Kernel Machines with Hard Shape Constraints

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Joint work with: Pierre-Cyril Aubin-Frankowski @ MINES ParisTech

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3. convexity: $\boxed{0 \leq f''(x)}$,
4. n-monotonicity: $\boxed{0 \leq f^{(n)}(x)}$,
5. $(n-1)$-alternating monotonicity: for $n \geq 2$

$$\boxed{(-1)^j f^{(j)}} : \boxed{\geq 0}, \boxed{\nearrow} \text{ and } \boxed{\text{convex}} \ \forall j \in [\![0, n-2]\!].$$

Example: generator of a d-variate Archimedean copula is $(d-2)$-alternating monotone.

Examples continued

6. Monotonicity w.r.t. partial ordering ($\mathrm{u} \preccurlyeq \mathrm{v} \Rightarrow f(\mathrm{u}) \leq f(\mathrm{v})$):

$\mathrm{u} \preccurlyeq \mathrm{v}$ iff

- $u_i \leq v_i$ ($\forall i$; product ordering),
- $\sum_{j \in [i]} u_j \leq \sum_{j \in [i]} v_j$ ($\forall i$; unordered weak majorization).

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7. Supermodularity:

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

i.e. $f(\mathrm{u} \vee \mathrm{v}) + f(\mathrm{u} \wedge \mathrm{v}) \geq f(\mathrm{u}) + f(\mathrm{v})$ for all $\mathrm{u}, \mathrm{v} \in \mathbb{R}^d$.

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- Biology (monotone regression): identify genome interactions [Luss et al., 2012], dose-response studies [Hu et al., 2005].

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- Supply chain models, stochastic multi-period inventory problems, pricing models and game theory: supermodularity [Topkis, 1998, Simchi-Levi et al., 2014].

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Towards flexible $\mathcal{H}$-s . . .

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- In $\mathbb{R}^d$: $\langle \mathrm{x}, \mathrm{x}' \rangle = \sum_{i \in [d]} x_i x_i' \Rightarrow \left\| \mathrm{x} - \mathrm{x}' \right\|_2$ and $\sphericalangle\left(\mathrm{x}, \mathrm{x}'\right)$.

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$\langle \mathbf{x}, \mathbf{x}' \rangle^d = \langle \varphi(\mathbf{x}), \varphi(\mathbf{x}') \rangle$: $\varphi(\mathbf{x}) = d$-order polynomial. $\Rightarrow$ Explicit computation would be heavy!

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$$k(\cdot, x) \in \mathcal{H}, \qquad f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}}.$$

Constructively, $\mathcal{H}_k = \overline{\left\{\sum_{i=1}^n \alpha_i k(\cdot, x_i) \,:\, n \in \mathbb{N}, x_i \in \mathcal{X}\right\}}$.

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- All these definitions are equivalent, $k \overset{1:1}{\leftrightarrow} \mathcal{H}_k$.
- Included: Fourier analysis, polynomials, splines, ...

Kernel examples on $\mathbb{R}^d$ ($\gamma, \sigma, v > 0$, $c \geq 0$, $p \in \mathbb{Z}^+$)

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Or the flexible Matérn family:

$$k_M(\mathrm{x},\mathrm{y}) = \frac{2^{1-v}}{\Gamma(v)}\left(\frac{\sqrt{2v}\,\|\mathrm{x}-\mathrm{y}\|_2}{\sigma}\right)^v K_v\left(\frac{\sqrt{2v}\,\|\mathrm{x}-\mathrm{y}\|_2}{\sigma}\right),$$

where

- K_v: modified Bessel function of the second kind of order v,
- Specific cases: For $v = \frac{1}{2}$ one gets $k(\mathrm{x},\mathrm{y}) = e^{-\frac{\|\mathrm{x}-\mathrm{y}\|_2}{\sigma}}$.
  Gaussian kernel: $v \to \infty$.

