Two Tales, One Resolution for Physics-Informed Inference-time Scaling

Debiasing and Precondition

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Ruihan Xu (Uchicago)

My Journey

- Undergrad: Peking University: 2015-2019
  - Work with Prof. Bin Dong and Prof. Liwei Wang
- Ph.D. Stanford University: 2019-2023
  - Work with Prof. Lexing Ying and Jose E

Beyond Finite Layer Neural Networks: Bridging Deep Architectures and Numerical Differential Equations

Yiping Lu [1] **Aoxiao Zhong** [2] **Quanzheng Li** [2 3 4] **Bin Dong** [5 6 4]

Abstract

Deep neural networks have become the state-of-the-art models in numerous machine learning tasks. However, general guidance to network architecture design is still missing. In our work, we bridge deep neural network design with numerical differential equations. We show that many effective networks, such as ResNet, PolyNet, FractalNet and RevNet, can be interpreted as different numerical discretizations of differential equations. This finding brings us a brand new perspective on the design of effective deep architectures. We can take advantage of the rich knowledge in numerical analysis to guide us in de- s while maintaining a similar performance. This can be explained mathematically using the concept of modified equation from numerical analysis. Last but not least, we also establish a connection between stochastic control and noise injection in the training process which helps to improve generalization of the networks. Furthermore, by relating stochastic training strategy with stochastic dynamic system, we can easily apply stochastic training to the networks with the LM-architecture. As an example, we introduced stochastic depth to LM-ResNet and achieve significant improvement over the original LM-ResNet on CIFAR10.

PDE-NET: LEARNING PDES FROM DATA

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Machine Learning For Elliptic PDEs:
Fast Rate Generalization Bound, Neural Scaling Law and Minimax Optimality

Yiping Lu*, Haoxuan Chen†, Jianfeng Lu ‡, Lexing Ying§, and Jose Blanchet ¶

Abstract. In this paper, we study the statistical limits of deep learning techniques for solving elliptic partial differential equations (PDEs) from random samples using the Deep Ritz Method (DRM) and Physics-Informed Neural Networks (PINNs). To simplify the problem, we focus on a prototype elliptic PDE: the Schrödinger equation on a hypercube with zero Dirichlet boundary condition, which is applied in quantum-mechanical systems. We establish upper and lower bounds for both methods, which improve upon concurrently developed upper bounds for this problem via a fast rate generalization bound. We discover that the current Deep Ritz Method is sub-optimal and propose a modified version of it. We also prove that PINN and the modified version of DRM can achieve minimax optimal bounds over Sobolev spaces. Empirically, following recent work which has shown that the deep model accuracy will improve with growing training sets according to a power law, we supply computational experiments to show similar-behavior of dimension dependent power law for deep PDE solvers.

Minimax Optimal Kernel Operator Learning via Multilevel Training

Jikai Jin,[*,1] Yiping Lu,[*,2] Jose Blanchet,[*,3] and Lexing Ying[*,4]

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Do you trust your theorem?

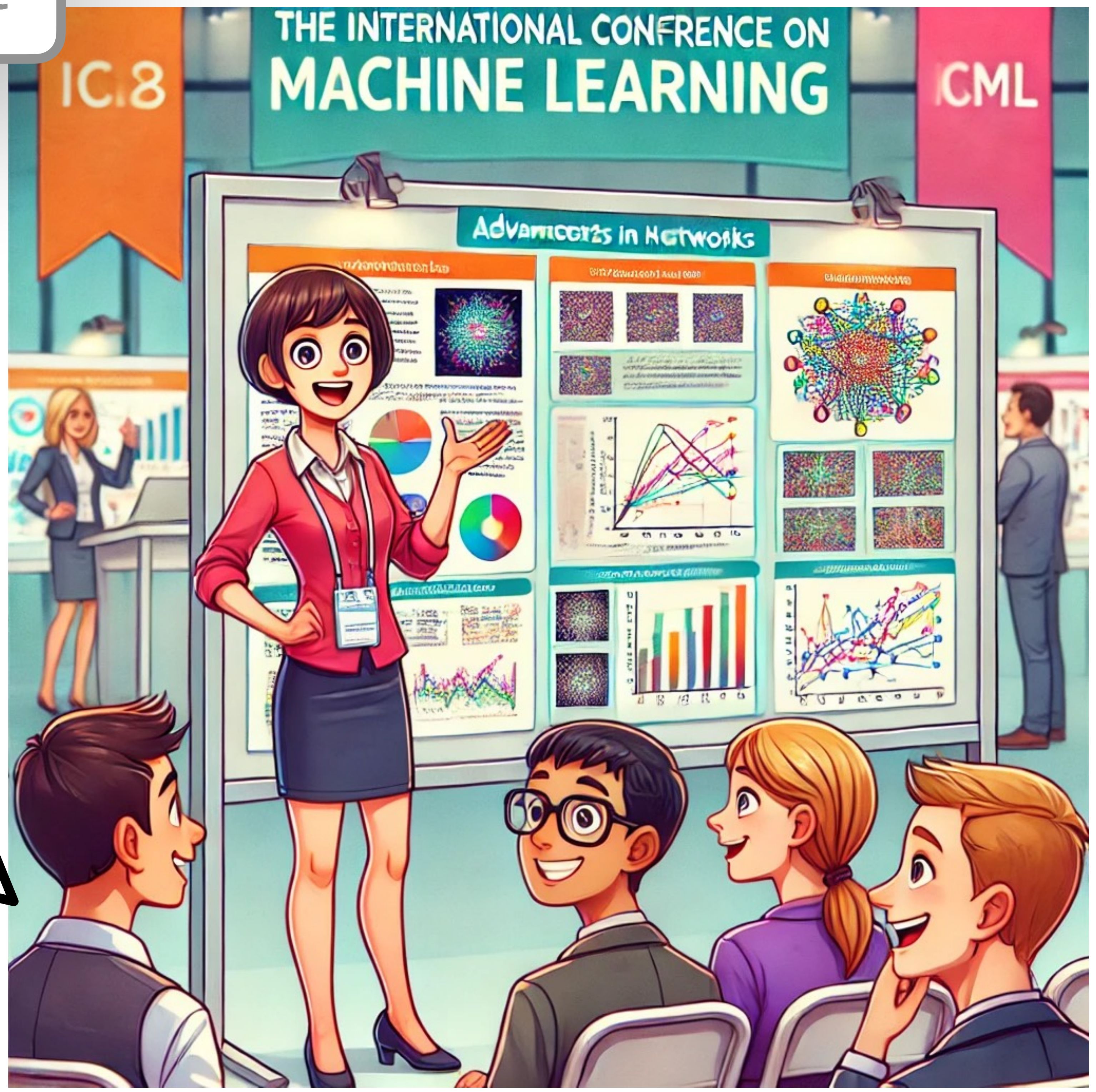
Big Constant

Theorem If you randomly collect ( ) data, then you can achieve ( ) accuracy with your AI!

Relu network is optimal for function regression
PINN is optimal for differential equation solving
Diffusion Model is optimal for density estimation
Transformer is optimal for in-context learning
…

Global optimization, the structure of target function,
The smoothness of ReLU, lower bound of $p(x)$…

Does Optimal results really gives me guarantee?



Consider How you use ChatGPT…

What is the most efficient route from Times Square to Chelsea Market that minimizes walking?

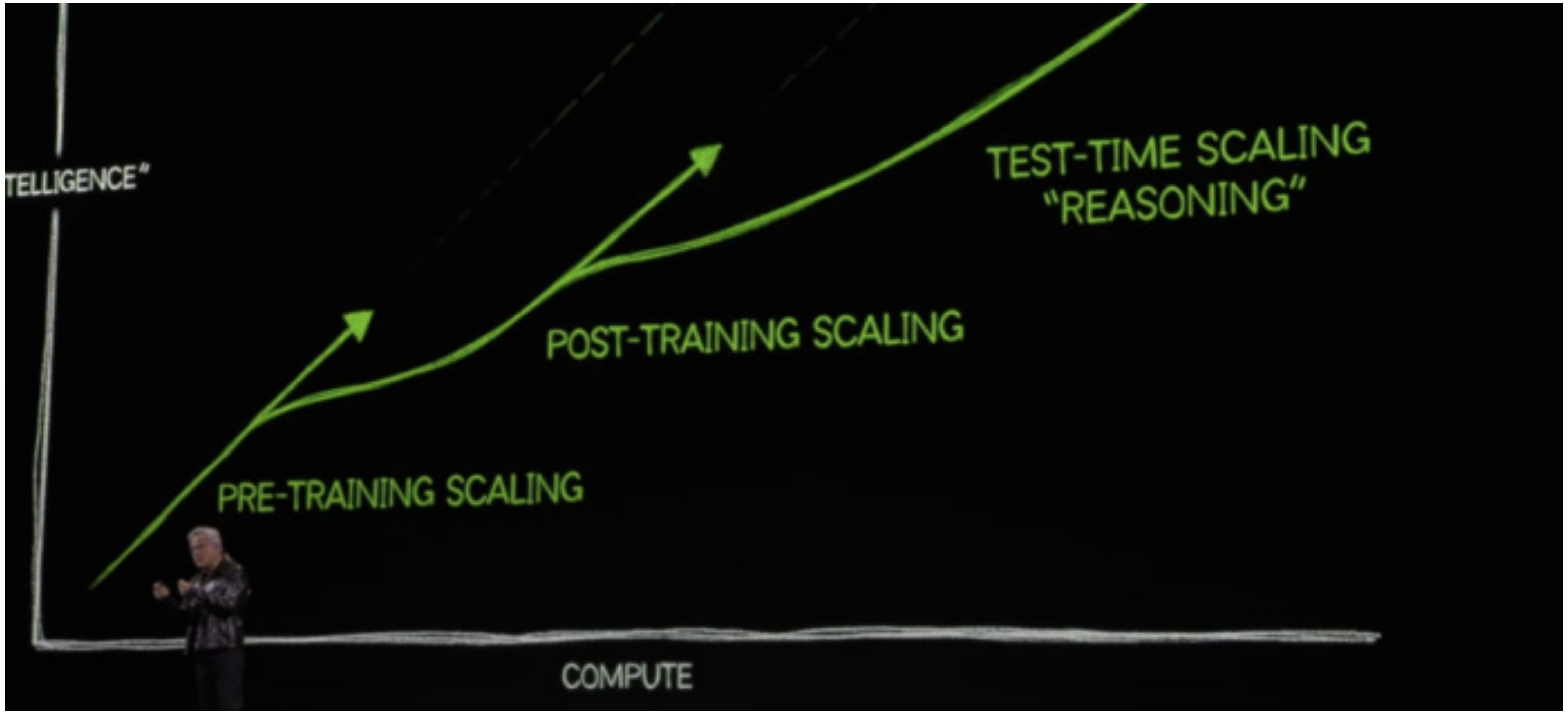
Option 1: Subway

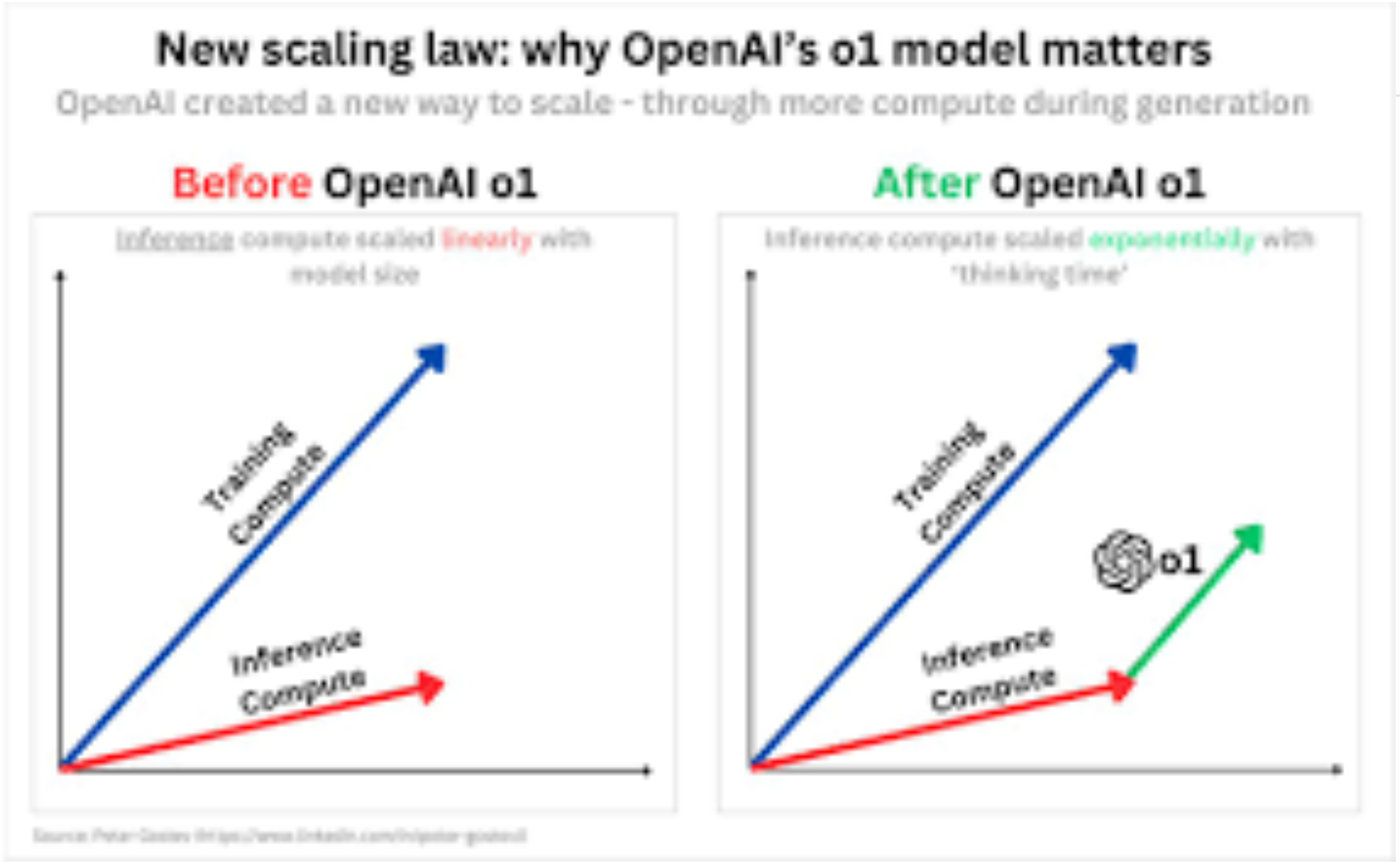
1. **Walk to a Nearby Subway Entrance:** Head to the Times Sq–42nd Street station.
2. **Board the E Train:** Catch an E train heading downtown (toward World Trade Center).
3. **Ride to 8th Avenue–14th Street Station:** Get off at this station (roughly 4 stops).
4. **Walk to Chelsea Market:** Exit the station and walk east on 14th Street for a few blocks until you reach Chelsea Market at 75 9th Avenue.

double-check with a map

1. **At Times Square:** Enter the Times Square–42nd Street station.
2. **Board the 1 Train:** Hop on a downtown 1 train (the red line).
3. **Ride to 14th Street:** Stay on until you reach the 14th Street station.
4. **Exit Appropriately:** Use the exit that leads toward 9th Avenue—this drop-off point is just a short walk from Chelsea Market (located at 75 9th Ave).

Inference Time Scaling Law





How can we perform Inference-Time Scaling for Scientific Machine Learning?

With trustworthy garuntee

don’t fine-tune/retrain/add a new surrogate model

How can we perform Inference-Time Scaling for Scientific Machine Learning?

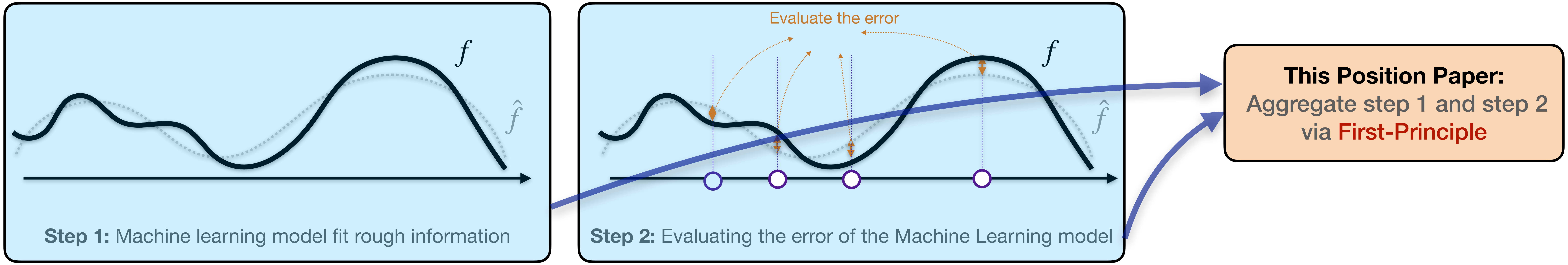
“Physics-informed”

With trustworthy garuntee

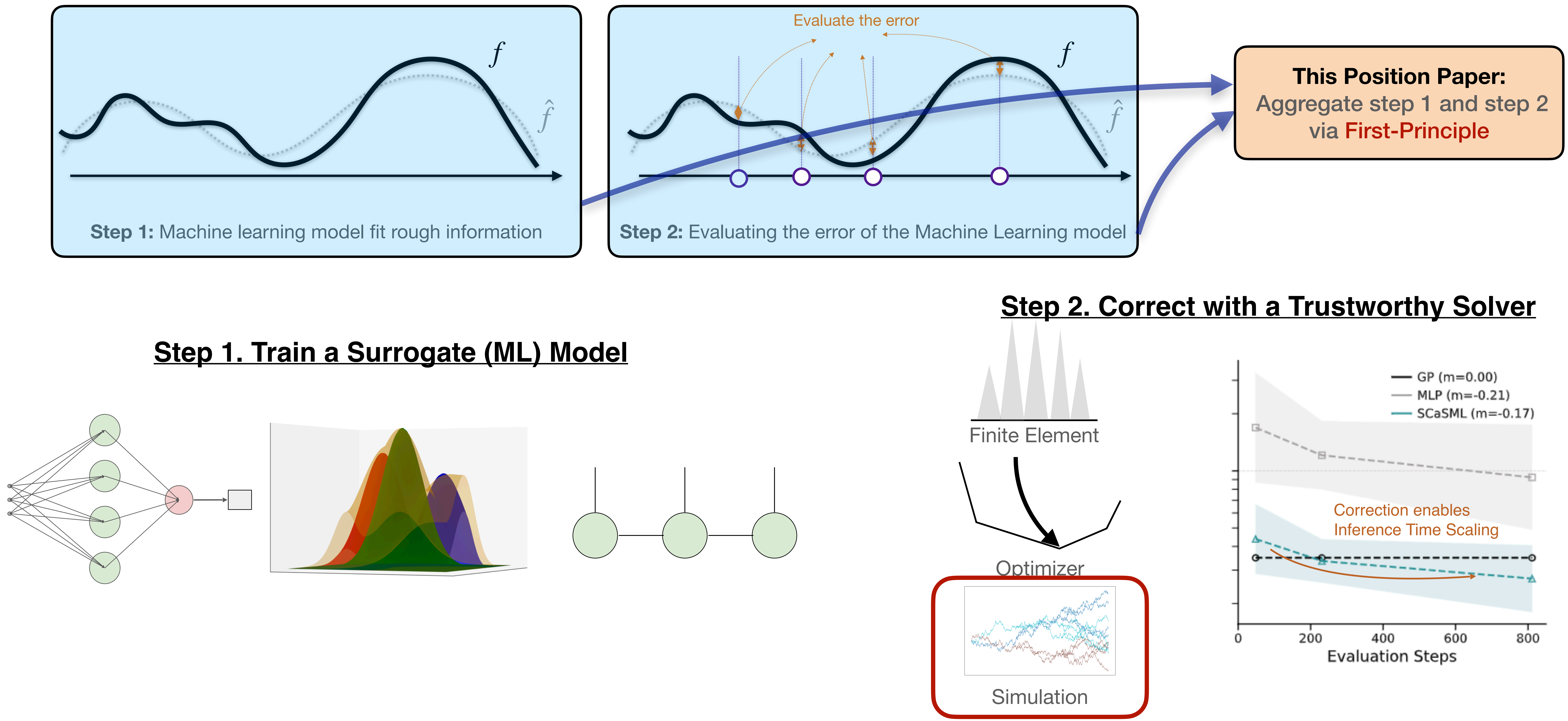
Tale 1: Debiasing

Hybrid Scientific Computing and Machine Learning

Physics-Informed Inference Time Scaling



Physics-Informed Inference Time Scaling



Our Framework

Step 1: Sceintific Computing as Machine Learning

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \hat{\theta} \to \Phi(\hat{\theta})$$

Scientific Machine Learning

Example 1

$$\theta = f, \quad X_i = (x_i, f(x_i))$$

Function fitting

Example 2

$$\theta = \Delta^{-1} f, \quad X_i = (x_i, f(x_i))$$

Solving $\Delta u = f$

Solving PDE

Example 3

$$\theta = A, \quad X_i = (x_i, Ax_i)$$

Estimation $\hat{A}$ via Randomized SVD

Our Framework

Step 2: Consider a Downstream Application

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \rightarrow \hat{\theta} \rightarrow \Phi(\hat{\theta})$$

Scientific Machine Learning — Downstream application

Example 1 $\theta = f, \quad X_i = (x_i, f(x_i))$ $\Phi(\theta) = \int f(x)dx$

Example 2 $\theta = \Delta^{-1}f, \quad X_i = (x_i, f(x_i))$ $\Phi(\theta) = (\Delta^{-1}f)(x)$

Example 3 $\theta = A, \quad X_i = (x_i, Ax_i)$ $\Phi(\theta) = \text{tr}(A), \text{eigs}(A)$

Our Framework

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \hat{\theta} \to \Phi(\hat{\theta})$$

Scientific Machine Learning   Downstream application

AIM: Unbiased prediction even with biased machine learning estimator

AIM: Compute $\Phi(\hat{\theta}) - \Phi(\theta)$ during Inference time

Using (stochastic) simulation to calibrate the (scientific) machine learning output !

