Data-Driven System Identification and Surrogate Modeling

Ben Russo

Oak Ridge National Laboratory

Mathematics in Computation

Joint work with Paul Laiu

System Identification:

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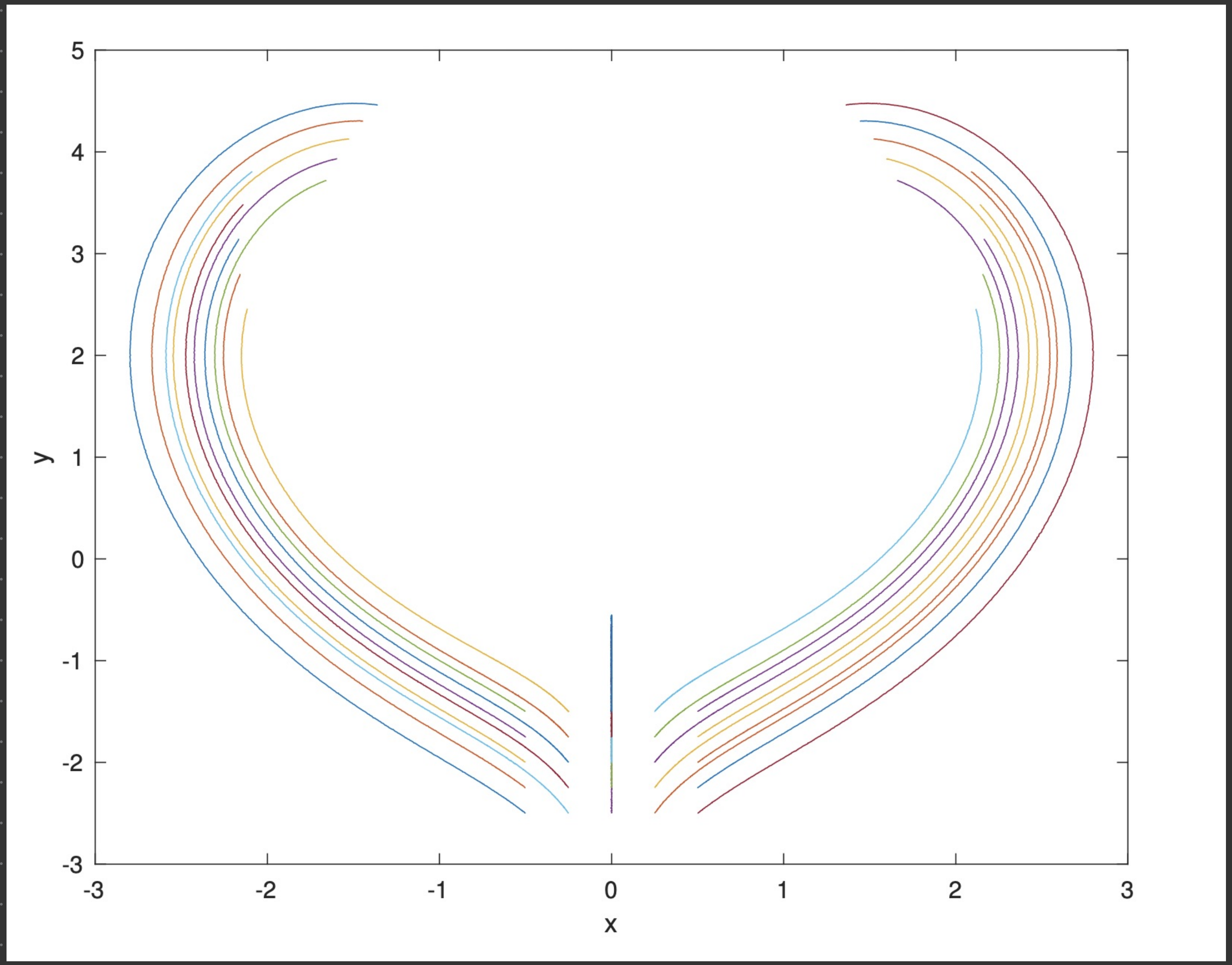

Observed data

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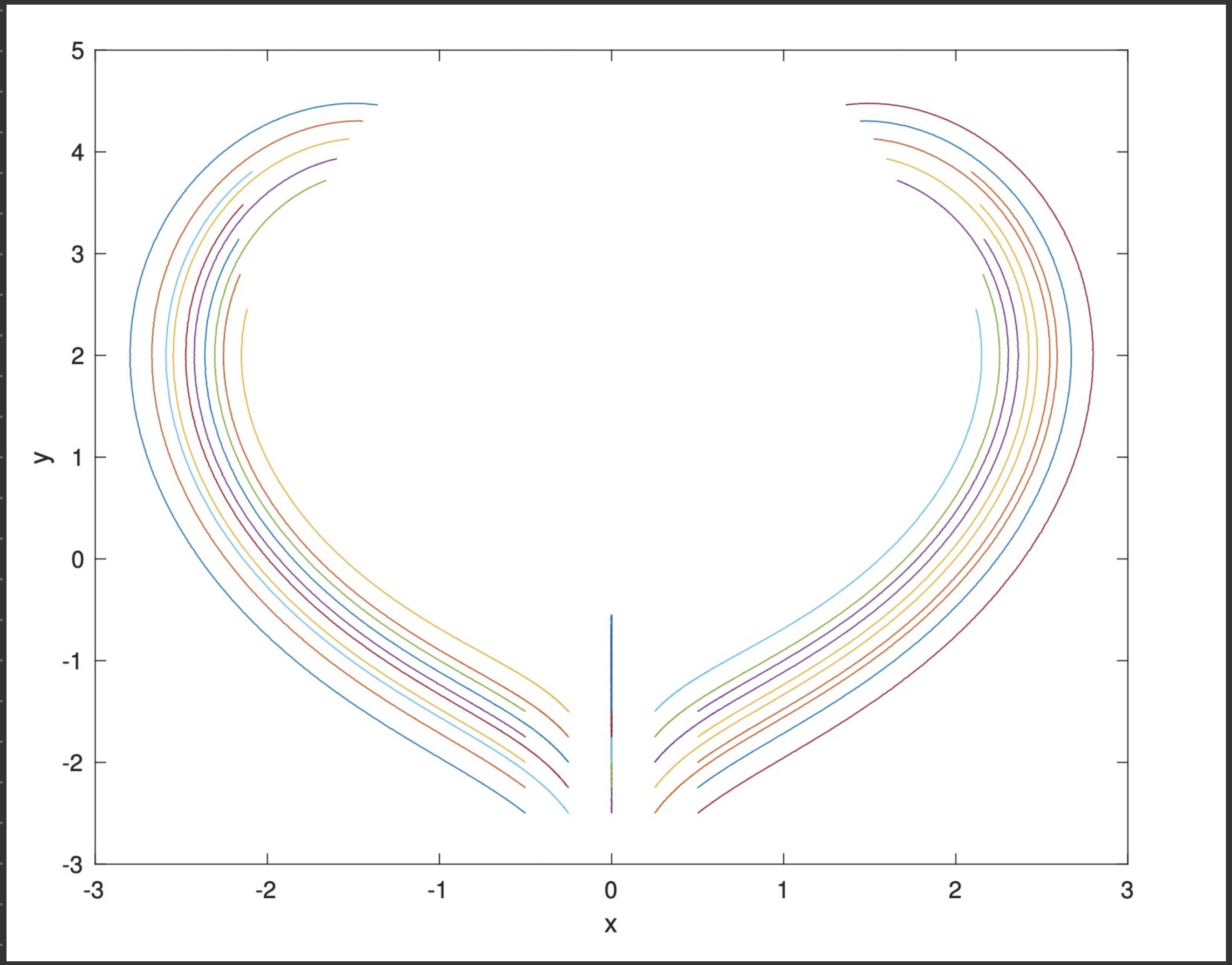

