta_m, t_m + \delta_m] \cap [0, T]} \|K(\cdot, t_m)c_i(t_m) - K(\cdot, t)c_i(t)\|_K,$$

$$d_i(\delta_m, t_m) := \inf_{t \in [t_m - \delta_m, t_m + \delta_m] \cap [0, T]} d_i(t).$$

We have strengthened SOC constraints that enable a representer theorem

$$\eta_i(\delta_m, t_m) \|x(\cdot)\|_K + c_i(t_m)^\top x(t_m) \leq d_i(\delta_m, t_m), \forall m \in \llbracket 1, N_P \rrbracket, \forall i \in \llbracket 1, P \rrbracket$$

\Downarrow

$$c_i(t)^\top x(t) \leq d_i(t), \forall t \in [0, T], \forall i \in \llbracket 1, P \rrbracket$$

Lemma (Uniform continuity of tightened constraints)

As $K(\cdot, \cdot)$ is UC, if $c_i(\cdot)$ and $d_i(\cdot)$ are C^0 -continuous, when $\delta \rightarrow 0^+$, $\eta_i(\cdot, t)$ converges to 0 and $d_i(\cdot, t)$ converges to $d_i(t)$, uniformly w.r.t. t .

Main theorem

(H-gen) $A(\cdot) \in L^1(0, T)$ and $B(\cdot) \in L^2(0, T)$, $c_i(\cdot)$ and $d_i(\cdot)$ are \mathcal{C}^0 .

(H-sol) $c_i(0)x_0 < d_i(0)$ and there exists a trajectory $x^\epsilon(\cdot) \in \mathcal{S}$ satisfying strictly the affine constraints, as well as the initial condition.³

(H-obj) $g(\cdot)$ is convex and continuous.

Theorem (Existence and Approximation by SOC constraints)

Both the original problem and its strengthening have unique optimal solutions. For any $\rho > 0$, there exists $\bar{\delta} > 0$ such that for all $(\delta_m)_{m \in \llbracket 1, N_0 \rrbracket}$, with $[0, T] \subset \cup_{m \in \llbracket 1, N_0 \rrbracket} [t_m - \delta_m, t_m + \delta_m]$ satisfying $\bar{\delta} \geq \max_{m \in \llbracket 1, N_0 \rrbracket} \delta_m$,

$$\frac{1}{\gamma_K} \cdot \sup_{t \in [0, T]} \|\bar{x}_\eta(t) - \bar{x}(t)\| \leq \|\bar{x}_\eta(\cdot) - \bar{x}(\cdot)\|_K \leq \rho.$$

with $\gamma_K := \sup_{t \in [0, T], p \in \mathbb{B}_N} \sqrt{p^\top K(t, t)p}$.

³(H-sol) is implied for instance by an inward-pointing condition at the boundary.

Numerical example: constrained pendulum - definition

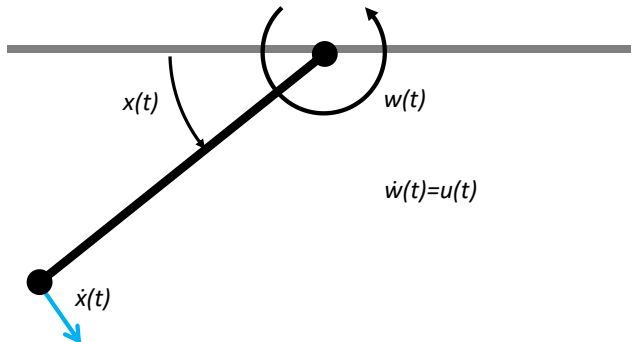
Constrained pendulum when controlling the third derivative of the angle

$$\min_{x(\cdot), w(\cdot), u(\cdot)} -\dot{x}(T) + \lambda \|u(\cdot)\|_{L^2(0,T)}^2 \quad \lambda \ll 1$$

$$x(0) = 0.5, \quad \dot{x}(0) = 0, \quad w(0) = 0, \quad x(T/3) = 0.5, \quad x(T) = 0$$

$$\ddot{x}(t) = -10x(t) + w(t), \quad \dot{w}(t) = u(t), \text{ a.e. in } [0, T]$$

$$\dot{x}(t) \in [-3, +\infty[, \quad w(t) \in [-10, 10], \quad \forall t \in [0, T]$$



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$$\dot{x}(t) \in [-3, +\infty[, \quad w(t) \in [-10, 10], \quad \forall t \in [0, T]$$