Our Framework

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \rightarrow \hat{\theta} \rightarrow \Phi(\hat{\theta})$$

Scientific Machine Learning　　　　Downstream application

AIM: Unbiased prediction even with biased machine learning estimator

How to estimate $\Phi(\hat{\theta}) - \Phi(\theta)$?

Physics-Informed! (Structure of Φ)

Why it is easier than directly estimate $\Phi(\theta)$?

Variance Reduction

Our Framework

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \hat{\theta} \to \Phi(\hat{\theta})$$

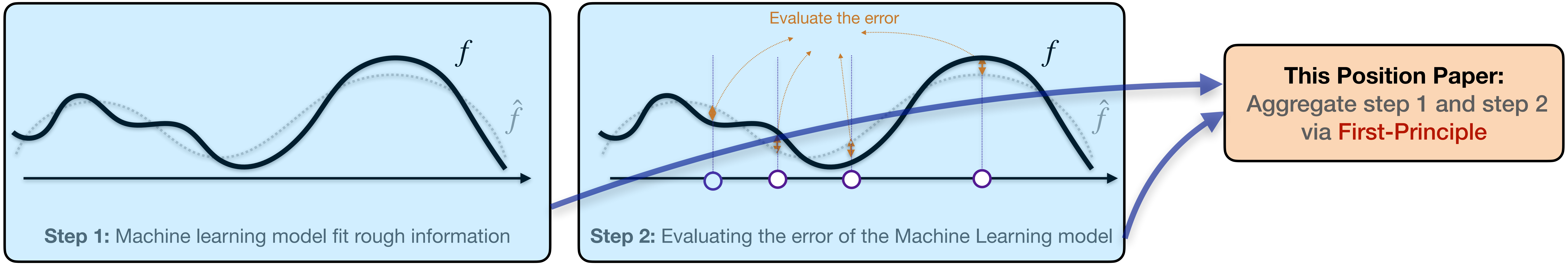
Scientific Machine Learning

Downstream application

AIM: Unbiased prediction even with biased machine learning estimator

- Qudrature Rule
- PDE Solver
- Eigenvalue Solver

Debiasing a Machine Learning Solution



$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \hat{\theta} \to \Phi(\hat{\theta})$$

Scientific Machine Learning

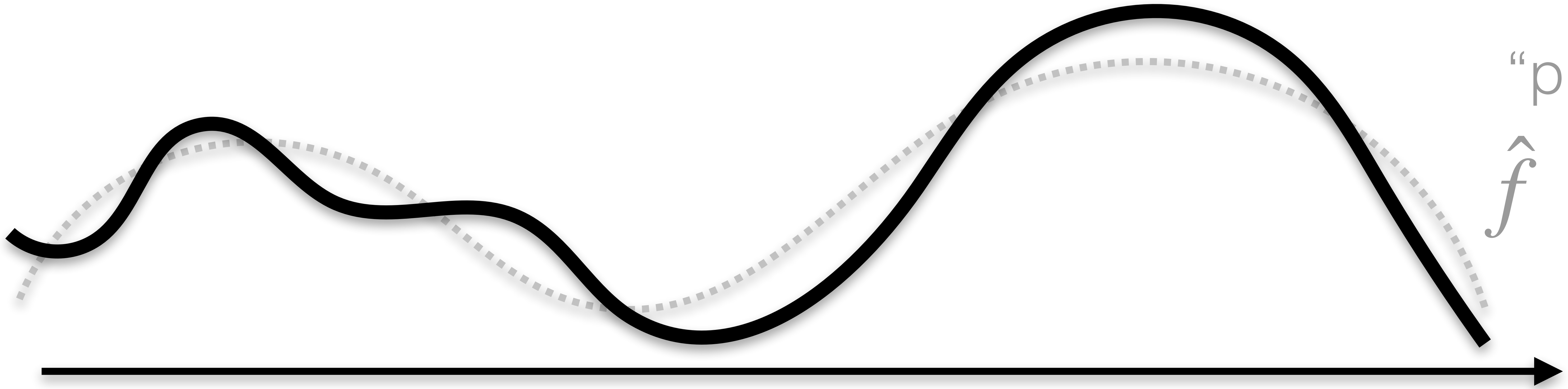
Downstream application

Example 1

$$\theta = f, \quad X_i = (x_i, f(x_i)) \qquad \Phi(\theta) = \int f^q(x)dx$$

Temperature, overall velocity…

Debiasing a Machine Learning Solution



$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \rightarrow \hat{\theta} \rightarrow \Phi(\hat{\theta})$$

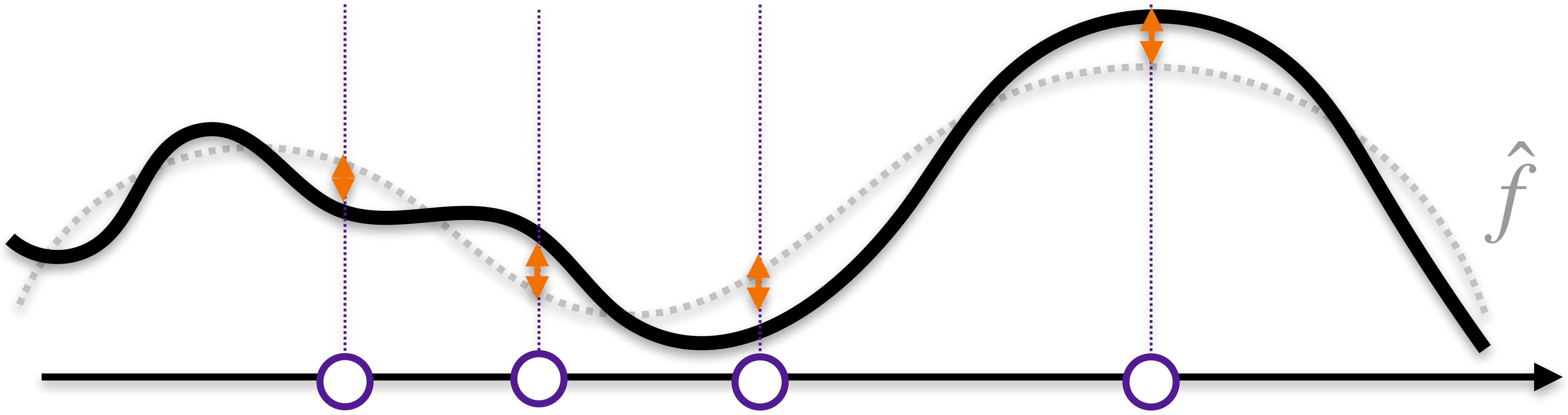
Scientific Machine Learning

Downstream application

Example 1 $\theta = f, \quad X_i = (x_i, f(x_i))$ $\quad \Phi(\theta) = \int f^q(x)dx$

Temperature, overall velocity…

Debiasing a Machine Learning Solution



Our Approah

Estimate $\mathbb{E}_P f \approx \mathbb{E}_P \hat{f}$
$+\mathbb{E}_{\hat{P}} f - \hat{f}$

An estimate to $\Phi(\hat{\theta}) - \Phi(\theta)$

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \hat{\theta} \to \Phi(\hat{\theta})$$

Scientific Machine Learning

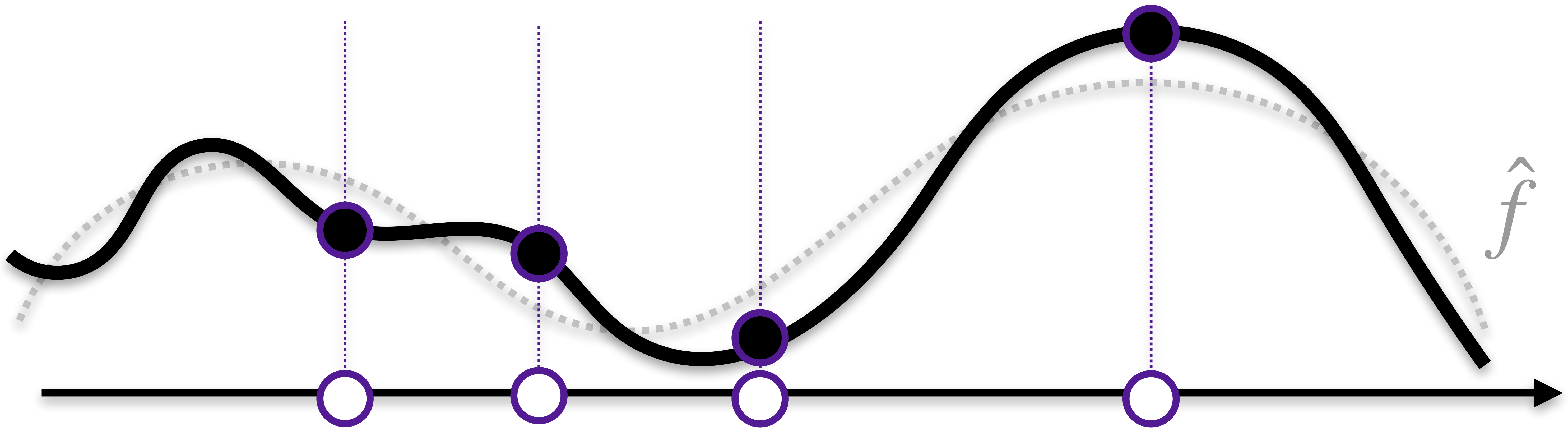
Downstream application

Example 1

$$\theta = f, \quad X_i = (x_i, f(x_i)) \qquad \Phi(\theta) = \int f^q(x)dx$$

Temperature, overall velocity…

Debiasing a Machine Learning Solution



Monte Carlo?

Estimate $\mathbb{E}_P f \approx \mathbb{E}_{\hat{P}} f$

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \hat{\theta} \to \Phi(\hat{\theta})$$

Scientific Machine Learning

Downstream application

Example 1 $\theta = f, \quad X_i = (x_i, f(x_i))$ $\Phi(\theta) = \int f^q(x)dx$

Temperature, overall velocity…

Debiasing a Machine Learning Solution

Regression-adjusted Control Variates | **Doubly Robust Estimator** | **Multi-fidelity monte carlo** | …

- Investigated the optimality of the SCaSML Framework
  - Jose Blanchet, Haoxuan Chen, Yiping Lu, Lexing Ying. When can Regression-Adjusted Control Variates Help? Rare Events, Sobolev Embedding and Minimax Optimality Neurips 2023

- Extend to nonlinear functional estimation using iterative methods **Later**

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \hat{\theta} \to \Phi(\hat{\theta})$$

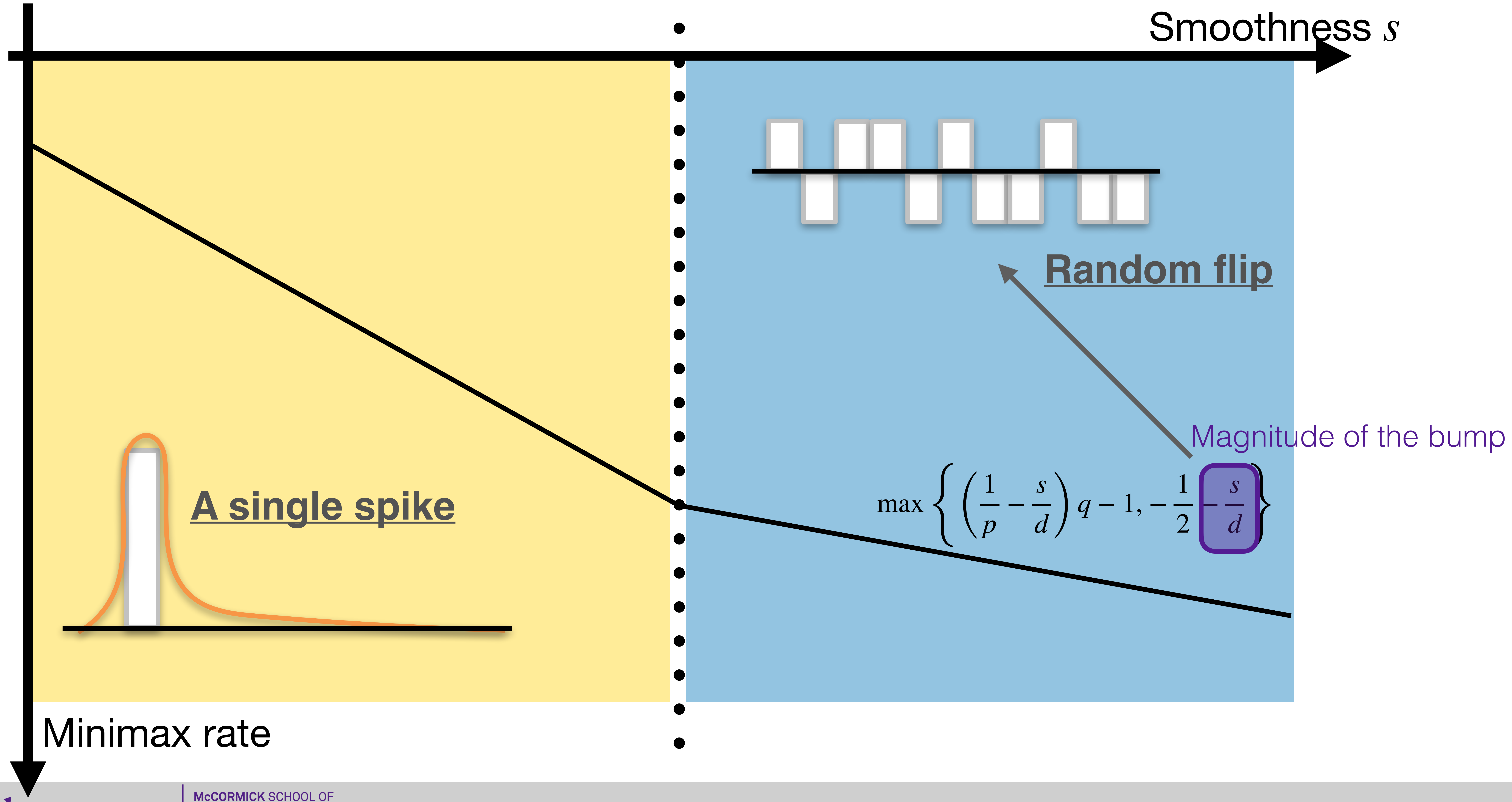
Scientific Machine Learning — Downstream application

Example 1 $\theta = f, \quad X_i = (x_i, f(x_i))$ $\quad \Phi(\theta) = \int f^q(x)dx$

Temperature, overall velocity…

Lower Bound

Hardest Examples



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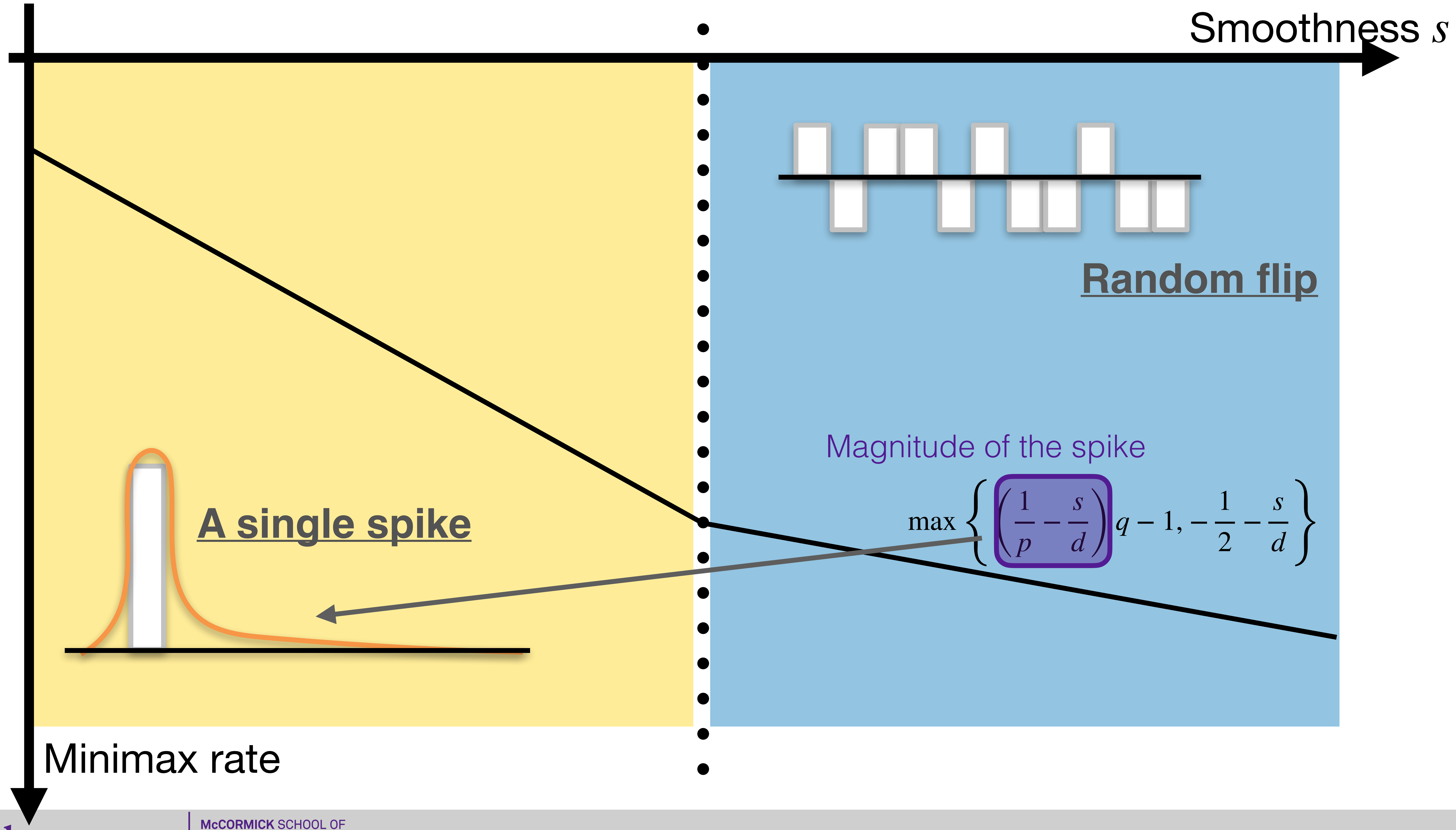
Hardest Examples



