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" $x(t) \in [x_{low}, x_{high}]$
- "abide by the speed limit" $x'(t) \in [v_{low}, v_{high}]$
- "do not stress the pilot" x" $(t) \in [a_{low}, a_{high}]$

Physical constraints

 $\stackrel{\hookrightarrow}{\rightarrow} \text{ provides feasible trajectories in} \\ \text{ path-planning}$

This consists in an infinite number of pointwise constraints!

Examples of constraints in function optimization - 2



Shape constraints

- nonnegativity $f(x) \ge 0$
- directional monotonicity $\partial_i f(x) \ge 0$
- directional convexity $\partial_{i,i}^2 f(x) \ge 0$

Side information/Requirements

 $\hookrightarrow \mbox{ compensates small number of samples} \\ \mbox{ or excessive noise }$

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:

 $\max_{\substack{c \in \mathbb{R} \\ c \ge g(x), \forall x \in \mathcal{X}}} c \qquad (= \min_{x \in \mathcal{X}} g(x))$

• Density estimation with relative entropy:

$$\min_{\substack{f \in \mathcal{C}(\mathcal{X},\mathbb{R}), \int_{\mathcal{X}} f(x) dx = 1 \\ f(x) \ge 0, \forall x \in \mathcal{X}}} - \int_{\mathcal{X}} \log(f(x)) d\mu(x) \qquad (= \mathsf{KL}(\mu, \mu_f) + \mathsf{cst})$$

• Optimal transport in its dual formulation:

$$\max_{\substack{u,v\in C(\mathfrak{X},\mathbb{R})\\ u(x)+v(y)\leq c(x,y), \forall x,y\in\mathfrak{X}\times\mathfrak{X}}} \int_{\mathfrak{X}} u(x) \mathrm{d}\mu(x) + \int_{\mathfrak{X}} v(y) \mathrm{d}\nu(y) \qquad (=\mathsf{OT}_{c}(\mu,\nu))$$

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] 4/28

Dealing with an infinite number of constraints: an overview

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

Relaxing

- Discretize constraint at "virtual" samples $\{\tilde{x}_m\}_{m \in [M]} \subset \mathcal{K}$, \hookrightarrow no guarantees out-of-samples [Agrell, 2019, Takeuchi et al., 2006]
- Add constraint-inducing penalty, R_{cons}(f) = −λ ∫_K min(0, f(x))dx
 → no guarantees, changes the problem objective [Brault et al., 2019]
- Replace inequality by equality to nonnegative function Φ(x)^TAΦ(x) then <u>discretize</u>
 → generic: bounded amount of violation, extra SDP variable A [Muzellec et al., 2021]

Tightening

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

- 1 Introduction to constrained problems
- 2 Kernel methods for problem approximation
- Oeriving bounds on the optimization error

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

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

 $\exists k : \mathfrak{X} \times \mathfrak{X} \to \mathbb{R} \text{ s.t. } k_x(\cdot) = k(x, \cdot) \in \mathfrak{H}_k \text{ and } f(x) = \langle f(\cdot), k_x(\cdot) \rangle_{\mathfrak{H}_k} \text{ for all } x \in \mathfrak{X} \text{ and } f \in \mathfrak{H}_k \text{ (reproducing property)}$

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

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

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

Two essential tools for computations

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

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

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

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

 \hookrightarrow Optimal solutions lie in a finite dimensional subspace of \mathcal{H}_k .

