Probabilistic operator learning:
Generative modeling and uncertainty quantification for foundation models of differential equations

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Sampling, Inference, and Data-driven Physical Modeling in Scientific Machine Learning
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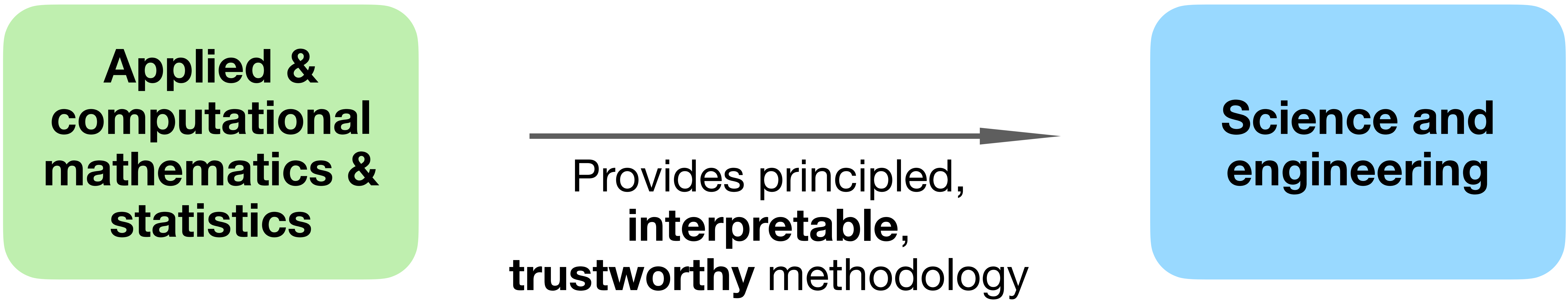
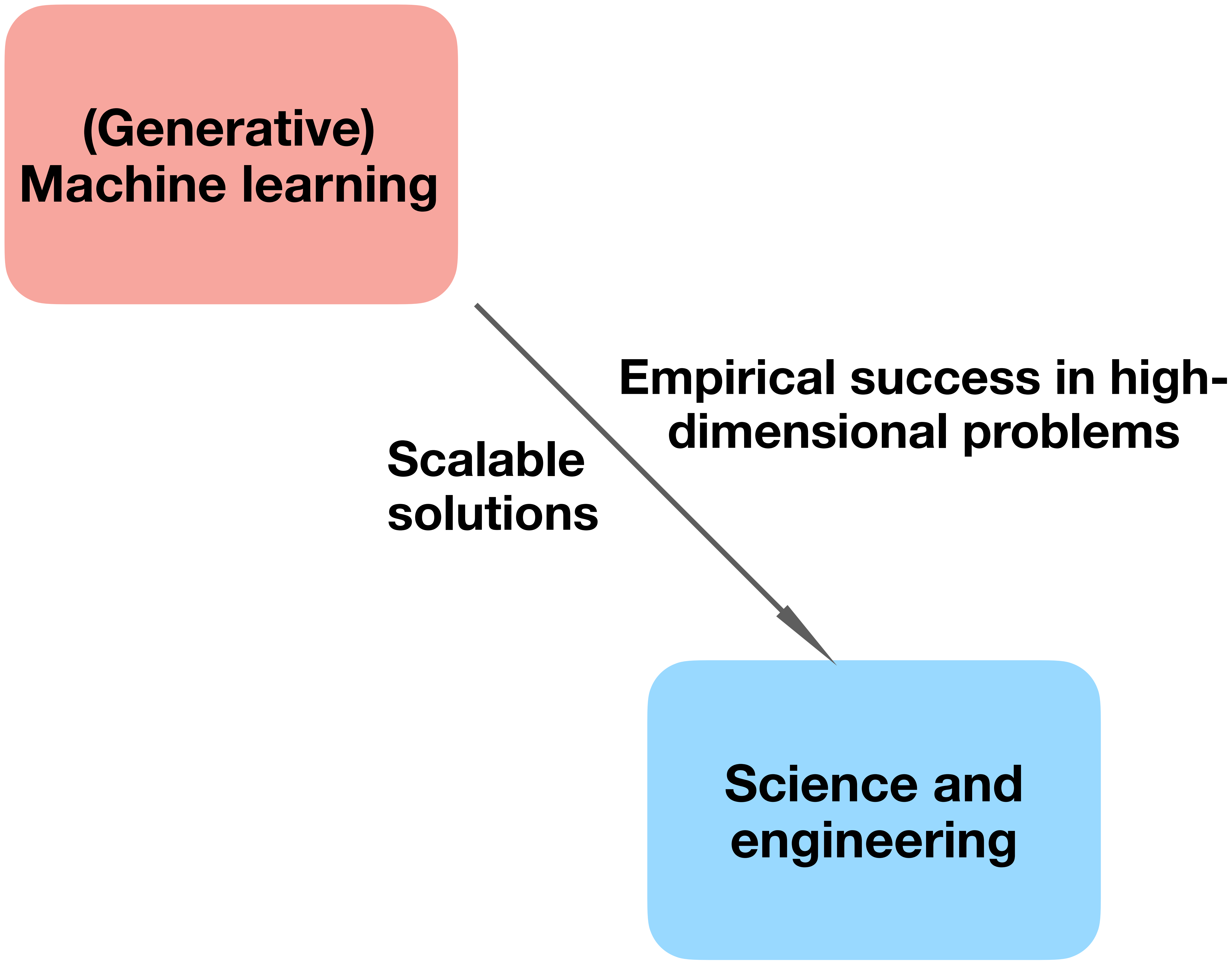
The establishment