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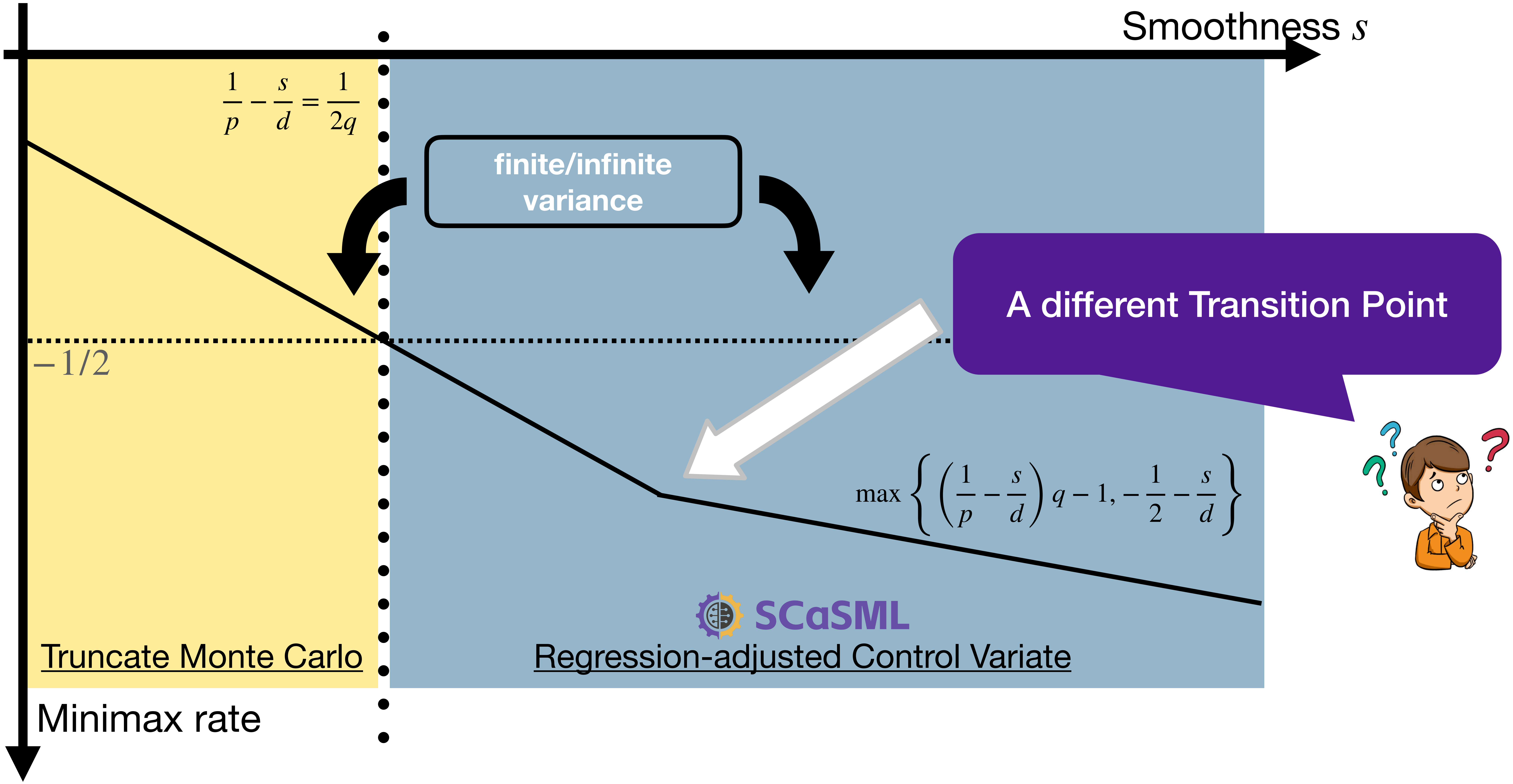
Optimal Algorithms

Easiest Understanding



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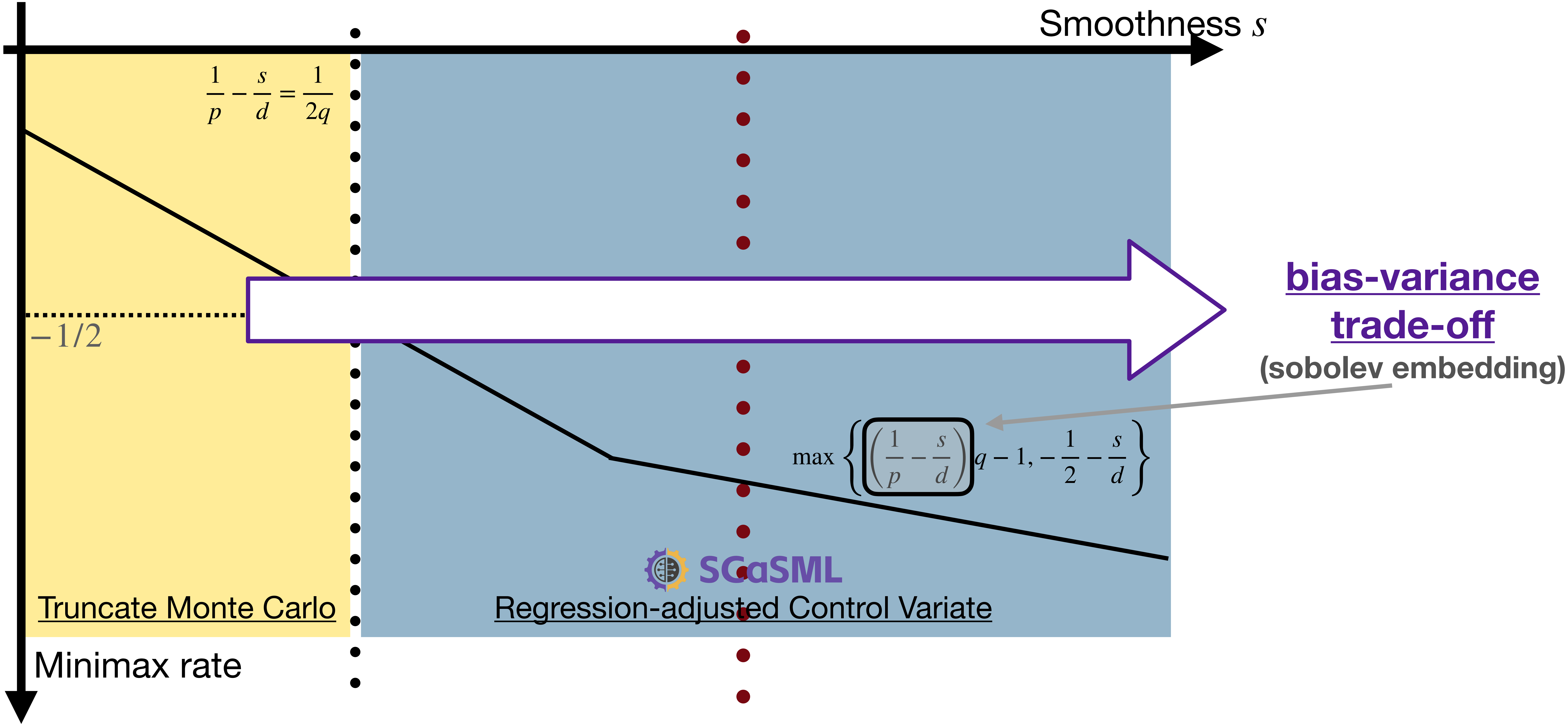
Easiest Understanding



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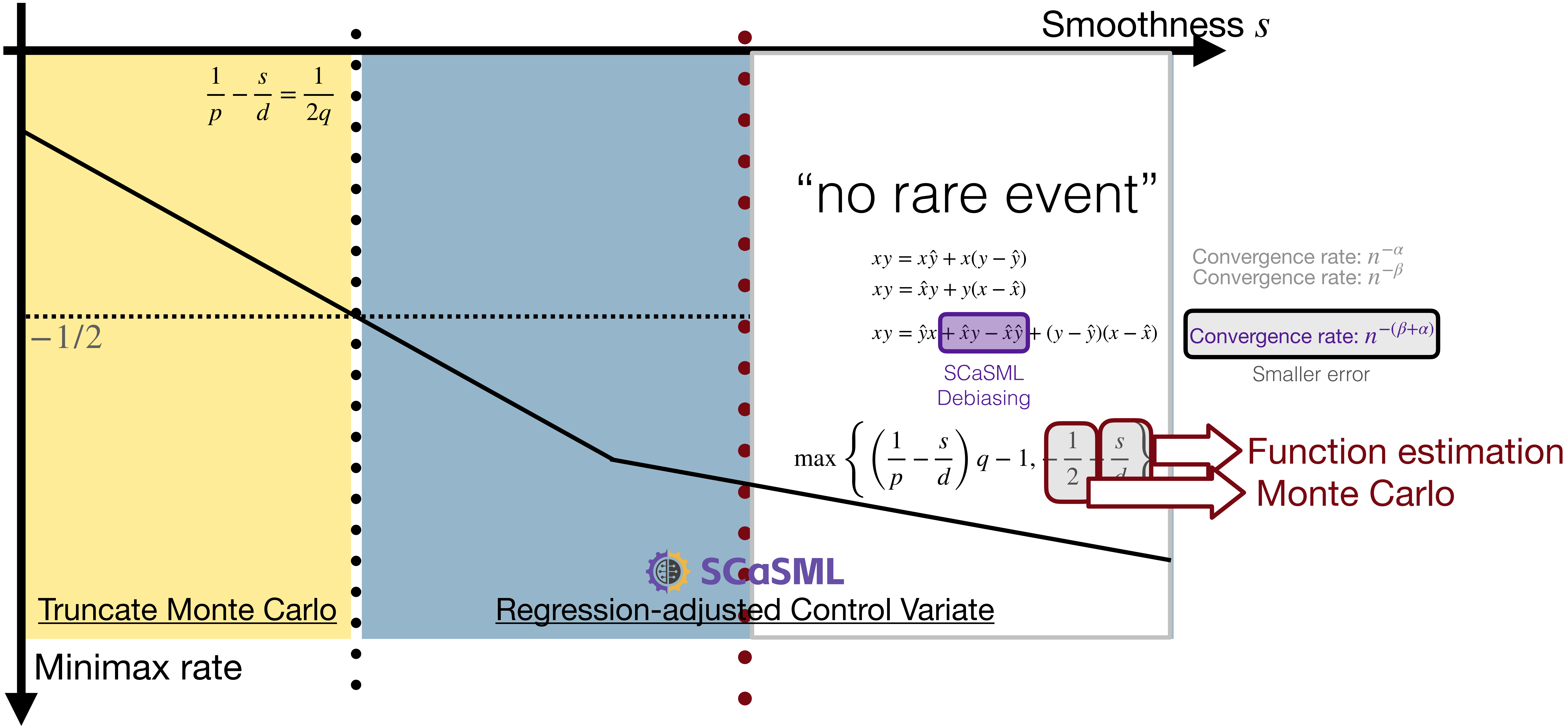
Easiest Understanding

SCaSML



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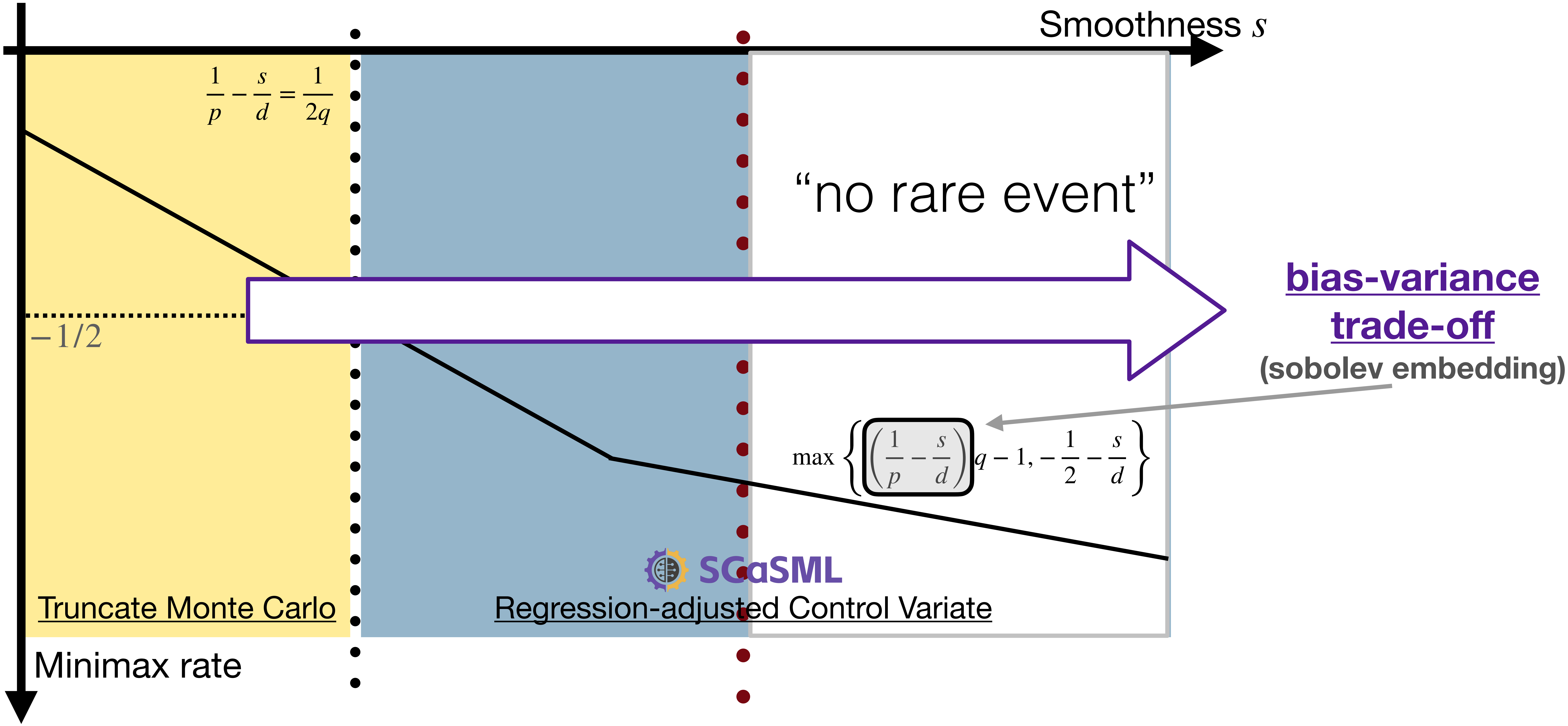
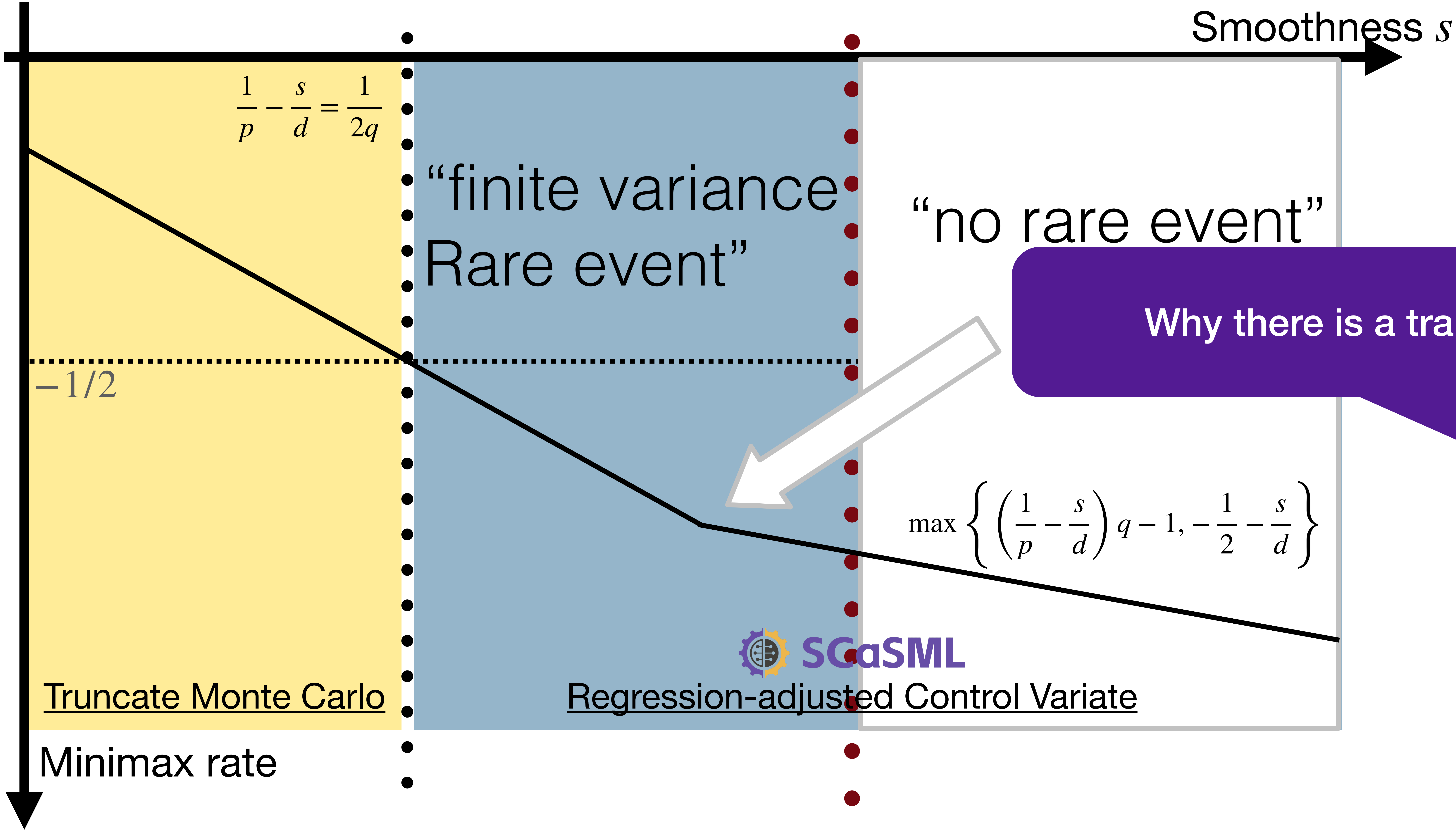
Easiest Understanding



Why…



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Analysis of Error propagation

SCaSML

SCaSML estimate of $\mathbb{E}_P f^q, f \in W^{s,p}$

Step 1 Using half of the data to estimate $\hat{f}$

Step 2 $\mathbb{E}_P f^q = \mathbb{E}_P(\hat{f}^q) + \mathbb{E}_P(f^q - \hat{f}^q)$

How does step2 variance depend on estimation error?

Hardness = The variance of the debasing step

Analysis of Error propagation

SCaSML estimate of $\mathbb{E}_P f^q, f \in W^{s,p}$

Step 1 Using half of the data to estimate $\hat{f}$

Step 2 $\mathbb{E}_P f^q = \mathbb{E}_P(\hat{f}^q) + \mathbb{E}_P(f^q - \hat{f}^q)$

How does step2 variance depend on estimation error?

Low order term: $f^q - \hat{f}^q$

$f^{q-1}(f-\hat{f}) + (f-\hat{f})^q$

"influnce function" (gradient): $f^{q-1}(f-\hat{f})$

Error propagation: $(f-\hat{f})^q$

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Analysis of Error propagation

SCaSML

SCaSML estimate of $\mathbb{E}_P f^q, f \in W^{s,p}$

Step 1 Using half of the data to estimate $\hat{f}$

Step 2 $\mathbb{E}_P f^q = \mathbb{E}_P(\hat{f}^q) + \mathbb{E}_P(f^q - \hat{f}^q)$

Low order term

$f^{q-1}(f - \hat{f}) + (f - \hat{f})^q$

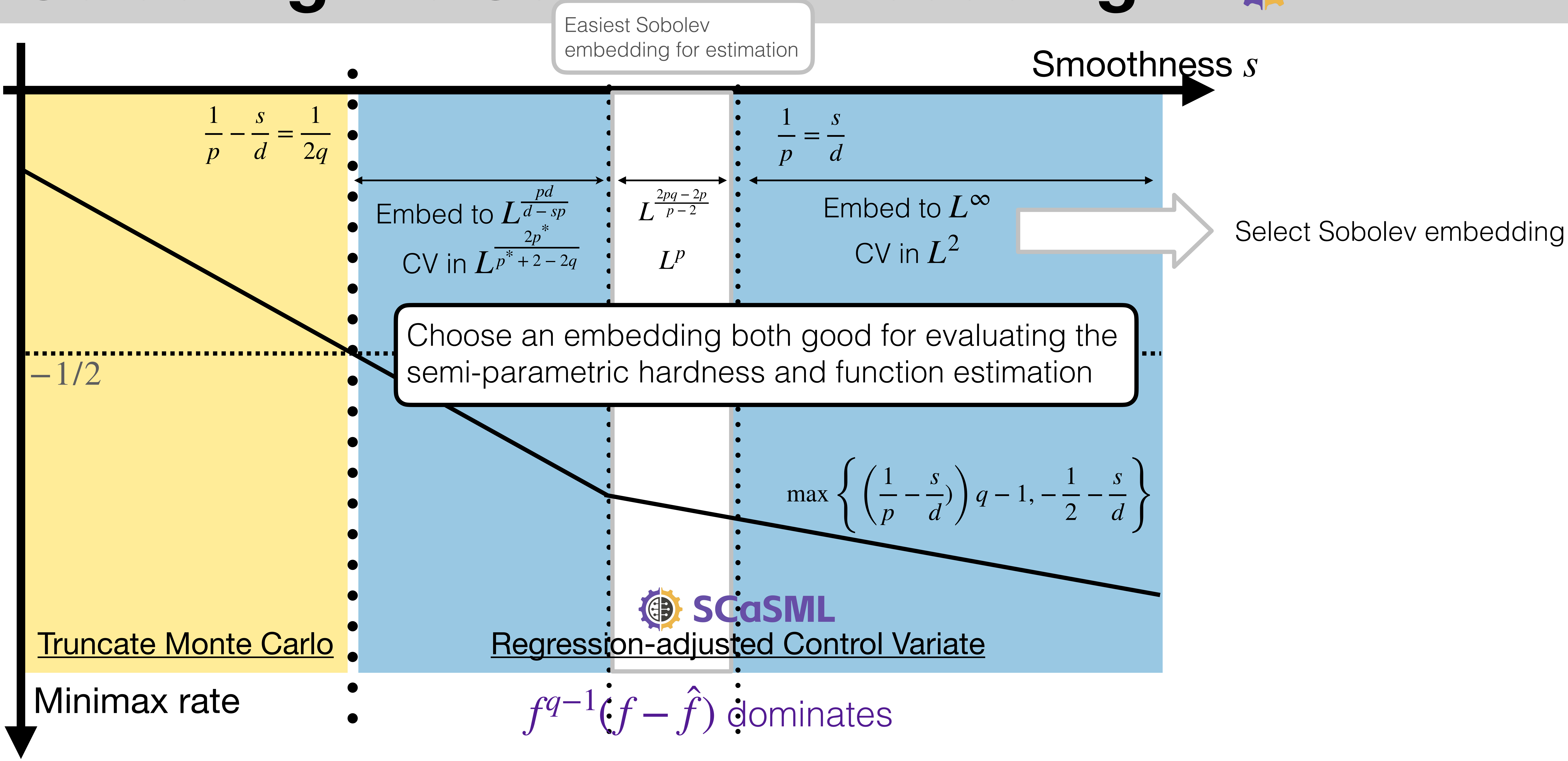
"influence function" (gradient)

Error p

Embed f^{q-1} and $f - \hat{f}$ into "dual" space

How to select the Sobolev emebedding?