Converting affine state constraints to SOC constraints, applying rep. thm

$$\eta_{\dot{x}} \|x(\cdot)\|_K - \dot{x}(t_m) \leq -3,$$

$$\eta_w \|x(\cdot)\|_K + w(t_m) \leq 10,$$

$$\eta_w \|x(\cdot)\|_K - w(t_m) \leq 10$$

$$\bar{x}(\cdot) = K(\cdot, 0)p_0 + K(\cdot, T/3)p_{T/3}$$

$$+ K(\cdot, T)p_T + \sum_{m=1}^M K(\cdot, t_m)p_m$$

Most of computational cost is related to the “controllability Gramians”

$K_1(s, t) = \int_0^{\min(s,t)} e^{(s-\tau)A} B B^T e^{(t-\tau)A^T} d\tau$ which we have to approximate.

Numerical example: constrained pendulum - illustration

Optimal solutions of the constrained pendulum “path-planning” problem. Red circles: equality constraints. Grayed areas: constraints over $[0, T]$.

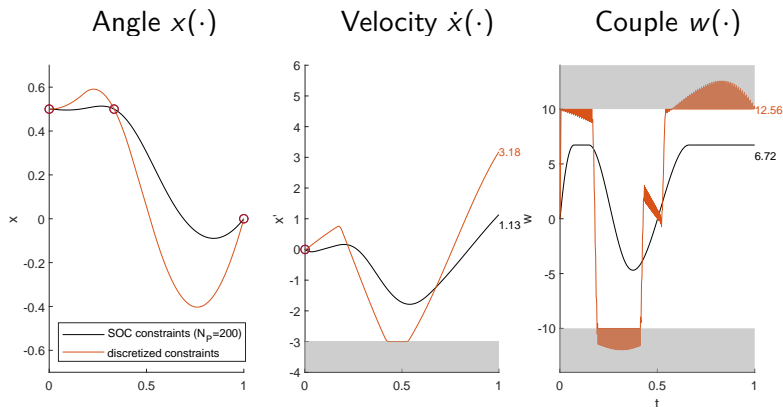


Figure: Comparison of SOC constraints (guaranteed η_w) vs discretized constraints ($\eta_w = 0$) for $N_P = 200$.

Numerical example: constrained pendulum - illustration

Optimal solutions of the constrained pendulum “path-planning” problem. Red circles: equality constraints. Grayed areas: constraints over $[0, T]$.

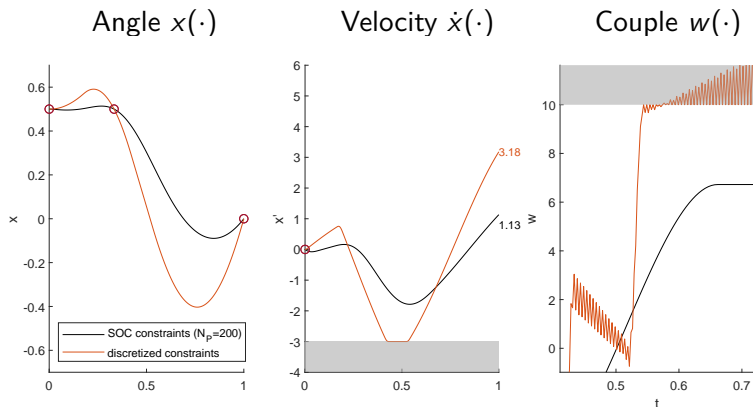


Figure: Comparison of SOC constraints (guaranteed η_w) vs discretized constraints ($\eta_w = 0$) for $N_p = 200$ - **Chattering phenomenon!**

Numerical example: constrained pendulum - illustration

Optimal solutions of the constrained pendulum “path-planning” problem. Red circles: equality constraints. Grayed areas: constraints over $[0, T]$.

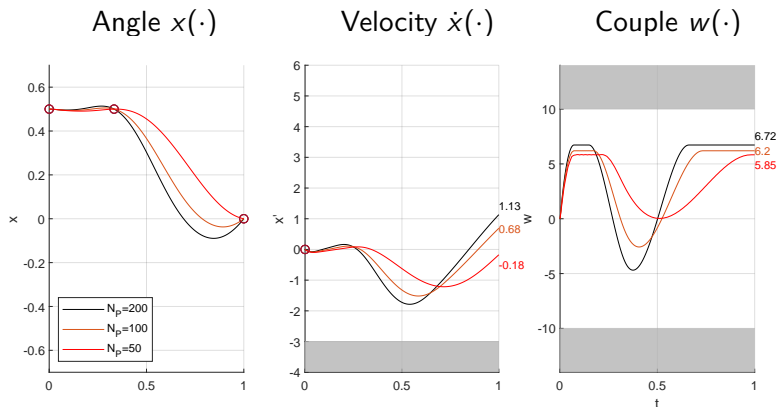


Figure: Comparison of SOC constraints for varying N_P and guaranteed η_w .

