Kernel representation of non-negative functions with applications in non-convex optimization and beyond

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## Examples of constraints in function optimization - 1

Optimal control


## State constraints

- "avoid the wall" $x(t) \in\left[x_{\text {low }}, x_{\text {high }}\right]$
- "abide by the speed limit" $x^{\prime}(t) \in\left[v_{\text {low }}, v_{\text {high }}\right]$
- "do not stress the pilot" $x^{\prime \prime}(t) \in\left[a_{\text {low }}, a_{\text {high }}\right]$

Physical constraints
$\hookrightarrow$ provides feasible trajectories in path-planning

This consists in an infinite number of pointwise constraints!

## Examples of constraints in function optimization - 2

Nonparametric estimation


## Shape constraints

- nonnegativity

$$
f(x) \geq 0
$$

- directional monotonicity

$$
\partial_{i} f(x) \geq 0
$$

- directional convexity

$$
\partial_{i, i}^{2} f(x) \geq 0
$$

## Side information/Requirements

$\hookrightarrow$ compensates small number of samples or excessive noise

Applied in many fields: Biology, Chemistry, Statistics, Economics,... With many techniques: Isotonic regression, density estimation with splines,...

## Examples of constraints in function optimization - 3

- Global optimization of smooth (nonconvex) $g$ :

$$
\max _{c \in \mathbb{R}} c \quad\left(=\min _{x \in X} g(x)\right)
$$

- Density estimation with relative entropy:

$$
\min _{\substack{f \in \mathcal{C}(x, \mathbb{R}), \int_{x} f(x) \mathrm{d} x=1 \\ f(x) \geq 0, \forall x \in X}}-\int_{x} \log (f(x)) \mathrm{d} \mu(x) \quad\left(=\mathrm{KL}\left(\mu, \mu_{f}\right)+\mathrm{cst}\right)
$$

- Optimal transport in its dual formulation:

$$
\max _{\substack{u, v \in C(X, \mathbb{R}) \\ u(x)+v(y) \leq c(x, y), \forall x, y \in X \times x}} \int_{X} u(x) \mathrm{d} \mu(x)+\int_{X} v(y) \mathrm{d} \nu(y) \quad\left(=\mathrm{OT}_{c}(\mu, \nu)\right)
$$

Other problems/extensions: Joint Quantile Regression (JQR), handling constrained derivatives, vector or SDP-valued functions, . . . methods presented in this talk used in [Aubin-Frankowski and Sz Marteau-Ferey et al., 2020a, Vacher et al., 2021, Rudi et al., 2020, Muzellec et al., 2021]

## Dealing with an infinite number of constraints: an overview

$$
\bar{f} \in \operatorname{argmin}_{f \in \mathcal{H}_{k}} \mathcal{L}(f) \text { s.t. " } 0 \leq f(x), \forall x \in \mathcal{K}^{\prime \prime}, \mathcal{K} \subset \mathbb{R}^{d} \text { non-finite (compact) }
$$

## Relaxing

- Discretize constraint at "virtual" samples $\left\{\tilde{x}_{m}\right\}_{m \in[M]} \subset \mathcal{K}$, $\hookrightarrow$ no guarantees out-of-samples [Agrell, 2019, Takeuchi et al., 2006]
- Add constraint-inducing penalty, $R_{\text {cons }}(f)=-\lambda \int_{\mathcal{K}} \min (0, f(x)) \mathrm{d} x$ $\hookrightarrow$ no guarantees, changes the problem objective [Brault et al., 2019]
- Replace inequality by equality to nonnegative function $\Phi(x)^{\top} A \Phi(x)$ then discretize $\hookrightarrow$ generic: bounded amount of violation, extra SDP variable $A$ [Muzellec et al., 2021]


## Tightening

- Replace inequality by equality to nonnegative function $\Phi(x)^{\top} A \Phi(x)$ and optimize over $A$ $\hookrightarrow$ non-generic: only specific classes of functions [Marteau-Ferey et al., 2020b];
- Discretize but replace 0 by $\eta_{m}\|f\|$ [Aubin-Frankowski and Szabó, 2020a] $\hookrightarrow$ generic: no violation, second-order cone constraints, but extra tightening


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(1) Introduction to constrained problems
(2) Kernel methods for problem approximation
(3) Deriving bounds on the optimization error