Selecting the Sobolev Embedding



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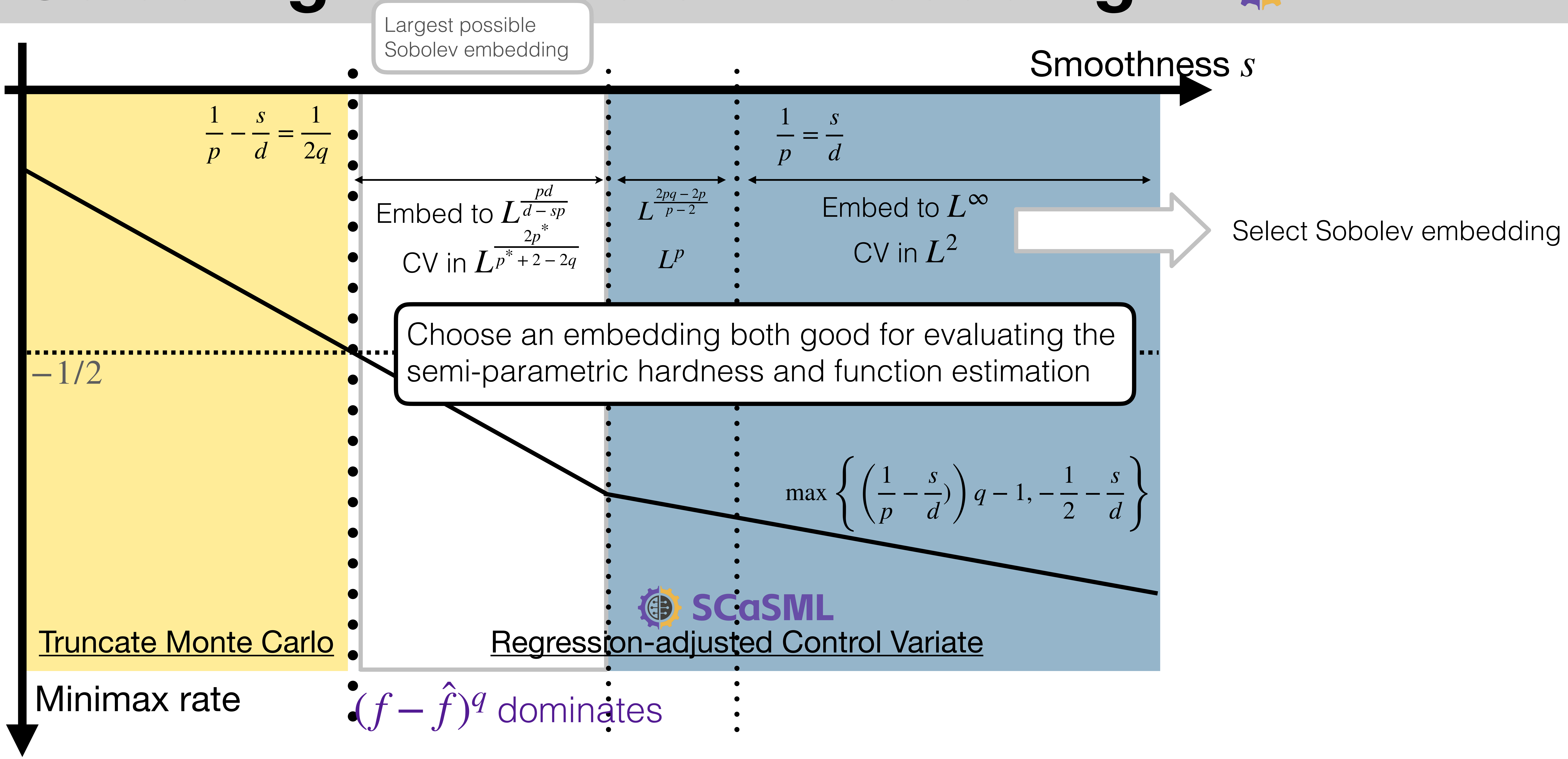
Selecting the Sobolev Embedding

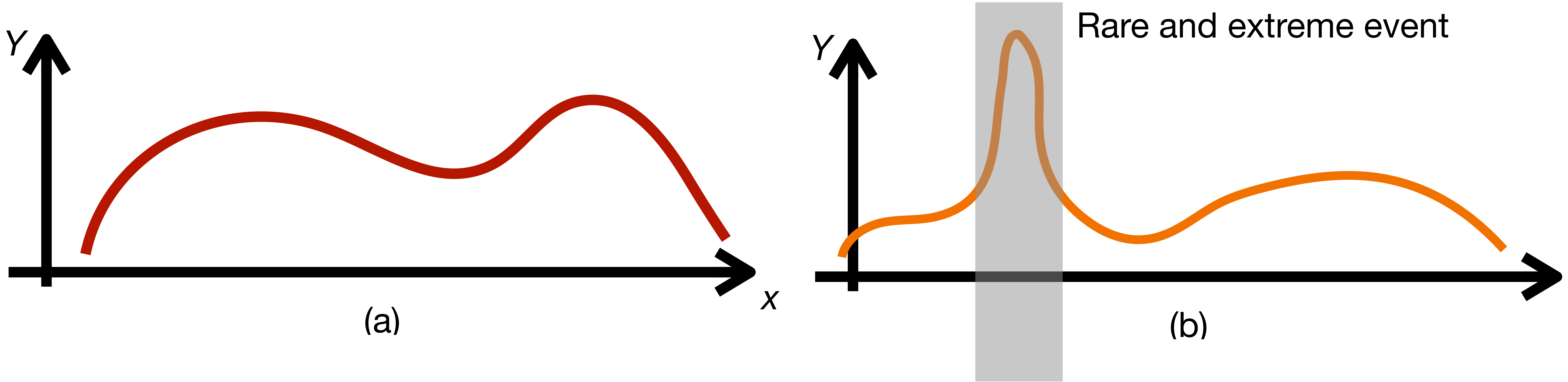


Take Home Message on the Theory

SCaSML

a) Statistical optimal regression is the optimal control variate
b) It helps only if there isn't a hard to simulate (infinite variance)
Rare and extreme event

<u>*q* control the extremeness</u>



Neurips 2023

When can Regression-Adjusted Control Variates Help?

Rare Events, Sobolev Embedding and Minimax Optimality

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PDE Solver

High Dimensional PDE-Solving

Let's consider $\Delta u = f$

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \theta \to \Phi(\theta)$$

$X_i = (x_i, \Delta u(x_i))$ — PDE R.h.s

u — PDE solution

PINN/DRM/Neural Galerkin

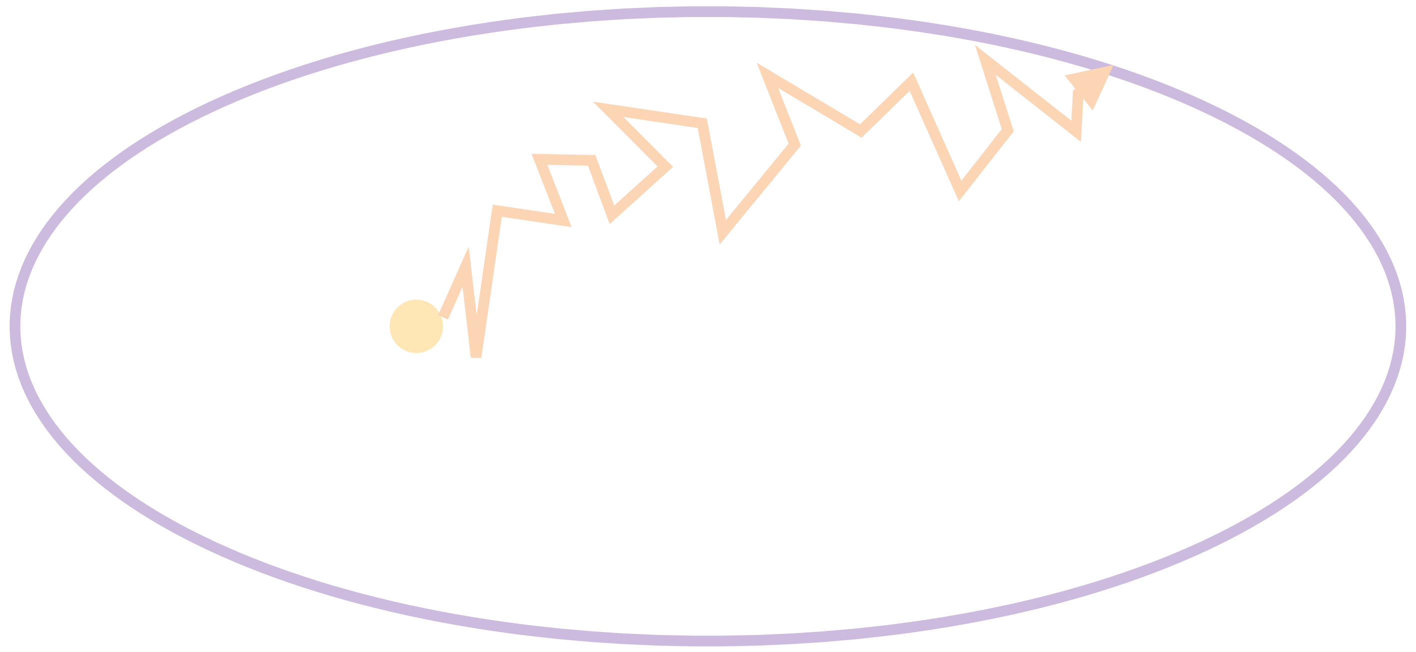
Mean/Variance/$u(x)$

$$(u - \hat{u})(x) = \mathbb{E}\int (f - \hat{f})(X_t)dt$$

$\Delta u = f$

$\Delta \hat{u} = \hat{f}$

$$\Delta(u - \hat{u}) = f - \hat{f}$$



High Dimensional PDE-Solving

Let's consider $\Delta u = f$

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \rightarrow \theta \rightarrow \Phi(\theta)$$

$X_i = (x_i, \Delta u(x_i))$ — PDE R.h.s

u — PDE solution

PINN/DRM/Neural Galerkin

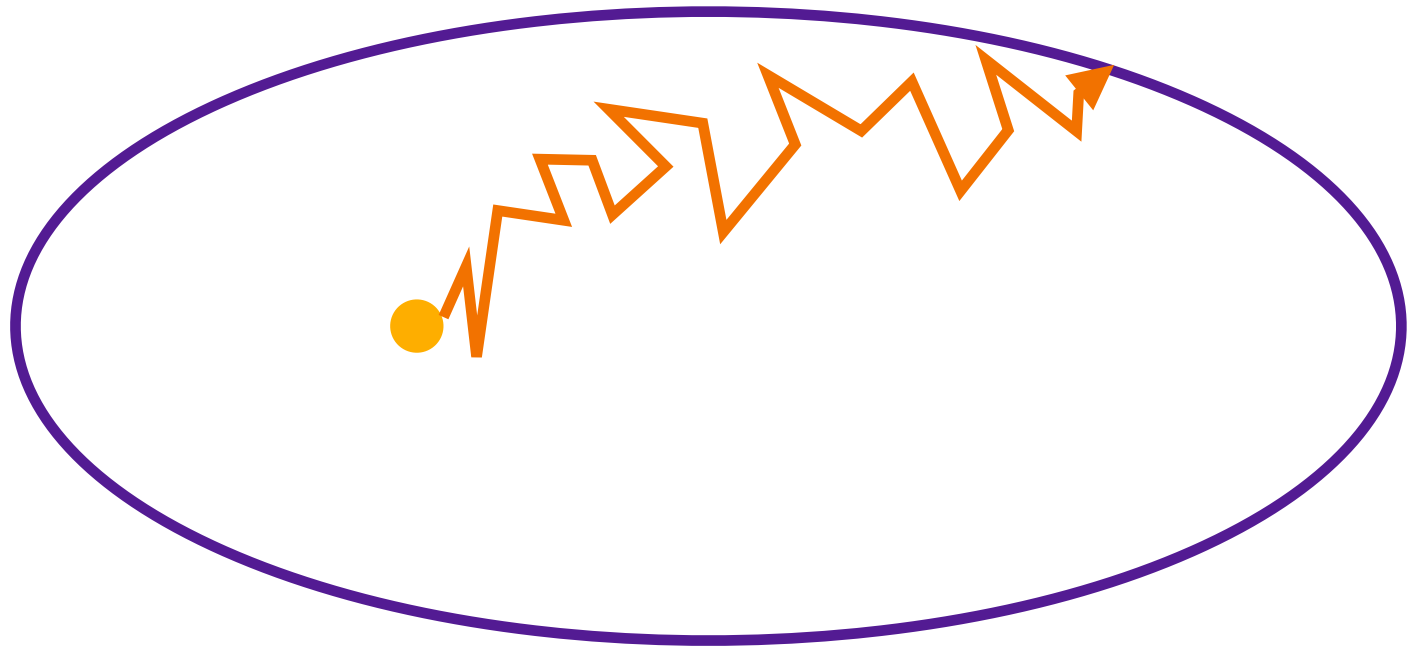
Mean/Variance/$u(x)$

$$\Delta u = f$$

$$\Delta \hat{u} = \hat{f}$$

$$\Delta(u - \hat{u}) = f - \hat{f}$$

$$(u - \hat{u})(x) = \mathbb{E} \int (f - \hat{f})(X_t) dt$$



Works for Semi-linear PDE

$$\frac{\partial U}{\partial t}(x,t) + \Delta U(x,t) + f(U(x,t)) = 0$$

Keeps the structure to enable brownian motion simulation

Can you do simulation for nonlinear equation?

Δ is linear!

Works for Semi-linear PDE

$$\frac{\partial U}{\partial t}(x,t) + \Delta U(x,t) + f(U(x,t)) = 0$$

Keeps the structure to enable brownian motion simulation

NN

$$\frac{\partial \hat{U}}{\partial t}(x,t) + \Delta \hat{U}(x,t) + f(\hat{U}(x,t)) = g(x,t)$$

$g(x,t)$ is the error made by NN

Works for Semi-linear PDE

$$\frac{\partial U}{\partial t}(x,t) + \Delta U(x,t) + f(U(x,t)) = 0$$

Keeps the structure to enable brownian motion simulation

NN

$$\frac{\partial \hat{U}}{\partial t}(x,t) + \Delta \hat{U}(x,t) + f(\hat{U}(x,t)) = g(x,t)$$

$g(x,t)$ is the error made by NN

Subtract two equations

Keeps the linear structure

$$\frac{\partial (U-\hat{U})}{\partial t}(x,t) + \Delta(U-\hat{U})(x,t)) + \underbrace{f(t, \hat{U}(x,t) + U(x,t) - \hat{U}(x,t)) - f(t, \hat{U}(x,t))}_{G\left(t, (U-\hat{U})(x,t)\right)} = g(x,t)\,.$$