Numerical example: constrained pendulum - illustration

Optimal solutions of the constrained pendulum “path-planning” problem. Red circles: equality constraints. Grayed areas: constraints over $[0, T]$.

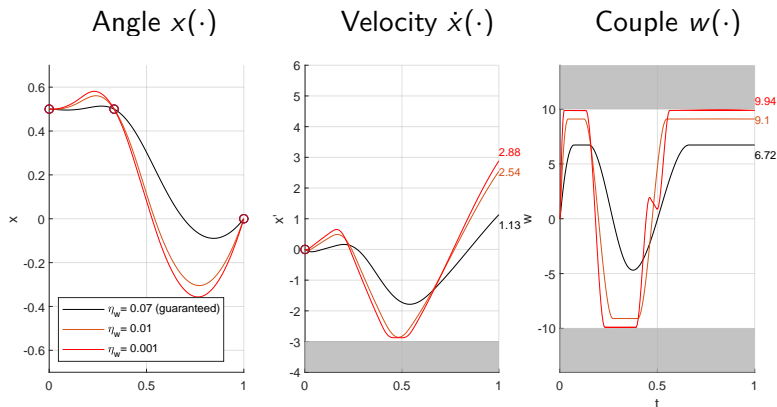


Figure: Comparison of SOC constraints for varying η_w and $N_P = 200$.

Pushing RKHSs beyond/Revisiting classical LQR

For RKHSs

- **Control constraints do not correspond to continuous evaluations**
↪ limits of RKHS pointwise theory (e.g. $x' = u \in L^2([0, T], [-1, 1])$ a.e.)
- **Successive linearizations of nonlinear system lead to changing kernels**
↪ a single kernel may not be sufficient (e.g. $x' = f_{[x_n(\cdot)]}x + f_{[u_n(\cdot)]}u$ a.e.)
- **Non-quadratic costs for linear systems do not lead to Hilbert spaces**
↪ you may need Banach kernels (e.g. $\|u(\cdot)\|_{L^2(0, T)}^2 \rightarrow \|u(\cdot)\|_{L^1(0, T)}$)

For control theory

- **To each evaluation at time t corresponds a covector $p_t \in \mathbb{R}^N$**
↪ Representer theorem well adapted for state constraints, but unsuitable for control constraints. Reverts the difficulty w.r.t. PMP approach.
- **The Gramian of controllability generates trajectories**
↪ This allows for close-form solutions in continuous-time

Shape constraints in RKHSs

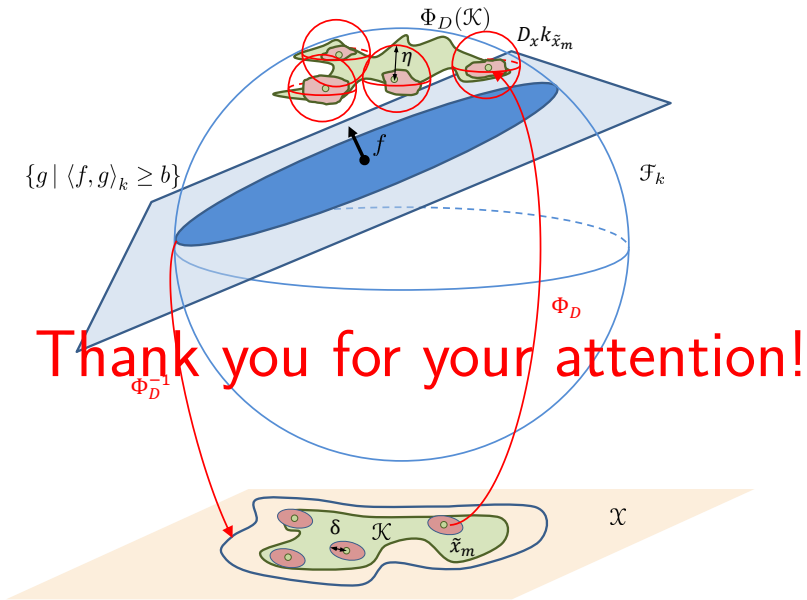
We have seen how to tighten in RKHSs an **infinite number of pointwise affine constraints over a compact set into finitely many SOC constraints.**

