Kernel Methods and Machine Learning

Workshop: The Mathematics of Scientific Machine Learning and Digital Twins

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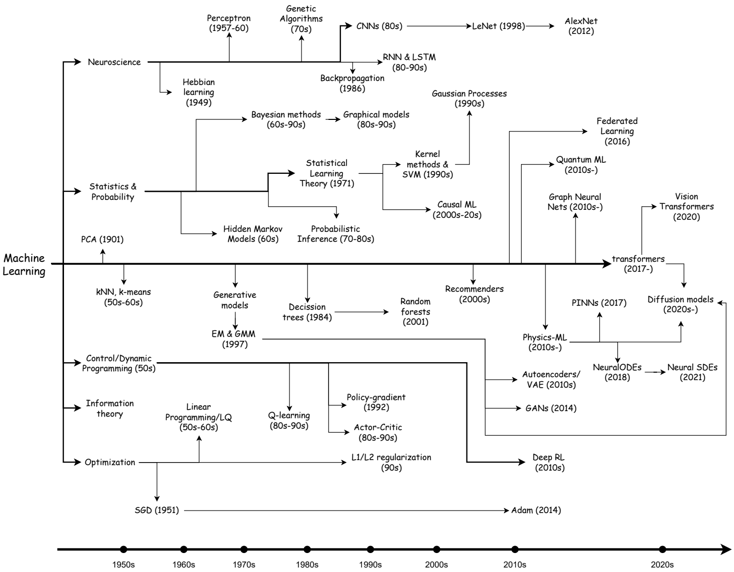
Overview

History of Machine Learning



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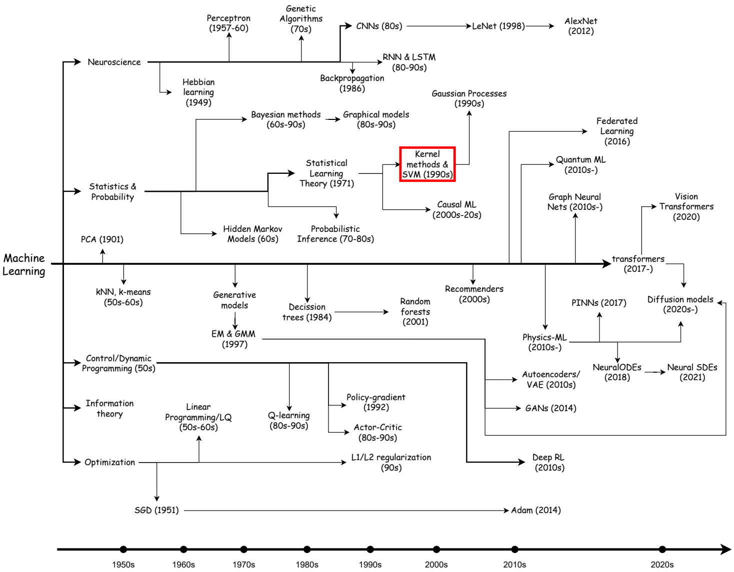


Introduction

Definition

A kernel $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is said to be positive definite if

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j \kappa(x_i, x_j) \geq 0 \qquad c_1, \ldots, c_n \in \mathbb{R},\ x_1, \ldots, x_n \in \mathcal{X}$$

Examples of kernels:

$$\kappa(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right) \qquad \text{(Gaussian kernel)}$$

$$\kappa(x, x') = \exp\langle x, x' \rangle \qquad \text{(Exponential kernel)}$$

$$\kappa(x, x') = (\langle x, x' \rangle + c)^d \qquad \text{(Polynomial kernel)}$$

Introduction: Reproducing Kernel Hilbert Space

We want to take the closure of linear combinations of kernel functions.

$$f := \sum_{i=1}^{n} \alpha_i \kappa(\cdot, x_i), \qquad \alpha_i \in \mathbb{R}, x_i \in \mathcal{X}$$

And we take the inner product as

$$\langle f, g \rangle_{\mathcal{H}_\kappa} \equiv \left\langle \sum_{i=1}^{n} \alpha_i \kappa(\cdot, x_i), \sum_{j=1}^{m} \beta_j \kappa(\cdot, y_j) \right\rangle_{\mathcal{H}_\kappa} := \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j \kappa(x_i, y_j)$$

Theorem (Aronszajn 1950)

Let κ be a symmetric positive definite kernel, then there exists a unique Hilbert space $\mathcal{H}_\kappa$.