## Our battle horse: the Reproducing kernel Hilbert space (RKHS)

A RKHS $\left(\mathcal{H}_{k},\langle\cdot, \cdot\rangle_{\mathcal{H}_{k}}\right)$ is a Hilbert space of real-valued functions over a set $\mathcal{X}$ if one of the following equivalent conditions is satisfied [Aronszajn, 1950]
$\exists k: X \times X \rightarrow \mathbb{R}$ s.t. $k_{x}(\cdot)=k(x, \cdot) \in \mathcal{H}_{k}$ and $f(x)=\left\langle f(\cdot), k_{x}(\cdot)\right\rangle_{\mathcal{H}_{k}}$ for all $x \in \mathcal{X}$ and $f \in \mathcal{H}_{k}$ (reproducing property)

$$
\left|f(x)-f_{n}(x)\right|=\left|\left\langle f-f_{n}, k_{x}\right\rangle_{k}\right| \leq\left\|f-f_{n}\right\|_{k}\left\|k_{x}\right\|_{k}=\left\|f-f_{n}\right\|_{k} \sqrt{k(x, x)}
$$

$k$ is s.t. $\exists \Phi_{k}: \mathcal{X} \rightarrow \mathcal{H}_{k}$ s.t. $k(x, y)=\left\langle\Phi_{k}(x), \Phi_{k}(y)\right\rangle_{\mathcal{H}_{k}}, \Phi_{k}(x)=k_{x}(\cdot)$
$k$ is s.t. $\mathbf{G}=\left[k\left(x_{i}, x_{j}\right)\right]_{i, j=1}^{n} \succcurlyeq 0$ and $\mathcal{H}_{k}:=\overline{\operatorname{span}\left(\left\{k_{x}(\cdot)\right\}_{x \in x}\right)}$, i.e. the completion for the pre-scalar product $\left\langle k_{x}(\cdot), k_{y}(\cdot)\right\rangle_{k, 0}=k(x, y)$

## Two essential tools for computations

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

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

$$
\bar{f} \in \underset{f \in \mathcal{H}_{k}}{\operatorname{argmin}} L\left(\left(f\left(x_{n}\right)\right)_{n \in[N]}\right)+\Omega\left(\|f\|_{k}\right)
$$

Then $\exists\left(a_{n}\right)_{n \in[N]} \in \mathbb{R}^{N}$ s.t. $\bar{f}(\cdot)=\sum_{n \in[N]} a_{n} k\left(\cdot, x_{n}\right)$
$\hookrightarrow$ Optimal solutions lie in a finite dimensional subspace of $\mathcal{H}_{k}$.
Finite number of evaluations $\Longrightarrow$ finite number of coefficients

## Kernel trick

$$
\left\langle\sum_{n \in[N]} a_{n} k\left(\cdot, x_{n}\right), \sum_{m \in[M]} b_{m} k\left(\cdot, y_{m}\right)\right\rangle_{\mathscr{H}_{k}}=\sum_{n \in[N]} \sum_{m \in[M]} a_{n} b_{m} k\left(x_{n}, y_{m}\right)
$$

$\hookrightarrow$ On this finite dimensional subspace, no need to know $\left(\mathcal{H}_{k},\langle\cdot, \cdot\rangle_{\mathcal{H}_{k}}\right)$.

## A nice class of nonnegative functions: kernel Sum-of-Squares/PSD models

How to build a nonnegative function given a kernel $\Phi_{k}(x)=k(\cdot, x)$ ? Square it!

$$
f: x \mapsto\left\langle\Phi_{k}(x), \Phi_{k}(x)\right\rangle_{\mathcal{H}_{k}}=k(x, x) \geq 0
$$

More generally take a positive semidefinite operator $A \in S^{+}\left(\mathcal{H}_{k}\right)$,

$$
\begin{gathered}
f_{A}: x \mapsto\left\langle\Phi_{k}(x), A \Phi_{k}(x)\right\rangle_{\mathcal{H}_{k}} \geq 0 \\
(\text { PSD model }) A=\sum_{i, j=1}^{N} a_{i j} \Phi_{k}\left(x_{i}\right) \otimes \Phi_{k}\left(x_{j}\right) \Longrightarrow f_{A}(x)=\sum_{i, j=1}^{N} a_{i j} k\left(x, x_{i}\right) k\left(x, x_{j}\right) \\
\text { (kernel SoS) }\left[a_{i j}\right]_{i, j}=\sum_{i} \mathbf{u}_{i} \mathbf{u}_{i}^{\top}(\text { SVD }) \Longrightarrow f_{A}(x)=\sum_{i=1}^{N}\left(\sum_{j=1}^{N} u_{i, j} k\left(x, x_{j}\right)\right)^{2}
\end{gathered}
$$