- tightening intractable constraints is the only way to have guarantees
- compact coverings in infinite dimensional spaces provide a solution

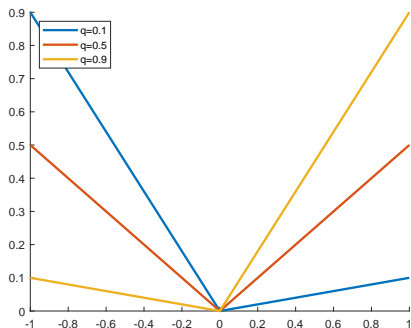
Linear Quadratic Regulator as a kernel regression

We have seen that **state-constrained LQR is a non-trivial 1D example of shape constraints** that

- allows to revisit classical notions from the kernel viewpoint
- allows to deal with the difficult problem of state constraints



Appendix: Joint Quantile Regression (JQR)



$f_\tau(x)$ conditional quantile over (X, Y) :
 $P(Y \leq f_\tau(x) | X = x) = \tau \in]0, 1[.$

Estimation through convex optimization over “pinball loss” $l_\tau(\cdot)$ (i.e. tilted absolute value [Koenker, 2005]).

Known fact: quantile functions can cross when estimated independently.

Joint quantile regression with non-crossing constraints, over $(f_q)_{q \in [Q]}$:

$$\mathcal{L}(f_1, \dots, f_Q) = \frac{1}{N} \sum_{q \in [Q]} \sum_{n \in [N]} l_{\tau_q}(y_n - f_q(x_n)) + \lambda_f \sum_{q \in [Q]} \|f_q\|_k^2$$

$$\text{s.t. } f_{q+1}(x) \geq f_q(x), \forall q \in [Q - 1], \forall x \in [\min x_n, \max x_n]^d.$$

Appendix: JQR performance over UCI datasets

- PDCD = Primal-Dual Coordinate Descent [Sangnier et al., 2016], JQR with parallel/heteroscedatic quantile penalization (see also ITL [Brault et al., 2019] for noncrossing inducer)
- mean \pm std of $100 \times$ value of the pinball loss (smaller is better)

Dataset	d	N	PDCD	SOC
engel	1	235	48 ± 8	53 ± 9
GAGurine	1	314	61 ± 7	65 ± 6
geyser	1	299	105 ± 7	108 ± 3
mcycle	1	133	66 ± 9	62 ± 5
ftcollinssnow	1	93	154 ± 16	148 ± 13
CobarOre	2	38	159 ± 24	151 ± 17
topo	2	52	69 ± 18	62 ± 14
caution	2	100	88 ± 17	98 ± 22
ufc	3	372	81 ± 4	87 ± 6

Annex: Green kernels and RKHSs

Let D be a differential operator, D^* its formal adjoint. Define the Green function $G_{D^*D,x}(y) : \Omega \rightarrow \mathbb{R}$ s.t. $D^*D G_{D^*D,x}(y) = \delta_x(y)$ then, if the integrals over the boundaries in Green's formula are null, for any $f \in \mathcal{F}_k$

$$f(x) = \int_{\Omega} f(y) D^* D G_{D^*D,x}(y) dy = \int_{\Omega} Df(y) D G_{D^*D,x}(y) dy =: \langle f, G_{D^*D,x} \rangle_{\mathcal{F}_k},$$

so $k(x, y) = G_{D^*D,x}(y)$ [Saitoh and Sawano, 2016, p61]. For vector-valued contexts, e.g. $\mathcal{F}_K = W^{s,2}(\mathbb{R}^d, \mathbb{R}^d)$ and $D^*D = (1 - \sigma^2 \Delta)^s$ component-wise, see [Micheli and Glaunès, 2014, p9].

Alternatively, in 1D, $D G_{D,x}(y) = \delta_x(y)$, the kernel associated to the inner product $\int_{\Omega} Df(y) Dg(y) dy$ for the space of f "null at the border" writes as

$$k(x, y) = \int_{\Omega} G_{D,x}(z) G_{D,y}(z) dz$$

see [Berlinet and Thomas-Agnan, 2004, p286] and [Heckman, 2012].