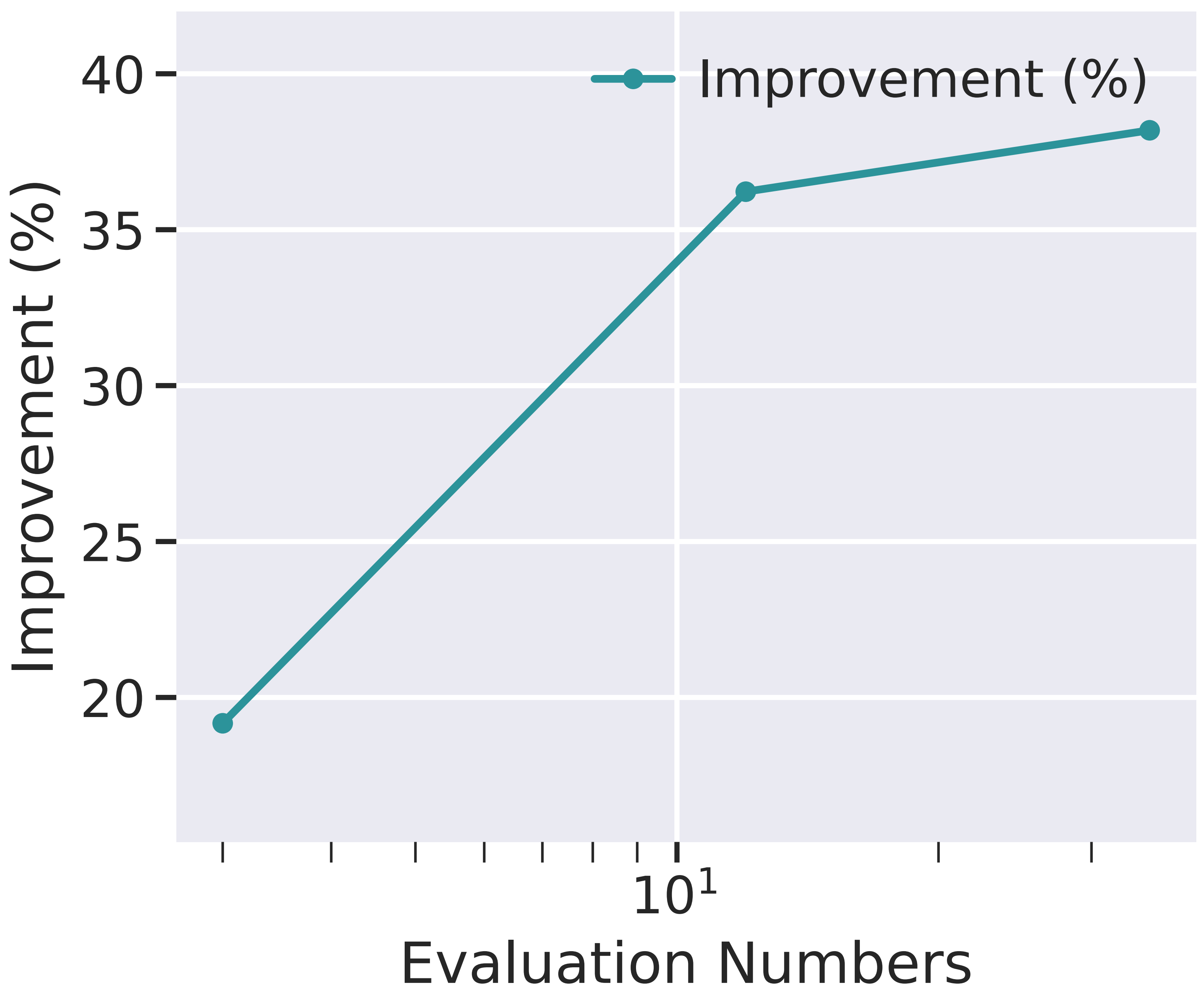
Numerical Results

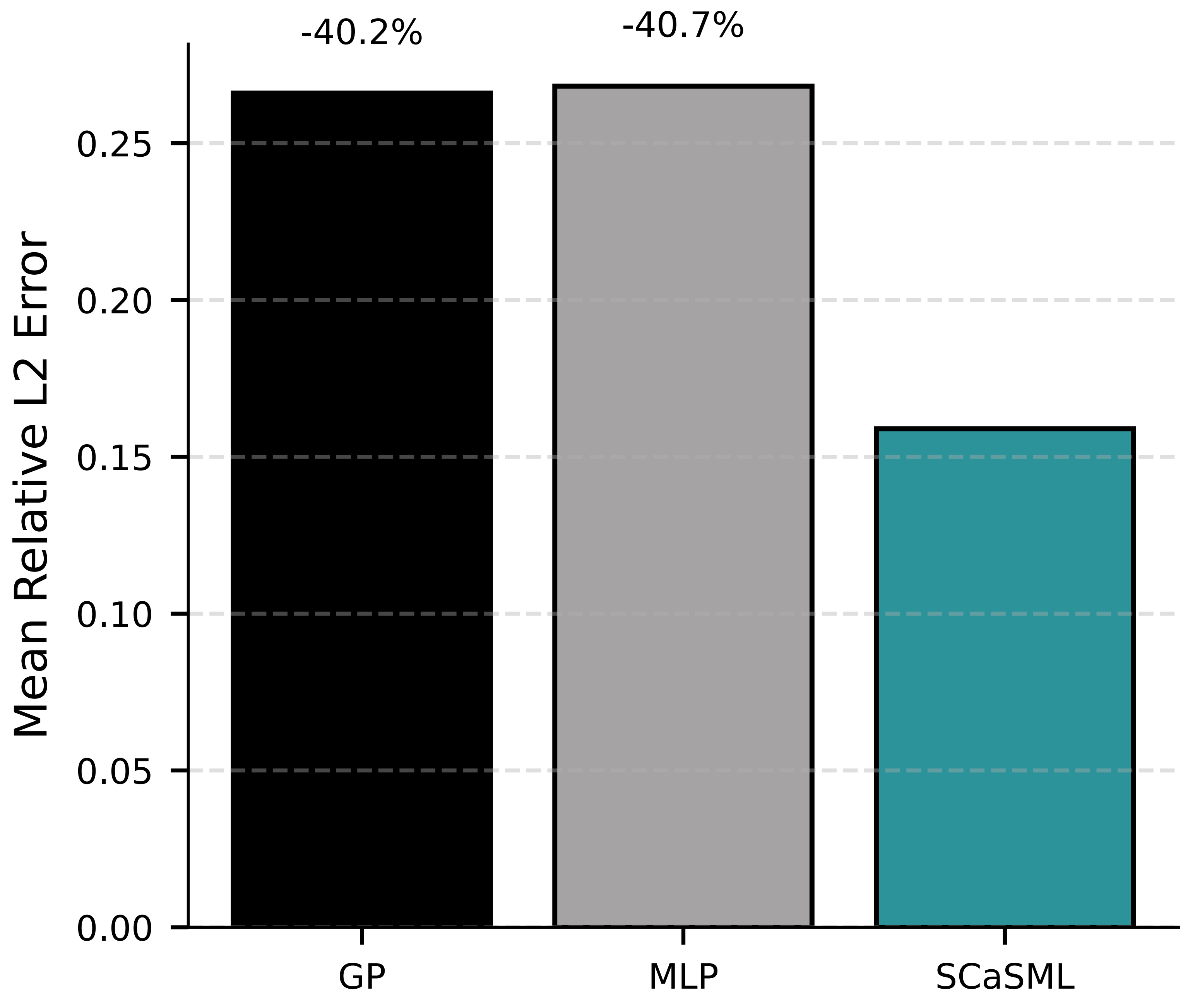
		Time (s)			Relative L^2 Error			L^∞ Error			L^1 Error		
		SR	MLP	SCaSML	SR	MLP	SCaSML	SR	MLP	SCaSML	SR	MLP	SCaSML
LCD	10d	2.64	11.24	23.75	5.24E-02	2.27E-01	**2.73E-02**	2.50E-01	9.06E-01	**1.61E-01**	3.43E-02	1.67E-01	**1.78E-02**
	20d	1.14	7.35	17.59	9.09E-02	2.35E-01	**4.73E-02**	4.52E-01	1.35E+00	**3.28E-01**	9.47E-02	2.37E-01	**4.52E-02**
	30d	1.39	7.52	25.33	2.30E-01	2.38E-01	**1.84E-01**	4.73E+00	1.59E+00	**1.49E+00**	**1.75E-01**	2.84E-01	1.91E-01
	60d	1.13	7.76	35.58	3.07E-01	2.39E-01	**1.32E-01**	3.23E+00	2.05E+00	**1.55E+00**	5.24E-01	4.07E-01	**2.06E-01**
VB-PINN	20d	1.15	7.05	13.82	1.17E-02	8.36E-02	**3.97E-03**	3.16E-02	2.96E-01	**2.16E-02**	5.37E-03	3.39E-02	**1.29E-03**
	40d	1.18	7.49	16.48	3.99E-02	1.04E-01	**2.85E-02**	8.16E-02	3.57E-01	**7.16E-02**	1.97E-02	4.36E-02	**1.21E-02**
	60d	1.19	7.57	19.83	3.97E-02	1.17E-01	**2.90E-02**	8.10E-02	3.93E-01	**7.10E-02**	1.95E-02	4.82E-02	**1.24E-02**
	80d	1.32	7.48	21.99	6.78E-02	1.19E-01	**5.68E-02**	1.89E-01	3.35E-01	**1.79E-01**	3.24E-02	4.73E-02	**2.49E-02**
VB-GP	20d	1.97	10.66	65.46	1.47E-01	8.32E-02	**5.52E-02**	3.54E-01	**2.22E-01**	2.54E-01	7.01E-02	3.50E-02	**1.91E-02**
	40d	1.68	10.14	49.38	1.81E-01	1.05E-01	**7.95E-02**	4.01E-01	3.47E-01	**3.01E-01**	9.19E-02	4.25E-02	**3.43E-02**
	60d	1.01	7.25	35.14	2.40E-01	2.57E-01	**1.28E-01**	3.84E-01	9.50E-01	**7.10E-02**	1.27E-01	9.99E-02	**6.11E-02**
	80d	1.00	7.00	38.26	2.66E-01	3.02E-01	**1.52E-01**	3.62E-01	1.91E+00	**2.62E-01**	1.45E-01	1.09E-01	**7.59E-02**
LQG	100d	1.54	8.67	26.95	7.96E-02	5.63E+00	**5.51E-02**	7.78E-01	1.26E+01	**6.78E-01**	1.40E-01	1.21E+01	**8.68E-02**
	120d	1.25	8.17	27.46	9.37E-02	5.50E+00	**6.64E-02**	9.02E-01	1.27E+01	**8.02E-01**	1.73E-01	1.22E+01	**1.05E-01**
	140d	1.80	8.27	29.72	9.79E-02	5.37E+00	**6.78E-02**	1.00E+00	1.27E+01	**9.00E-01**	1.91E-01	1.23E+01	**1.11E-01**
	160d	1.74	9.07	32.08	1.11E-01	5.27E+00	**9.92E-02**	1.38E+00	1.28E+01	**1.28E+00**	2.15E-01	1.23E+01	**1.79E-01**
DR	100d	1.62	7.75	60.86	9.52E-03	8.99E-02	**8.87E-03**	7.51E-02	6.37E-01	**6.51E-02**	1.13E-02	9.74E-02	**1.11E-02**
	120d	1.26	7.28	65.66	1.11E-02	9.13E-02	**9.90E-03**	7.10E-02	5.74E-01	**6.10E-02**	1.40E-02	9.97E-02	**1.23E-02**
	140d	2.38	7.82	76.90	3.17E-02	8.97E-02	**2.94E-02**	1.79E-01	8.56E-01	**1.69E-01**	3.96E-02	9.77E-02	**3.67E-02**
	160d	1.75	7.42	82.40	3.46E-02	9.00E-02	**3.23E-02**	2.08E-01	8.02E-01	**1.98E-01**	4.32E-02	9.75E-02	**4.02E-02**

Inference-Time Scaling

$$\frac{\partial}{\partial t}u + \left[\sigma^2 u - \frac{1}{d} - \frac{\bar{\sigma}^2}{2}\right](\nabla \cdot u) + \frac{\bar{\sigma}^2}{2}\Delta u = 0$$

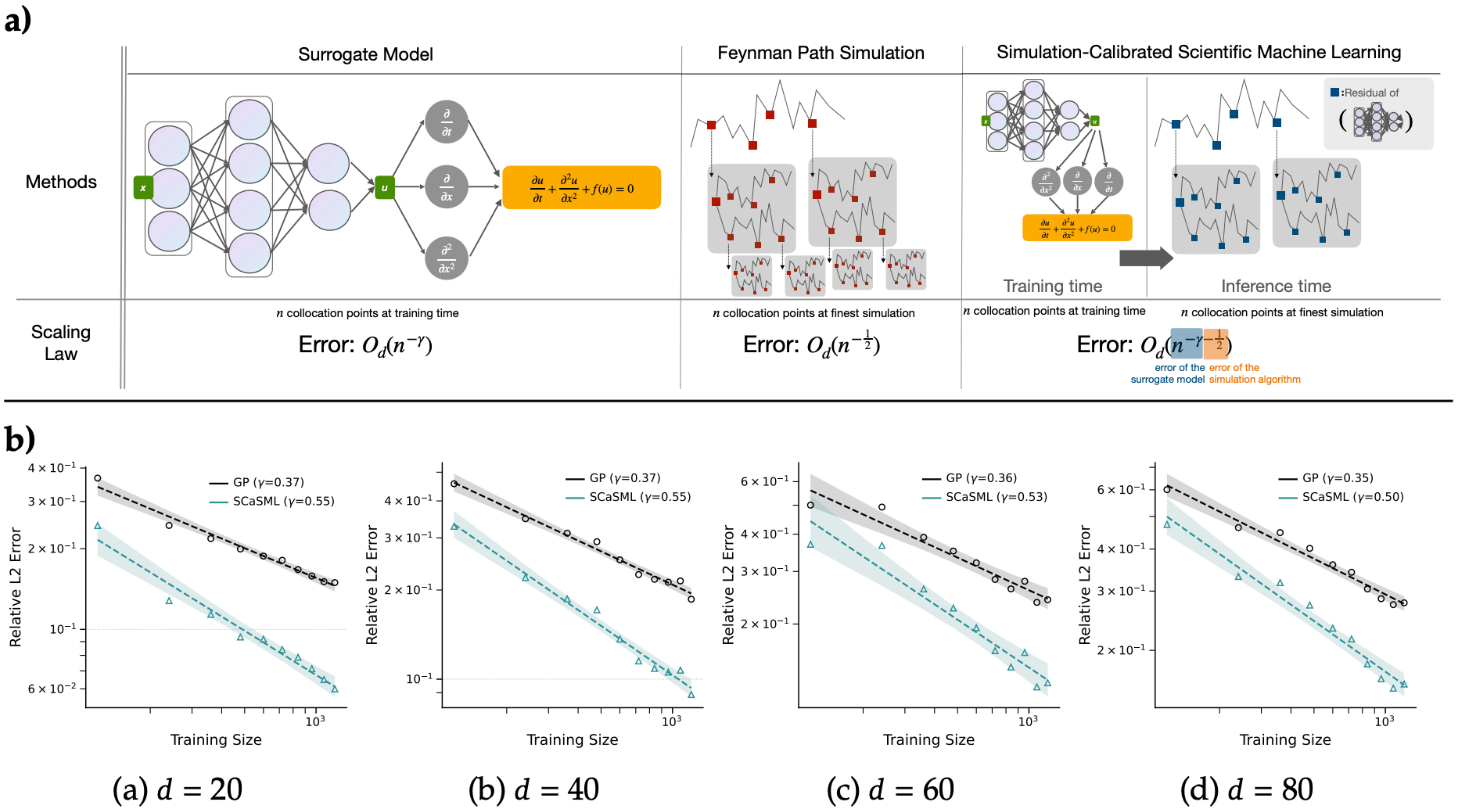
have closed-form solution $g(x) = \frac{\exp(T + \sum_i x_i}{1 + \exp(T + \sum_i x_i)}$





Method	Convergence Rate
PINN	$O(n^{-s/d})$
MLP	$O(n^{-1/4})$
ScaSML	$O(n^{-1/4-s/d})$

Better Scaling Law



SCaSML
Simulation-Calibrated Scientific Machine Learning

Arxiv

Physics-Informed Inference Time Scaling via Simulation-Calibrated Scientific Machine Learning

Zexi Fan[1], Yan Sun [2], Shihao Yang[3], Yiping Lu*[4]

[1] **Peking University** [2] **Visa Inc.** [3] **Georgia Institute of Technology** [4] **Northwestern University**

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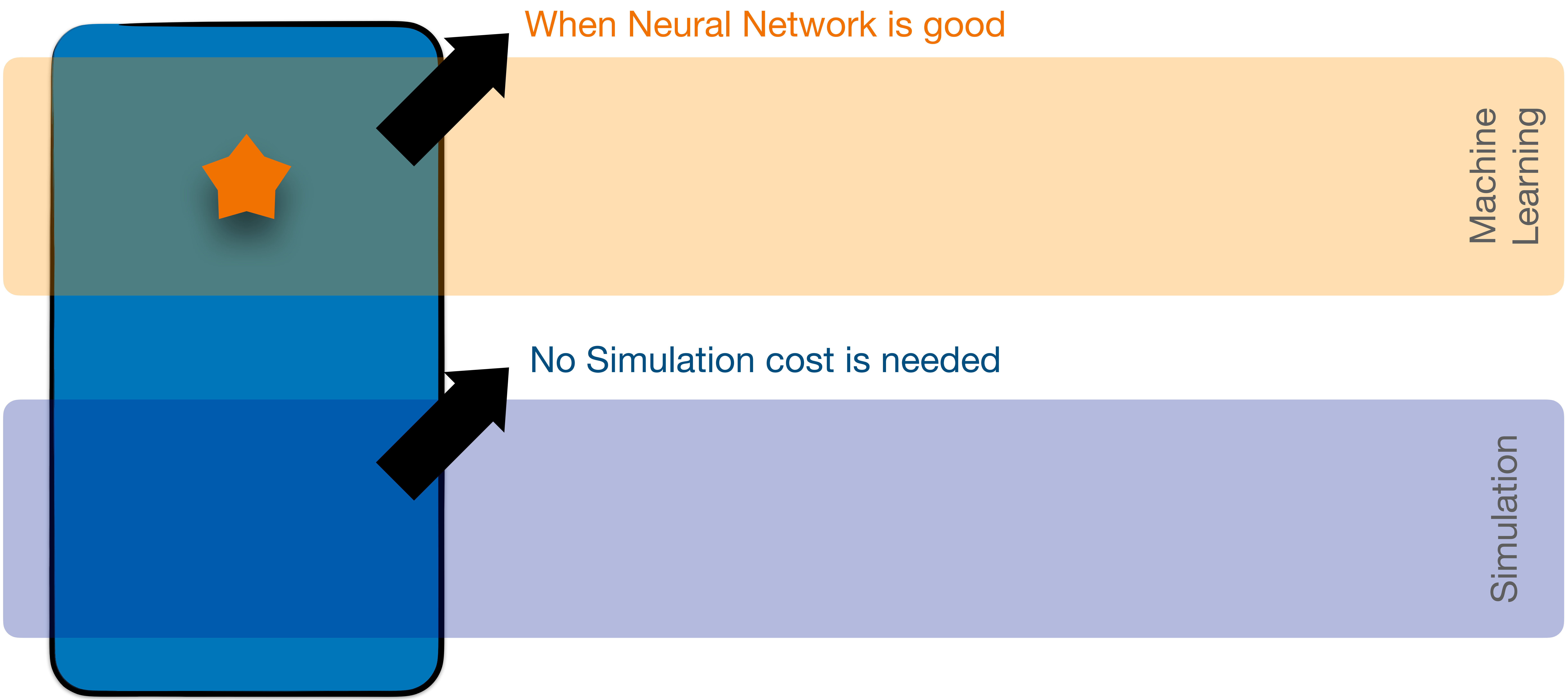
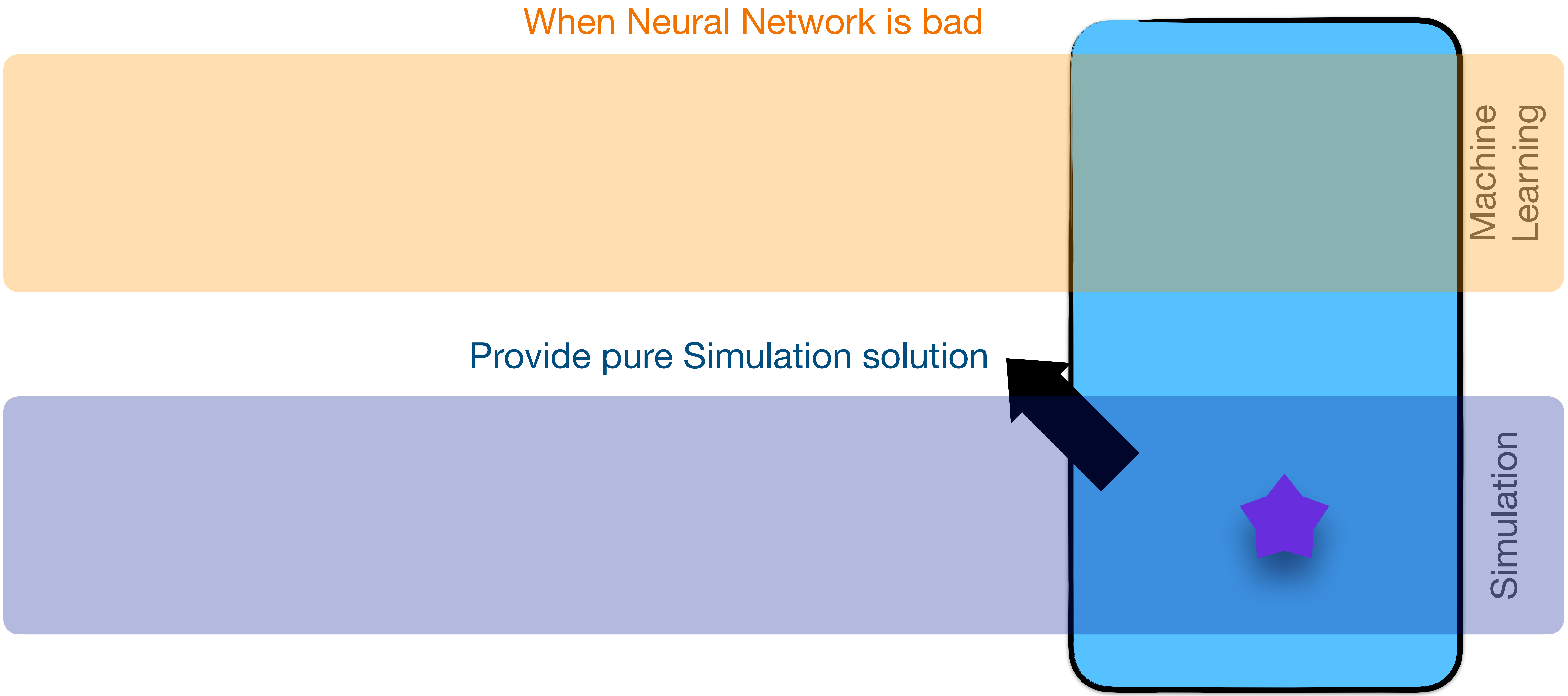
https://2prime.github.io/files/scasml_techreport.pdf