Finite number of evaluations \implies finite number of coefficients

Kernel trick

$$\langle \sum_{n \in [N]} a_n k(\cdot, x_n), \sum_{m \in [M]} b_m k(\cdot, y_m) \rangle_{\mathfrak{H}_k} = \sum_{n \in [N]} \sum_{m \in [M]} a_n b_m k(x_n, y_m)$$

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

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!

$$f:x\mapsto \langle \Phi_k(x),\Phi_k(x)
angle_{\mathcal{H}_k}=k(x,x)\geq 0$$

More generally take a positive semidefinite operator $A \in S^+(\mathfrak{H}_k)$,

$$f_{A}: x \mapsto \langle \Phi_{k}(x), A\Phi_{k}(x) \rangle_{\mathcal{H}_{k}} \geq 0$$

(PSD model) $A = \sum_{i,j=1}^{N} a_{ij} \Phi_{k}(x_{i}) \otimes \Phi_{k}(x_{j}) \implies f_{A}(x) = \sum_{i,j=1}^{N} a_{ij}k(x,x_{i})k(x,x_{j})$
(kernel SoS) $[a_{ij}]_{i,j} = \sum_{i} \mathbf{u}_{i} \mathbf{u}_{i}^{\top}$ (SVD) $\implies f_{A}(x) = \sum_{i=1}^{N} (\sum_{i=1}^{N} u_{i,j}k(x,x_{j}))^{2}$

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

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

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

$$\begin{split} \min_{\substack{\mathbf{f} = [f_1; \ldots; f_P] \in \mathcal{F}^P \\ \text{ s.t. }}} & \int l(x, \mathbf{f}(x)) d\mu(x) \\ \text{ s.t. } \\ \mathbf{f}(x) \in \mathbf{F}(x), \, \forall x \in \mathcal{K} \end{split}$$

What I am looking for: an approximation framework

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

Optimization over $\mathcal{F} \stackrel{e.g}{=} \mathcal{C}(\mathcal{X}, \mathbb{R})$ or $L(\mu)$ $\mathbf{f} = [f_1; \dots; f_P] \in \mathcal{F}^P \qquad \int l(x, \mathbf{f}(x)) d\mu(x)$ s.t. $\mathbf{c}_i(x)^\top \mathbf{f}(x) + d_i(x) \ge 0, \forall i \in [I], \forall x \in \mathcal{K}$

Infinite number of affine constraints!

What I am looking for: an approximation framework

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Optimization over $\mathfrak{F}\stackrel{e.g}{=}\mathcal{C}(\mathfrak{X},\mathbb{R})$ or $L(\mu)$	Empirical approx. through RKHS \mathfrak{H}_k
$ \begin{split} \min_{ \mathbf{f} = [f_1; \dots; f_P] \in \mathcal{F}^P } & \int l(x, \mathbf{f}(x)) \mathrm{d} \mu(x) \\ & \text{s.t.} \end{split} $	$ \min_{\mathbf{f} \in \mathcal{H}_{k}^{P}} \sum_{n \in [N]} I(x_{n}, \mathbf{f}(x_{n})) + \lambda \ \mathbf{f}\ _{\mathcal{H}_{k}^{P}}^{2} $ s.t.
$\mathbf{c}_i(x)^{ op}\mathbf{f}(x) + d_i(x) \ge 0, \forall i \in [I], \forall x \in \mathcal{K}$	$\mathbf{c}_i(x_m)^{\top}\mathbf{f}(x_m) + d_i(x_m) \stackrel{\geq}{=} ?, \forall i \in [I], \forall m \in [M]$
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Infinite number of affine constraints!	Finite number of constraints for $\{x_m\}_m \subset \mathcal{K}!$

Statement of simpler problem

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

$$ar{f}^0 \in \mathop{\mathrm{arg\ min}}_{f \in \mathcal{H}_k} \mathcal{L}(f) = L\left((f(x_n))_{n \in [N]}\right) + R\left(\|f\|_{\mathcal{H}_k}
ight)$$