Kernels on other domains ($\mathcal{X}$)

- Strings [Watkins, 1999, Lodhi et al., 2002, Leslie et al., 2002, Kuang et al., 2004, Leslie and Kuang, 2004, Saigo et al., 2004, Cuturi and Vert, 2005],
- time series [Rüping, 2001, Cuturi et al., 2007, Cuturi, 2011, Király and Oberhauser, 2019],
- trees [Collins and Duffy, 2001, Kashima and Koyanagi, 2002],
- groups and specifically rankings [Cuturi et al., 2005, Jiao and Vert, 2016],
- sets [Haussler, 1999, Gärtner et al., 2002],
- various generative models [Jaakkola and Haussler, 1999, Tsuda et al., 2002, Seeger, 2002, Jebara et al., 2004],
- fuzzy domains [Guevara et al., 2017], or
- graphs [Kondor and Lafferty, 2002, Gärtner et al., 2003, Kashima et al., 2003, Borgwardt and Kriegel, 2005, Shervashidze et al., 2009, Vishwanathan et al., 2010, Kondor and Pan, 2016, Bai et al., 2020].

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   - encode probability measures injectively [Fukumizu et al., 2008, Sriperumbudur et al., 2010]

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   - characterize independence of random variables [Bach and Jordan, 2002, Blanchard et al., 2011, Gretton, 2015, Szabó and Sriperumbudur, 2018].

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3. Computationally tractable: $k(x_i, x_j)$.
4. Hilbert structure $\Rightarrow$ statistical analysis.

Why kernel and RKHSs?

1. Numerous data types.
2. RKHS can
   - be dense in various function spaces [Steinwart, 2001, Micchelli et al., 2006, Sriperumbudur et al., 2011, Simon-Gabriel and Schölkopf, 2018],
   - encode probability measures injectively [Fukumizu et al., 2008, Sriperumbudur et al., 2010]

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3. Computationally tractable: $k(x_i, x_j)$.
4. Hilbert structure $\Rightarrow$ statistical analysis.
5. Vector-valued RKHSs [Pedrick, 1957, Micchelli and Pontil, 2005, Carmeli et al., 2006].

Task-1: joint quantile regression (JQR)

- Given: $(\tau_q)_{q\in[Q]} \subset (0,1)$ levels $\nearrow$, $\{(\mathrm{x}_n, y_n)\}_{n\in[N]}$ samples.
- Estimate jointly the τ_q-quantiles of $\mathbb{P}(Y|X=\mathrm{x})$.

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- Objective:

$$\mathcal{L}(\mathrm{f},\mathrm{b}) = \frac{1}{N}\sum_{q\in[Q]}\sum_{n\in[N]} l_{\tau_q}\left(y_n - [f_q(\mathrm{x}_n) + b_q]\right) + \lambda_{\mathrm{b}}\|\mathrm{b}\|_2^2 + \lambda_f \sum_{q\in[Q]} \|f_q\|_k^2,$$

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Constraints

function values (f_q) with interaction $(f_{q+1} - f_q)$, bias terms (b_q) with interaction $(b_q - b_{q+1})$.

Task-2: convoy localization, one vehicle ($Q = 1$)

- Given: noisy time-location samples $\{(t_n, x_n)\}_{n\in[N]} \subset \underbrace{[0, T]}_{=:\mathcal{T}} \times \mathbb{R}$.
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$$\begin{aligned}
&\min_{b \in \mathbb{R}, f \in \mathcal{H}_k} \left[\frac{1}{N} \sum_{n\in[N]} |x_n - (b + f(t_n))|^2 + \lambda \|f\|^2_{\mathcal{H}_k} \right] \\
&\text{s.t.} \\
&v_{\min} \le f'(t), \quad \forall t \in \mathcal{T}.
\end{aligned}$$

Task-2b: convoy localization, multiple vehicles ($Q \geq 1$)

- Data: $\left\{ (t_{q,n}, x_{q,n})_{n \in [N_q]} \right\}_{q \in [Q]} \subseteq \mathcal{T} \times \mathbb{R}$.
- Constraints: speed ($v_{\min}$), inter-vehicular distance ($d_{\min}$).
- Objective:

$$\min_{\substack{f_1,\ldots,f_Q \in \mathcal{H}_k, \\ b_1,\ldots,b_Q \in \mathbb{R}}} \frac{1}{Q} \sum_{q=1}^{Q} \left[\left(\frac{1}{N_q} \sum_{n=1}^{N_q} |x_{q,n} - (b_q + f_q(t_{q,n}))|^2 \right) + \lambda \|f_q\|_{\mathcal{H}_k}^2 \right]$$

s.t.

$$d_{\min} + b_{q+1} + f_{q+1}(t) \leq b_q + f_q(t), \forall q \in [Q-1], \; t \in \mathcal{T},$$

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Constraints

function values (f_q) and derivatives (f_q') with interaction ($f_q - f_{q+1}$), bias terms (b_q) with interaction ($b_{q+1} - b_q$).