Note that in general $f_{A} \notin \mathcal{H}_{k}$ but $f_{A} \in \mathcal{H}_{k} \odot \mathcal{H}_{k}$ (Hadamard product). If $\operatorname{span}\left(\left\{k_{x}(\cdot)\right\}_{x \in X}\right)$ is dense in continuous functions, so are the $\left\{f_{A}\right\}_{A \in S^{+}\left(\mathcal{H}_{k}\right)}$ in nonnegative functions

## What I am looking for: an approximation framework

Example: optimizing over vector fields $\mathbf{f}: \mathbb{R}^{d} \rightarrow \mathbb{R}^{P}$ constrained over compact set $\mathcal{K}$ to belong to a set $\mathbf{F}(x)$

Optimization over $\mathcal{F} \stackrel{e . g}{=} \mathcal{C}(X, \mathbb{R})$ or $L(\mu)$

$$
\begin{aligned}
& \min _{\mathbf{f}=}^{\left[f_{1} ; \ldots ; f_{P}\right] \in \mathcal{F}^{P} \quad \int I(x, \mathbf{f}(x)) \mathrm{d} \mu(x)} \begin{array}{l}
\text { s.t. } \\
\mathbf{f}(x) \in \mathbf{F}(x), \forall x \in \mathcal{K}
\end{array}
\end{aligned}
$$

## What I am looking for: an approximation framework

Example: optimizing over vector fields $\mathbf{f}: \mathbb{R}^{d} \rightarrow \mathbb{R}^{P}$ constrained over compact set $\mathcal{K}$ to belong to a convex set $\mathbf{F}(x)$

Optimization over $\mathcal{F} \stackrel{e, g}{=} \mathcal{C}(X, \mathbb{R})$ or $L(\mu)$

$$
\min _{\mathbf{f}=\left[f_{1} ; \ldots ; f_{P}\right] \in \mathcal{F}^{P}} \int I(x, \mathbf{f}(x)) \mathrm{d} \mu(x)
$$

s.t.
$\mathbf{c}_{i}(x)^{\top} \mathbf{f}(x)+d_{i}(x) \geq 0, \forall i \in[I], \forall x \in \mathcal{K}$

Infinite number of affine constraints!

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Empirical approx. through RKHS $\mathcal{H}_{k}$

$$
\begin{aligned}
& \min _{\mathbf{f} \in \mathcal{H}_{k}^{P}} \sum_{n \in[N]} I\left(x_{n}, \mathbf{f}\left(x_{n}\right)\right)+\lambda\|\mathbf{f}\|_{\mathcal{H}_{k}^{P}}^{2} \\
& \quad \text { s.t. } \\
& \mathbf{c}_{i}\left(x_{m}\right)^{\top} \mathbf{f}\left(x_{m}\right)+d_{i}\left(x_{m}\right) \underset{=}{=} ?, \forall i \in[I], \forall m \in[M]
\end{aligned}
$$

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& \quad \text { s.t. } \\
& \mathbf{c}_{i}\left(x_{m}\right)^{\top} \mathbf{f}\left(x_{m}\right)+d_{i}\left(x_{m}\right) \underset{=}{=} ?, \forall i \in[I], \forall m \in[M]
\end{aligned}
$$

## Statement of simpler problem

Given points $\left(x_{n}\right)_{n \in[N]} \in X^{N}$, a loss $L: \mathbb{R}^{N} \rightarrow \mathbb{R} \cup\{\infty\}$, a regularizer $R: \mathbb{R}_{+} \rightarrow \mathbb{R}$, a RKHS $\mathcal{H}_{k}$ of smooth functions from $\mathcal{X}$ to $\mathbb{R}$ and a compact set $\mathcal{K} \subset \mathcal{X}$.

$$
\begin{aligned}
\bar{f}^{0} \in \underset{f \in \mathcal{H}_{k}}{\arg \min } & \mathcal{L}(f)=L\left(\left(f\left(x_{n}\right)\right)_{n \in[\mathcal{N}]}\right)+R\left(\|f\|_{\mathcal{H}_{k}}\right) \\
& \text { s.t. }
\end{aligned} \quad 0 \leq f(x), \quad \forall x \in \mathcal{K} . \quad .
$$

Idea to overcome non-finiteness: Discretize constraint at "virtual" samples $\left\{\tilde{x}_{m}\right\}_{m \in[M]} \subset \mathcal{K}$, use the fill distance: $h_{M}=\sup _{x \in \mathcal{K}} d\left(x,\left\{\tilde{x}_{m}\right\}_{m \in[M]}\right)$ to bound $\left|L\left(\overline{\mathbf{f}}^{\text {approx }}\right)-L\left(\overline{\mathbf{f}}^{0}\right)\right|$

