Support Vector Machines with Hard Shape Constraints

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- *n*-monotonicity: $0 \le f^{(n)}(x)$,
- **1** (n-1)-alternating monotonicity: for $n \ge 2$

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

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

Examples continued

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

```
\mathbf{u} \preccurlyeq \mathbf{v} iff

• u_i \leq v_i (\forall i; product ordering),

• \sum_{i \in [i]} u_j \leq \sum_{i \in [i]} v_i (\forall i; unordered weak majorization).
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$$\frac{0 \le \partial^{\mathbf{e}_j} f(\mathbf{x})}{0 \le \partial^{\mathbf{e}_d} f(\mathbf{x})}, \quad (\forall j \in [d], \forall \mathbf{x}),$$
$$0 \le \partial^{\mathbf{e}_d} f(\mathbf{x}) \le \dots \le \partial^{\mathbf{e}_1} f(\mathbf{x}) \quad (\forall \mathbf{x}).$$

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

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

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

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

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- Supply chain models, game theory: supermodularity [Topkis, 1998, Simchi-Levi et al., 2014].

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Towards flexible H-s . . .

Kernel

• Def-1 (feature space): $k: \mathfrak{X} \times \mathfrak{X} \to \mathbb{R}$ kernel if

$$k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}.$$

• Examples $(\gamma > 0, c \ge 0, p \in \mathbb{Z}^+)$:

$$k_p(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + c)^p, \qquad k_G(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x} - \mathbf{y}\|_2^2},$$

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

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

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- Equivalent definitions, $k \stackrel{1:1}{\leftrightarrow} \mathcal{H}_k$.
- Included: Fourier analysis, polynomials, splines, ...
- Examples $(\gamma > 0, c \ge 0, p \in \mathbb{Z}^+)$:

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- Given: $(\tau_q)_{q \in [Q]} \subset (0,1)$ levels \nearrow , $\{(\mathbf{x}_n, y_n)\}_{n \in [N]}$ samples.
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- Objective:

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

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• Constraint (non-crossing): $K := \text{smallest rectangle containing } \{\mathbf{x}_n\}_{n \in [N]}$

$$f_q(\mathbf{x}) + b_q \le f_{q+1}(\mathbf{x}) + b_{q+1}, \, \forall q \in [Q-1], \, \forall \mathbf{x} \in K.$$

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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 $\{(t_n, x_n)\}_{n \in [N]} \subset [0, T] \times \mathbb{R}$. • Goal: learn the (t, x) relation.
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- Objective:

$$\min_{b \in \mathbb{R}, f \in \mathcal{H}_k} \left[\frac{1}{N} \sum_{n \in [N]} |x_n - [b + f(t_n)]|^2 + \lambda \|f\|_{\mathcal{H}_k}^2 \right]$$
s.t.
$$V_{\min} \leq f'(t), \quad \forall t \in \mathcal{T}.$$

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

- 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:

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

$$t \in \mathcal{T} := [0,1] \mapsto [x(t);z(t)] \in \mathbb{R}^2.$$

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

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

Task-3: safety-critical control – continued

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

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

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

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

and the task is

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