Task-3: safety-critical control

- Trajectory of an underwater vehicle:

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- Initial condition: $z(0) = 0$ and $\dot{z}(0) = 0$.
- Control task (LQ = linear dynamics & quadratic cost):

$$\begin{aligned} &\min_{u \in L^2(\mathcal{T},\mathbb{R})} \quad \int_{\mathcal{T}} |u(t)|^2 \mathrm{d}t \\ &\text{s.t.} \\ &z(0) = 0, \quad \dot{z}(0) = 0, \\ &\ddot{z}(t) = -\dot{z}(t) + u(t), \, \forall t \in \mathcal{T}, \\ &z_{\text{low}}(t) \leq z(t) \leq z_{\text{up}}(t), \, \forall \, t \in \mathcal{T}. \end{aligned}$$

Task-3: safety-critical control – continued

- With full state $\mathsf{f}(t) := [z(t); \dot{z}(t)] \in \mathbb{R}^2$

$$\dot{\mathsf{f}}(t) = \mathsf{A}\mathsf{f}(t) + \mathsf{B}u(t), \quad \mathsf{f}(0) = 0, \quad \mathsf{A} = \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix} \in \mathbb{R}^{2\times 2}, \quad \mathsf{B} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \in \mathbb{R}^2$$

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- The controlled trajectories f belong to a $\mathbb{R}^2$-valued RKHS with kernel

$$k(s,t) := \int_0^{\min(s,t)} e^{(s-\tau)\mathsf{A}}\mathsf{B}\mathsf{B}^\top e^{(t-\tau)\mathsf{A}^\top} \mathrm{d}\tau, \quad s,t \in \mathcal{T},$$

and the task is

$$\begin{aligned} \min_{\mathsf{f}=[f_1;f_2]\in\mathcal{H}_k} \quad & \|\mathsf{f}\|_k^2 \\ \text{s.t.} \quad & \\ z_{\mathrm{low}}(t) \le f_1(t) \le z_{\mathrm{up}}(t),\ & \forall\, t \in \mathcal{T}. \end{aligned}$$

Task-3: safety-critical control – finished

- Assume for simplicity: z_{low} and z_{up} are piece-wise constant.
- Task:

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Constraints

linear transformation of functions (f_1), with matrix-valued kernel.

Our task

$$(\bar{\mathrm{f}}, \bar{\mathrm{b}}) = \mathop{\arg\min}_{\substack{\mathrm{f}=(f_q)_{q\in[Q]} \in (\mathcal{H}_k)^Q, \\ \mathrm{b}=(b_q)_{q\in[Q]} \in \mathcal{B}, \\ (\mathrm{f},\mathrm{b}) \in C}} \mathcal{L}(\mathrm{f}, \mathrm{b}),$$

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$$C = \{(\mathrm{f}, \mathrm{b}) \,|\, (\mathrm{b}_0 - \mathrm{U}\mathrm{b})_i \leq D_i(\mathrm{W}\mathrm{f} - \mathrm{f}_0)_i(\mathrm{x}), \quad \forall \mathrm{x} \in K_i, \forall i \in [I]\},$$

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$$(\mathrm{W}\mathrm{f})_i = \sum_{q\in[Q]} W_{i,q} f_q,$$

$$D_i = \sum_{j\in[n_{i,j}]} \gamma_{i,j} \partial^{\mathrm{r}_{i,j}},\ |\mathrm{r}_{i,j}| \le s,\ \gamma_{i,j} \in \mathbb{R},\ \partial^{\mathrm{r}} f(\mathrm{x}) = \frac{\partial^{|\mathrm{r}|} f(\mathrm{x})}{\partial^{r_1}_{x_1} \cdots \partial^{r_d}_{x_d}}.$$

Blanket assumptions

1. Domain $\mathcal{X} \subseteq \mathbb{R}^d$: open. Kernel $k \in \mathcal{C}^s(\mathcal{X} \times \mathcal{X})$.
2. $K_i \subset \mathcal{X}$: compact, $\forall i$.
3. $\mathrm{f}_{0,i} \in \mathcal{H}_k$ for $\forall i$.
4. Bias domain $\mathcal{B} \subseteq \mathbb{R}^Q$: convex.
5. Loss L restricted to $\mathcal{B}$: strictly convex in b.
6. Regularizer Ω: strictly increasing in each of its argument.

