When Shape Constraints Meet Kernel Machines

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

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

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

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

Examples continued

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

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

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

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

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

$$0 \leq \partial^{\mathbf{e}_d} f(\mathbf{x}) \leq \ldots \leq \partial^{\mathbf{e}_1} f(\mathbf{x}) \quad (\forall \mathbf{x}).$$

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7. Supermodularity:

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

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

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  - European and American call option prices: convex & monotone in the underlying stock price and $\nearrow$ in volatility [Aït-Sahalia and Duarte, 2003].

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

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

Kernel

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

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

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

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

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

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

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Task-1: joint quantile regression (JQR)

- 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:

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

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

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

$$\min_{b \in \mathbb{R}, f \in \mathcal{H}_k} \left[\frac{1}{N} \sum_{n\in[N]} |x_n - [b + f(t_n)]|^2 + \lambda \|f\|^2_{\mathcal{H}_k} \right]$$

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

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

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:

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

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

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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 ($b_{q+1} - b_q$).

Our task

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

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

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

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

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

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. $\mathbf{f}_{0,i} \in \mathcal{H}_k$ 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.

Our strenghtened SOC-constrained formulation

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

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

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

where

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

Tightening idea

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

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

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- η is obtained as the minimal radius.

Theorem

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

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Then,

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

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

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

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

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

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

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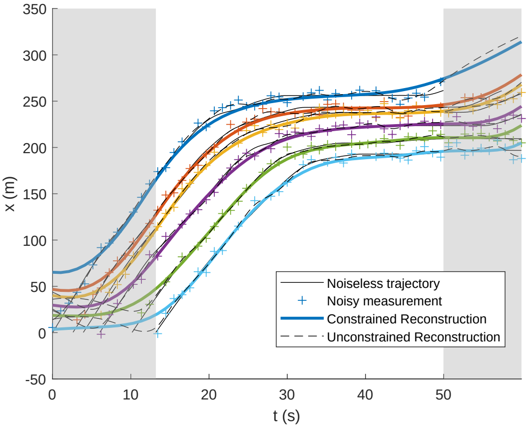
1st bound: computable. 2nd: Larger $M_i \Rightarrow$ smaller $\delta_i \Rightarrow$ smaller η_i $\Rightarrow$ tighter bound.

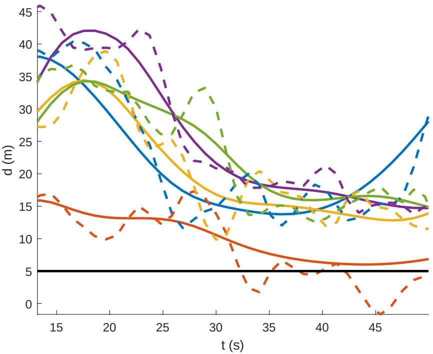
Demo (task-1): convoy localization with traffic jam

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



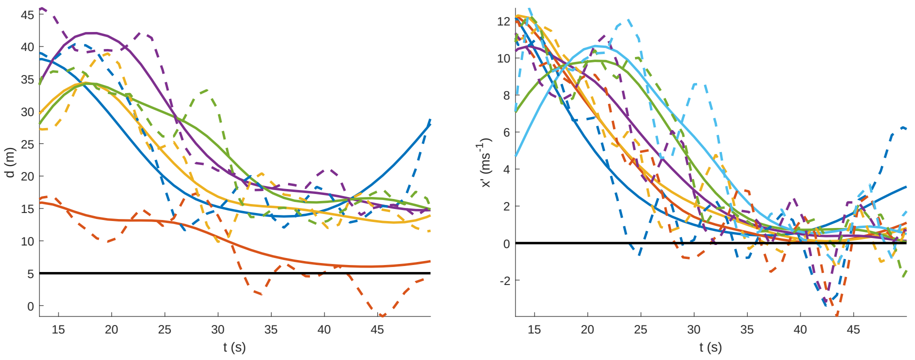
Demo (task-1): continued

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

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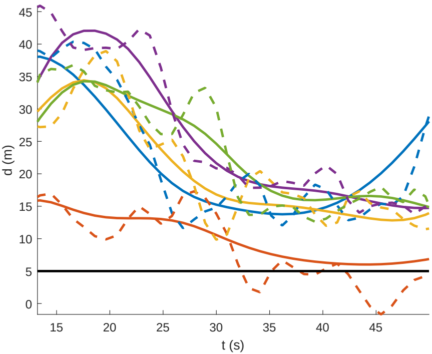
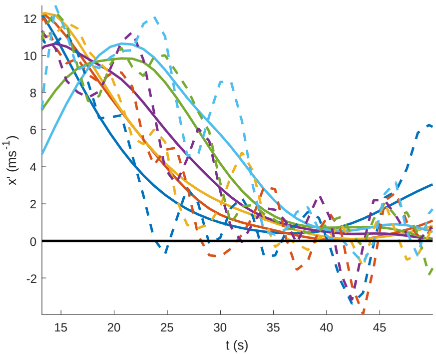


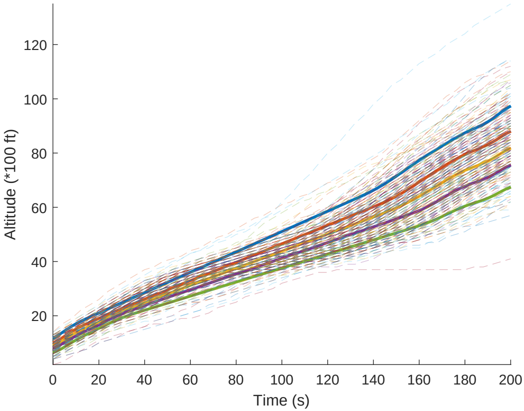


Shape constraints: especially relevant in noisy situations.

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, $\nearrow$ (takeoff).



Summary

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

References & acknowledgements

- Transportation systems [Aubin-Frankowski et al., 2020].
- Method:
  - $dim(y) = 1$: [Aubin-Frankowski and Szabó, 2020]. Code @ GitHub.
  - $dim(y) \geq 1$ (ex: safety-critical control) and SDP constraints (ex: production functions $\rightarrow$ joint convexity): [Aubin-Frankowski and Szabó, 2021].

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