When Kernel Machines Meet Shape Constraints

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

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

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

Examples continued

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

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

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

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7. Supermodularity:

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

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

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Today: optimization framework

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

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

$$k_L(\mathbf{x}, \mathbf{y}) = e^{-\gamma \|\mathbf{x}-\mathbf{y}\|_1}, \qquad k_e(\mathbf{x}, \mathbf{y}) = e^{\gamma \langle \mathbf{x}, \mathbf{y} \rangle}.$$

Kernel, RKHS

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

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- Equivalent definitions, $k \overset{1:1}{\leftrightarrow} \mathcal{H}_k$.
- Included: Fourier analysis, polynomials, splines, ...
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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], probability distributions [Berlinet and Thomas-Agnan, 2004, Hein and Bousquet, 2005, Smola et al., 2007, Sriperumbudur et al., 2010],
- 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].

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:

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

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

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

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:

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

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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Task-3: safety-critical control

- Trajectory of an underwater vehicle:

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$$z(t) \in [z_{\text{low}}(t), z_{\text{up}}(t)] \;\; \forall t \in \mathcal{T}.$$

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

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

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

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

and the task is

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

Task-3: safety-critical control – finished

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

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

Task-3: safety-critical control – finished

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Constraints

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

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

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

Our task

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

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

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. $\mathbf{f}_{0,i} \in \mathcal{H}_k$ 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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$$\boxed{\Phi(K)} := \{k(\mathbf{x},\cdot) : \mathbf{x} \in K\} \boxed{\subseteq H^{+}_{\phi,\beta}} := \Big\{g \in \mathcal{H}_k \mid \beta \leq \langle \phi, g\rangle_{\mathcal{H}_k}\Big\}$$

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

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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

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

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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.

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

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

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

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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

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

Theorem – continued

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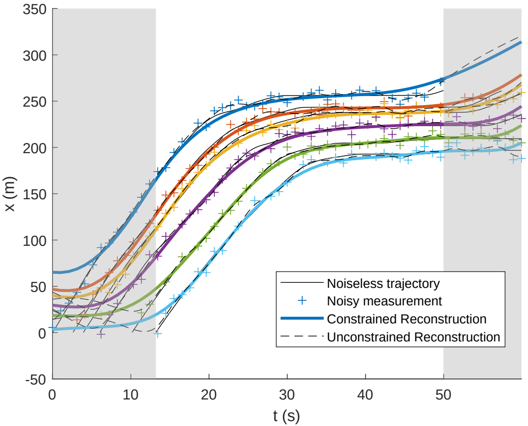
1st bound: computable. 2nd: Larger $M_i \Rightarrow$ smaller $\delta_i \Rightarrow$ smaller η_i $\Rightarrow$ tighter bound.

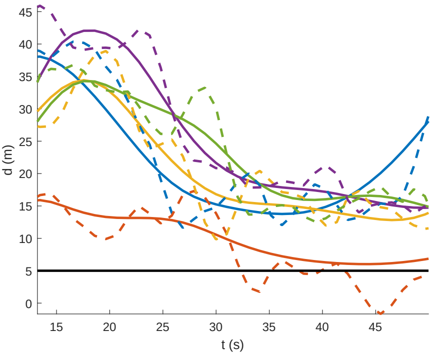
Demo (task-1): convoy localization with traffic jam

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

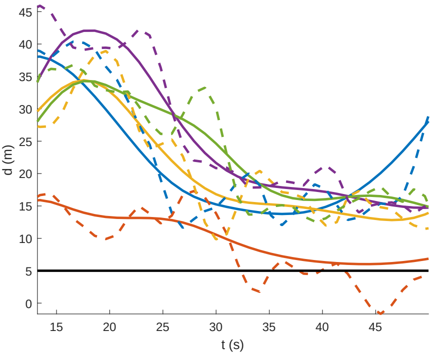


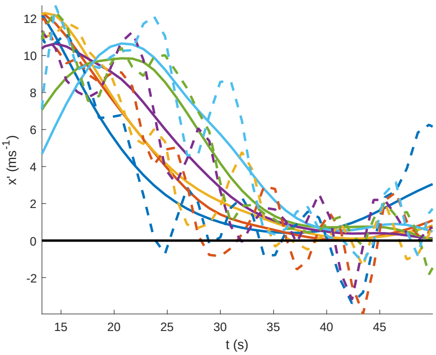
Demo (task-1): continued

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



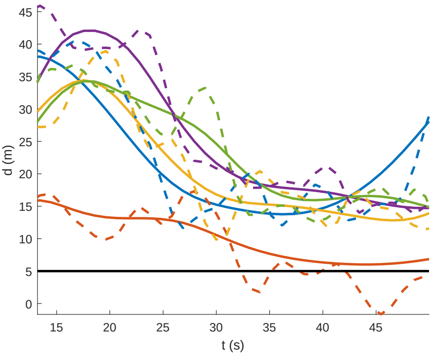
Pairwise distances: $t \mapsto f_q(t) - f_{q+1}(t)$ Speed: $t \mapsto f_q'(t)$