Our strenghtened SOC-constrained formulation

$$(\mathsf{f}_{\boldsymbol{\eta}}, \mathsf{b}_{\boldsymbol{\eta}}) = \underset{\mathsf{f} \in (\mathcal{H}_k)^Q,\, \mathsf{b} \in \mathcal{B}}{\arg\min} \quad \mathcal{L}(\mathsf{f}, \mathsf{b}) \qquad (\mathcal{P}_{\boldsymbol{\eta}})$$

$$\text{s.t.}$$

$$(\mathsf{b}_0 - \mathsf{U}\mathsf{b})_i + \eta_i \|(\mathsf{W}\mathsf{f} - \mathsf{f}_0)_i\|_{\mathcal{H}_k} \leq \min_{m \in [M_i]} D_i(\mathsf{W}\mathsf{f} - \mathsf{f}_0)_i\left(\tilde{\mathsf{x}}_{i,m}\right), \ \forall i \in [I], \qquad (\mathcal{C}_{\boldsymbol{\eta}})$$

where

- $\{\tilde{\mathsf{x}}_{i,m}\}_{m \in [M_i]}$: a δ_i-net of K_i in $\|\cdot\|_{\mathcal{X}}$,
- $\eta_i = \sup_{m \in [M_i], \mathsf{u} \in \mathbb{B}_{\|\cdot\|_{\mathcal{X}}}(0,1)} \|D_{i,\mathsf{x}} k(\tilde{\mathsf{x}}_{i,m}, \cdot) - D_{i,\mathsf{x}} k(\tilde{\mathsf{x}}_{i,m} + \delta_i \mathsf{u}, \cdot)\|_{\mathcal{H}_k}$.

Theorem

- Minimal values: v_{disc} = value of $(\mathcal{P}_{\boldsymbol{\eta}})$ with '$\boldsymbol{\eta} = 0$', $\bar{v} = \mathcal{L}\left(\bar{\mathrm{f}}, \bar{\mathrm{b}}\right)$, $v_{\boldsymbol{\eta}} = \mathcal{L}\left(\mathrm{f}_{\boldsymbol{\eta}}, \mathrm{b}_{\boldsymbol{\eta}}\right)$.
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- Let $\mathrm{f}_{\boldsymbol{\eta}} = \left(f_{\boldsymbol{\eta},q}\right)_{q \in [Q]}$.

Then,

- (i) Tightening: any (f, b) satisfying $(\mathcal{C}_{\boldsymbol{\eta}})$ also satisfies $(\mathcal{C})$, hence

$$v_{\text{disc}} \leq \bar{v} \leq v_{\boldsymbol{\eta}}.$$

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- (ii) Representer theorem: For $\forall q \in [Q]$, $\exists \tilde{a}_{i,0,q}, \tilde{a}_{i,m,q}, a_{n,q} \in \mathbb{R}$ s.t.

$$f_{\boldsymbol{\eta},q} = \sum_{i\in[I]} \left[\tilde{a}_{i,0,q} f_{0,i} + \sum_{m\in[M_i]} \tilde{a}_{i,m,q} D_{i,\mathrm{x}} k\left(\tilde{\mathrm{x}}_{i,m}, \cdot\right)\right] + \sum_{n\in[N]} a_{n,q} k(\mathrm{x}_n, \cdot).$$

Theorem – continued

- (iii) Performance guarantee: if $\mathcal{L}$ is $(\mu_{f_q}, \mu_{\mathrm{b}})$-strongly convex w.r.t. (f_q, b) for any $q \in [Q]$, then

$$\|f_{\boldsymbol{\eta},q} - \bar{f}_q\|_{\mathcal{H}_k} \leq \sqrt{\frac{2(v_{\boldsymbol{\eta}} - v_{\mathrm{disc}})}{\mu_{f_q}}}, \quad \|\mathrm{b}_{\boldsymbol{\eta}} - \bar{\mathrm{b}}\|_2 \leq \sqrt{\frac{2(v_{\boldsymbol{\eta}} - v_{\mathrm{disc}})}{\mu_{\mathrm{b}}}}.$$