1. **Gaussian and exponential kernels:** $\mathcal{H}_\kappa \subseteq C(\mathcal{X})$ dense.

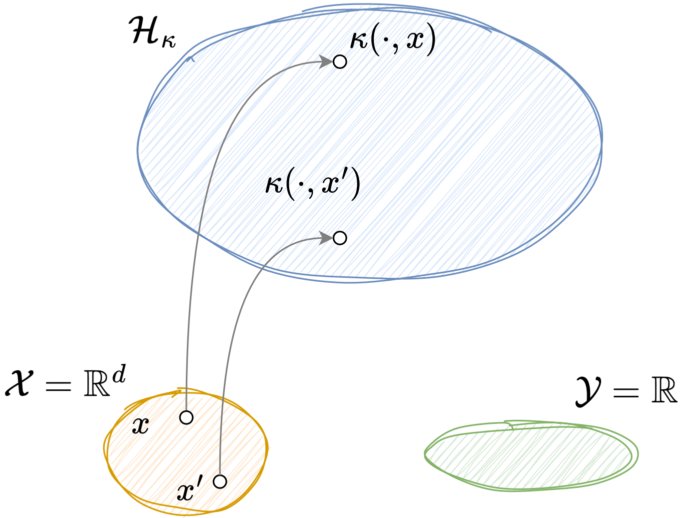
$$\kappa(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right), \qquad \kappa(x, x') = \exp\langle x, x'\rangle$$

2. **Sobolev kernels:** $\mathcal{H}_{\kappa_\nu} \subseteq H^s(\mathbb{R}^d)$ is dense for $s < \nu + d/2$. And for $s = \nu + d/2$, they coincide.

$$\kappa_\nu(x, x') = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\|x - x'\|}{\ell}\right)^\nu K_\nu\left(\frac{\|x - x'\|}{\ell}\right),$$

where K_ν is the modified Bessel function of the second kind.

Idea of Kernel Methods



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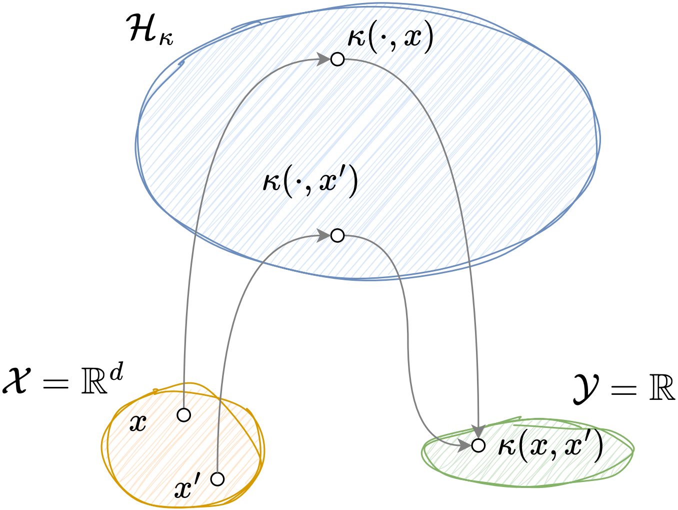