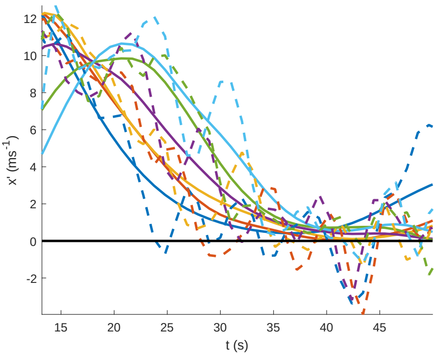




Demo (task-1): continued

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



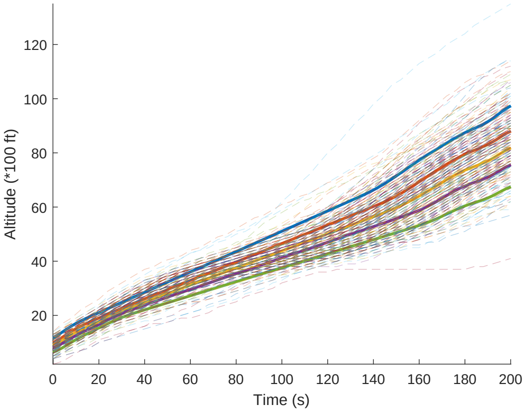


Shape constraints: especially relevant in noisy situations.

Demo (task-2): joint quantile regression

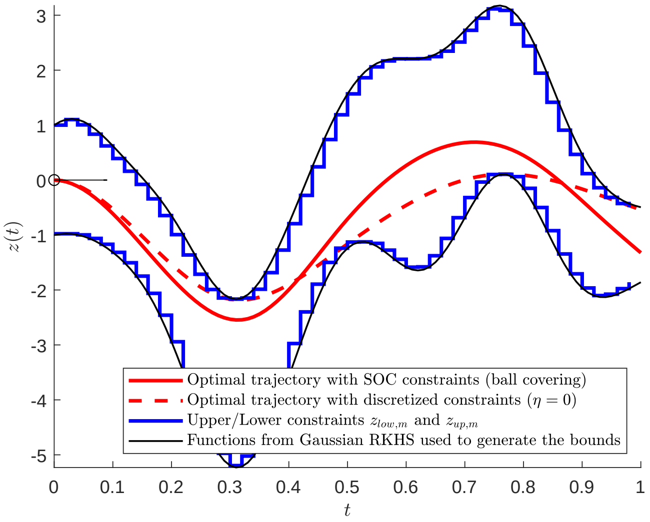
Analysis of aircraft trajectories, ENAC [Nicol, 2013]

- 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, $\nearrow$ (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: 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.
  - $dim(y) \geq 1$ and SDP constraints (say joint convexity, production functions): [Aubin-Frankowski and Szabó, 2021].

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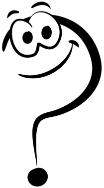

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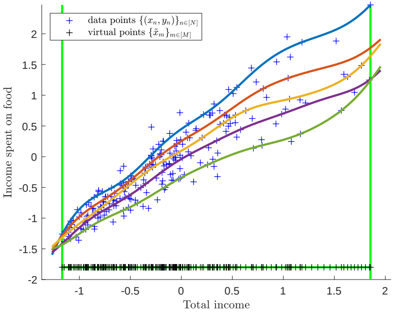
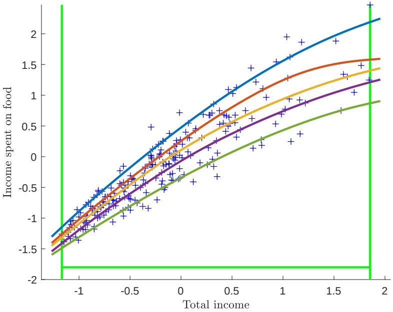
Demo (task-2): joint quantile regression

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.





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