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If in addition U is surjective, $\mathcal{B} = \mathbb{R}^Q$, and $\mathcal{L}(\bar{\mathrm{f}}, \cdot)$ is L_b–Lipschitz continuous on $\mathbb{B}_{\|\cdot\|_2}\left(\bar{\mathrm{b}}, c_f\|\boldsymbol{\eta}\|_\infty\right)$ where $c_f \;=\; \sqrt{d}\left\|\left(\mathrm{U}^T\mathrm{U}\right)^{-1}\mathrm{U}^T\right\| \max_{i\in[I]} \left\|(\mathrm{W}\bar{\mathrm{f}} - \mathrm{f}_0)_i\right\|_{\mathcal{H}_k}$, then

$$\|f_{\boldsymbol{\eta},q} - \bar{f}_q\|_{\mathcal{H}_k} \leq \sqrt{\frac{2L_b c_f\|\boldsymbol{\eta}\|_\infty}{\mu_{f_q}}}, \|\mathrm{b}_{\boldsymbol{\eta}} - \bar{\mathrm{b}}\|_2 \leq \sqrt{\frac{2L_b c_f\|\boldsymbol{\eta}\|_\infty}{\mu_{\mathrm{b}}}}.$$

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1st bound: computable. 2nd: Larger $M_i \Rightarrow$ smaller $\delta_i \Rightarrow$ smaller η_i $\Rightarrow$ tighter bound.

Tightening idea

Let $s = 0$, $l = 1$. Recall constraint $(\mathcal{C})$:

$$\left\{(\mathrm{f}, \mathrm{b}) \mid \underbrace{(b_0 - \mathrm{Ub})}_{\beta} \leq \underbrace{\underbrace{(\mathrm{Wf} - f_0)}_{\phi}(\mathrm{x})}_{\langle \phi, k(\mathrm{x}, \cdot) \rangle_{\mathcal{H}_k}}, \quad \forall \mathrm{x} \in K\right\}$$

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$$\boxed{\Phi(K)} := \{k(\mathrm{x},\cdot) : \mathrm{x} \in K\} \boxed{\subseteq H^+_{\phi,\beta}} := \Big\{g \in \mathcal{H}_k \,|\, \beta \le \langle \phi, g\rangle_{\mathcal{H}_k}\Big\}$$

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Let $s = 0$, $l = 1$. Recall constraint $(\mathcal{C})$:

$$\Big\{(\mathrm{f}, \mathrm{b}) \mid \underbrace{(b_0 - \mathrm{Ub})}_{\beta} \leq \underbrace{\underbrace{(\mathrm{Wf} - f_0)}_{\phi}(\mathrm{x})}_{\langle \phi, k(\mathrm{x}, \cdot)\rangle_{\mathcal{H}_k}}, \quad \forall \mathrm{x} \in K\Big\}, \text{ i.e.}$$

$$\boxed{\Phi(K)} := \{k(\mathrm{x}, \cdot) : \mathrm{x} \in K\} \boxed{\subseteq H^{+}_{\phi,\beta}} := \Big\{g \in \mathcal{H}_k \mid \beta \leq \langle \phi, g\rangle_{\mathcal{H}_k}\Big\}$$

- $(\mathcal{C}_{\boldsymbol{\eta}})$ means: covering of $\Phi(K)$ by balls with η-radius centered at the $k(\tilde{\mathrm{x}}_m, \cdot)$ is in the halfspace $H^{+}_{\phi,\beta}$; hence it is tightening.

Tightening idea

Let $s = 0$, $l = 1$. Recall constraint $(\mathcal{C})$:

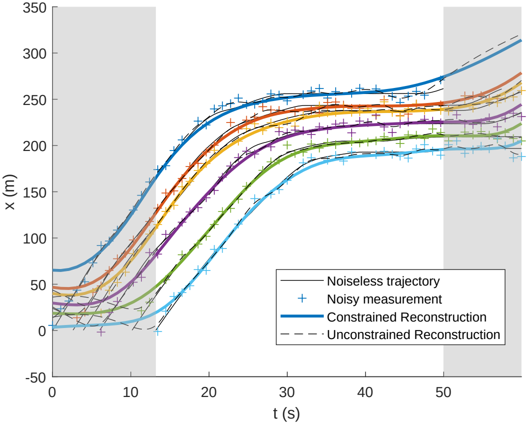
$$\Big\{(\mathrm{f},\mathrm{b}) \,|\, \underbrace{(b_0 - \mathrm{Ub})}_{\beta} \le \underbrace{\underbrace{({\color{red}\mathrm{Wf}} - f_0)}_{\phi}(\mathrm{x})}_{\langle \phi, k(\mathrm{x},\cdot)\rangle_{\mathcal{H}_k}}, \quad \forall \mathrm{x} \in K\Big\}, \text{i.e.}$$