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$$
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Second-order cone (SOC) tightening
[Aubin-Frankowski and Szabó, 2020a]

$$
\eta_{M}\|f\| \leq f\left(\tilde{x}_{m}\right)
$$

e.g. for $k(x, y)=\psi(x-y)$
$\eta_{M}:=\sqrt{\psi(0)-\psi\left(h_{M}\right)} \propto h_{M} \ll 1$
Tighten constraint by at most $C\|f\| \cdot h_{M}$

Semi-positive definite (SDP) relaxation [Rudi et al., 2020]

$$
\left\langle\Phi\left(\tilde{x}_{m}\right), A \Phi\left(\tilde{x}_{m}\right)\right\rangle_{k}=f\left(\tilde{x}_{m}\right)
$$

with extra variable $A \in S^{+}\left(\mathcal{H}_{k}\right)$
Relax by at most $C(\|f\|+\operatorname{Tr}(A)) \cdot\left(h_{M}\right)^{s}$ for $s$-smooth Sobolev spaces

## Deriving SOC constraints through continuity moduli

Take $\delta \geq 0$ and $x$ s.t. $\left\|x-\tilde{x}_{m}\right\| \leq \delta$

$$
\begin{aligned}
\left|f(x)-f\left(\tilde{x}_{m}\right)\right| & =\left|\left\langle f(\cdot), k(x, \cdot)-k\left(\tilde{x}_{m}, \cdot\right)\right\rangle_{k}\right| \\
& \leq\|f(\cdot)\|_{k} \underbrace{\sup _{\left\{x \mid\left\|x-\tilde{x}_{m}\right\| \leq \delta\right\}}\left\|k(x, \cdot)-k\left(\tilde{x}_{m}, \cdot\right)\right\|_{k}}_{\eta_{m}(\delta)} \\
\omega_{m}(f, \delta) & :=\sup _{\left\{x \mid\left\|x-\tilde{x}_{m}\right\| \leq \delta\right\}}\left|f(x)-f\left(\tilde{x}_{m}\right)\right| \leq \eta_{m}(\delta)\|f(\cdot)\|_{k}
\end{aligned}
$$

For a covering $\mathcal{K}=\bigcup_{m \in[M]} \mathbb{B}_{X}\left(\tilde{x}_{m}, \delta_{m}\right)$

$$
" 0 \leq f(x), \forall x \in \mathcal{K}^{\prime \prime} \Leftarrow " \omega_{m}(f, \delta) \leq f\left(\tilde{x}_{m}\right), \forall m \in[M] "
$$

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& \leq\|f(\cdot)\|_{k} \underbrace{\eta_{m}(\delta)}_{\sup _{\left\{x \mid\left\|x-\tilde{x}_{m}\right\| \leq \delta\right\}}\left\|k(x, \cdot)-k\left(\tilde{x}_{m}, \cdot\right)\right\|_{k}} \\
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\end{aligned}
$$

For a covering $\mathcal{K} \subset \bigcup_{m \in[M]} \mathbb{B}_{X}\left(\tilde{x}_{m}, \delta_{m}\right)$

$$
\begin{aligned}
" 0 \leq f(x), \forall x \in \mathcal{K}^{\prime \prime} & \Leftarrow " \omega_{m}(f, \delta) \leq f\left(\tilde{x}_{m}\right), \forall m \in[M] " \\
& \Leftarrow " \eta_{m}(\delta)\|f(\cdot)\| \leq f\left(\tilde{x}_{m}\right), \forall m \in[M]
\end{aligned}
$$

Since the kernel is smooth, $\delta \rightarrow 0$ gives $\eta_{m}(\delta) \rightarrow 0$.
There is also a geometrical interpretation for this choice of $\eta_{m}$.


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


Using the nonlinear embedding $\Phi: x \mapsto D_{x} k(x, \cdot)$, the idea is the same. With only the green points, it is a one-class SVM [Schölkopf et al., 2001b]


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


The image $\Phi(\mathcal{K})$ is not convex...


The image $\Phi(\mathcal{K})$ is not convex, can we cover it by balls of radius $\eta$ ?


First cover $\mathcal{K} \subset \bigcup\left\{\tilde{x}_{m}+\delta \mathbb{B}\right\}$, and then look at the images $\Phi\left(\left\{\tilde{x}_{m}+\delta \mathbb{B}\right\}\right)$


Cover the $\Phi\left(\left\{\tilde{x}_{m}+\delta \mathbb{B}\right\}\right)$ with tiny balls! This is how SOC was defined.


For SDP relaxation (a.k.a. kernel Sum-Of-Squares), it is rather like inflating an ellipsis...