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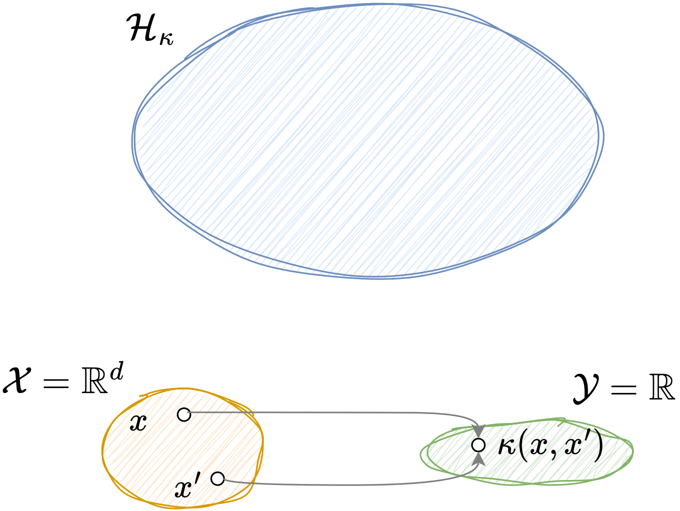

Representer Theorem

Theorem (Schölkopf, Herbrich, et al. 2001)

Suppose we are given training data:

$$(x_1, y_1), \ldots, (x_n, y_n) \in \mathcal{X} \times \mathbb{R}.$$

We consider optimization problems of the form:

$$\min_{f \in \mathcal{H}_\kappa} L((x_1, y_1, f(x_1)), \ldots, (x_n, y_n, f(x_n))) + \lambda \|f\|^2_{\mathcal{H}_\kappa}.$$

Then, any minimizer $f^* \in \mathcal{H}_\kappa$ admits a representation of the form

$$f^*(\cdot) = \sum_{i=1}^{n} \alpha_i \kappa(\cdot, x_i)$$

for some coefficients $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$.

Self-Attention as a Kernel Method

Given a positive semi-definite matrix $\mathbf{A}$, define the kernel

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) := \exp\{-(\mathbf{x}_i - \mathbf{x}_j)^\top \mathbf{A}(\mathbf{x}_i - \mathbf{x}_j)\}$$

where $\mathbf{A} = \frac{1}{2}\mathbb{Q}^\top\mathbb{K}$ and let the value projection be $\mathbf{y} = \mathbb{V}\mathbf{x}$.

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The Nadaraya-Watson smoothing kernel (Nadaraya 1964; Watson 1964):

$$\sum_j \frac{\kappa(\mathbf{x}_i, \mathbf{x}_j)\mathbf{y}_j}{\sum_k \kappa(\mathbf{x}_i, \mathbf{x}_k)}$$

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Key, query, and value matrices are given by $\mathbb{K}, \mathbb{Q}, \mathbb{V}$ respectively.

Proof that Self-Attention is Kernel Regression

Proof.

Expand the exponent:

$$-(\mathbf{x}_i - \mathbf{x}_j)^\top \mathbf{A}(\mathbf{x}_i - \mathbf{x}_j) = -\mathbf{x}_i^\top \mathbf{A}\mathbf{x}_i - \mathbf{x}_j^\top \mathbf{A}\mathbf{x}_j + 2\mathbf{x}_i^\top \mathbf{A}\mathbf{x}_j$$

Then,

$$\begin{aligned}\frac{\kappa(\mathbf{x}_i, \mathbf{x}_j)}{\sum_k \kappa(\mathbf{x}_i, \mathbf{x}_k)} &= \frac{\exp\{-\mathbf{x}_j^\top \mathbf{A}\mathbf{x}_j + 2\mathbf{x}_i^\top \mathbf{A}\mathbf{x}_j\}}{\sum_k \exp\{-\mathbf{x}_k^\top \mathbf{A}\mathbf{x}_k + 2\mathbf{x}_i^\top \mathbf{A}\mathbf{x}_k\}} \\ &= \frac{e^{\langle \mathbb{Q}\mathbf{x}_i, \mathbb{K}\mathbf{x}_j \rangle}}{\sum_k e^{\langle \mathbb{Q}\mathbf{x}_i, \mathbb{K}\mathbf{x}_k \rangle}}\end{aligned}$$

where we have assumed that $\mathbf{x}_j^\top \mathbf{A}\mathbf{x}_j$ is constant for all j. □