s.t. $0 \leq f(x), \quad \forall x \in \mathcal{K}.$

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

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$$ar{f}^0 \in \mathop{\mathrm{arg\ min}}_{f \in \mathcal{H}_k} \mathcal{L}(f) = L\left(\left(f(x_n)\right)_{n \in [N]}\right) + R\left(\|f\|_{\mathcal{H}_k}
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Second-order cone (SOC) tightening [Aubin-Frankowski and Szabó, 2020a]	Semi-positive definite (SDP) relaxation [Rudi et al., 2020]
$\eta_{\mathcal{M}}\ f\ \leq f(\tilde{x}_m)$	$\langle \Phi(\tilde{x}_m), A \Phi(\tilde{x}_m) \rangle_k = f(\tilde{x}_m)$
e.g. for $k(x, y) = \psi(x - y)$	with extra variable ${oldsymbol A}\in S^+({{\mathfrak H}_k})$
$\eta_{\mathcal{M}} := \sqrt{\psi(0) - \psi(h_{\mathcal{M}})} \propto h_{\mathcal{M}} \ll 1$	Relax by at most $C(f + \operatorname{Tr}(A)) \cdot (h_M)^s$ for
Tighten constraint by at most $C \ f\ \cdot h_M$	s-smooth Sobolev spaces

Deriving SOC constraints through continuity moduli

Take $\delta \ge 0$ and x s.t. $||x - \tilde{x}_m|| \le \delta$ $|f(x) - f(\tilde{x}_m)| = |\langle f(\cdot), k(x, \cdot) - k(\tilde{x}_m, \cdot) \rangle_k|$ $\le ||f(\cdot)||_k \sup_{\substack{\{x \mid ||x - \tilde{x}_m|| \le \delta\}}} ||k(x, \cdot) - k(\tilde{x}_m, \cdot)||_k}{\eta_m(\delta)}$ $\omega_m(f, \delta) := \sup_{\{x \mid ||x - \tilde{x}_m|| \le \delta\}} |f(x) - f(\tilde{x}_m)| \le \eta_m(\delta) ||f(\cdot)||_k}$ For a covering $\mathcal{K} = \bigcup_{m \in [M]} \mathbb{B}_{\mathcal{X}}(\tilde{x}_m, \delta_m)$

" $0 \leq f(x), \forall x \in \mathcal{K}$ " \Leftarrow " $\omega_m(f, \delta) \leq f(\tilde{x}_m), \forall m \in [M]$ "

Deriving SOC constraints through continuity moduli

Take $\delta \ge 0$ and x s.t. $||x - \tilde{x}_m|| \le \delta$ $|f(x) - f(\tilde{x}_m)| = |\langle f(\cdot), k(x, \cdot) - k(\tilde{x}_m, \cdot) \rangle_k|$ $\le ||f(\cdot)||_k \sup_{\substack{\{x \mid ||x - \tilde{x}_m|| \le \delta\}}} ||k(x, \cdot) - k(\tilde{x}_m, \cdot)||_k}{\eta_m(\delta)}$ $\omega_m(f, \delta) := \sup_{\{x \mid ||x - \tilde{x}_m|| \le \delta\}} |f(x) - f(\tilde{x}_m)| \le \eta_m(\delta) ||f(\cdot)||_k}$

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

$$"0 \le f(x), \, \forall x \in \mathcal{K}" \Leftarrow "\omega_m(f, \delta) \le f(\tilde{x}_m), \, \forall m \in [M]" \\ \Leftarrow "\eta_m(\delta) \| f(\cdot) \| \le f(\tilde{x}_m), \, \forall m \in [M]$$

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 $\Phi : x \mapsto D_x k(x, \cdot)$, the idea is the same. With only the green points, it is a one-class SVM [Schölkopf et al., 2001b] 13/28



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



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



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



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



Cover the $\Phi({\tilde{x}_m + \delta \mathbb{B}})$ 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 \implies extra computational price