Why do we trust computational methods?



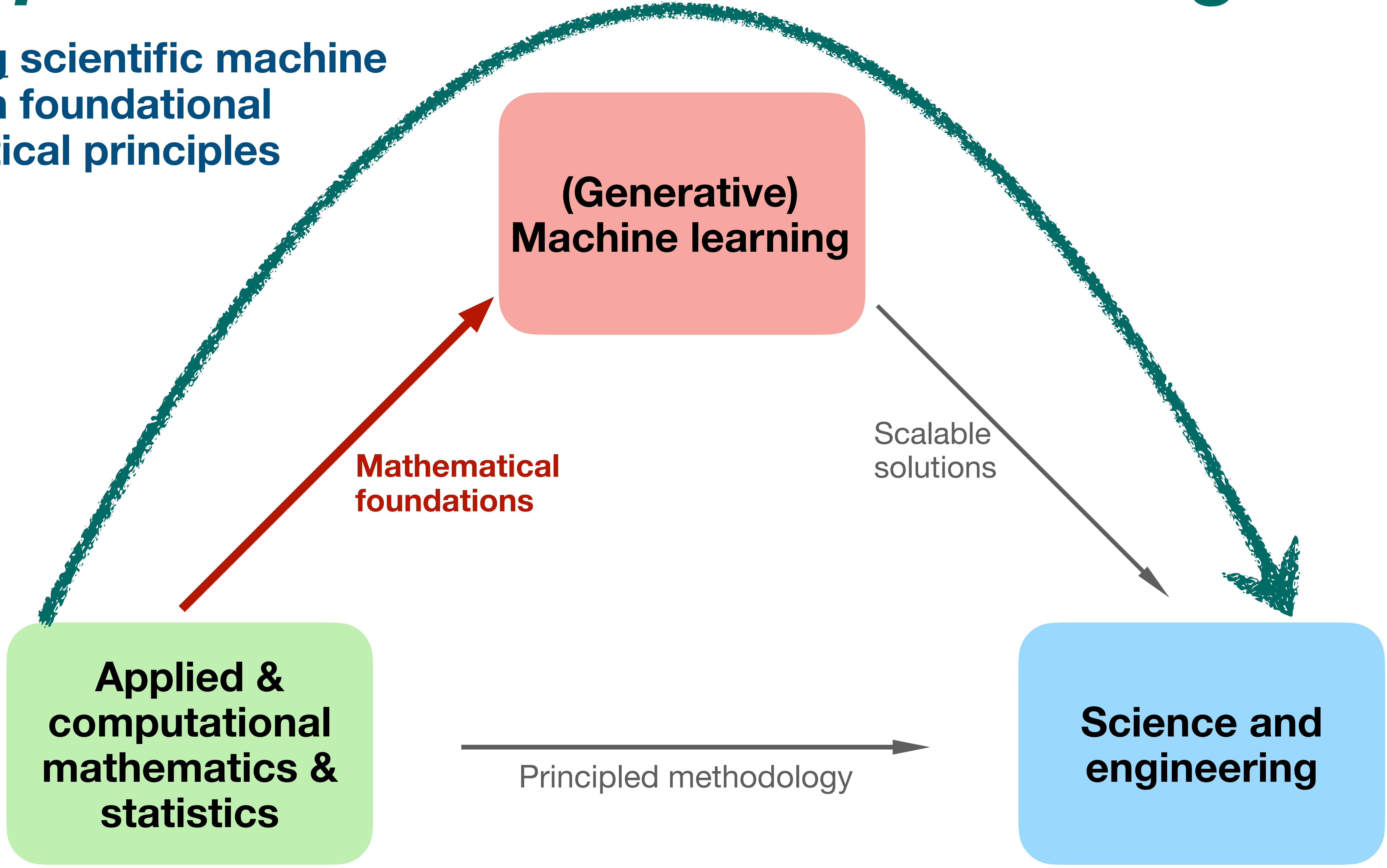
The insurgent

Why is machine learning attractive?