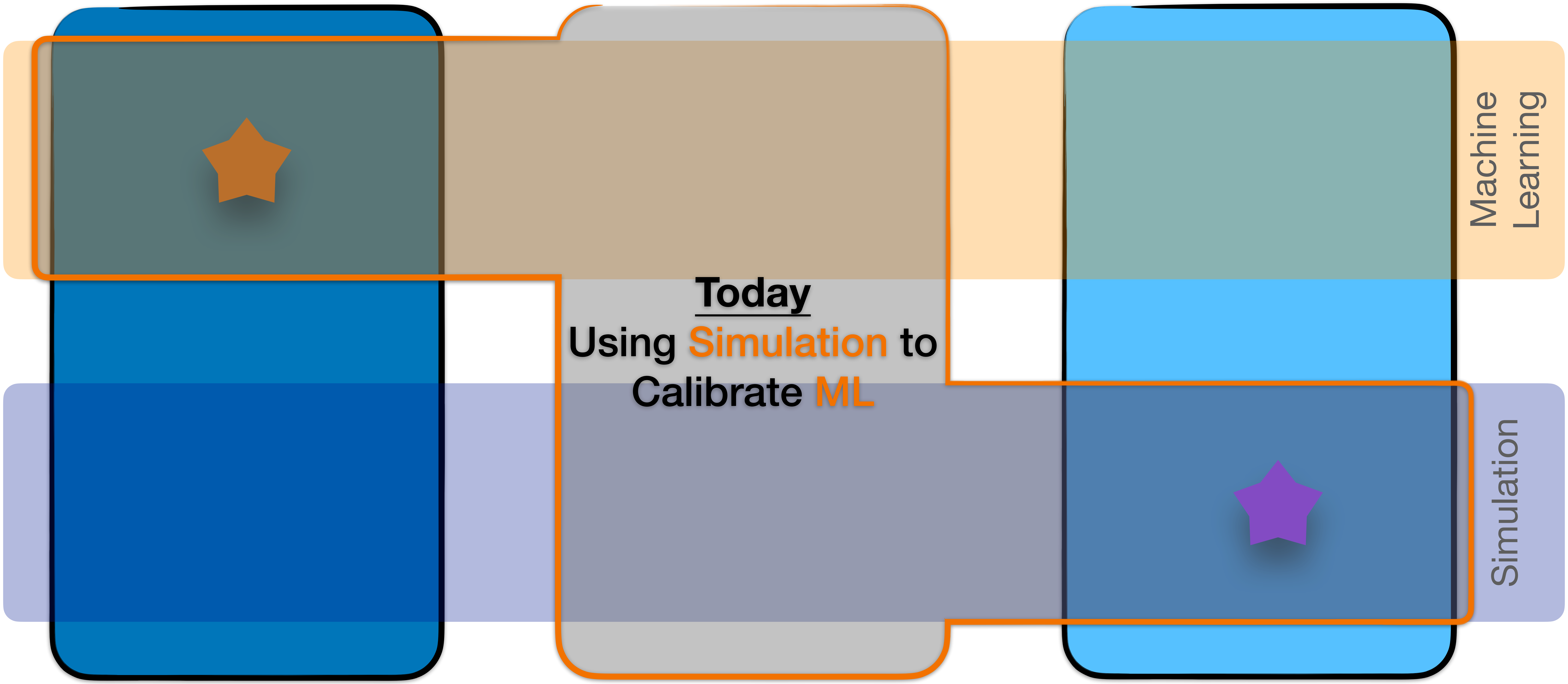
Our Aim Today : A Marriage



Our Aim Today : A Marriage



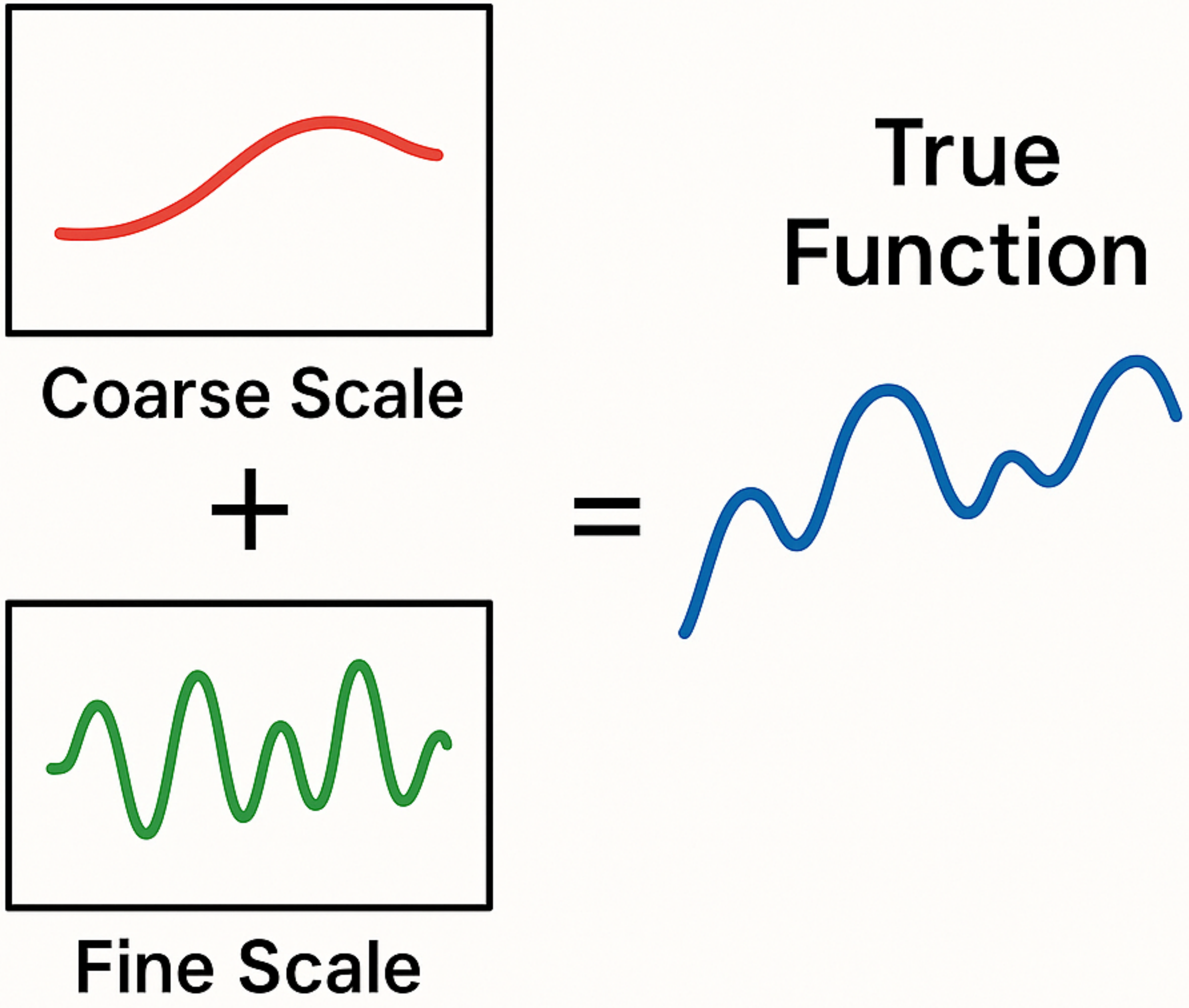
Our AIM Today: A Marriage



A multiscale view

Capture via surrogate model

Capture via Monte-Carlo



More Examples…

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \hat{\theta} \to \Phi(\hat{\theta})$$

Scientific Machine Learning — Downstream application

Example 1 $\theta = f, \quad X_i = (x_i, f(x_i))$ $\Phi(\theta) = \int f^q(x)dx$

Example 2 $\theta = \Delta^{-1}f, \quad X_i = (x_i, f(x_i))$ $\Phi(\theta) = \theta(x)$

Example 3 $\theta = A, \quad X_i = (x_i, Ax_i)$ $\Phi(\theta) = \mathrm{tr}(A)$

Estimation $\hat{A}$ via Randomized SVD

Estimate tr$(A - \hat{A})$ via Hutchinson's estimator

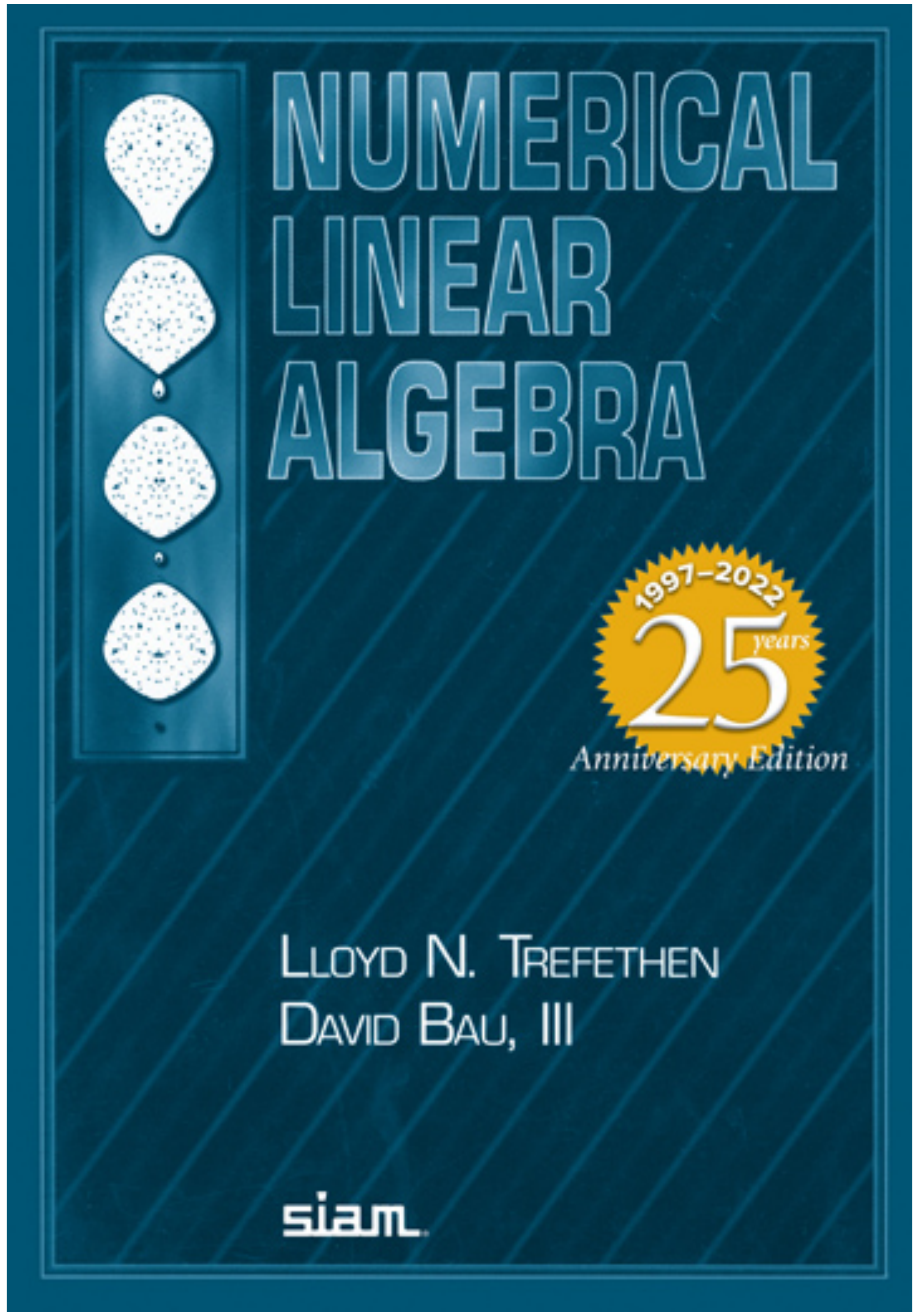
Lin 17 Numerische Mathematik and Mewyer-Musco-Musco-Woodruff 20

Application in graph theory, quantum …

Tale 2: Pre-condition

with a surprising connection with debiasing

Tale 2: Preconditioning



> *"In ending this book with the subject of preconditioners, we find ourselves at the philosophical center of the scientific computing of the future."*
>
> — **L. N. Trefethen and D. Bau III**, `Numerical Linear Algebra` [TB22]

Nothing will be more central to computational science in the next century than the art of transforming a problem that appears intractable into another whose solution can be approximated rapidly.

What is precondition

- Solving $Ax = b$ is equivalent to solving $B^{-1}Ax = B^{-1}b$

hardness depend on $\kappa(A)$

hardness depend on $\kappa(B^{-1}A)$

Become easier when $B \approx A$

A New Way to Implement **Precondition**

- Debiasing is a way of solving $Ax = b$
  - Using an approximate solver $Bx_1 = b$

Error depends on $\|A^{-1}(A - B)\|$

A New Way to Implement **Precondition**

- Debiasing is a way of solving $Ax = b$
  - Using an approximate solver $Bx_1 = b$
  - $x - x_1$ satisfies the equation $A(x - x_1) = b - Ax_1$
  - Using the approximate solver to approximate $x - x_1$ via $Bx_2 = b - Ax_1$

Easy to solve for $b - Ax_1$ is small

A New Way to Implement Precondition

- Debiasing is a way of solving $Ax = b$
  - Using an approximate solver $Bx_1 = b$

Iterative Refinement Algorithm

- $x - \sum_{i=1}^{t} x_i$ satisfies the equation $A(x - \sum_{i=1}^{t} x_i) = b - A\sum_{i=1}^{t} x_i$
- Using the approximate solver to approximate $x - \sum_{i=1}^{t} x_i$ via $Bx_{i+1} = b - A\sum_{i=1}^{t} x_i$

A New Way to Implement Precondition

- Debiasing is a way of solving $Ax = b$
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Iterative Refinement Algorithm

- $x - \sum_{i=1}^{t} x_i$ satisfies the equation $A(x - \sum_{i=1}^{t} x_i) = b - A\sum_{i=1}^{t} x_i$
- Using the approximate solver to approximate $x - \sum_{i=1}^{t} x_i$ via $Bx_{i+1} = b - A\sum_{i=1}^{t} x_i$

$$x_{i+1} = (I - B^{-1}A)x_i + B^{-1}b$$

Preconditioned Jacobi Iteration

This Talk: A New Way to Implement Precondition

Via Debiasing

- **Step 1:** Aim to solve (potentially nonlinear) equation $A(u) = b$
- **Step 2:** Build an approximate solver $A(\hat{u}) \approx b$
  - Via machine learning/sketching/finite element….
- **Step 3:** Solve $u - \hat{u}$

use Machine Learning

Unrealiable approximate solver as preconditioner

Connection with control variate, doubly robust estimator, Multifidelity Monte Carlo

AIM: Debiasing a Learned Solution = Using Learned Solution as preconditioner!

Randomized NLA as Machine Learning

AIM: using matrix-vector multiplication to compute eigenvalue/least square problem

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \theta \to \Phi(\theta)$$

$X_i = (x, Ax)$ $\quad A$

$$\Phi(A) = \begin{cases} A^{-1}b \\ \text{Eigenvalue of } A \end{cases}$$

"Randomized Numerical Linear Algebra"/Sketching

➡

"Sketch-and-Solve"

Randomized NLA as Machine Learning

AIM: using matrix-vector multiplication to compute eigenvalue/least square problem

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \theta \to \Phi(\theta)$$

$X_i = (x, Ax)$ $\qquad$ A

$$\Phi(A) = \begin{cases} A^{-1}b \\ \text{Eigenvalue of } A \end{cases}$$

Structure here: Φ is the solution of a fixed point equation

$$\Phi(\hat\theta) - \Phi(\theta) - \nabla\Phi(\hat\theta)(\hat\theta - \theta) = O(\epsilon^2)$$

"A Newton Step"

Radomized estimation $\qquad$ Exact estimation

(In)exact Sub-sample Newton Method/Sketch-and-Precondtion

Relationship with Inverse Power Methods

(Approximate) Inverse Power Method	Our Method
$X_{n+1} = (\lambda I - A)^{\dagger} X_n$	$X_{n+1} = \underbrace{(\lambda I - \hat{A})^{\dagger}}_{\nabla \Phi(\hat{\theta})} \underbrace{(A - \hat{A}) X_n}_{(\theta - \hat{\theta})}$

Relationship with Inverse Power Methods

(Approximate) Inverse Power Method	Our Method
$X_{n+1} = (\lambda I - A)^{\dagger} X_n$	$X_{n+1} = (\lambda I - \hat{A})^{\dagger} (A - \hat{A}) X_n$

Replace with an approximate solver $\hat{A}$ changes the fixed point

Ture eigenvector is the fix point for every approximate solver $\hat{A}$

Relationship with Inverse Power Methods

(Approximate) Inverse Power Method	Our Method
$X_{n+1} = (\lambda I - A)^{\dagger} X_n$	$X_{n+1} = (\lambda I - \hat{A})^{\dagger} (A - \hat{A}) X_n$

Replace with an approximate solver $\hat{A}$ changes the fixed point

Ture eigenvector is the fix point for every approximate solver $\hat{A}$

How you construct such iteration?
What is the rule of $\hat{A}$?

Take Hoem Message 1:
Power the Residual but not Power the vector

Why better than Directly DMD

“Sketch-and-Solve” VS “Sketch-and-Precondition”

	Sketch-and-Solve	Sketch-and-Precondition
Least Square		Sketch-and-precondition, Sketch-and-project, Iterataive Sketching, ….
Low rank Approx	Idea 1: plug in a SVD Solver: Random SVD Idea 2: plug in a inverse power method	 ***Our Work!***

Use sketched matrix $\hat{A}$ as an approximation to A

Use sketched matrix $\hat{A}$ as an precondition to the probelm

Sorry… but I can’t see the relationship….

Ruihan Xu, **Yiping Lu**. What is a Sketch-and-Precondition Derivation for Low-Rank Approximation? Power Error or Power Estimation?

Why better than Directly DMD

“Sketch-and-Solve” VS “Sketch-and-Precondition”

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Use sketched matrix $\hat{A}$ as an approximation to A

Use sketched matrix $\hat{A}$ as an precondition to the probelm

We only sketch the Hessian

Idea: using (approximate) Newton method to solve the Lagrange from

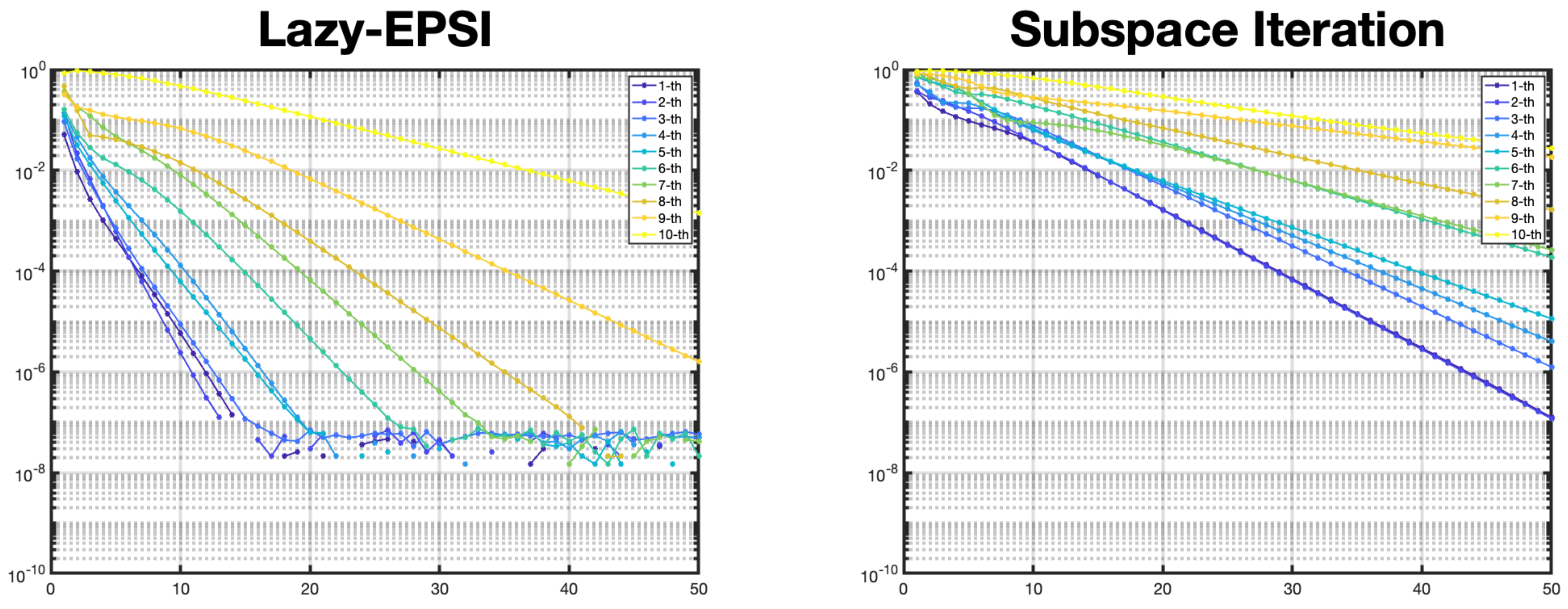
$$\min_u u^\top A u - \lambda(x^\top x - 1)$$

Thus Our convergence is linear-quadratic

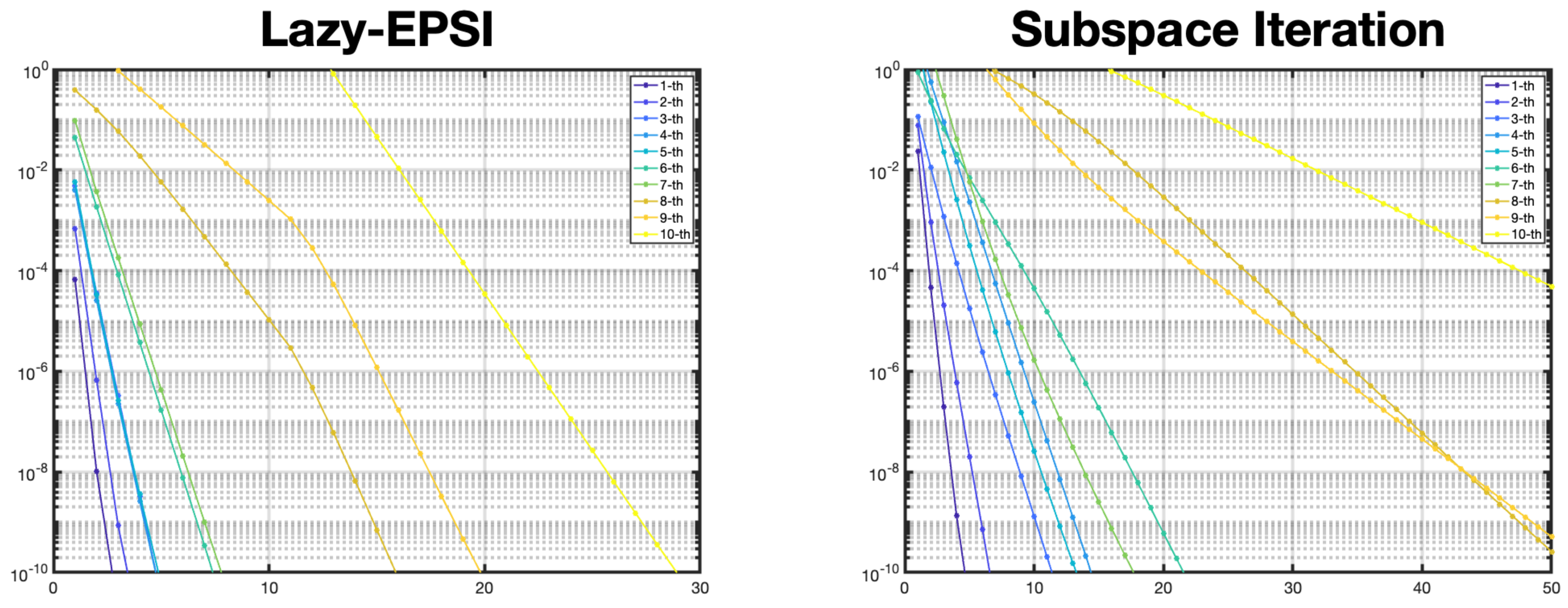
Contraction coefficient improves when sketching quality increases

Ruihan Xu, **Yiping Lu**. What is a Sketch-and-Precondition Derivation for Low-Rank Approximation? Power Error or Power Estimation?