Nested constraint sets

$$\begin{array}{ll} \text{Fill distance:} & h_{M} = \sup_{x \in \mathcal{K}} d(x, \{\tilde{x}_{m}\}_{m \in [M]}) \\ \mathcal{V}_{-\epsilon} := \{f \in \mathcal{H}_{k} \, | \, f(x) \geq -\epsilon, \, \forall \, x \in \mathcal{K} \} \\ \mathcal{V}_{SDP} := \{f \in \mathcal{H}_{k} \, | \, \exists A \in S^{+}(\mathcal{H}_{k}), \, f(\tilde{x}_{m}) = \langle \Phi(\tilde{x}_{m}), A \Phi(\tilde{x}_{m}) \rangle_{k}, \, \forall \, m \in [M] \}, \\ \mathcal{V}_{0} := \{f \in \mathcal{H}_{k} \, | \, f(x) \geq 0, \, \forall \, x \in \mathcal{K} \}, \\ \mathcal{V}_{SOC} := \{f \in \mathcal{H}_{k} \, | \, f(\tilde{x}_{m}) \geq \eta_{M} \| f \|_{K}, \, \forall \, m \in [M] \}, \\ \mathcal{V}_{\epsilon} := \{f \in \mathcal{H}_{k} \, | \, f(x) \geq \epsilon, \, \forall \, x \in \mathcal{K} \}. \end{array}$$

Nested constraint sets

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Proposition (Informal nestedness)

Under some assumptions on the kernel (e.g. Sobolev), there exists explicit constants C_{SOC} and C_{SDP} , such that for $h_M = \sup_{x \in \mathcal{K}} d(x, \{\tilde{x}_m\}_{m \in [M]})$ and any $R \ge 0$ $\epsilon \ge C_{SOC} \cdot R \cdot h_M \implies (\mathcal{V}_{\epsilon} \cap R\mathbb{B}_k) \subset \mathcal{V}_{SOC} \subset \mathcal{V}_0$ $\epsilon \ge C_{SDP} \cdot R \cdot (h_M)^s \implies (R\mathbb{B}_k \cap \mathcal{V}_0) \subset (R\mathbb{B}_k \cap \mathcal{V}_{SDP}) \subset \mathcal{V}_{-\epsilon}$ If \mathcal{L} is β -Lipschitz, then $|\mathcal{L}(\bar{f}^0) - \mathcal{L}(\bar{f}^{SOC})| \le \beta C_{SOC} \cdot R \cdot h_M$. If \bar{f}^0 has a quadratic expression, then $|\mathcal{L}(\bar{f}^0) - \mathcal{L}(\bar{f}^{SDP})| < \beta C_{SDP} \cdot R \cdot (h_M)^s$

Nested constraint sets - decreasing optima sequence



$$\begin{split} \mathcal{V}_{-\epsilon} &:= \{ f \in \mathcal{H}_k \,|\, f(x) \geq -\epsilon, \,\forall \, x \in \mathcal{K} \} \\ \mathcal{V}_{SDP} &:= \{ f \in \mathcal{H}_k \,|\, \exists A \in S^+(\mathcal{H}_k), \\ f(\tilde{x}_m) &= \langle \Phi(\tilde{x}_m), A \Phi(\tilde{x}_m) \rangle_k, \,\forall \, m \in [M] \}, \\ \mathcal{V}_0 &:= \{ f \in \mathcal{H}_k \,|\, f(x) \geq 0, \,\forall \, x \in \mathcal{K} \}, \\ \mathcal{V}_{SOC} &:= \{ f \in \mathcal{H}_k \,|\, f(\tilde{x}_m) \geq \eta_M \|f\|_{\mathcal{K}}, \,\forall \, m \in [M] \}, \\ \mathcal{V}_\epsilon &:= \{ f \in \mathcal{H}_k \,|\, f(x) \geq \epsilon, \,\forall \, x \in \mathcal{K} \}. \\ & \text{For } R \geq \|\bar{f}^0\|_k, \,\text{we have} \\ \mathcal{L}(\bar{f}^{-\epsilon}) \leq \mathcal{L}(\bar{f}_R^{SDP}) \leq \mathcal{L}(\bar{f}^0) \leq \mathcal{L}(\bar{f}^{SOC}) \leq \mathcal{L}(\bar{f}^\epsilon) \end{split}$$

Nested constraint sets - decreasing optima sequence



$$\mathcal{L}(\bar{f}^{-\epsilon}) \leq \mathcal{L}(\bar{f}^{SDP}_{R}) \leq \mathcal{L}(\bar{f}^{0}) \leq \mathcal{L}(\bar{f}^{SOC}) \leq \mathcal{L}(\bar{f}^{\epsilon})$$