Neural Tangent Kernel (Jacot et al. 2018)

- **Training data:** $\mathcal{D} = \{(X_i, Y_i)\}_{i=1}^n$
- **Model:**

$$f_\theta(x) = \sum_{j=1}^m a_j \sigma(w_j^\top x + b_j)$$

- **Squared loss:**

$$\mathcal{L}(\theta) = \frac{1}{2}\sum_{i=1}^n (f_\theta(X_i) - Y_i)^2$$

- **Gradient flow:**

$$\begin{aligned} \dot{\theta}_t &:= -\nabla_\theta \mathcal{L}(\theta_t) \\ &= -\nabla_\theta f_{\theta_t}(X)^\top (f_{\theta_t}(X) - Y) \end{aligned}$$

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This is exactly kernel regression!

Mean-Field Neural Networks (Barron Spaces)

Finite-width NN:

$$f_\theta(x) = \sum_{i=1}^{n} a_i \sigma(w_i^\top x + b_i) \tag{1}$$

where $\theta_i = (a_i, w_i, b_i) \in \mathbb{R}^{d+2}$.

Mean-Field NN:

$$f_\pi(x) = \int_{\mathbb{R}^{d+2}} a\sigma(w^\top x + b) d\pi(a, w, b)$$

where $\pi \in \mathcal{P}(\mathbb{R}^{d+2})$ is a probability measure.

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Consider the norm

$$\|f\|_{\mathcal{B}_\sigma} := \inf_{f = f_\pi} \int_{\mathbb{R}^{d+2}} |a|(1 + \|w\|_1 + |b|) d\pi$$

Theorem (Spek et al. 2023)

The space of mean-field NN with norm $\|\cdot\|_{\mathcal{B}_\sigma}$ is a reproducing kernel Banach space.

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Theorem (Bartolucci et al. 2021)

Let $\{(x_i, y_i)\}_{i=1}^n$ be training data. Then

$$\inf_{f \in \mathcal{B}_\sigma} \frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i)) + \lambda \|f\|_{\mathcal{B}_\sigma}$$

admits a minimizer of the form (1).

Neural Networks vs. Kernel Methods

We want to compare kernel methods with neural networks

$$\sum_i a_i \sigma(w_i^\top x + b_i) \qquad \text{vs} \qquad \sum_i \alpha_i \kappa(x, x_i)$$

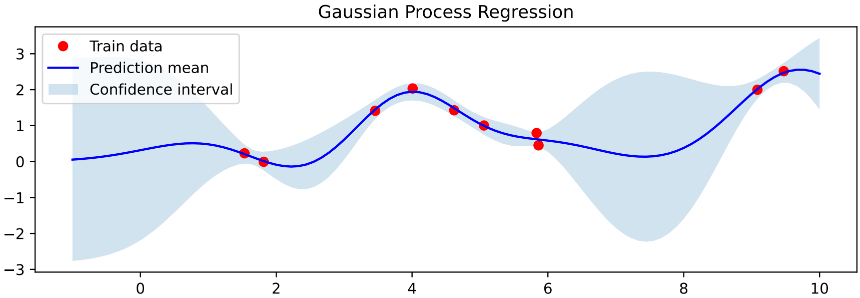
	Neural Networks	**Kernel Methods**
Universal Approximation	✓	✓
Representer Theorem	✓	✓
Compatibility	✓	✓
Interpretability	✗	**?**
Scalability	✓	**?**
Experiments	✓	**?**

Interpretability of Kernel Methods

Decomposability:

$$f(x) = \sum_i \overbrace{\alpha_i}^{\text{weight}} \underbrace{\kappa(x, x_i)}_{\text{similarity}}$$

Uncertainty Quantification:



Experiments: Kernel Methods and Digital Twins

Data: $\{y_{t,i}\}_{i=1}^{n}$.
Goal: learn the vector field $f \in \mathcal{F}$ so that $z_t \approx y_t$ with

$$\dot{z}_t = f(z_t), \qquad z_0 = y_0$$

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$$\boxed{\begin{aligned} &\inf_{f \in \mathcal{F}} \quad \frac{1}{2n} \sum_{i=1}^{n} \int_0^T \|z_{t,i} - y_{t,i}\|^2 dt + \frac{\lambda}{2} \|f\|_{\mathcal{F}}^2 \\ &\quad \text{s.t. } \dot{z}_{t,i} = f(z_{t,i}), \quad z_{0,i} = y_{0,i}. \end{aligned}}$$

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NeuralODE (Chen et al. 2018)

- Model:

$$f_\theta \in \mathsf{NN}(\Theta)$$

- Regularization:

$$\|f_\theta\|_{\mathcal{F}} := \|\theta\|_2$$

KernelODE (Owhadi 2020)

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$$f \in \mathcal{H}_\kappa$$

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NeuralODE (Chen et al. 2018)

$$\begin{aligned} \dot{z}_{t,i} &= f_\theta\big(z_{t,i}\big), \\ \dot{p}_{t,i} &= (z_{t,i} - y_{t,i}) - \big(Df_\theta(z_{t,i})\big)^\top p_{t,i}, \\ \theta &= -\frac{1}{\lambda n}\sum_{j=1}^n \int_0^T (\partial_\theta f_\theta(z_{s,j}))^\top p_{s,j}\, ds. \end{aligned}$$

KernelODE (Owhadi 2020),
Mean-Field NeuralODE (Jabir et al. 2021)

$$\begin{aligned} \dot{z}_{t,i} &= f\big(z_{t,i}\big), \\ \dot{p}_{t,i} &= (z_{t,i} - y_{t,i}) - \big(Df(z_{t,i})\big)^\top p_{t,i}, \\ f(\cdot) &= -\frac{1}{\lambda n}\sum_{j=1}^n \int_0^T K\big(\cdot, z_{s,j}\big)\, p_{s,j}\, ds. \end{aligned}$$

where $z_{0,i} = y_{0,i}$ and $p_{T,i} = 0$.

FitzHugh–Nagumo

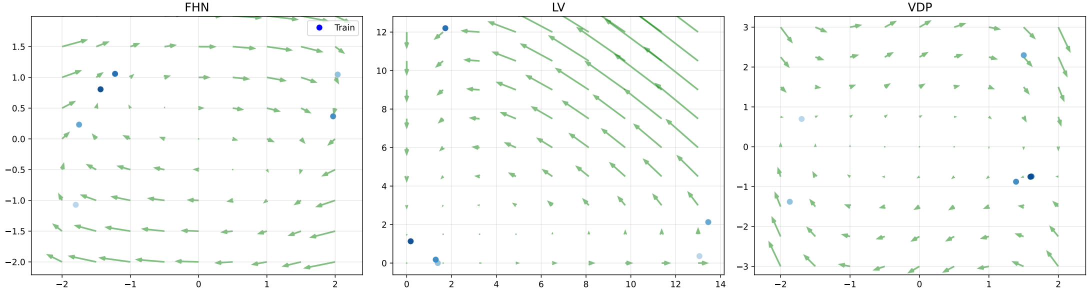
$$\dot{x}_1 = 3\left(x_1 - \frac{x_1^3}{3} + x_2\right),$$
$$\dot{x}_2 = \frac{0.2 - 3x_1 - 0.2x_2}{3}$$