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System Id techniques

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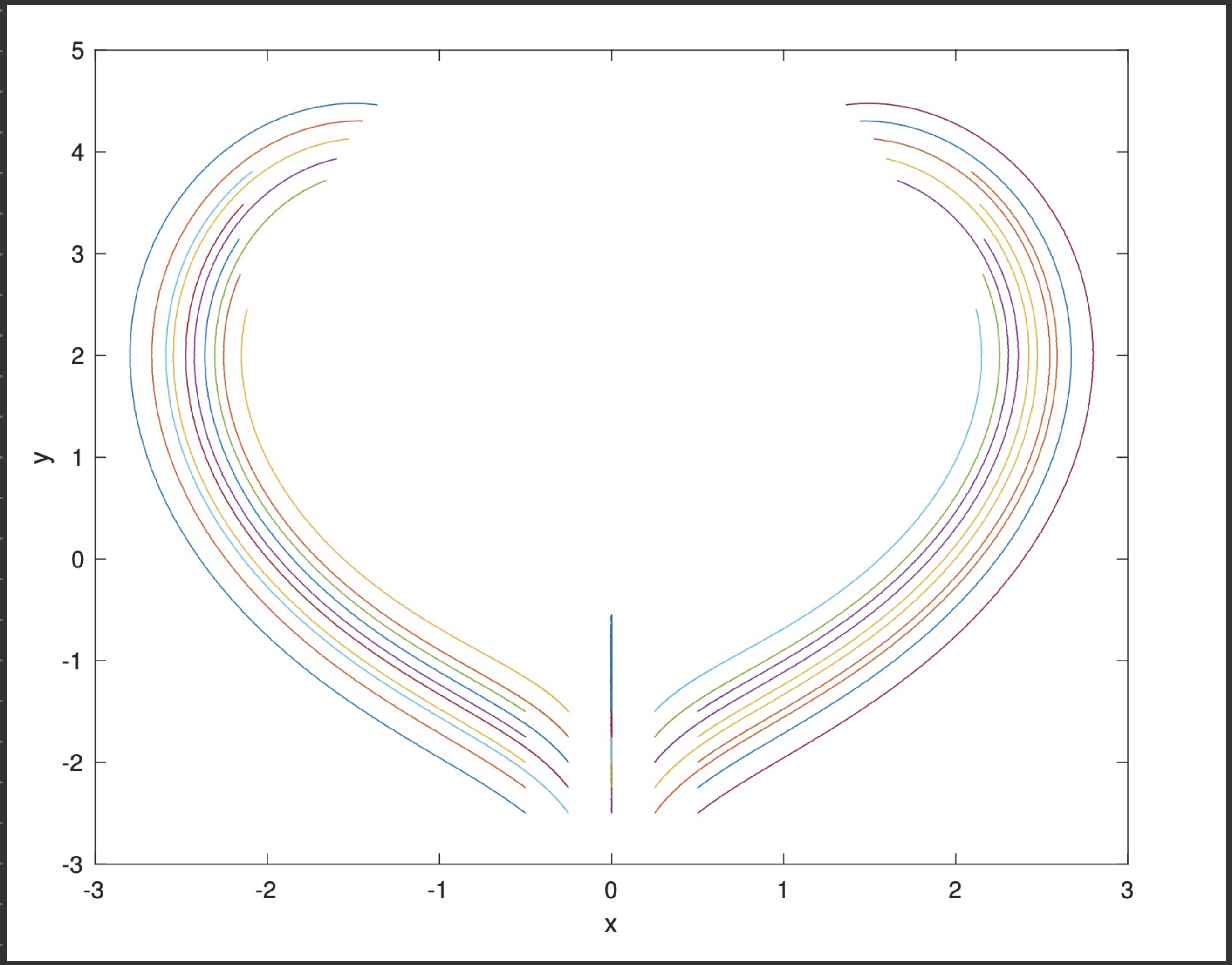