Idea: find a $g_{\epsilon} \in \mathcal{H}_k$ such that $||g_{\epsilon}||_k \leq \omega(\epsilon)$ where $\omega : \mathbb{R}_+ \to \mathbb{R}_+ \nearrow$, and such that $\overline{f}^{-\epsilon} + g_{\epsilon} \in \mathcal{V}_0$, thus under some β -Lipschitz assumption on \mathcal{L} ,

$$\begin{split} \mathcal{L}(\bar{f}^{-\epsilon}) &\leq \mathcal{L}(\bar{f}_{R}^{SDP}) \\ &\leq \mathcal{L}(\bar{f}^{0}) \\ &\leq \mathcal{L}(\bar{f}^{-\epsilon} + g_{\epsilon}) \\ &\leq \mathcal{L}(\bar{f}^{-\epsilon}) + \beta \omega(\epsilon). \end{split}$$

$$\begin{split} \mathsf{SOC:} \ \epsilon &\geq C_{SOC} \cdot R \cdot h_{M} \\ \mathsf{SDP}/\mathsf{kSoS:} \ \epsilon &\approx C_{SDP} \cdot R \cdot (h_{M})^{s} \end{split}$$

Example 1: solving LQ control with state constraints through KRR



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)



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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
 - $\hookrightarrow \mathsf{Coming} \text{ in soon!}$

More to be found on https://pcaubin.github.io/

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Thank you for your attention!

Example 3: 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

$$\min_{f_q)_{q\in[Q]}\in\mathcal{H}_k^Q} \mathcal{L}\left(f_1,\ldots,f_Q\right) = \frac{1}{N} \sum_{q\in[Q]} \sum_{n\in[N]} l_{\tau_q}\left(y_n - f_q(\mathbf{x}_n)\right) + \lambda_f \sum_{q\in[Q]} \|f_q\|_k^2$$









Time-varying state-constrained LQ optimal control

$$\begin{split} \min_{\mathbf{x}(\cdot),\mathbf{u}(\cdot)} \quad & \chi_{\mathbf{x}_0}(\mathbf{x}(t_0)) + g(\mathbf{x}(\mathcal{T})) \\ + \mathbf{x}(t_{ref})^\top \mathbf{J}_{ref} \mathbf{x}(t_{ref}) + \int_{t_0}^{\mathcal{T}} \left[\mathbf{x}(t)^\top \mathbf{Q}(t) \mathbf{x}(t) + \mathbf{u}(t)^\top \mathbf{R}(t) \mathbf{u}(t) \right] \mathrm{d}t \\ \text{s.t.} \quad & \mathbf{x}'(t) = \mathbf{A}(t) \mathbf{x}(t) + \mathbf{B}(t) \mathbf{u}(t), \text{ a.e. in } [t_0, \mathcal{T}], \\ & \mathbf{c}_i(t)^\top \mathbf{x}(t) \le d_i(t), \forall t \in \mathcal{T}_c, \forall i \in [\mathcal{I}] = \llbracket 1, \mathcal{I} \rrbracket, \end{split}$$

- state $\mathbf{x}(t) \in \mathbb{R}^Q$, control $\mathbf{u}(t) \in \mathbb{R}^P$,
- reference time $t_{ref} \in [t_0, T]$, set of constraint times $\mathfrak{T}_c \subset [t_0, T]$,
- $\mathbf{x}(\cdot): [t_0, T] \to \mathbb{R}^Q$ absolutely continuous, $\mathbf{R}(\cdot)^{1/2} \mathbf{u}(\cdot) \in L^2([t_0, T])$