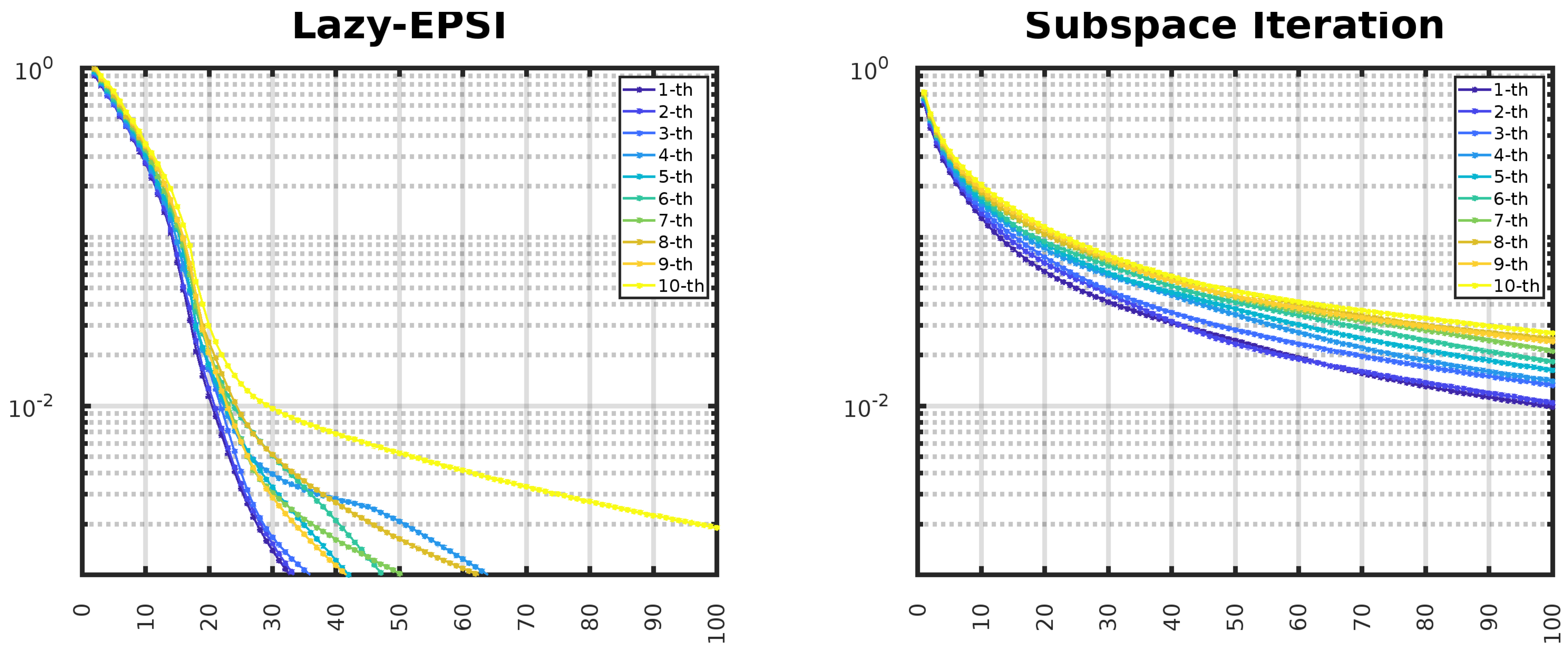
Eigenvalue Computation



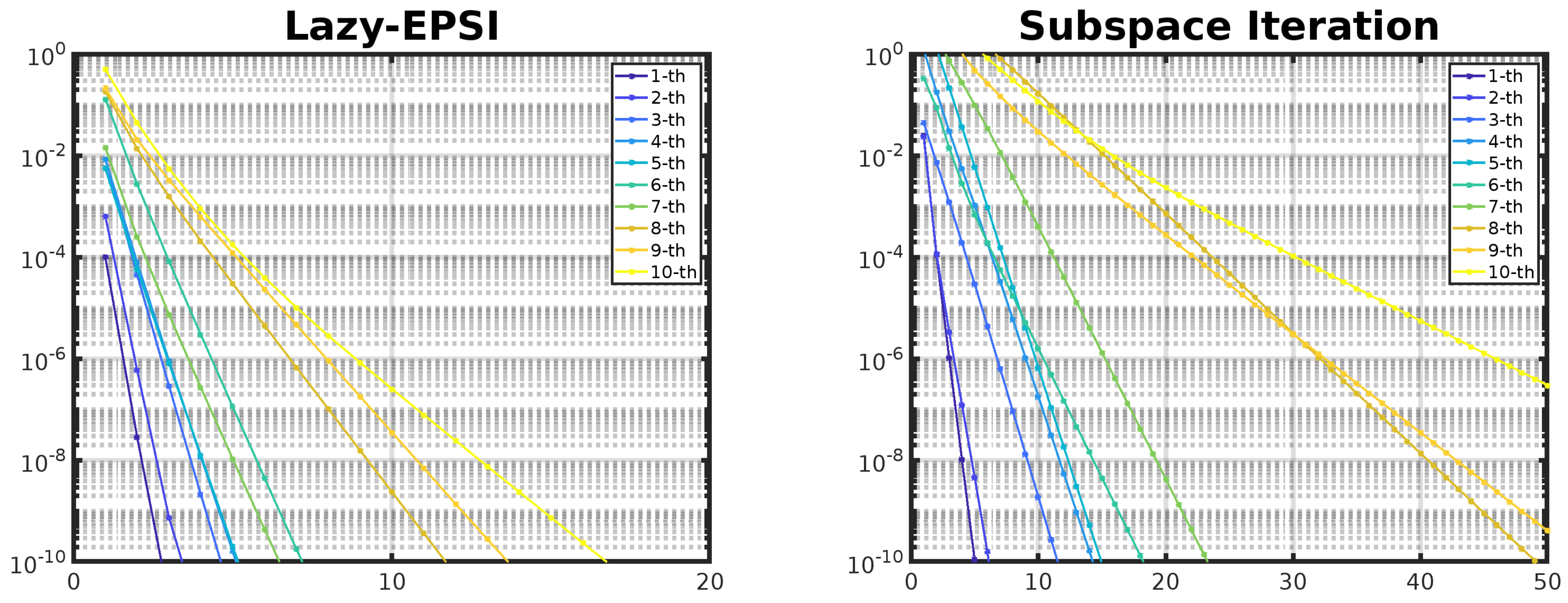
Random ill-conditioned matrix



Amazon (SNAP)

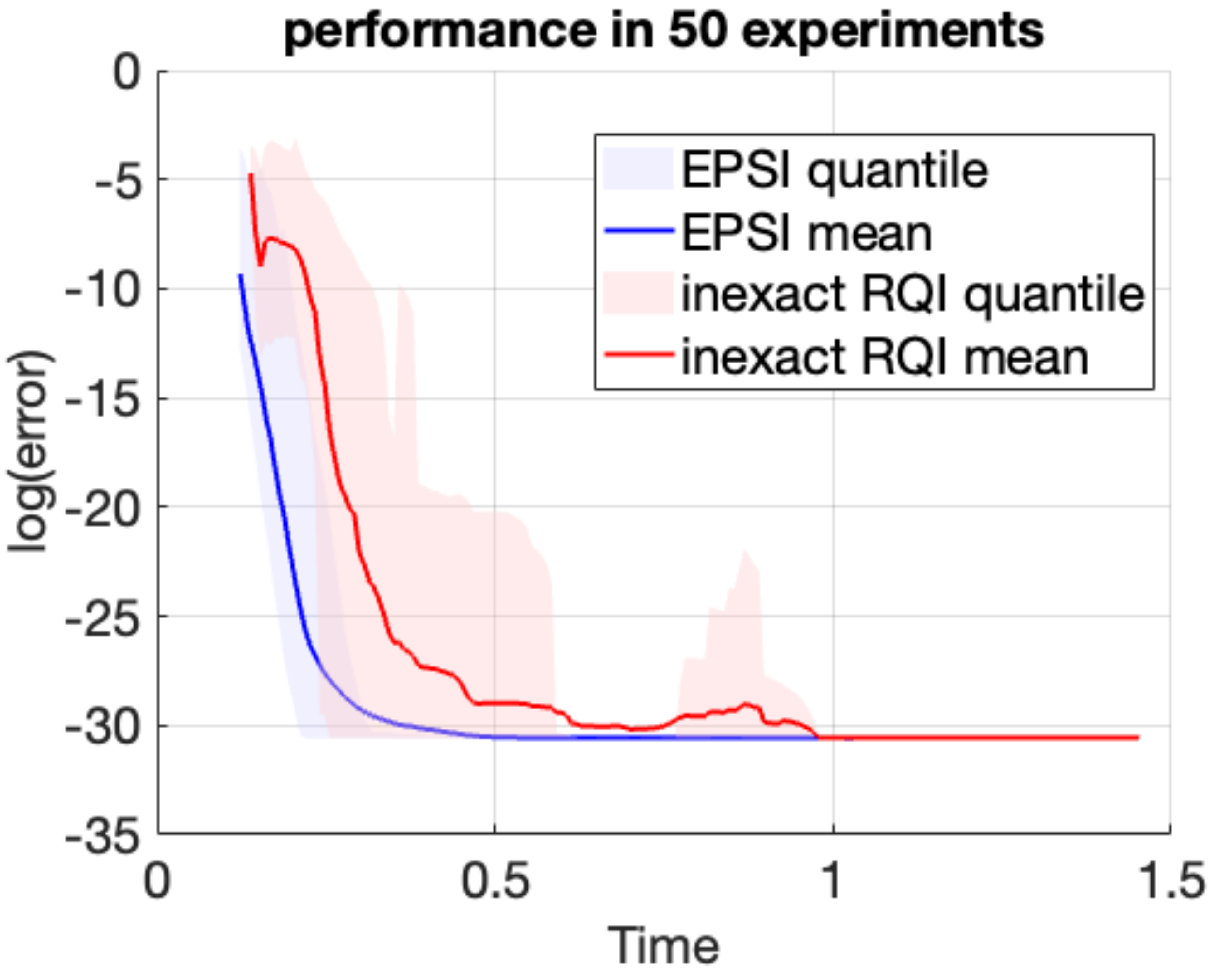


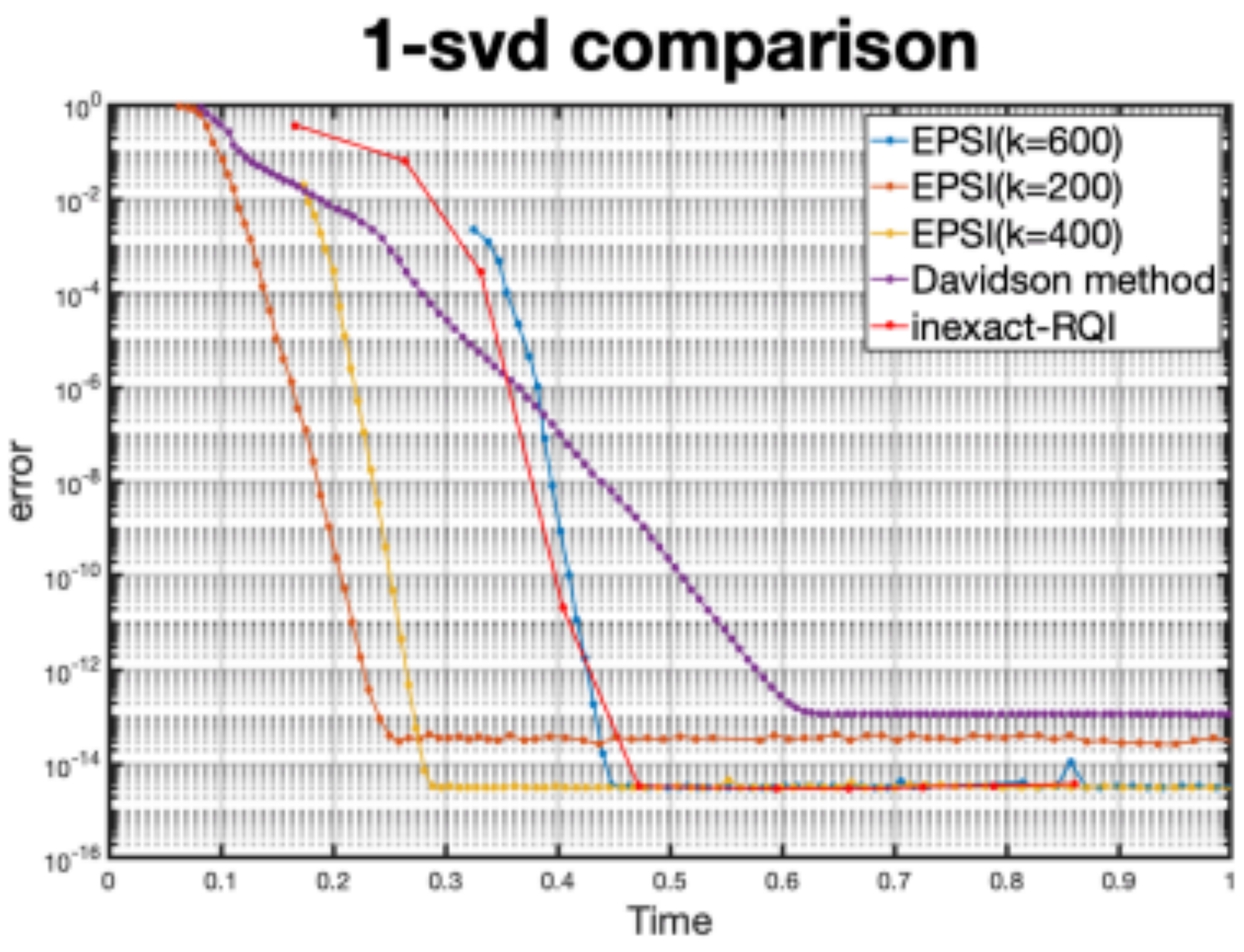
PDE (Laplacian)



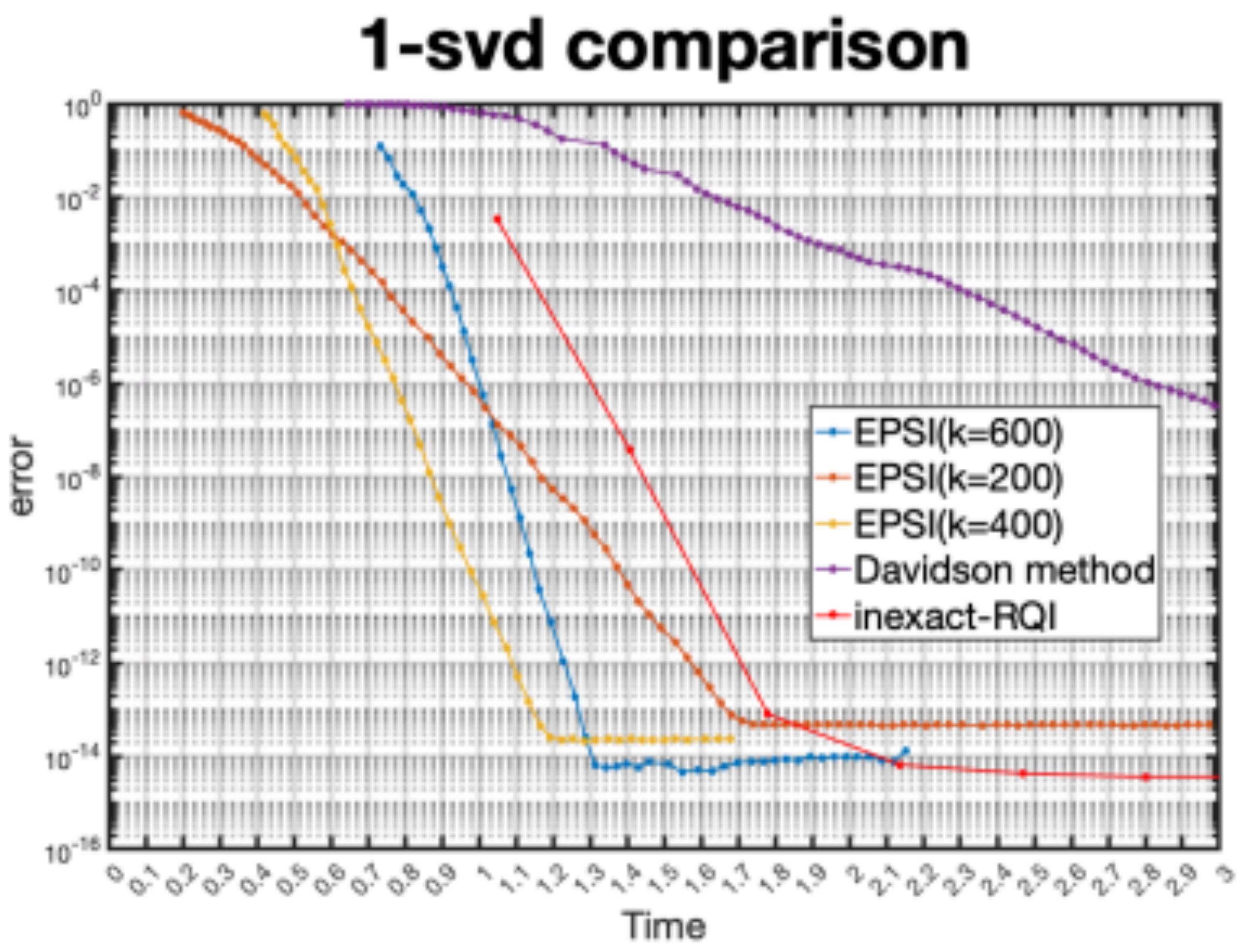
Web Stanford (SNAP)

Runing Time





(b) $n = 2000, \kappa = 10^{-6}$



(c) $n = 4000, \kappa = 10^{6}$

What is a Sketch-and-Precondition Derivation for Low-Rank Approximation? Inverse Power Error or Inverse Power Estimation?