For SDP relaxation (a.k.a. kernel Sum-Of-Squares), it is rather like inflating an ellipsis until it reaches all the points to interpolate


Second-order-cone (SOC) tightening Ball covering in the RKHS

Protecting the points from all sides, thus
"slower" convergence


Semi-positive definite (SDP) relaxation Kernel Sum-Of-Squares (kSOS)

Leverages smooth interpolation and relaxing, thus "faster" convergence

In both cases, SOC or SDP constraints instead of affine $\Longrightarrow$ extra computational price

## Nested constraint sets

Fill distance: $\quad h_{M}=\sup _{x \in \mathcal{K}} d\left(x,\left\{\tilde{x}_{m}\right\}_{m \in[M]}\right)$

$$
\begin{aligned}
\mathcal{V}_{-\epsilon} & :=\left\{f \in \mathcal{H}_{k} \mid f(x) \geq-\epsilon, \forall x \in \mathcal{K}\right\} \\
\mathcal{V}_{S D P} & :=\left\{f \in \mathcal{H}_{k} \mid \exists A \in S^{+}\left(\mathcal{H}_{k}\right), f\left(\tilde{x}_{m}\right)=\left\langle\Phi\left(\tilde{x}_{m}\right), A \Phi\left(\tilde{x}_{m}\right)\right\rangle_{k}, \forall m \in[M]\right\}, \\
\mathcal{V}_{0} & :=\left\{f \in \mathcal{H}_{k} \mid f(x) \geq 0, \forall x \in \mathcal{K}\right\}, \\
\mathcal{V}_{\text {SOC }} & :=\left\{f \in \mathcal{H}_{k} \mid f\left(\tilde{x}_{m}\right) \geq \eta_{M}\|f\|_{K}, \forall m \in[M]\right\}, \\
\mathcal{V}_{\epsilon} & :=\left\{f \in \mathcal{H}_{k} \mid f(x) \geq \epsilon, \forall x \in \mathcal{K}\right\} .
\end{aligned}
$$

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\mathcal{V}_{0} & :=\left\{f \in \mathcal{H}_{k} \mid f(x) \geq 0, \forall x \in \mathcal{K}\right\}, \\
\mathcal{V}_{S O C} & :=\left\{f \in \mathcal{H}_{k} \mid f\left(\tilde{x}_{m}\right) \geq \eta_{M}\|f\|_{K}, \forall m \in[M]\right\}, \\
\mathcal{V}_{\epsilon} & :=\left\{f \in \mathcal{H}_{k} \mid f(x) \geq \epsilon, \forall x \in \mathcal{K}\right\} .
\end{aligned}
$$

## Proposition (Informal nestedness)

Under some assumptions on the kernel (e.g. Sobolev), there exists explicit constants CsOC and $C_{S D P}$, such that for $h_{M}=\sup _{x \in \mathcal{K}} d\left(x,\left\{\tilde{x}_{m}\right\}_{m \in[M]}\right)$ and any $R \geq 0$

$$
\begin{aligned}
\epsilon \geq C_{S O C} \cdot R \cdot h_{M} & \Longrightarrow\left(\mathcal{V}_{\epsilon} \cap R \mathbb{B}_{k}\right) \subset \mathcal{V}_{S O C} \subset \mathcal{V}_{0} \\
\epsilon \geq C_{S D P} \cdot R \cdot\left(h_{M}\right)^{s} & \Longrightarrow\left(R \mathbb{B}_{k} \cap \mathcal{V}_{0}\right) \subset\left(R \mathbb{B}_{k} \cap \mathcal{V}_{S D P}\right) \subset \mathcal{V}_{-\epsilon}
\end{aligned}
$$

If $\mathcal{L}$ is $\beta$-Lipschitz, then $\left|\mathcal{L}\left(\bar{f}^{0}\right)-\mathcal{L}\left(\bar{f}{ }^{S O C}\right)\right| \leq \beta C_{S O C} \cdot R \cdot h_{M}$. If $\bar{f}^{0}$ has a quadratic expression, then $\left|\mathcal{L}\left(\bar{f}^{0}\right)-\mathcal{L}\left(\bar{f}^{S D P}\right)\right| \leq \beta C_{S D P} \cdot R \cdot\left(h_{M}\right)^{s}$