Time-varying state-constrained LQ optimal control

$$\begin{split} \min_{\mathbf{x}(\cdot),\mathbf{u}(\cdot)} \quad &\chi_{\mathbf{x}_{0}}(\mathbf{x}(t_{0})) + g(\mathbf{x}(\mathcal{T})) \qquad \rightarrow \mathcal{L}(\mathbf{x}(t_{j})_{j\in[\mathcal{I}]}) \\ + \mathbf{x}(t_{ref})^{\top} \mathbf{J}_{ref} \mathbf{x}(t_{ref}) + \int_{t_{0}}^{\mathcal{T}} \left[\mathbf{x}(t)^{\top} \mathbf{Q}(t) \mathbf{x}(t) + \mathbf{u}(t)^{\top} \mathbf{R}(t) \mathbf{u}(t) \right] \mathrm{d}t \qquad \rightarrow \|\mathbf{x}(\cdot)\|_{\mathcal{S}}^{2} \\ \text{s.t.} \quad \mathbf{x}'(t) = \mathbf{A}(t) \mathbf{x}(t) + \mathbf{B}(t) \mathbf{u}(t), \text{ a.e. in } [t_{0}, \mathcal{T}], \\ \mathbf{c}_{i}(t)^{\top} \mathbf{x}(t) \leq d_{i}(t), \forall t \in \mathcal{T}_{c}, \forall i \in [\mathcal{I}] = \llbracket 1, \mathcal{I} \rrbracket, \end{split}$$

- state $\mathbf{x}(t) \in \mathbb{R}^Q$, control $\mathbf{u}(t) \in \mathbb{R}^P$,
- reference time $t_{ref} \in [t_0, T]$, set of constraint times $\mathfrak{T}_c \subset [t_0, T]$,
- $\mathbf{x}(\cdot) : [t_0, T] \to \mathbb{R}^Q$ absolutely continuous, $\mathbf{R}(\cdot)^{1/2} \mathbf{u}(\cdot) \in L^2([t_0, T])$

 $\mathcal{S} := \{ \mathbf{x} : [t_0, \mathcal{T}] \to \mathbb{R}^Q \, | \, \exists \, \mathbf{R}(\cdot)^{1/2} \mathbf{u}(\cdot) \in L^2(t_0, \mathcal{T}) \text{ s.t. } \mathbf{x}'(t) = \mathbf{A}(t) \mathbf{x}(t) + \mathbf{B}(t) \mathbf{u}(t) \text{ a.e. } \}$

Given $\mathbf{x}(\cdot) \in S$, for the pseudoinverse $\mathbf{B}(t)^{\ominus}$ for $\|\cdot\|_{\mathbf{R}}$, set $\mathbf{u}(t) \stackrel{\text{a.e.}}{=} \mathbf{B}(t)^{\ominus}[\mathbf{x}'(t) - \mathbf{A}(t)\mathbf{x}(t)]$. ($S, \langle \cdot, \cdot \rangle_{S}$) 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

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$$\begin{array}{c} \min_{x(\cdot),w(\cdot),u(\cdot)} -\dot{x}(T) + \lambda \| u(\cdot) \|_{L^{2}(0,T)}^{2} & \lambda \ll 1 \\ \hline x(0) = 0.5, \quad \dot{x}(0) = 0, \quad w(0) = 0, \quad x(T/3) = 0.5, \quad x(T) = 0 \\ \hline \dot{x}(t) = -10 \, x(t) + w(t), \quad \dot{w}(t) = u(t), \text{ a.e. in } [0,T] \\ \hline \dot{x}(t) \in [-3, +\infty[, \quad w(t) \in [-10, 10], \forall t \in [0,T]] \\ \hline & & \downarrow \\ \hline & & \downarrow \\ &$$

Optimal control: constrained pendulum - definition

Constrained pendulum when controlling the third derivative of the angle

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

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

Most of computational cost is related to the "controllability Gramians" $K_1(s, t) = \int_0^{\min(s,t)} \mathbf{e}^{(s-\tau)\mathbf{A}} \mathbf{B} \mathbf{B}^\top \mathbf{e}^{(t-\tau)\mathbf{A}^\top} d\tau$ which we have to approximate.







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