Ruihan Xu * Yiping Lu †

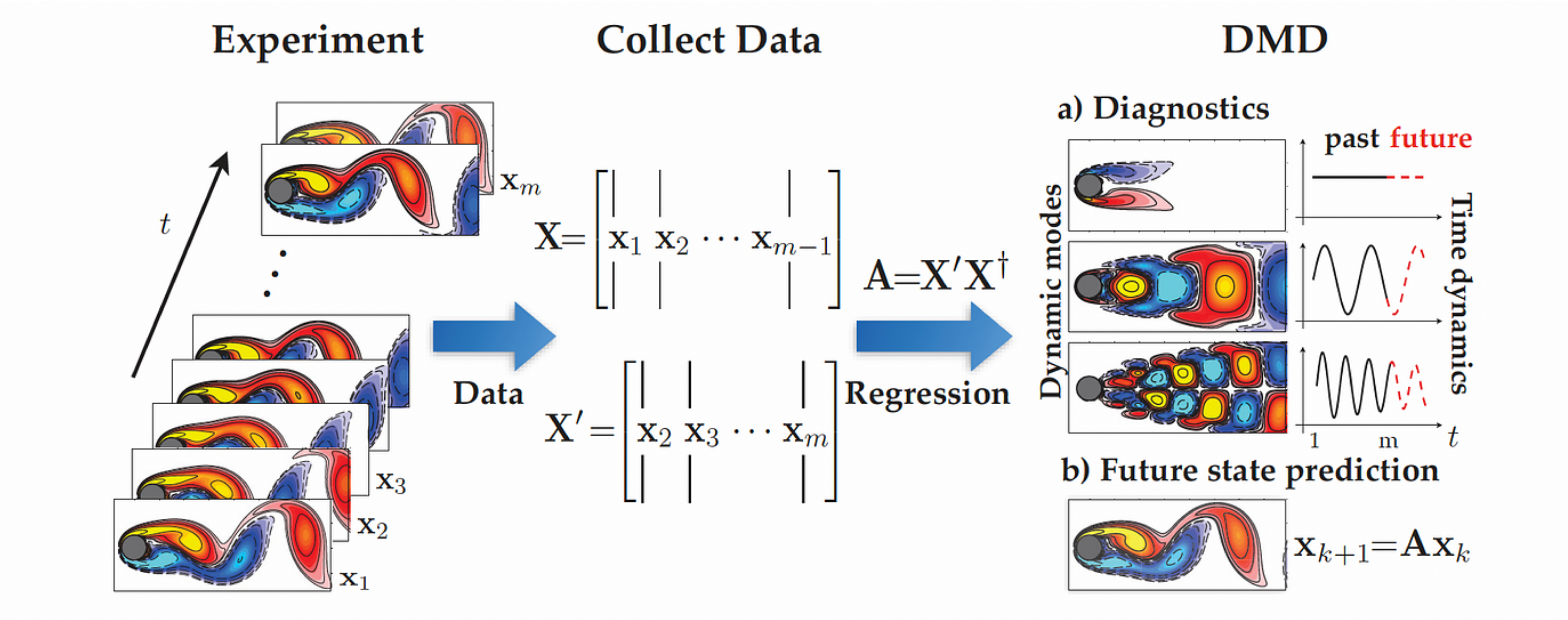
Abstract

Randomized sketching accelerates large-scale numerical linear algebra by reducing computational complexity. While the traditional sketch-and-solve approach reduces the problem size directly through sketching, the sketch-and-precondition method leverages sketching to construct a computational friendly preconditioner. This preconditioner improves the convergence speed of iterative solvers applied to the original problem, maintaining accuracy in the full space. Furthermore, the convergence rate of the solver improves at least linearly with the sketch size. Despite its potential, developing a sketch-and-precondition framework for randomized algorithms in low-rank matrix approximation remains an open challenge. We introduce the *Error-Powered Sketched Inverse Iteration* (`EPSI`) Method via run sketched Newton iteration for the Lagrange form as a sketch-and-precondition variant for randomized low-rank approximation. Our method achieves theoretical guarantees, including a convergence rate that improves at least linearly with the sketch size.

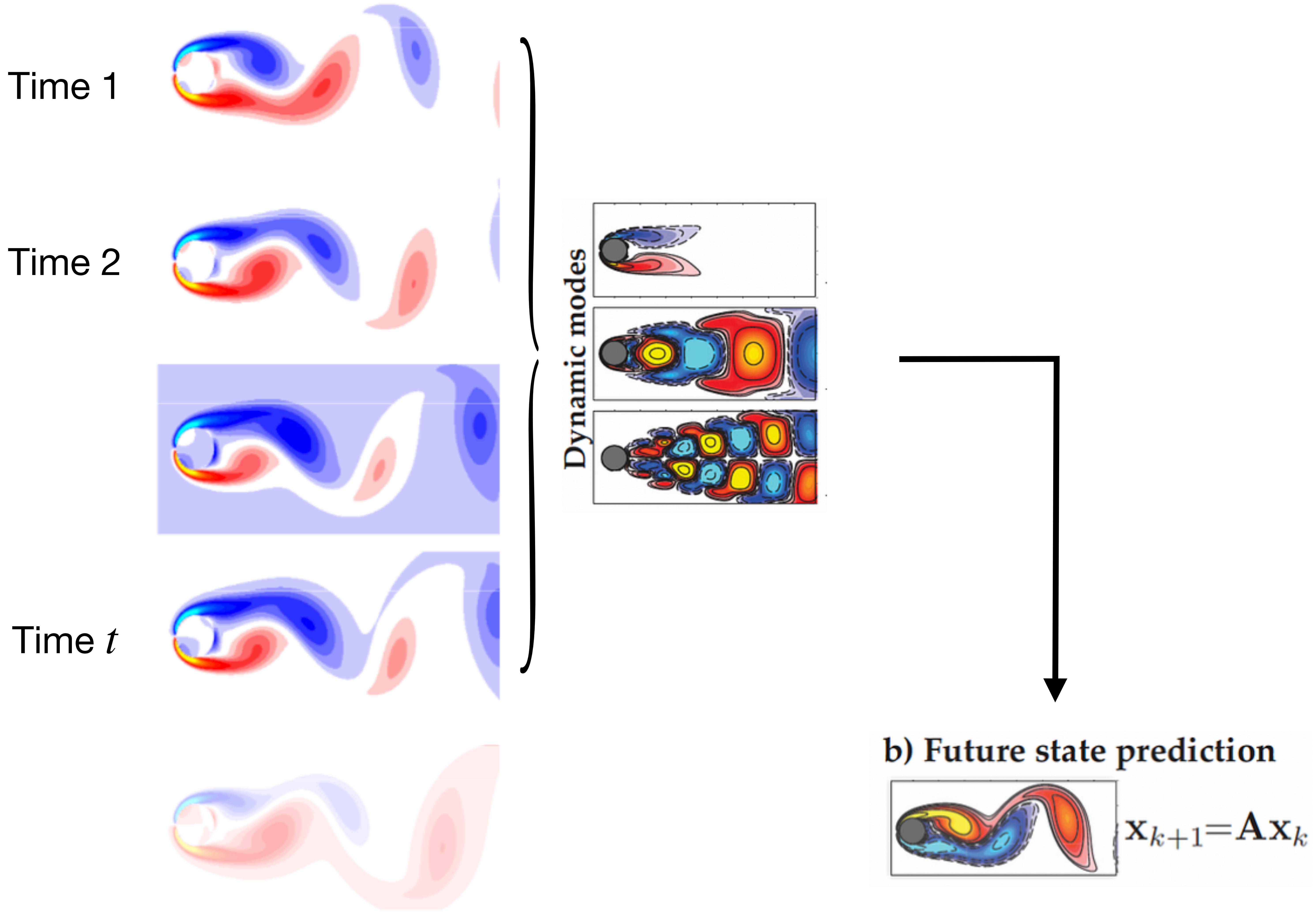
Another Supersing Fact…

Iteration lies in the Krylov Subspace

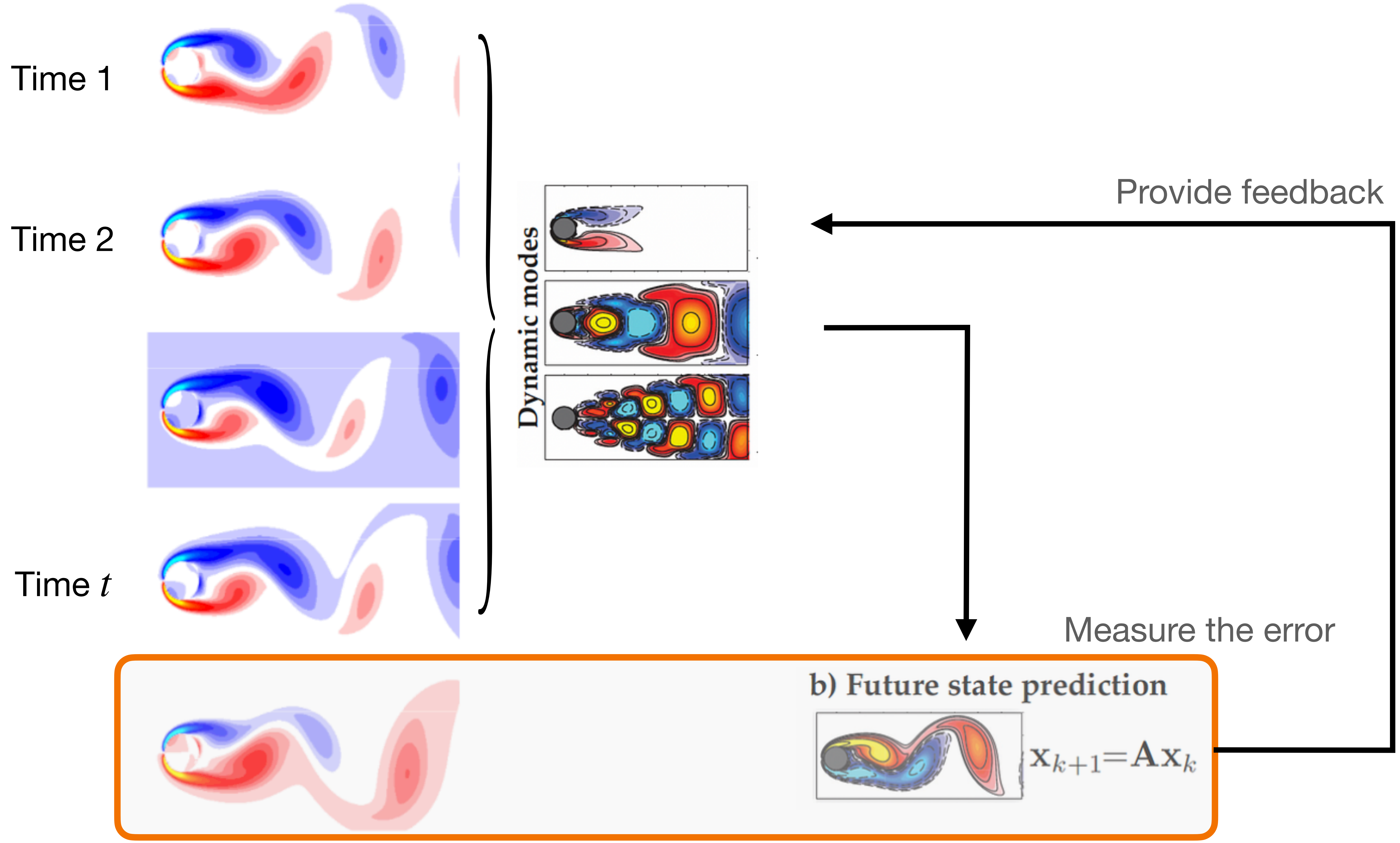
- enable dynamic mode decomposition
- Online fast update
- Much better than DMD



Dynamic Mode Decomposition with Feedback



Dynamic Mode Decomposition with Feedback



Another Supersing Fact…

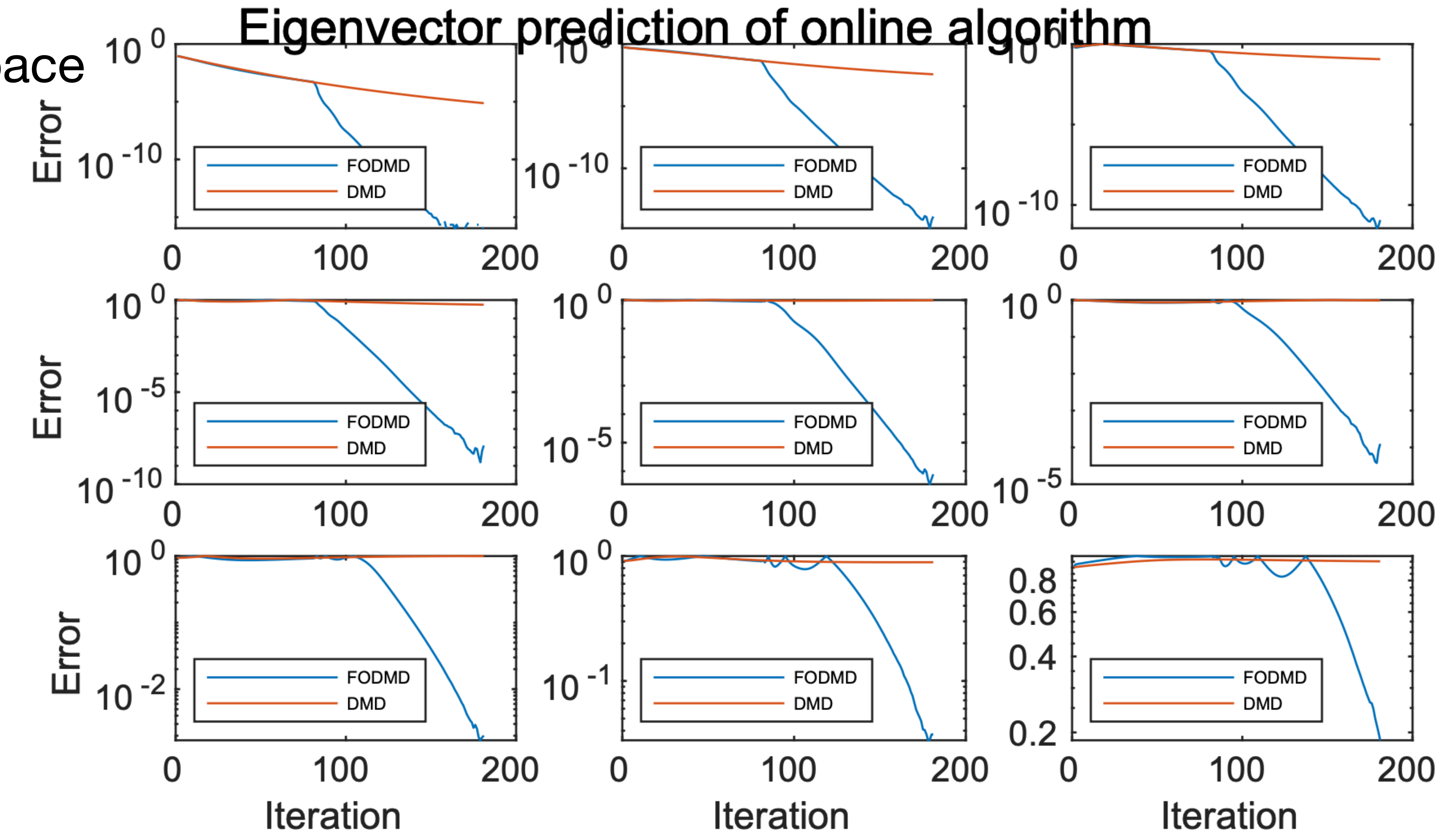
Iteration lies in the Krylov Subspace

- enable dynamic mode decomposition
- Online fast update
- Much better than DMD

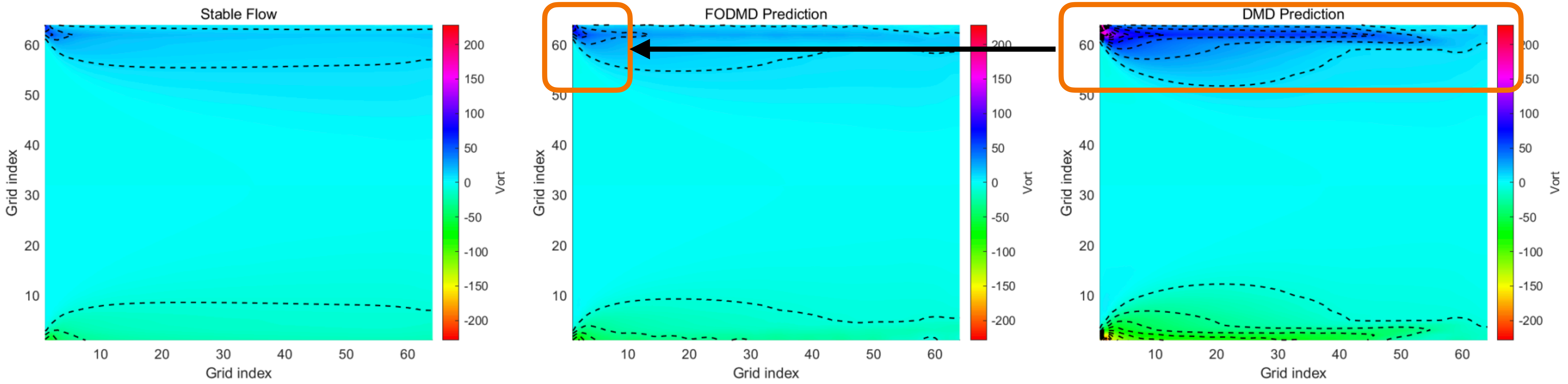
No matrix inverse, No SVD computation

Only a $n \times r$ QR decomposition

(Everything has a closed-form solution)



Prediction of Tube Flow



One more thing…

Iterative debiasing

Easier for numerical stability computation
Algorithms can do online computation

⇕

Newton Methods

Easier for convergence analysis

AISTATS 2025

Randomized Iterative Solver as Iterative Refinement
A Simple Fix Towards Backward Stability

Ruihan Xu
University of Chicago

Yiping Lu
Northwestern University

Abstract

Iterative sketching and sketch-and-precondition are well-established randomized algorithms for solving large-scale over-determined linear least-squares problems. In this paper, we introduce a new perspective that interprets Iterative Sketching and Sketching-and-Precondition as forms of Iterative Refinement. We also examine the numerical stability of two distinct refinement strategies: iterative refinement and recursive refinement, which progressively improve

tive tools for developing approximate matrix factorizations. These methods are remarkable for their simplicity and efficiency, often producing surprisingly accurate results.

In this paper, we consider randomized algorithms to solve the overdetermined linear least-squares problem

$$x = \arg\min_{y\in\mathbb{R}^n} \|b - Ay\| \quad (A \in \mathbb{R}^{m\times n}, b \in \mathbb{R}^m) \tag{1}$$

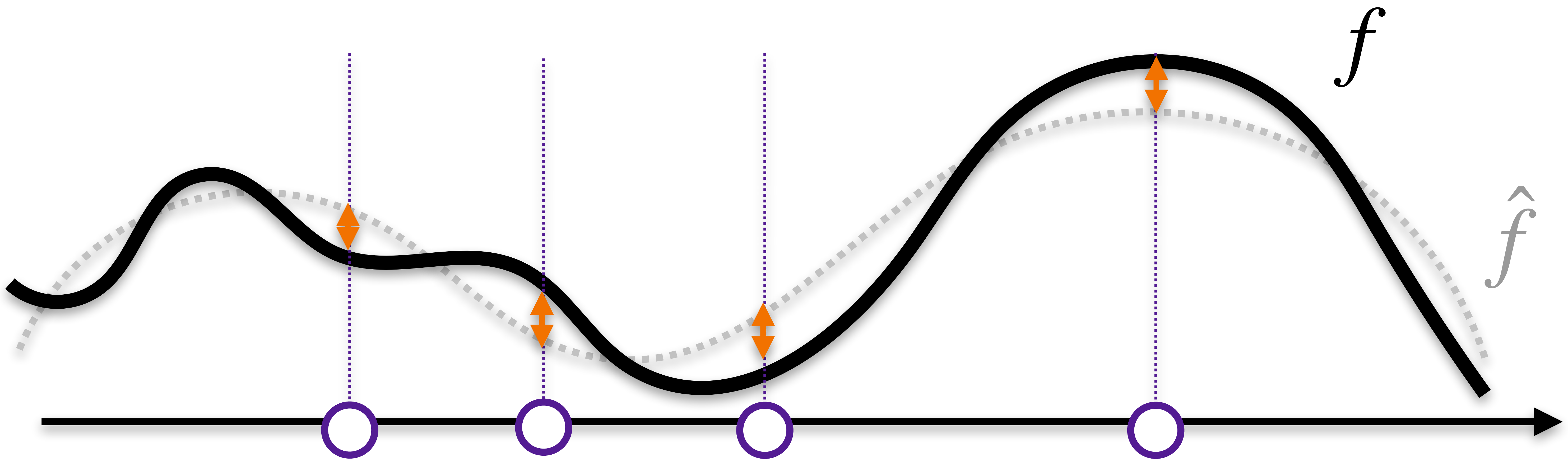
What is SCaSML about?

SCaSML

$$\{X_1, \cdots, X_n\} \sim \mathbb{P}_\theta \to \theta \to \Phi(\theta)$$

Step 1: Using Machine Learning to fit the rough function/environment

Step 2: Using validation dataset to know how much mistake machine learning algorithm has made



Step 3: Using Simulation algorithm to estimate $\Phi(\theta) - \Phi(\hat{\theta})$

Examples Later!

Using ML surrogate during inference time to improve ML solution

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