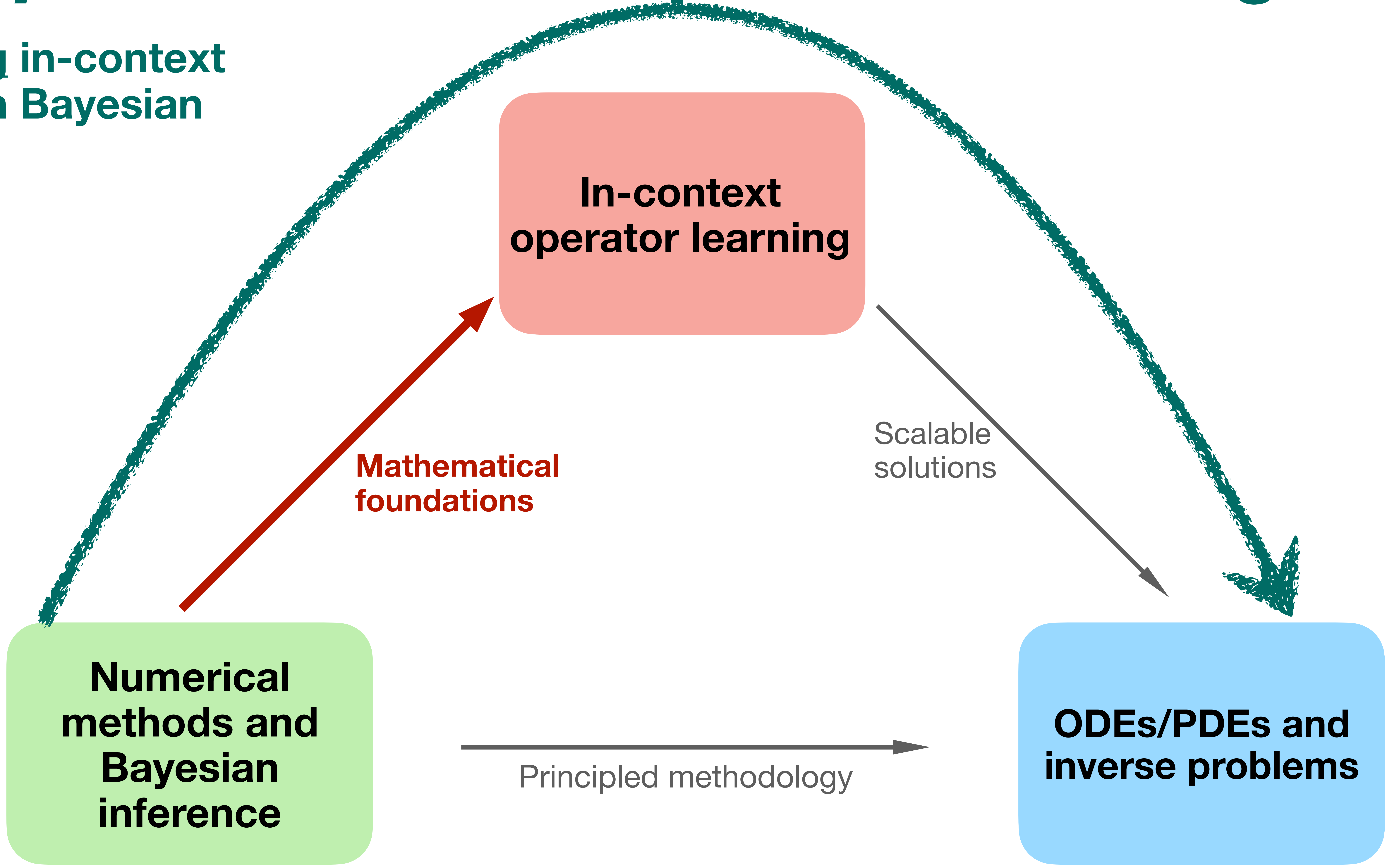
Principled scientific machine learning

<u>Grounding</u> scientific machine learning in foundational mathematical principles



Principled in-context operator learning

<u>Grounding</u> in-context learning in Bayesian inference



“Traditional” operator learning

Standard information flow for traditional operator learning

Operator Learning: algorithms and Analysis, Kovachki et al. 2024

Parameters: $\boldsymbol{\alpha}$ **Conditions: y** **Quantities-of-interest: z**

$\mathscr{A}(\alpha)z = 0,$ in D $\mathscr{B}(\alpha)z = y,$ on ∂D

Initial value problems:

$z'(t) = f(z(t); \alpha)$

$z(0) = y$

Boundary value problems:

$-\nabla \cdot (\alpha_1(x)\nabla z(x)) = \alpha_2(x)$ in D

$z(x) = y$ on ∂D

Inverse problems:

$-\nabla \cdot (\alpha_1(x)\nabla y(x)) = \alpha_2(x)$ in D

$y(x) = z$ on ∂D

Training data: $\{(\boldsymbol{\alpha}^{(i)}, y^{(i)}, z^{(i)})\}_{i=1}^N$

Model: $z = \mathscr{F}_\theta(y; \boldsymbol{\alpha})$

