

# Shape-Constrained Kernel Machines

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

$$(-1)^j f^{(j)} : \geq 0, \nearrow \text{ and } \text{convex} \quad \forall j \in \llbracket 0, n-2 \rrbracket.$$

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

- ⑥ Monotonicity w.r.t. partial ordering ( $u \preceq v \Rightarrow f(u) \leq f(v)$ ):

$u \preceq v$  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).



## Examples continued

- ⑥ Monotonicity w.r.t. partial ordering ( $u \preceq v \Rightarrow f(u) \leq f(v)$ ):

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

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

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- 7 Supermodularity:

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

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

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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  $\mathbb{R}^d$ :  $\langle \mathbf{x}, \mathbf{x}' \rangle = \sum_{i \in [d]} x_i x'_i \Rightarrow \|\mathbf{x} - \mathbf{x}'\|_2$  and  $\angle(\mathbf{x}, \mathbf{x}')$ .

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- Nonlinear features ( $d = 2$ ):

$$\varphi(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2),$$

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Explicit computation would be heavy!

# Kernel, RKHS: definition

- Def-1 (feature space):  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  kernel if

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- Def-4 (reproducing kernel):

$$k(\cdot, x) := [x' \mapsto k(x', x)] \in \mathcal{H}, \quad f(x) = \langle f, k(\cdot, x) \rangle_{\mathcal{H}}.$$

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

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

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

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$$k_C(x, y) = \frac{1}{1 + \gamma \|x - y\|_2^2},$$

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Or the flexible Matérn family:

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

where

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

## 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, Borgwardt et al., 2020].

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[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]

$$\mathbb{P} \mapsto \int_{\mathcal{X}} \varphi(x) d\mathbb{P}(x) \in \mathcal{H}_k,$$

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

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- ➌ Computationally tractable:  $k(x_i, x_j)$ .

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[Bach and Jordan, 2002, Blanchard et al., 2011, Gretton, 2015, Szabó and Sriperumbudur, 2018].
- 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:  $k(x_i, x_j)$ .
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  - 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  $\nearrow$ ,  $\{(x_n, y_n)\}_{n \in [N]}$  samples.
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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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$$\min_{b \in \mathbb{R}, f \in \mathcal{H}_k} \left[ \frac{1}{N} \sum_{n \in [N]} |x_n - (b + f(t_n))|^2 + \lambda \|f\|_{\mathcal{H}_k}^2 \right]$$

s.t.

$$v_{\min} \leq f'(t), \quad \forall t \in \mathcal{T}.$$

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

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

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

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



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

$$\min_{u \in L^2(\mathcal{T}, \mathbb{R})} \int_{\mathcal{T}} |u(t)|^2 dt$$

s.t.

$$z(0) = 0, \quad \dot{z}(0) = 0,$$

$$\ddot{z}(t) = -\dot{z}(t) + u(t), \quad \forall t \in \mathcal{T},$$

$$z_{\text{low}}(t) \leq z(t) \leq z_{\text{up}}(t), \quad \forall t \in \mathcal{T}.$$

## Task-3: safety-critical control – continued

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

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

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

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

and the task is

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

## Task-3: safety-critical control – finished

- Assume for simplicity:  $z_{\text{low}}$  and  $z_{\text{up}}$  are piece-wise constant.
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$$\min_{f=[f_1;f_2]\in\mathcal{H}_k} \|f\|_k^2$$

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### Constraints

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

# Our task

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

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

# 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  $f_{0,i} \in \mathcal{H}_k$  for  $\forall i$ .
- 4 Bias domain  $\mathcal{B} \subseteq \mathbb{R}^Q$ : convex.
- 5 Loss  $L$  restricted to  $\mathcal{B}$ : strictly convex in  $\mathbf{b}$ .
- 6 Regularizer  $\Omega$ : strictly increasing in each of its argument.