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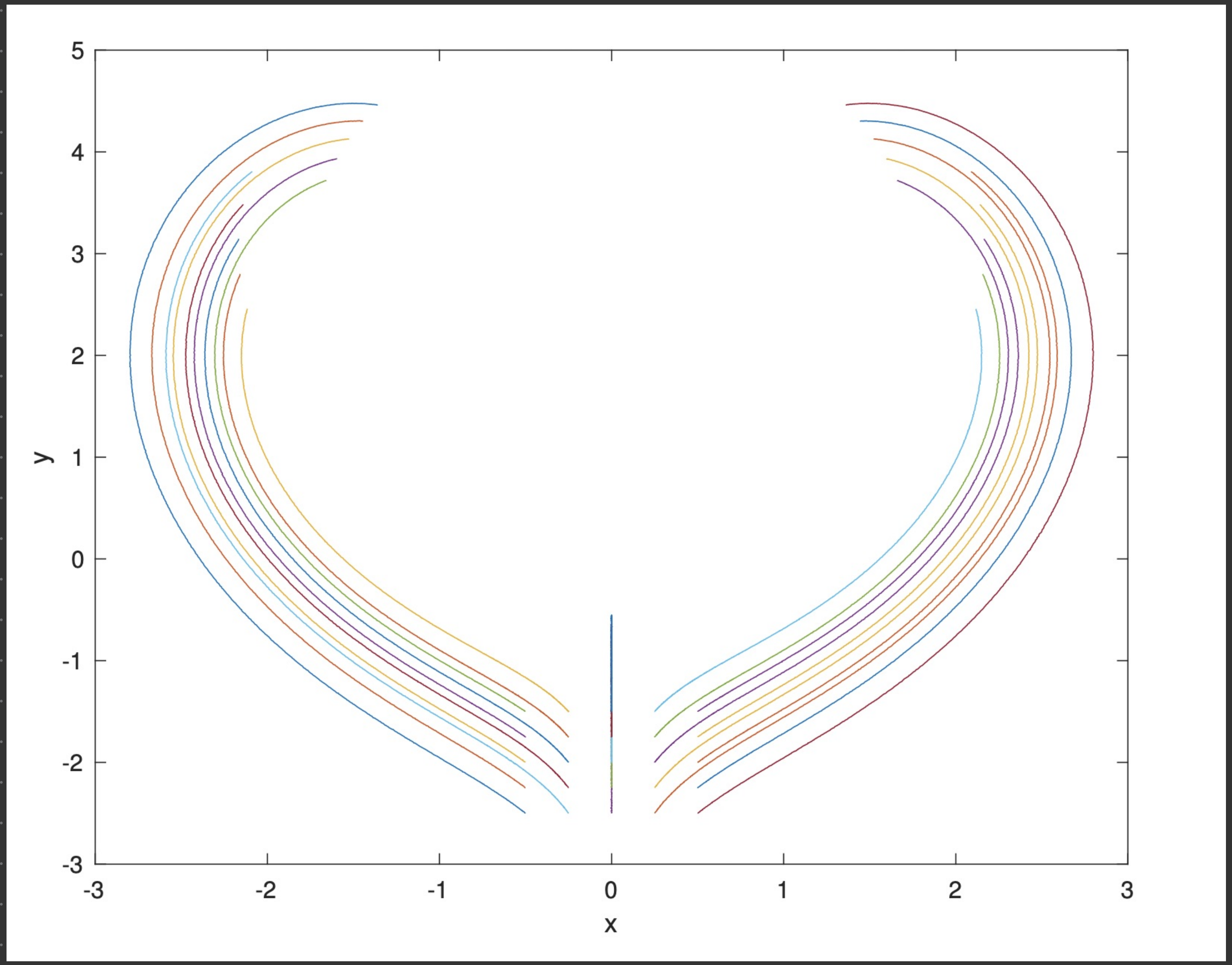

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Unknown: $\dot{x}(t) = f(x(t))$

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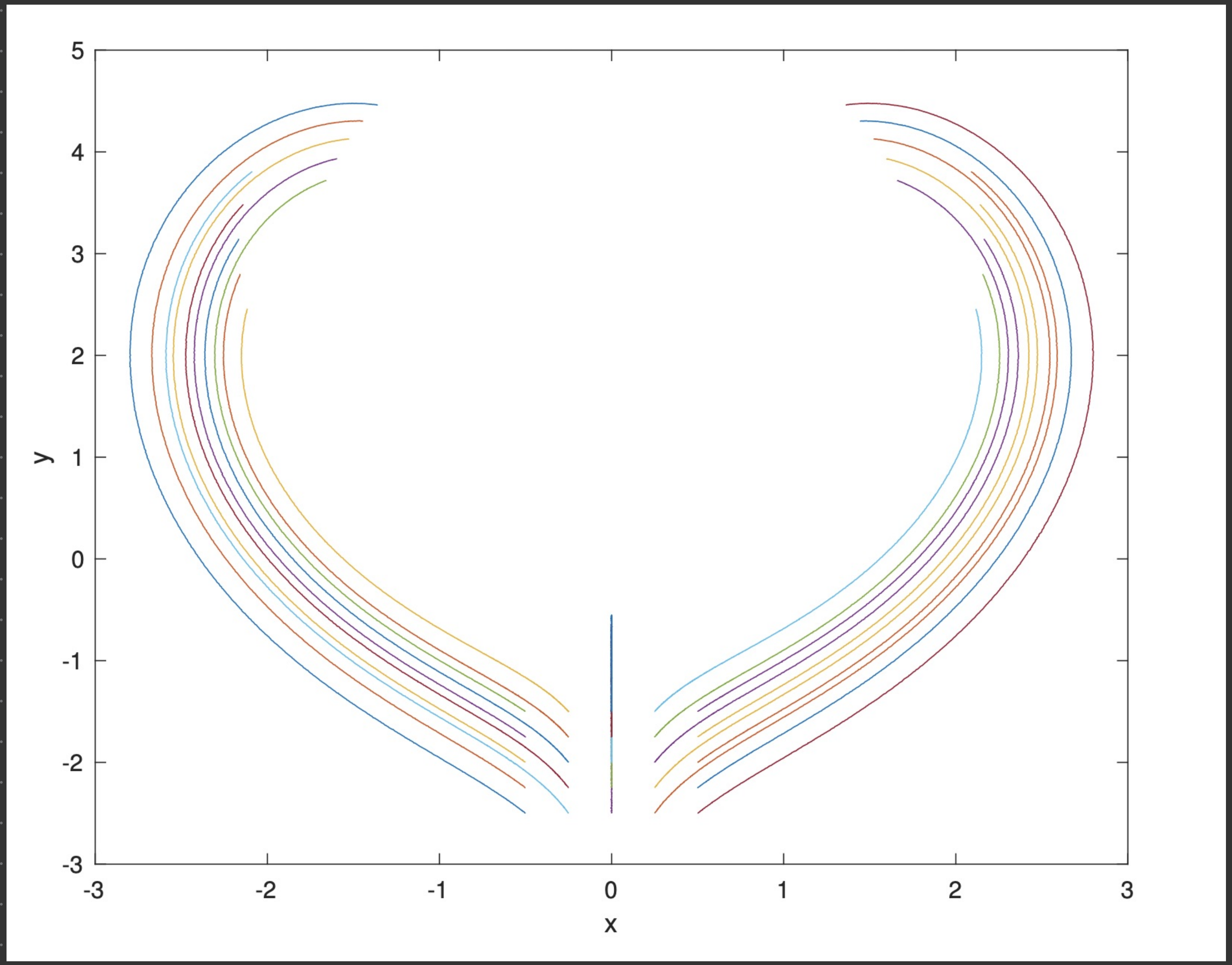