## Nested constraint sets - decreasing optima sequence



$$
\begin{aligned}
\mathcal{V}_{-\epsilon} & :=\left\{f \in \mathcal{H}_{k} \mid f(x) \geq-\epsilon, \forall x \in \mathcal{K}\right\} \\
\mathcal{V}_{S D P} & :=\left\{f \in \mathcal{H}_{k} \mid \exists A \in S^{+}\left(\mathcal{H}_{k}\right),\right. \\
& \left.f\left(\tilde{x}_{m}\right)=\left\langle\Phi\left(\tilde{x}_{m}\right), A \Phi\left(\tilde{x}_{m}\right)\right\rangle_{k}, \forall m \in[M]\right\}, \\
\mathcal{V}_{0} & :=\left\{f \in \mathcal{H}_{k} \mid f(x) \geq 0, \forall x \in \mathcal{K}\right\}, \\
\mathcal{V}_{S O C} & :=\left\{f \in \mathcal{H}_{k} \mid f\left(\tilde{x}_{m}\right) \geq \eta_{M}\|f\|_{K}, \forall m \in[M]\right\}, \\
\mathcal{V}_{\epsilon} & :=\left\{f \in \mathcal{H}_{k} \mid f(x) \geq \epsilon, \forall x \in \mathcal{K}\right\} .
\end{aligned}
$$

For $R \geq\left\|\bar{f}^{0}\right\|_{k}$, we have

$$
\mathcal{L}\left(\bar{f}^{-\epsilon}\right) \leq \mathcal{L}\left(\bar{f}_{R}^{S D P}\right) \leq \mathcal{L}\left(\bar{f}^{0}\right) \leq \mathcal{L}\left(\bar{f}^{S O C}\right) \leq \mathcal{L}\left(\bar{f}^{\epsilon}\right)
$$

## Nested constraint sets - decreasing optima sequence



$$
\mathcal{L}\left(\bar{f}^{-\epsilon}\right) \leq \mathcal{L}\left(\bar{f}_{R}^{S D P}\right) \leq \mathcal{L}\left(\bar{f}^{0}\right) \leq \mathcal{L}\left(\bar{f}^{S O C}\right) \leq \mathcal{L}\left(\bar{f}^{\epsilon}\right)
$$

Idea: find a $g_{\epsilon} \in \mathcal{H}_{k}$ such that $\left\|g_{\epsilon}\right\|_{k} \leq \omega(\epsilon)$ where $\omega: \mathbb{R}_{+} \rightarrow \mathbb{R}_{+} \nearrow$, and such that $\bar{f}^{-\epsilon}+g_{\epsilon} \in \mathcal{V}_{0}$, thus under some $\beta$-Lipschitz assumption on $\mathcal{L}$,

$$
\begin{aligned}
& \mathcal{L}\left(\bar{f}^{-\epsilon}\right) \leq \mathcal{L}\left(\bar{f}_{R}^{S D P}\right) \\
& \leq \mathcal{L}\left(\bar{f}^{0}\right) \\
& \leq \mathcal{L}\left(\bar{f}^{-\epsilon}+g_{\epsilon}\right) \\
& \leq \mathcal{L}\left(\bar{f}^{-\epsilon}\right)+\beta \omega(\epsilon) \\
& \text { SOC: } \epsilon \geq C_{S O C} \cdot R \cdot h_{M} \\
& \text { SDP } / \mathrm{kSoS}: \epsilon \approx C_{S D P} \cdot R \cdot\left(h_{M}\right)^{s}
\end{aligned}
$$

SOC: $\epsilon \geq C_{S O C} \cdot R \cdot h_{M}$

## Example 1: solving LQ control with state constraints through KRR

## Original control problem

$$
\begin{aligned}
& \min _{z(\cdot) \in W^{2,2}, u(\cdot) \in L^{2}} \quad \int_{0}^{1}|u(t)|^{2} \mathrm{~d} t \\
& \text { s.t. } \\
& z(0)=0, \quad \dot{z}(0)=0, \\
& \ddot{z}(t)=-\dot{z}(t)+u(t), \forall t \in[0,1] \\
& z(t) \in\left[z_{\text {low }}(t), z_{\text {up }}(t)\right], \forall t \in[0,1] .
\end{aligned}
$$



## Example 2: Estimation of monotone/convex production functions

Only 25 points selected out of 543 , checking generalization properties for various constraints (used as side information)

(a) NoCons

(b) SOC Monot.

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Figure: MSE as a function of incorporating shape constraints with the proposed SOC technique. NoCons: no constraint. SOC Monot.: two monotonicity constraints. SOC Conv.: one convexity constraint. SOC Conv.+Monot.: one convexity and two monotonicity constraints.
"Finite coverings in RKHSs can be used to turn an infinite number of pointwise affine constraints over a compact set into finitely many SOC inequality/SDP equality constraints."
"Bounding the constraint perturbation made by discretizing allows to easily assess rates of convergence."