$$\boxed{\Phi(K)} := \{k(\mathrm{x},\cdot) : \mathrm{x} \in K\} \boxed{\subseteq H^+_{\phi,\beta}} := \Big\{g \in \mathcal{H}_k \,|\, \beta \le \langle \phi, g\rangle_{\mathcal{H}_k}\Big\}$$

- $(\mathcal{C}_{\boldsymbol{\eta}})$ means: covering of $\Phi(K)$ by balls with η-radius centered at the $k(\tilde{\mathrm{x}}_m, \cdot)$ is in the halfspace $H^+_{\phi,\beta}$; hence it is tightening.
- η is obtained as the minimal radius.

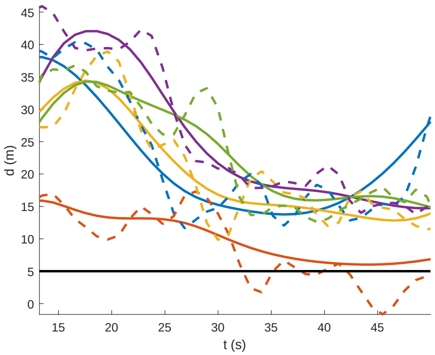
Demo (task-1): convoy localization with traffic jam

Setting: $Q = 6$, $d_{\min} = 5m$, $v_{\min} = 0$.



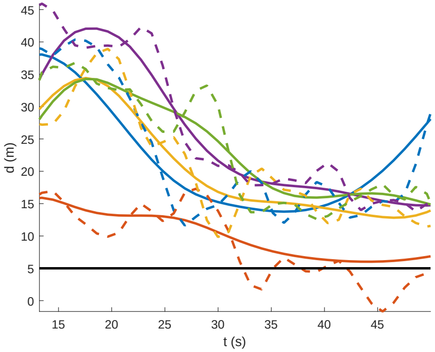
Demo (task-1): continued

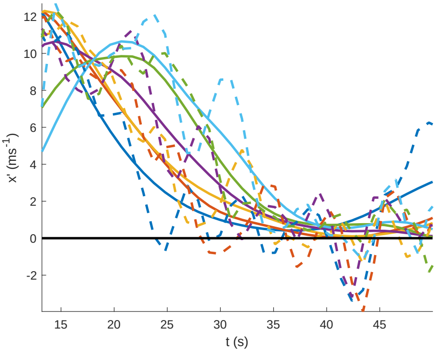
Pairwise distances: $t \mapsto f_q(t) - f_{q+1}(t)$



Demo (task-1): continued

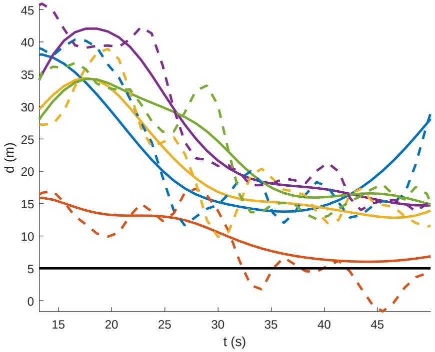
Pairwise distances: $t \mapsto f_q(t) - f_{q+1}(t)$ Speed: $t \mapsto f'_q(t)$