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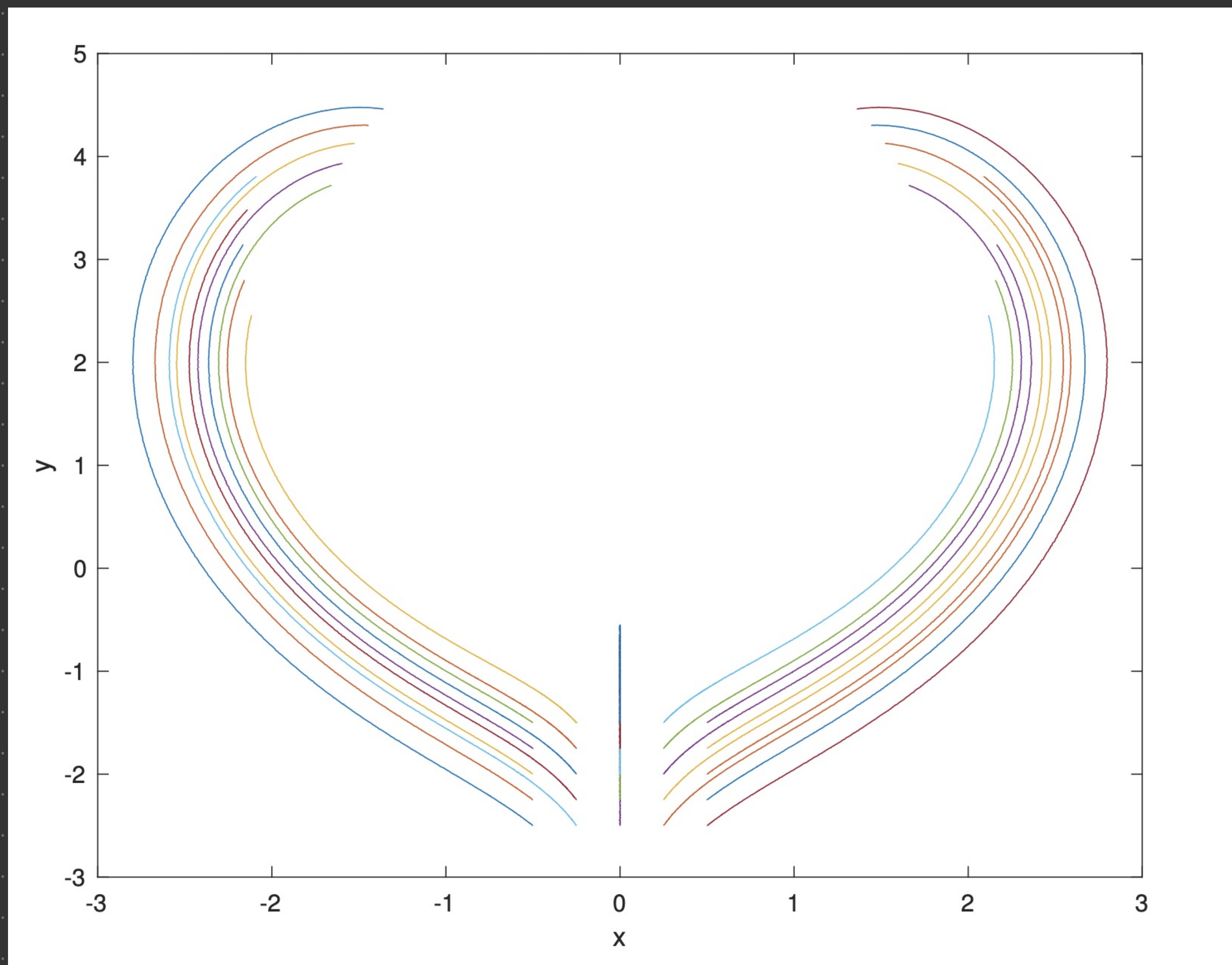

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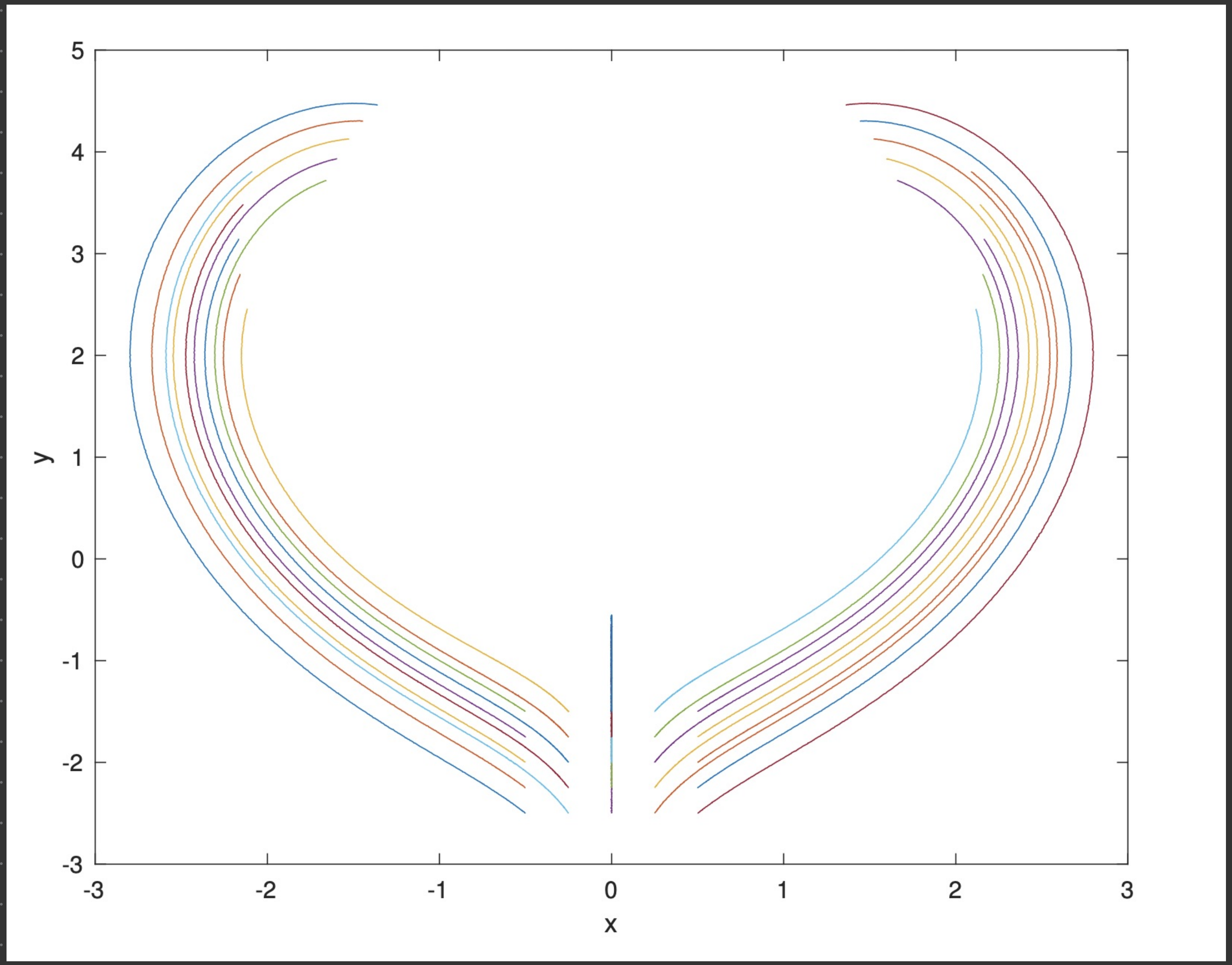

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SINDy : Brunton et al.