Task-3: safety-critical control – finished

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

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

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Constraints

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

$$\begin{split} \left(\overline{\mathbf{f}}, \overline{\mathbf{b}}\right) &= \underset{\substack{\mathbf{f} = (f_q)_{q \in [Q]} \in (\mathcal{H}_k)^Q, \\ \mathbf{b} = (b_q)_{q \in [Q]} \in \mathcal{B}, \\ (\mathbf{f}, \mathbf{b}) \in \mathcal{C}} } \\ \end{aligned}$$

$$\begin{split} \left(\overline{\mathbf{f}}, \overline{\mathbf{b}}\right) &= \underset{\mathbf{f} = (f_q)_{q \in [Q]} \in (\mathfrak{R}_k)^Q, \\ \mathbf{b} = (b_q)_{q \in [Q]} \in \mathfrak{B}, \\ (\mathbf{f}, \mathbf{b}) &\in \mathcal{C} \end{split}}{\mathbf{\mathcal{L}}(\mathbf{f}, \mathbf{b}), \\ \mathbf{b} = (b_q)_{q \in [Q]} \in \mathfrak{B}, \\ (\mathbf{f}, \mathbf{b}) &\in \mathcal{C} \end{split}$$

$$\mathcal{L}(\mathbf{f}, \mathbf{b}) = L\left(\mathbf{b}, \left(\mathbf{x}_n, y_n, (f_q(\mathbf{x}_n))_{q \in [Q]}\right)_{n \in [N]}\right) + \Omega\left(\left(\|f_q\|_{\mathfrak{H}_k}\right)_{q \in [Q]}\right), \end{split}$$

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$$\mathcal{C} &= \left\{\left(\mathbf{f}, \mathbf{b}\right) \mid \left(\mathbf{b}_0 - \mathbf{U}\mathbf{b}\right)_i \leq D_i(\mathbf{W}\mathbf{f} - \mathbf{f}_0)_i(\mathbf{x}), \quad \forall \mathbf{x} \in K_i, \forall i \in [I]\right\}, \end{split}$$

$$\begin{split} \left(\overline{\mathbf{f}},\overline{\mathbf{b}}\right) &= \underset{\mathbf{f} = (f_q)_q \in [Q]}{\arg\min} \, \mathcal{L}(\mathbf{f},\mathbf{b}), \\ &\underset{\mathbf{b} = (b_q)_q \in [Q]}{\mathbf{b} \in (\mathcal{H}_k)^Q}, \\ &\underset{(\mathbf{f},\mathbf{b}) \in \mathcal{C}}{\mathbf{b} = (b_q)_q \in [Q] \in \mathcal{B}}, \\ &\mathcal{L}(\mathbf{f},\mathbf{b}) = L\left(\mathbf{b}, \left(\mathbf{x}_n, y_n, (f_q(\mathbf{x}_n))_{q \in [Q]}\right)_{n \in [N]}\right) + \Omega\left(\left(\|f_q\|_{\mathcal{H}_k}\right)_{q \in [Q]}\right), \\ &\mathcal{C} = \left\{(\mathbf{f},\mathbf{b}) \mid (\mathbf{b}_0 - \mathbf{U}\mathbf{b})_i \leq D_i(\mathbf{W}\mathbf{f} - \mathbf{f}_0)_i(\mathbf{x}), \quad \forall \mathbf{x} \in \mathcal{K}_i, \forall i \in [I]\right\}, \\ &(\mathbf{W}\mathbf{f})_i = \sum_{q \in [Q]} W_{i,q} f_q, \end{split}$$

 $i \in [n_{i}]$

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$$\mathcal{L}(\mathbf{f},\mathbf{b}) &= L\left(\mathbf{b}, \left(\mathbf{x}_n, y_n, (f_q(\mathbf{x}_n))_{q \in [Q]}\right)_{n \in [N]}\right) + \Omega\left(\left(\|f_q\|_{\mathcal{H}_k}\right)_{q \in [Q]}\right), \\ \mathcal{C} &= \left\{\left(\mathbf{f},\mathbf{b}\right) \mid \left(\mathbf{b}_0 - \mathbf{U}\mathbf{b}\right)_i \leq D_i(\mathbf{W}\mathbf{f} - \mathbf{f}_0)_i(\mathbf{x}), \quad \forall \mathbf{x} \in K_i, \forall i \in [I]\right\}, \\ (\mathbf{W}\mathbf{f})_i &= \sum_{q \in [Q]} W_{i,q} f_q, \\ D_i &= \sum_{q \in [Q]} \gamma_{i,j} \partial^{\mathbf{r}_{i,j}}, \ |\mathbf{r}_{i,j}| \leq s, \ \gamma_{i,j} \in \mathbb{R}, \ \partial^{\mathbf{r}} f(\mathbf{x}) = \frac{\partial^{|\mathbf{r}|} f(\mathbf{x})}{\partial_{x_1}^{x_1} \cdots \partial_{x_d}^{x_d}}. \end{split}$$

Blanket assumptions

- **1** Domain $\mathfrak{X} \subseteq \mathbb{R}^d$: open. Kernel $k \in \mathcal{C}^s(\mathfrak{X} \times \mathfrak{X})$.
- **2** $K_i \subset \mathfrak{X}$: compact, $\forall i$.
- **3** $\mathbf{f}_{0,i} \in \mathcal{H}_k$ 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 Ω : strictly increasing in each of its argument.

$$(\mathbf{f}_{\eta}, \mathbf{b}_{\eta}) = \underset{\mathbf{f} \in (\mathcal{H}_{k})^{Q}, \mathbf{b} \in \mathcal{B}}{\operatorname{arg min}} \mathcal{L}(\mathbf{f}, \mathbf{b})$$

$$\operatorname{s.t.}$$