Training objective: $\min_\theta \sum_{i=1}^N \|z^{(i)} - \mathscr{F}_\theta(y^{(i)}; \boldsymbol{\alpha}^{(i)})\|_2^2$

$\mathscr{F}$ is a neural operator (Deep-O-net, FNO, PCA-net, etc.)

In-context operator learning

Information flow of ICON induces learning of ‘context’

Parameters: $\boldsymbol{\alpha}$ **Conditions:** y **Quantities-of-interest:** z

Group according to $\boldsymbol{\alpha}$: $\left\{ \left\{ (\boldsymbol{\alpha}^{(i)}, y^{(i,j)}, z^{(i,j)}) \right\}_{j=1}^{J} \right\}_{i=1}^{N}$

Training data omits $\boldsymbol{\alpha}$: $\left\{ \left\{ (y^{(i,j)}, z^{(i,j)}) \right\}_{j=1}^{J} \right\}_{i=1}^{N}$

$$\mathscr{A}(\alpha)z = 0, \text{ in } D$$

$$\mathscr{B}(\alpha)z = y, \text{ in } \partial D$$

Example Condition-QoI pairs

In-context operator network: $z = \mathscr{T}_\theta \left(y; \left\{ (y^{(j)}, z^{(j)}) \right\}_{j=1}^{J-1} \right)$

Query-prediction pair

Informs ‘context’

Training objective: $\min_\theta \sum_{i=1}^{N} \left\| z^{(J)} - \mathscr{T}_\theta \left(y^{(J)}; \left\{ (y^{(j)}, z^{(j)}) \right\}_{j=1}^{J-1} \right) \right\|_2^2$