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SINDy (Brunton et al.)

$$\dot{x}(t_k) = \sum_{j=0}^{J} w_j \varphi_j(x(t_k)) \implies \begin{bmatrix} \dot{x}(t_0) \\ \vdots \\ \dot{x}(t_K) \end{bmatrix} = \begin{bmatrix} \varphi_0(x(t_0)) & \cdots & \varphi_J(x(t_0)) \\ \vdots & \ddots & \vdots \\ \varphi_0(x(t_K)) & \cdots & \varphi_J(x(t_K)) \end{bmatrix} \begin{bmatrix} w_0 \\ \vdots \\ w_J \end{bmatrix}$$

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$$\langle \dot{x}, \psi_k \rangle = \left\langle \sum_{j=0}^{J} w_j \varphi_j(x(t_k)), \psi_k \right\rangle$$

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Weak-SINDy (Messenger & Bortz)

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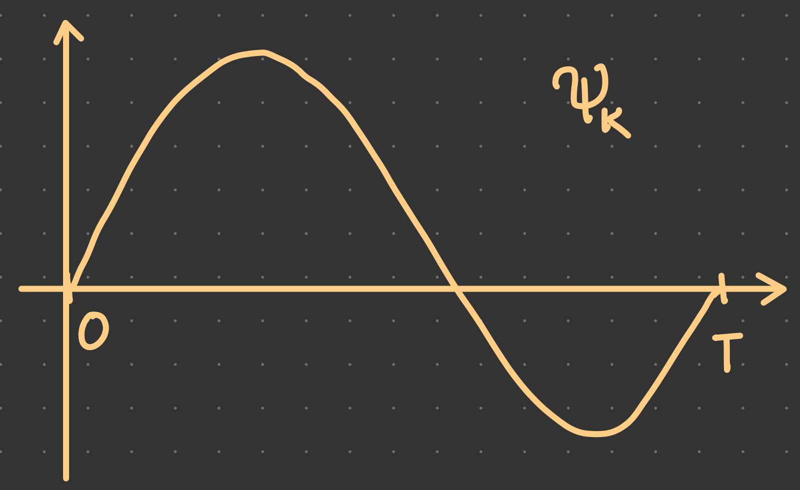

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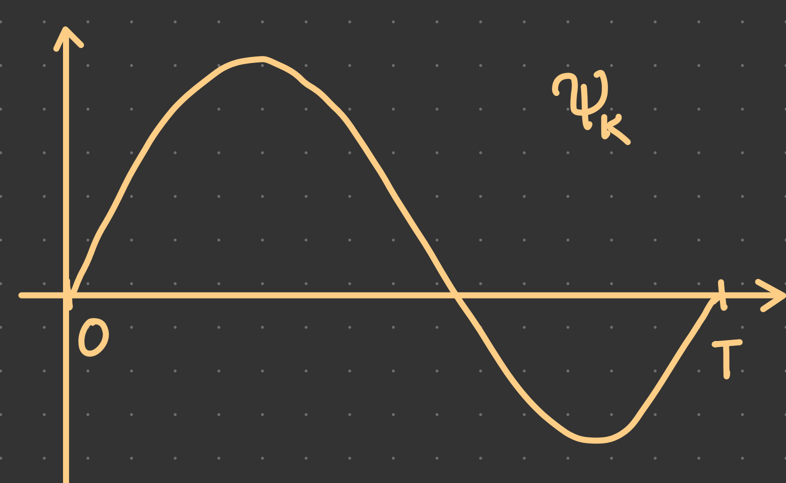

$$\langle \dot{x}, \psi_k \rangle = -\langle x, \dot{\psi}_k \rangle$$

Can be evaluated with derivatives of chosen test functions

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$$\langle \dot{x}, \dot{\psi}_k(x(t)) \rangle = \left\langle \sum_{j=0}^{J} w_j \varphi_j(x(t_k)), \dot{\psi}_k(x(t)) \right\rangle$$

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Occupation Kernel Method (Rosenfeld et al.)

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$$\int_0^T \dot{x}(t)\, \dot{\psi}_k(x(t))\, dt = \int_0^T d/dt \left[\psi_k(x(t)) \right] dt = \psi_k(x(T)) - \psi_k(x(0))$$

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Can be evaluated without derivative data

Operator Theoretic Viewpoint

Operator Theoretic Viewpoint

SINDy

$$\left[G_{jk} \right]_{k,j=0,0}^{K,J} = \left[\varphi_j(x(t_k)) \right]_{k,j=0,0}^{K,J}$$

Weak-SINDy

$$\left[G_{jk} \right]_{k,j=0,0}^{K,J} = \left[\langle \varphi_j(x), \psi_k \rangle \right]_{k,j=0,0}^{K,J}$$

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SINDy $\quad \left[G_{jk} \right]_{k,j=0,0}^{K,J} = \left[\varphi_j(x(t_k)) \right]_{k,j=0,0}^{K,J}$

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Operators:

$C_x(g) = g \circ x$ Koopman Operators

$A_f(g) = \dot{g} \cdot f$ Liouville Operators

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Hilbert Spaces:

- $\mathcal{L}^2$, $H^{k,2}$
- Reproducing Kernel Hilbert Spaces

$\hookrightarrow g(x) = \langle g, K_x \rangle \; ; \; \int_0^T g(x(t))\,dt = \langle g, \Gamma_x^T \rangle$

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SINDy $\quad \left[G_{jk} \right]_{k,j=0,0}^{K,J} = \left[\varphi_j(x(t_k)) \right]_{k,j=0,0}^{K,J} = \left[\langle C_x(\varphi_j), K_{t_k} \rangle \right]_{k,j=0,0}^{K,J}$

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Consider the following scalar ODE

$$\dot{x}(t) = f(x(t)) \;;\quad x(\xi) = \eta \,,\quad t \in [a,b],\quad f : X \longrightarrow \mathbb{R}.$$

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Goal: $f(x) \approx \sum_{j=0}^{J} w_j \varphi_j(x)$

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Proposition: Suppose the above ODE has a solution $x : [a,b] \longrightarrow X \subseteq \mathbb{R}$ where $\xi \in [a,b]$. Let $\hat{x} : [a,b] \longrightarrow X$ be a solution to

$$\dot{\hat{x}}(t) = p(\hat{x}(t)) \; ; \quad \hat{x}(\xi) = \eta, \quad p : X \longrightarrow \mathbb{R}.$$