Annex: IPC gives strictly feasible trajectories

(H-sol) $C(0)x_0 < d(0)$ and there exists a trajectory $x^\epsilon(\cdot) \in \mathcal{S}$ satisfying strictly the affine constraints, as well as the initial condition.

(H1) $A(\cdot)$ and $B(\cdot)$ are \mathcal{C}^0 . $C(\cdot)$ and $d(\cdot)$ are \mathcal{C}^1 and $C(0)x_0 < d(0)$.

(H2) There exists $M_u > 0$ s.t. , for all $t \in [0, T]$ and $x \in \mathbb{R}^N$ satisfying $C(t)x \leq d(t)$, and $\|x\| \leq (1 + \|x_0\|)e^{T\|A(\cdot)\|_{L^\infty(0,T)} + TM_u\|B(\cdot)\|_{L^\infty(0,T)}}$, there exists $u_{t,x} \in M_u\mathbb{B}_M$ such that

$$\forall i \in \{j \mid c_j(t)^\top x = d_j(t)\}, \quad c_i'(t)^\top x - d_i'(t) + c_i(t)^\top (A(t)x + B(t)u_{t,x}) < 0.$$

This is an **inward-pointing condition** (IPC) at the boundary.

Lemma (Existence of interior trajectories)

If (H1) and (H2) hold, then (H-sol) holds.

Annex: control proof main idea, nested property

$$\eta_i(\delta, t) := \sup \|K(\cdot, t)c_i(t) - K(\cdot, s)c_i(s)\|_K, \quad \omega_i(\delta, t) := \sup |d_i(t) - d_i(s)|, \\ d_i(\delta_m, t_m) := \inf d_i(s), \quad \text{over } s \in [t_m - \delta_m, t_m + \delta_m] \cap [0, T]$$

For $\vec{\epsilon} \in \mathbb{R}_+^P$, the constraints we shall consider are defined as follows

$$\mathcal{V}_0 := \{x(\cdot) \in \mathcal{S} \mid C(t)x(t) \leq d(t), \forall t \in [0, T]\}, \\ \mathcal{V}_{\delta, \text{fin}} := \{x(\cdot) \in \mathcal{S} \mid \vec{\eta}(\delta_m, t_m)\|x(\cdot)\|_K + C(t_m)x(t_m) \leq d(\delta_m, t_m), \forall m \in \llbracket 1, N_0 \rrbracket\}, \\ \mathcal{V}_{\delta, \text{inf}} := \{x(\cdot) \in \mathcal{S} \mid \vec{\eta}(\delta, t)\|x(\cdot)\|_K + \vec{\omega}(\delta, t) + C(t)x(t) \leq d(t), \forall t \in [0, T]\}, \\ \mathcal{V}_{\vec{\epsilon}} := \{x(\cdot) \in \mathcal{S} \mid \vec{\epsilon} + C(t)x(t) \leq d(t), \forall t \in [0, T]\}.$$

Proposition (Nested sequence)

Let $\delta_{\max} := \max_{m \in \llbracket 1, N_0 \rrbracket} \delta_m$. For any $\delta \geq \delta_{\max}$, if, for a given $y_0 \geq 0$, $\epsilon_i \geq \sup_{t \in [0, T]} [\eta_i(\delta, t)y_0 + \omega_i(\delta, t)]$, then we have a nested sequence

$$(\mathcal{V}_{\vec{\epsilon}} \cap y_0 \mathbb{B}_K) \subset \mathcal{V}_{\delta, \text{inf}} \subset \mathcal{V}_{\delta, \text{fin}} \subset \mathcal{V}_0.$$

Only the simpler $\mathcal{V}_{\vec{\epsilon}}$ constraints matter!

Annex: List of shape constraints

- **Monotonicity w.r.t. partial ordering:**

$$\partial^{e_1} f(x) \geq \dots \geq \partial^{e_d} f(x) \geq 0 \quad (\forall x).$$

$$\partial^{e_j} f(x) \geq 0, \quad (\forall j \in [d], \quad \forall x).$$

- **Supermodularity:** $f(u \vee v) + f(u \wedge v) \geq f(u) + f(v)$, $u, v \in \mathbb{R}^d$, where $u \vee v := (\max(u_j, v_j))_{j \in [d]}$ and $u \wedge v := (\min(u_j, v_j))_{j \in [d]}$. For $f \in C^2$

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} \geq 0 \quad (\forall i \neq j \in [d], \forall x).$$

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