## To go beyond

- Handle state constraint in LQ control through the LQ kernel
$\hookrightarrow$ PCAF, Linearly-constrained Linear Quadratic Regulator from the viewpoint of kernel methods, SIAM Journal on Control and Optimization, 2021
- Tackle SDP and derivative constraints with SOC constraints
$\hookrightarrow$ PCAF and Zoltán Szabó, Handling Hard Affine Shape Constraints in RKHSs, under review, 2021
- Use kernels for learning vector fields and nonlinear systems
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## Example 3: Joint Quantile Regression (JQR)


$f_{\tau}(x)$ conditional quantile over $(X, Y)$ : $\left.P\left(Y \leq f_{\tau}(x) \mid X=x\right)=\tau \in\right] 0,1[$.

Estimation through convex optimization over "pinball loss" $I_{\tau}(\cdot)$ (i.e. tilted absolute value [Koenker, 2005]).

Known fact: quantile functions can cross when estimated independently.

Joint quantile regression with non-crossing constraints

$$
\min _{\left(f_{q}\right)_{q \in\left[Q \in \in \mathcal{H}_{k}^{Q}\right.}} \mathcal{L}\left(f_{1}, \ldots, f_{Q}\right)=\frac{1}{N} \sum_{q \in[Q]} \sum_{n \in[N]} I_{\tau_{q}}\left(y_{n}-f_{q}\left(\mathbf{x}_{n}\right)\right)+\lambda_{f} \sum_{q \in[Q]}\left\|f_{q}\right\|_{k}^{2}
$$

## Pairing non-crossing quantiles with other shape constraints

Engel's law (1857): "As income rises, the proportion of income spent on food falls, but absolute expenditure on food rises."


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## Time-varying state-constrained LQ optimal control

$$
\begin{array}{ll}
\min _{\mathbf{x}(\cdot), \mathbf{u}(\cdot)} & \chi_{\mathbf{x}_{0}}\left(\mathbf{x}\left(t_{0}\right)\right)+g(\mathbf{x}(T)) \\
+\mathbf{x}\left(t_{r e f}\right)^{\top} \mathbf{J}_{r e f} \mathbf{x}\left(t_{r e f}\right)+\int_{t_{0}}^{T}\left[\mathbf{x}(t)^{\top} \mathbf{Q}(t) \mathbf{x}(t)+\mathbf{u}(t)^{\top} \mathbf{R}(t) \mathbf{u}(t)\right] \mathrm{d} t \\
\text { s.t. } & \mathbf{x}^{\prime}(t)=\mathbf{A}(t) \mathbf{x}(t)+\mathbf{B}(t) \mathbf{u}(t), \text { a.e. in }\left[t_{0}, T\right], \\
& \mathbf{c}_{i}(t)^{\top} \mathbf{x}(t) \leq d_{i}(t), \forall t \in \mathcal{T}_{c}, \forall i \in[\mathcal{I}]=\llbracket 1, \mathcal{I} \rrbracket,
\end{array}
$$

- state $\mathbf{x}(t) \in \mathbb{R}^{Q}$, control $\mathbf{u}(t) \in \mathbb{R}^{P}$,
- reference time $t_{r e f} \in\left[t_{0}, T\right]$, set of constraint times $\mathcal{T}_{c} \subset\left[t_{0}, T\right]$,
- $\mathbf{x}(\cdot):\left[t_{0}, T\right] \rightarrow \mathbb{R}^{Q}$ absolutely continuous, $\mathbf{R}(\cdot)^{1 / 2} \mathbf{u}(\cdot) \in L^{2}\left(\left[t_{0}, T\right]\right)$


## Time-varying state-constrained $L Q$ optimal control

$$
\begin{array}{cll}
\min _{\mathbf{x}(\cdot), \mathbf{u}(\cdot)} & \chi_{\mathbf{x}_{0}}\left(\mathbf{x}\left(t_{0}\right)\right)+g(\mathbf{x}(T)) & \rightarrow L\left(\mathbf{x}\left(t_{j}\right)_{j \in[J]}\right) \\
+\mathbf{x}\left(t_{r e f}\right)^{\top} \mathbf{J}_{r e f} \mathbf{x}\left(t_{r e f}\right)+\int_{t_{0}}^{T}\left[\mathbf{x}(t)^{\top} \mathbf{Q}(t) \mathbf{x}(t)+\mathbf{u}(t)^{\top} \mathbf{R}(t) \mathbf{u}(t)\right] \mathrm{d} t & \rightarrow\|\mathbf{x}(\cdot)\|_{\mathcal{S}}^{2} \\
\text { s.t. } & \mathbf{x}^{\prime}(t)=\mathbf{A}(t) \mathbf{x}(t)+\mathbf{B}(t) \mathbf{u}(t), \text { a.e. in }\left[t_{0}, T\right] \\
& \mathbf{c}_{i}(t)^{\top} \mathbf{x}(t) \leq d_{i}(t), \forall t \in \mathcal{T}_{c}, \forall i \in[\mathcal{I}]=\llbracket 1, \mathcal{I} \rrbracket
\end{array}
$$