# Our strengthened SOC-constrained formulation

$$(f_\eta, b_\eta) = \arg \min_{f \in (\mathcal{H}_k)^Q, b \in \mathcal{B}} \mathcal{L}(f, b) \quad (\mathcal{P}_\eta)$$

s.t.

$$\begin{aligned} & (b_0 - Ub)_i + \eta_i \|(Wf - f_0)_i\|_{\mathcal{H}_k} \\ & \leq \min_{m \in [M_i]} D_i(Wf - f_0)_i(\tilde{x}_{i,m}), \forall i \in [I], \end{aligned} \quad (\mathcal{C}_\eta)$$

where

- $\{\tilde{x}_{i,m}\}_{m \in [M_i]}$ : a  $\delta_i$ -net of  $K_i$  in  $\|\cdot\|_{\mathcal{X}}$ ,
- $\eta_i = \sup_{m \in [M_i], u \in \mathbb{B}_{\|\cdot\|_{\mathcal{X}}}(0,1)} \|D_{i,x}k(\tilde{x}_{i,m}, \cdot) - D_{i,x}k(\tilde{x}_{i,m} + \delta_i u, \cdot)\|_{\mathcal{H}_k}$ ,
- $D_{i,x}k(x_0, \cdot) := y \mapsto D_i(x \mapsto k(x, y))(x_0)$ .



# Theorem

- Minimal values:  $v_{\text{disc}} = \text{value of } (\mathcal{P}_\eta) \text{ with } '\eta = 0', \bar{v} = \mathcal{L}(\bar{f}, \bar{b}),$   
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Then,

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

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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.

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

## Theorem – continued

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

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

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

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

# Tightening idea

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

$$\{(f, b) \mid \underbrace{(b_0 - Ub)}_{\beta} \leq \underbrace{(\textcolor{red}{W}f - f_0)}_{\phi}(x), \quad \forall x \in K\}$$

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



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

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

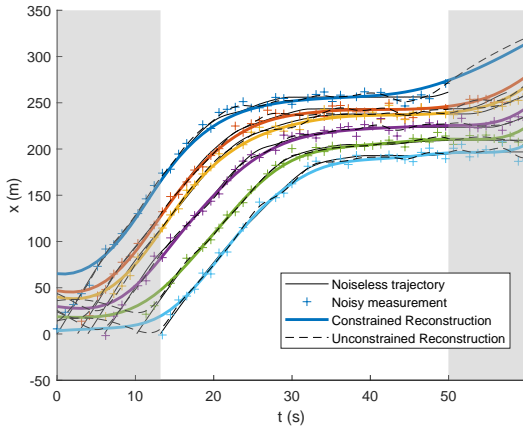
$$\{(f, b) \mid \underbrace{(b_0 - Ub)}_{\beta} \leq \underbrace{(\text{Wf} - f_0)(x)}_{\phi}, \quad \forall x \in K\}, \text{ i.e.}$$
$$\underbrace{\hspace{10em}}_{\langle \phi, k(x, \cdot) \rangle_{\mathcal{H}_k}}$$

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

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

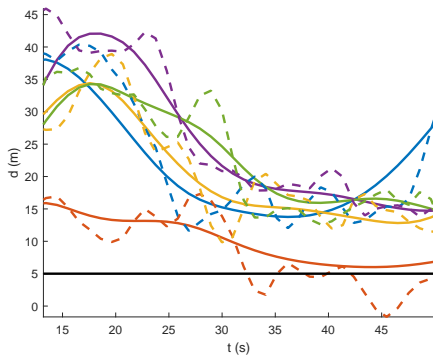
# Demo (task-1): convoy localization with traffic jam

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



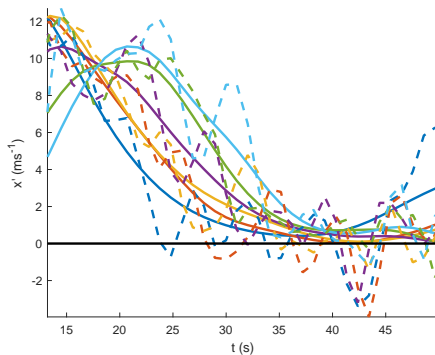
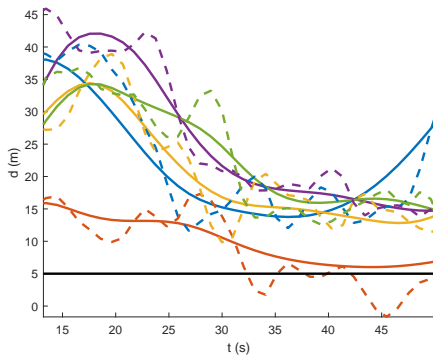
# Demo (task-1): continued