Then,

$$\| x - \hat{x} \|_{\mathcal{L}^\infty(a,b)} \leq (b-a)^{1/2} \, \| f \circ x - p \circ \hat{x} \|_{\mathcal{L}^2(a,b)}$$

$$\|f \circ x - p \circ \hat{x}\| \leq \|f \circ x - p \circ x\| + \|p \circ x - p \circ \hat{x}\|$$

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$$G = \left[G_{jk} \right]_{k,j=0,0}^{K,J} = \left[\langle \varphi_j(x), \psi_k \rangle \right]_{k,j=0,0}^{K,J}$$

$$b = [b_0 \dots b_K]^T = [\dots \langle f\circ x, \psi_k \rangle \dots]^T$$

$$\min_{w\in\mathbb{R}^{J+1}} \|Gw - b\|_2$$

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$$\Longleftrightarrow$$

Assuming $\{\psi_k\}_{k=0}^{K}$ is orthonormal and $\operatorname{span}\{\varphi_j\}_{j=0}^{J} = \mathbb{P}_J$

$$\min_{p\in\mathbb{P}_J(X)} \|P_K(f\circ x - p\circ x)\|_{L^2(a,b)}$$

We'll denote the minimizer as $p^*_{J,K}$

Theorem: Let Ω be a bounded cube in $\mathbb{R}^d$. Suppose $u \in H^m(\Omega)$, for any $m \geq 0$ then

$$\| u - P_J u \|_{H^s(\Omega)} \leq C J^{e(s,m)} \| u \|_{H^m(\Omega)}$$

with $e(s,m) = \begin{cases} 2s - m - \frac{1}{2} & s \geq 1 \\ \frac{3s}{2} - m & 0 \leq s \leq 1 \end{cases}$ and C independent of J and u.

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Here, P_J is projection onto polynomial space. We will assume the spaces spanned by $\{\varphi_j\}_{j=0}^{J}$ and $\{\psi_k\}_{k=0}^{K}$ to be polynomial spaces.

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$$\|f\circ X - p^*_{JK}\circ X\|_{\mathcal{L}^2} \leq \|f\circ X - \mathcal{P}_K(f\circ X)\|_{\mathcal{L}^2} + \|\mathcal{P}_K(f\circ X - p^*_{JK}\circ X)\|_{\mathcal{L}^2} + \|p^*_{JK}\circ X - \mathcal{P}_K(p^*_{JK}\circ X)\|_{\mathcal{L}^2}$$

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$$\|\mathcal{P}_K(f\circ X - p\circ X)\|_{\mathcal{L}^2} \le \|f\circ X - p\circ X\|_{\mathcal{L}^2} \le \|C_X\|_{op}\,\|f-p\|_{\mathcal{L}^2}$$

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Proposition: Let $f\in H^m(X)$ for some $m>0$ and $x:[a,b]\to X$, then

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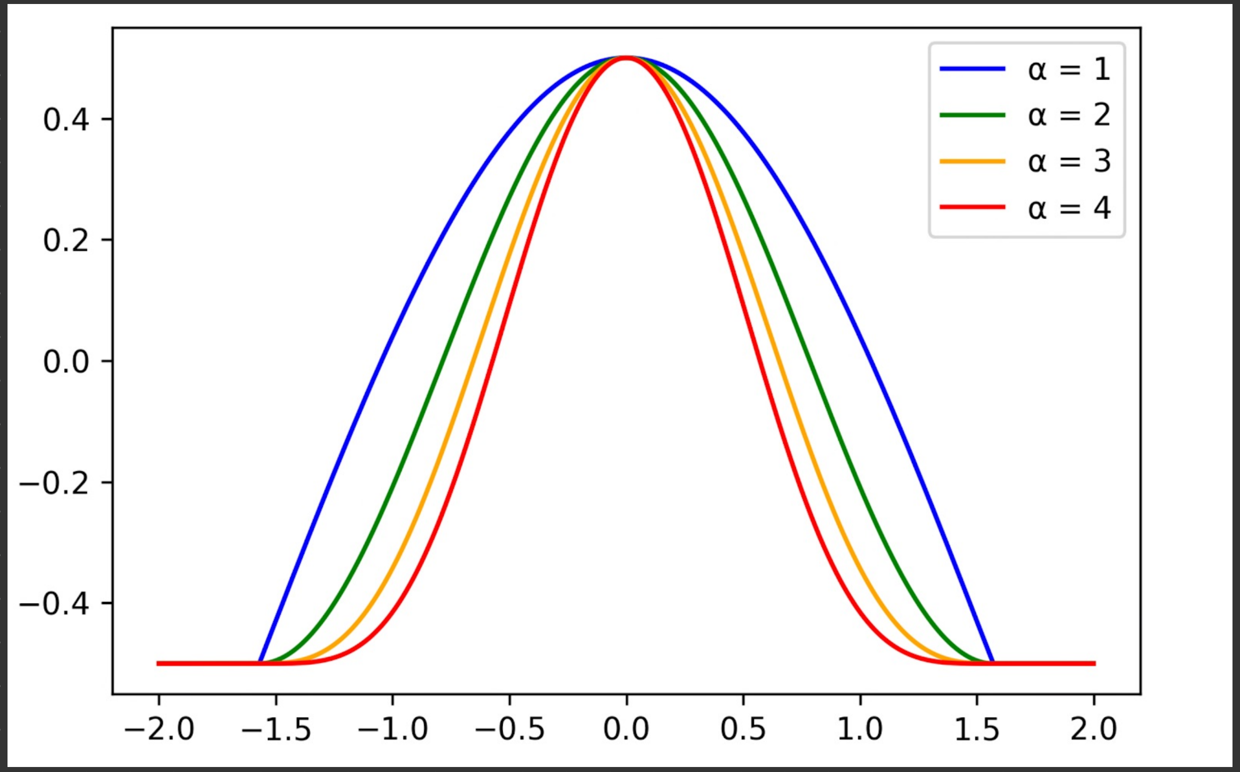
$$\| \mathcal{P}_K (f \circ x - P^*_{JK} \circ x) \|_{\ell^2} \leq C \| C_x \|_{op} J^{-m} \| f \|_{H^m(\Omega)}.$$