Lotka–Volterra

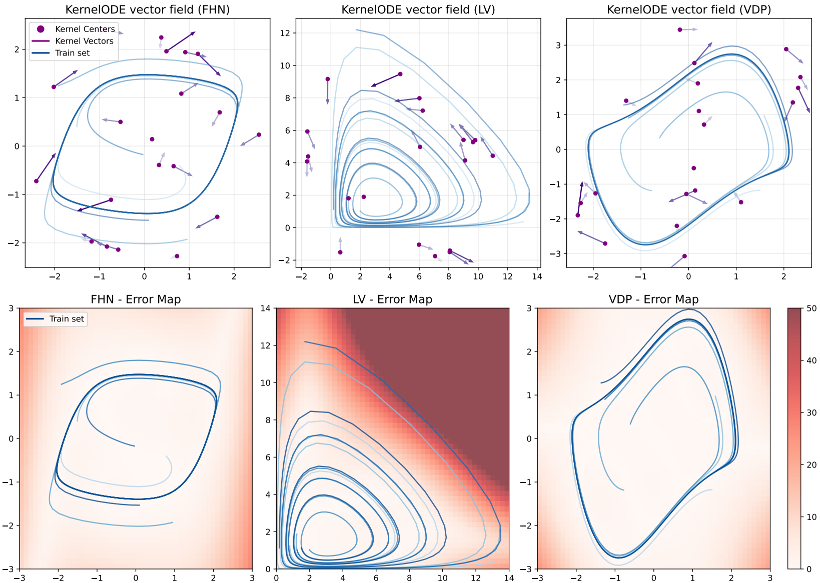
$$\dot{x}_1 = 1.5\,x_1 - x_1x_2,$$
$$\dot{x}_2 = -3\,x_2 + x_1x_2$$

Van der Pol

$$\dot{x}_1 = x_2,$$
$$\dot{x}_2 = (1 - x_1^2)\,x_2 - x_1$$



Experiments: Kernel Methods and Digital Twins



Experiments: Kernel Methods and Digital Twins

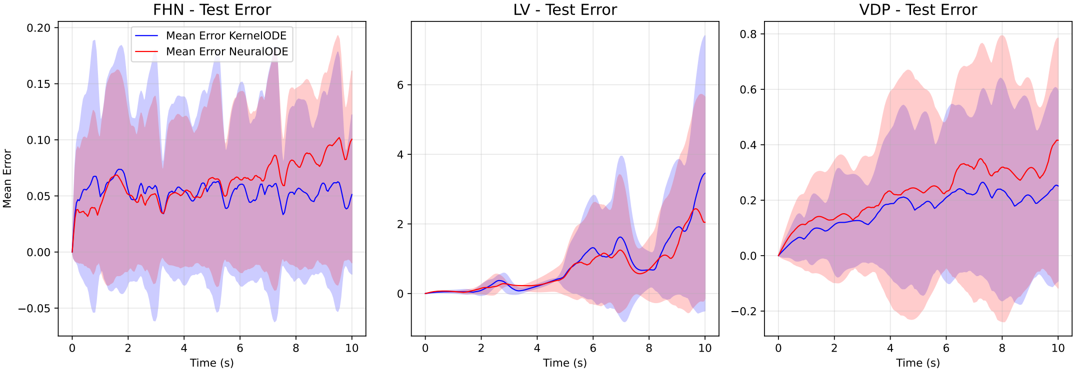


Figure: Comparison between NeuralODE and KernelODE.

Applications of Kernel Methods

Algorithms based on Kernel Methods:

- Gaussian Processes (Rasmussen et al. 2005)
- Support Vector Machines (Cortes et al. 1995)
- Kernel PCA (Schölkopf, Alexander Smola, et al. 1998)
- Kernel Mean Embeddings (Alex Smola et al. 2007)
- Neural Tangent Kernels (Jacot et al. 2018)
- Operator Learning (Batlle et al. 2023)
- Kernel-based Transformers (Choromanski et al. 2022; Peng et al. 2021)

Large Scale Applications:

- Large-scale kernel machines (Rahimi et al. 2007)
- Random Feature Attention (Peng et al. 2021): $\mathcal{O}(n^2)$ to $\mathcal{O}(nm)$.
- Rethinking Attention with Performers (Choromanski et al. 2022)
- Nyströmformer: A Nyström-Based Algorithm for Approximating Self-Attention (Xiong et al. 2021).
- Kernel Methods are Competitive for Operator Learning (Batlle et al. 2023)

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