$$(\mathbf{b}_{0} - \mathbf{U}\mathbf{b})_{i} + \underset{\eta_{i}}{\eta_{i}} \|(\mathbf{W}\mathbf{f} - \mathbf{f}_{0})_{i}\|_{\mathcal{H}_{k}}$$

$$\leq \min_{m \in [M_{i}]} D_{i}(\mathbf{W}\mathbf{f} - \mathbf{f}_{0})_{i}(\tilde{\mathbf{x}}_{i,m}), \ \forall i \in [I],$$

$$(\mathfrak{C}_{\eta})$$

where

- $\{\tilde{\mathbf{x}}_{i,m}\}_{m\in[M_i]}$: a δ_i -net of K_i in $\|\cdot\|_{\mathfrak{X}}$,
- $\bullet \ \eta_i = \sup_{m \in [M_i], \mathbf{u} \in \mathbb{B}_{\|\cdot\|_{\Upsilon}}(\mathbf{0}, \mathbf{1})} \|D_{i, \mathbf{x}} k(\tilde{\mathbf{x}}_{i, m}, \cdot) D_{i, \mathbf{x}} k(\tilde{\mathbf{x}}_{i, m} + \delta_i \mathbf{u}, \cdot)\|_{\mathcal{H}_k},$
- $\bullet \ D_{i,\mathbf{x}}k(\mathbf{x}_0,\cdot) := \mathbf{y} \mapsto D_i(\mathbf{x} \mapsto k(\mathbf{x},\mathbf{y}))(\mathbf{x}_0).$

Let
$$s = 0$$
, $l = 1$. Recall constraint (\mathcal{C}):
$$\{(\mathbf{f}, \mathbf{b}) \mid \underbrace{(b_0 - \mathbf{U}\mathbf{b})}_{\beta} \leq \underbrace{(\mathbf{W}\mathbf{f} - f_0)}_{\phi}(\mathbf{x}), \quad \forall \mathbf{x} \in \mathcal{K}\}$$

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$$\boxed{\Phi(K) := \left\{ k(\mathbf{x}, \cdot) : \mathbf{x} \in K \right\} \subseteq H_{\phi, \beta}^{+} := \left\{ g \in \mathfrak{H}_{k} \, | \, \beta \leq \langle \phi, g \rangle_{\mathfrak{H}_{k}} \right\}}$$

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

Theorem

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

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Then,

ullet (i) Tightening: any (\mathbf{f},\mathbf{b}) satisfying (\mathcal{C}_{η}) also satisfies (\mathcal{C}) , hence

$$v_{\rm disc} \leq \overline{v} \leq v_{\eta}$$
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ullet (ii) Representer theorem: For $\forall q \in [Q], \ \exists ilde{a}_{i,0,q}, ilde{a}_{i,m,q}, a_{n,q} \in \mathbb{R}$ s.t.

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

Theorem - continued

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

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

Theorem – continued

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

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

Theorem – continued

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

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

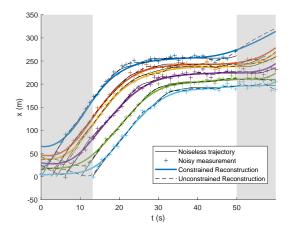
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1st bound: computable. 2nd: Larger $M_i \Rightarrow$ smaller $\delta_i \Rightarrow$ smaller $\eta_i \Rightarrow$ tighter bound.

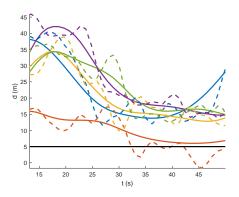
Demo (task-1): convoy localization with traffic jam

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



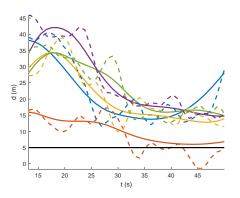
Demo (task-1): continued

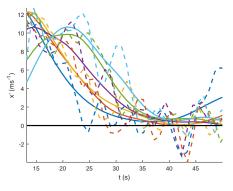
Pairwise distances: $t\mapsto f_q(t)-f_{q+1}(t)$



Demo (task-1): continued

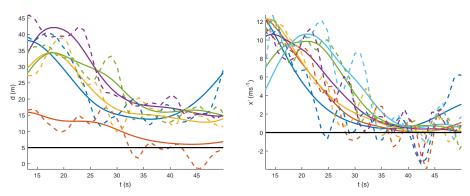
Pairwise distances: $t\mapsto f_q(t)-f_{q+1}(t)$ Speed: $t\mapsto f_q'(t)$





Demo (task-1): continued

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

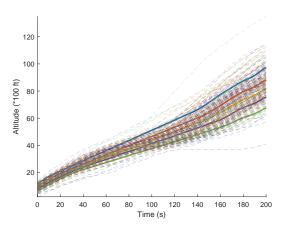


Shape constraints: especially relevant in noisy situations.

Demo (task-2): joint quantile regression

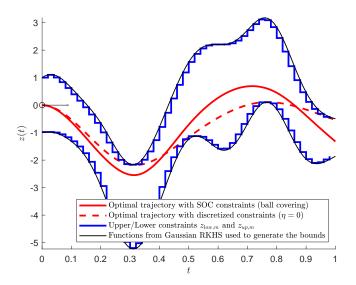
Analysis of aircraft trajectories, ENAC [Nicol, 2013]

- 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,
 \^ (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: aircraft trajectories,
 - safety-critical control.

References & acknowledgements

- Transportation systems [Aubin-Frankowski et al., 2020].
- Control aspect [Aubin-Frankowski, 2020].
- Method:
 - dim(y) = 1: [Aubin-Frankowski and Szabó, 2020]. Code @ GitHub.
 - dim(y) ≥ 1 (ex: safety-critical control) and SDP constraints (ex: production functions → joint convexity): [Aubin-Frankowski and Szabó, 2022].

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