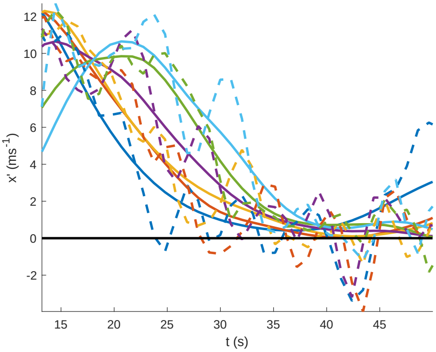




Demo (task-1): continued

Pairwise distances: $t \mapsto f_q(t) - f_{q+1}(t)$ Speed: $t \mapsto f_q'(t)$



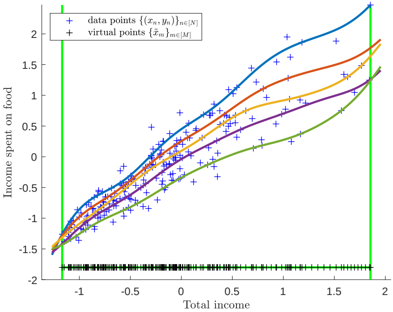


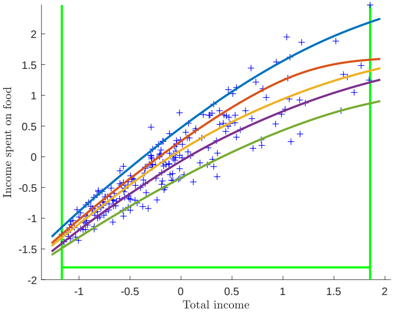
Shape constraints: especially relevant in noisy situations.

Demo (task-2): joint quantile regression

Economics :

- x: annual household income, y: food expenditure. $d = 1$, $N = 235$.
- Engel's law $\Rightarrow \nearrow$, concave.
- Demo: $\tau_q \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$.
- Left: non-crossing, $\nearrow$. Right: non-crossing, $\nearrow$, concave.

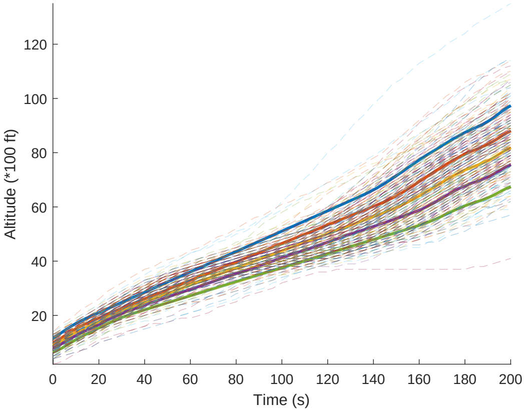




Demo (task-2): joint quantile regression

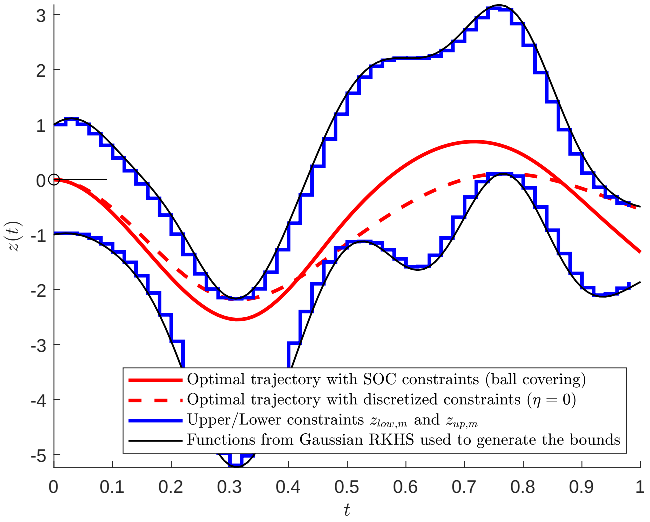
Analysis of aircraft trajectories, ENAC:

- y: radar-measured altitude of aircrafts flying between two cities (Paris & Toulouse); x: time. $d = 1$, $N = 15657$.
- Demo: $\tau_q \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$.
- Constraint: non-crossing, $\nearrow$ (takeoff).



Demo (task-3): control of underwater vehicle

Vs discretization-based approach (which might crash):



Summary

- Focus: hard affine shape constraints on derivatives & RKHS.
- Proposed framework: SOC-based tightening.
- Applications:
  - convoy localization,
  - joint quantile regression: economics, aircraft trajectories,
  - safety-critical control.

References & acknowledgements

Details:

- Transportation systems [Aubin-Frankowski et al., 2020],
- Control aspect [Aubin-Frankowski, 2020],
- Method [Aubin-Frankowski and Szabó, 2020], extension [under preparation to JMLR]. Code @ GitHub.

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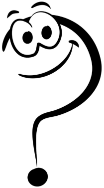

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