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



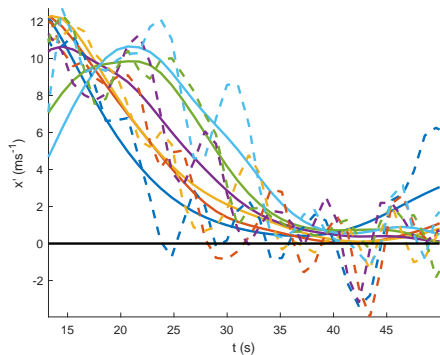
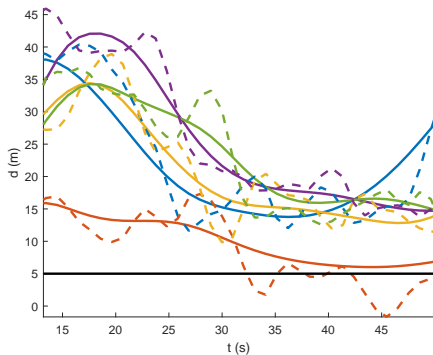
# Demo (task-1): continued

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:  $t \mapsto f'_q(t)$



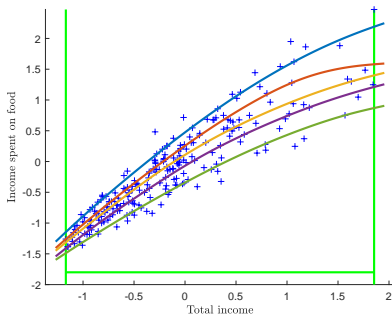
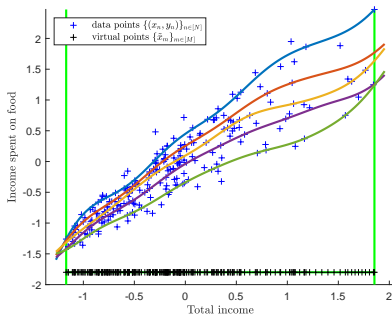
Shape constraints: especially relevant in **noisy** situations.

# 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,  $\nearrow$ .

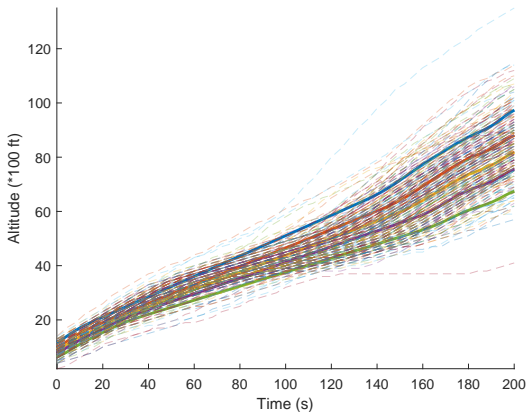
Right: non-crossing,  $\nearrow$ , concave.



# Demo (task-2): joint quantile regression

## Analysis of aircraft trajectories, ENAC:

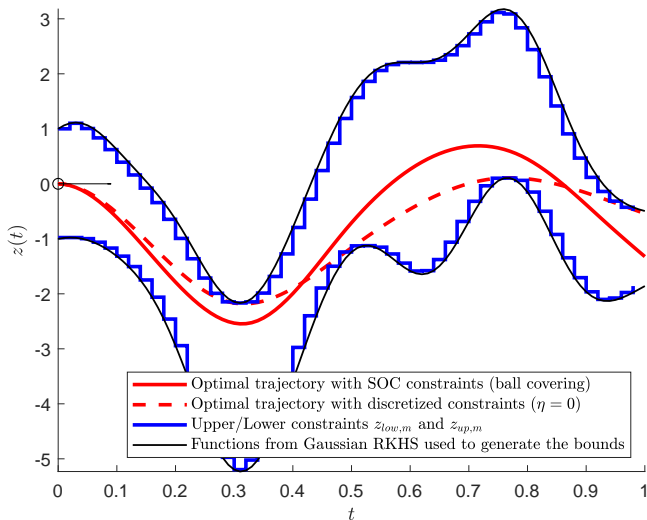
- $y$ : radar-measured altitude of aircrafts flying between two cities (Paris & Toulouse);  $x$ : time.  $d = 1$ ,  $N = 15657$ .
- Demo:  $\tau_q \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$ .
- Constraint: non-crossing,  $\nearrow$  (takeoff).





## 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

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- Control aspect [Aubin-Frankowski, 2020].
- Method:
  - $\dim(y) = 1$ : [Aubin-Frankowski and Szabó, 2020]. Code @ GitHub.
  - $\dim(y) \geq 1$  and SDP constraints (say joint convexity, production functions): [Aubin-Frankowski and Szabó, 2021].

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