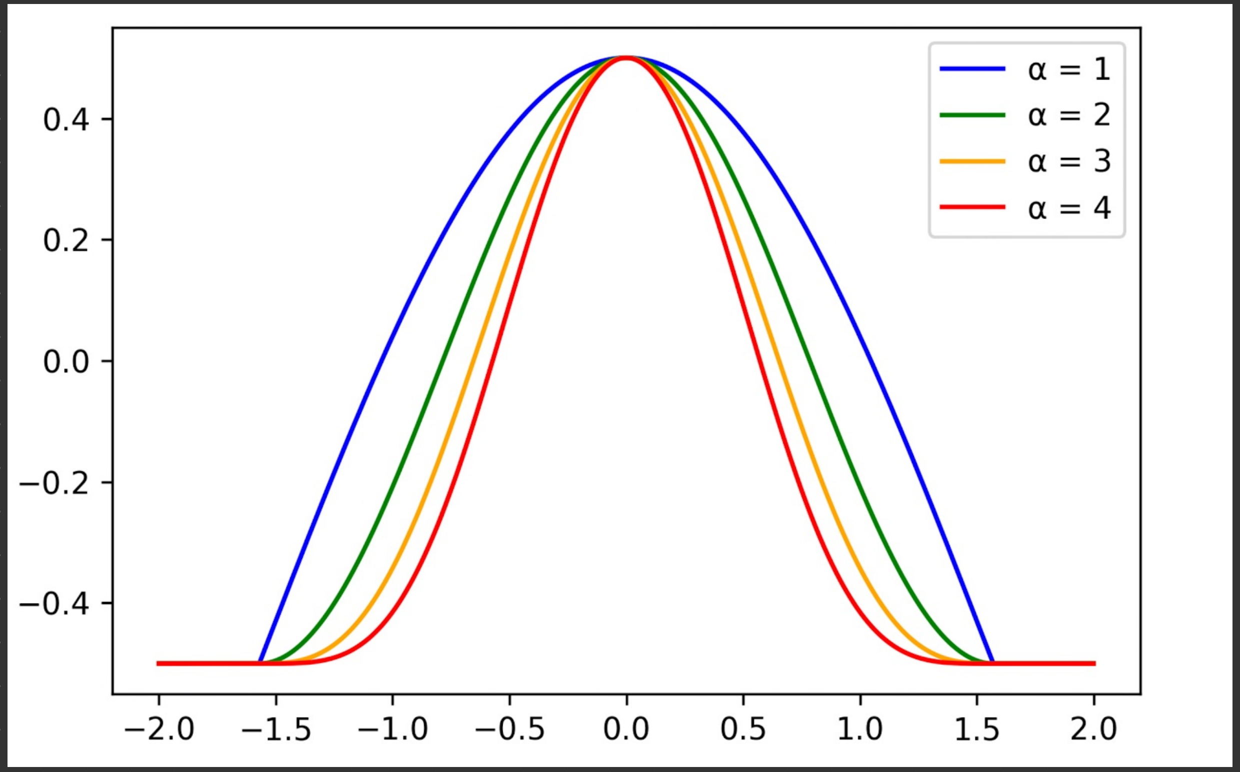
Ex// $\dot{x}(t) = g_\alpha(x(t))$; $x(0) = 2$ with $g_\alpha(x) = \mathbb{1}_{[-\pi/2, \pi/2]} \cdot \cos^\alpha(x) - 1/2$.



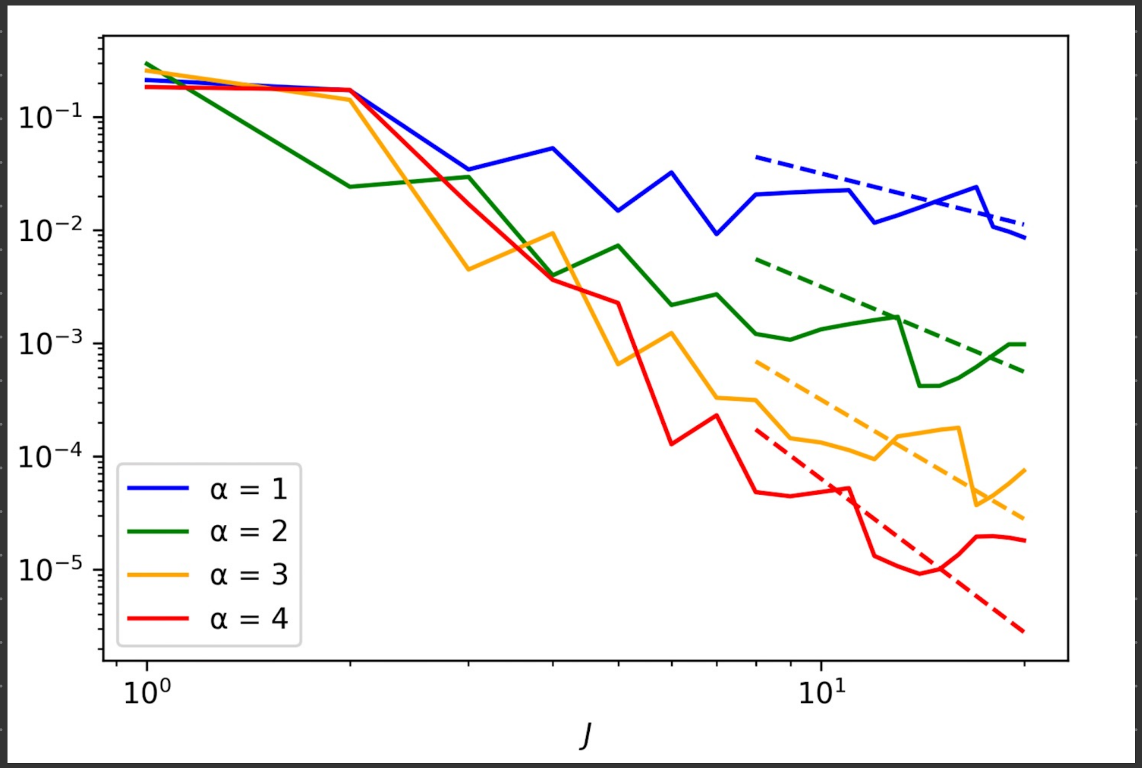
Proposition: Let $f \in H^m(X)$ for some $m > 0$ and $x : [a,b] \to X$, then

$$\| \mathcal{P}_K (f \circ x - p^*_{JK} \circ x) \|_{\ell^2} \leq C \| C_x \|_{op} J^{-m} \| f \|_{H^m(\Omega)}.$$

Ex// $\quad \dot{x}(t) = g_\alpha(x(t))\,; \quad x(0) = 2 \quad$ with $\quad g_\alpha(x) = \mathbb{1}_{[-\pi/2,\, \pi/2]} \cdot \cos^\alpha(x) - 1/2.$