- state $\mathbf{x}(t) \in \mathbb{R}^{Q}$, control $\mathbf{u}(t) \in \mathbb{R}^{P}$,
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$$
\mathcal{S}:=\left\{\mathbf{x}:\left[t_{0}, T\right] \rightarrow \mathbb{R}^{Q} \mid \exists \mathbf{R}(\cdot)^{1 / 2} \mathbf{u}(\cdot) \in L^{2}\left(t_{0}, T\right) \text { s.t. } \mathbf{x}^{\prime}(t)=\mathbf{A}(t) \mathbf{x}(t)+\mathbf{B}(t) \mathbf{u}(t) \text { a.e. }\right\}
$$

Given $\mathbf{x}(\cdot) \in \mathcal{S}$, for the pseudoinverse $\mathbf{B}(t)^{\ominus}$ for $\|\cdot\|_{\mathbf{R}}$, set $\mathbf{u}(t) \stackrel{\text { a.e. }}{=} \mathbf{B}(t)^{\ominus}\left[\mathbf{x}^{\prime}(t)-\mathbf{A}(t) \mathbf{x}(t)\right]$. $\left(\mathcal{S},\langle\cdot, \cdot\rangle_{\mathcal{S}}\right)$ is a (vector-valued) RKHS with an explicit kernel [Aubin-Frankowski, 2021]!

## Optimal control: constrained pendulum - definition

Constrained pendulum when controlling the third derivative of the angle

$$
\begin{gathered}
\underbrace{x(0)=0.5, \quad \dot{x}(0)=0, \quad w(0)=0, \quad x(T / 3)=0.5, \quad x(T)=0}_{\min _{x(\cdot), w(\cdot), u(\cdot)}-\dot{x}(T)+\lambda\|u(\cdot)\|_{L^{2}(0, T)}^{2} \quad \lambda \ll 1} \\
\underbrace{}_{\substack{\ddot{x}(t)=-10 x(t)+w(t), \quad \dot{w}(t)=u(t), \text { a.e. in }[0, T] \\
\dot{x}(t) \in[-3,+\infty[, \quad w(t) \in[-10,10], \forall t \in[0, T]}}
\end{gathered}
$$

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x(0)=0.5, \quad \dot{x}(0)=0, \quad w(0)=0, \quad x(T / 3)=0.5, \quad x(T)=0 \\
\dot{\ddot{x}(t)=-10 x(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], \forall t \in[0, T]
\end{gathered}
$$

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

$$
\begin{aligned}
\eta_{\dot{x}}\|\mathbf{x}(\cdot)\|_{K}-\dot{x}\left(t_{m}\right) & \leq 3 \\
\eta_{w}\|\mathbf{x}(\cdot)\|_{K}+w\left(t_{m}\right) & \leq 10 \\
\eta_{w}\|\mathbf{x}(\cdot)\|_{K}-w\left(t_{m}\right) & \leq 10
\end{aligned}
$$

$$
\begin{aligned}
& \overline{\mathbf{x}}(\cdot)=K(\cdot, 0) \mathbf{p}_{0}+K(\cdot, T / 3) \mathbf{p}_{T / 3} \\
& \quad+K(\cdot, T) \mathbf{p}_{T}+\sum_{m=1}^{M} K\left(\cdot, t_{m}\right) \mathbf{p}_{m}
\end{aligned}
$$

Most of computational cost is related to the "controllability Gramians" $K_{1}(s, t)=\int_{0}^{\min (s, t)} \mathbf{e}^{(s-\tau) \mathbf{A}} \mathbf{B} \mathbf{B}^{\top} \mathbf{e}^{(t-\tau) \mathbf{A}^{\top}} \mathrm{d} \tau$ which we have to approximate.

## Optimal control: constrained pendulum - illustration

Optimal solutions of the constrained pendulum "path-planning" problem. Red circles: equality constraints. Grayed areas: constraints over [0, T]., Angle $x(\cdot) \quad$ Velocity $\dot{x}(\cdot) \quad$ Couple $w(\cdot)$




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