$\| \mathcal{P}_K (f \circ x - p^*_{JK} \circ x) \|_{\ell^2}$



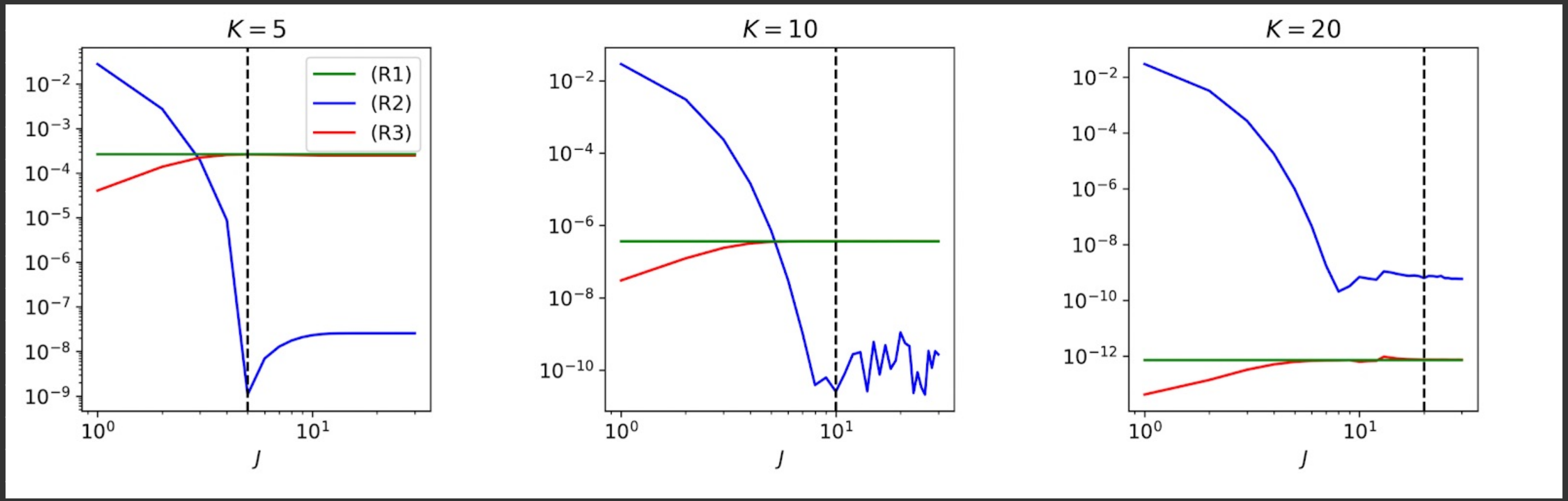
$$\|f\circ X - p^*_{JK}\circ X\|_{\mathcal{L}^2} \le \|f\circ X - \mathcal{P}_K(f\circ X)\|_{\mathcal{L}^2} + \|\mathcal{P}_K(f\circ X - p^*_{JK}\circ X)\|_{\mathcal{L}^2} + \|p^*_{JK}\circ X - \mathcal{P}_K(p^*_{JK}\circ X)\|_{\mathcal{L}^2}$$

$$\|f\circ x - p^*_{JK}\circ x\|_{\mathcal{L}^2} \leq \|f\circ x - \mathcal{P}_K(f\circ x)\|_{\mathcal{L}^2} + \|\mathcal{P}_K(f\circ x - p^*_{JK}\circ x)\|_{\mathcal{L}^2} + \|p^*_{JK}\circ x - \mathcal{P}_K(p^*_{JK}\circ x)\|_{\mathcal{L}^2}$$

Ex// $\dot{x}(t) = \exp(-2x(t))$; $x(0) = 0$.

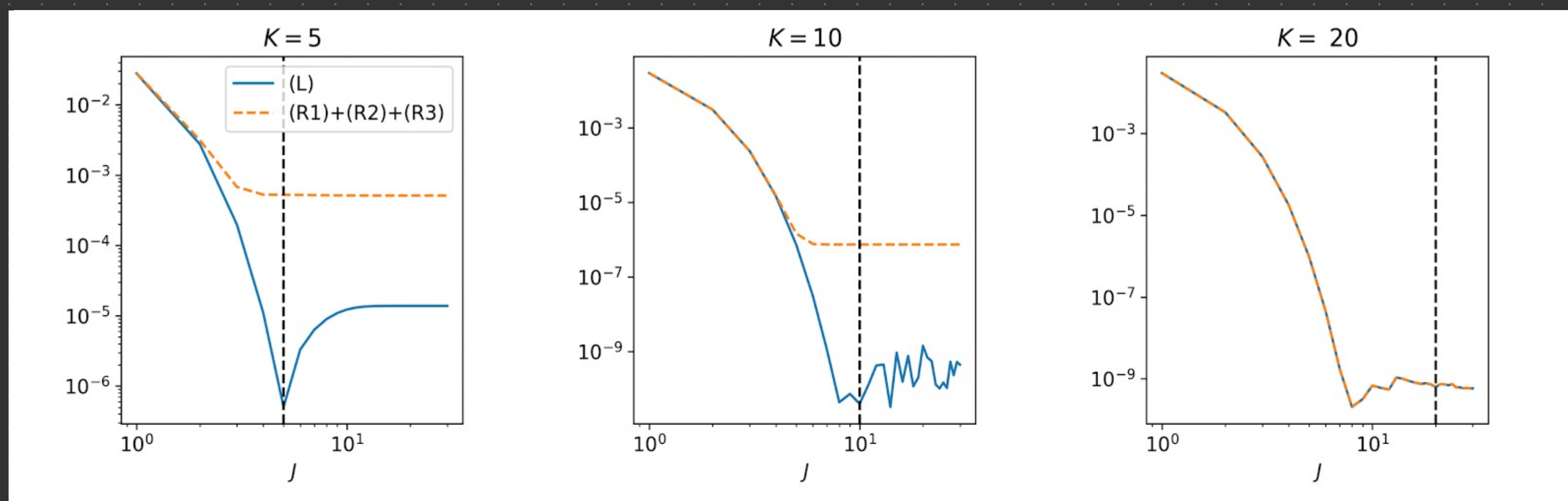
$$\| f\circ x - p^*_{JK}\circ x\|_{\mathcal{L}^2} \leq \| f\circ x - \mathcal{P}_K(f\circ x)\|_{\mathcal{L}^2} + \| \mathcal{P}_K(f\circ x - p^*_{JK}\circ x)\|_{\mathcal{L}^2} + \| p^*_{JK}\circ x - \mathcal{P}_K(p^*_{JK}\circ x)\|_{\mathcal{L}^2}$$

Ex// $\dot{x}(t) = \exp(-2x(t))$; $x(0) = 0$.



$$\| f\circ X - p^*_{JK}\circ X\|_{\mathcal{L}^2} \le \| f\circ X - \mathcal{P}_K(f\circ X)\|_{\mathcal{L}^2} + \|\mathcal{P}_K(f\circ X - p^*_{JK}\circ X)\|_{\mathcal{L}^2} + \|p^*_{JK}\circ X - \mathcal{P}_K(p^*_{JK}\circ X)\|_{\mathcal{L}^2}$$

Ex// $\dot{x}(t) = \exp(-2x(t))$; $x(0) = 0$.



Thanks!