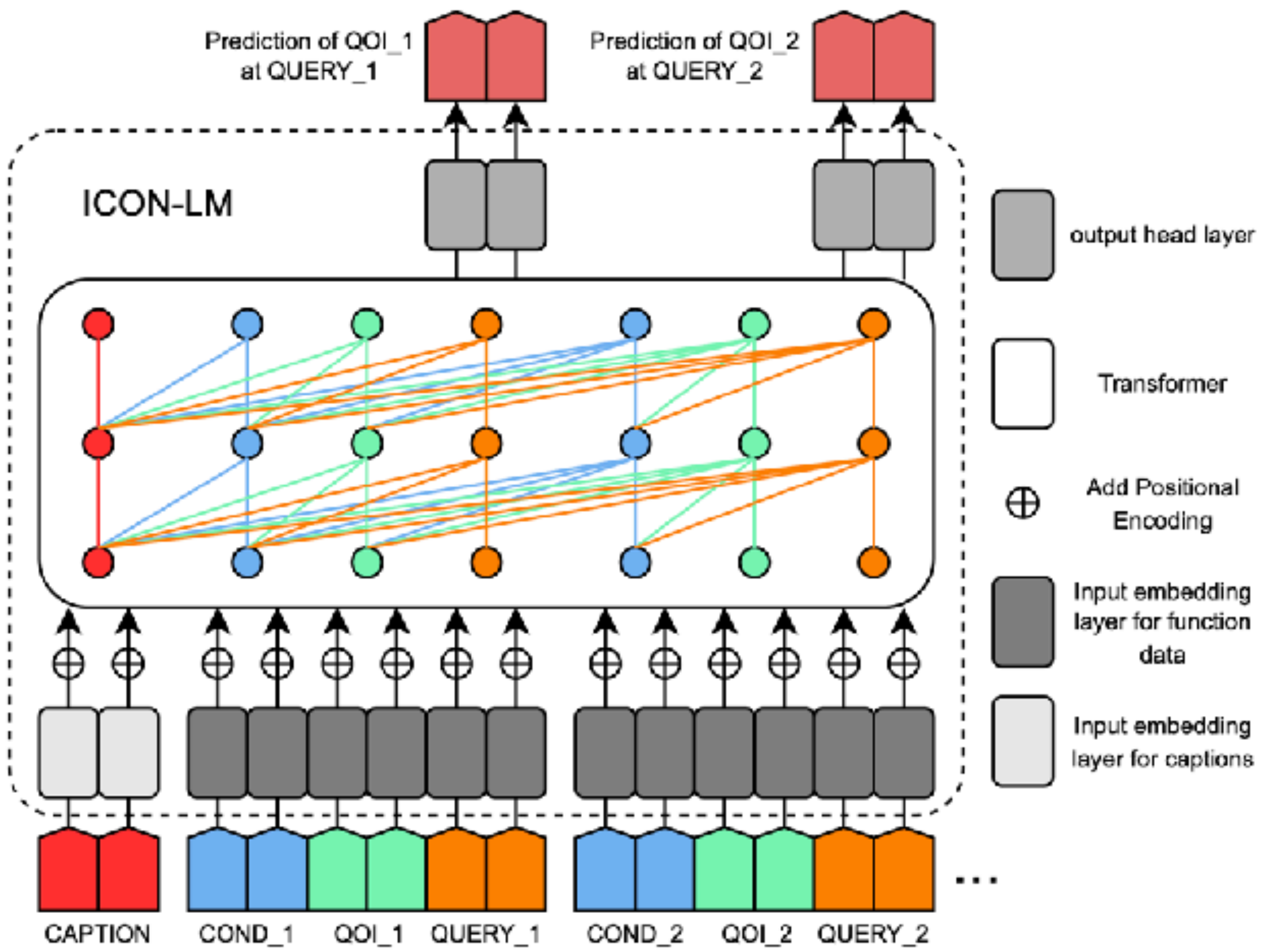
Note training does not involve $\boldsymbol{\alpha}$

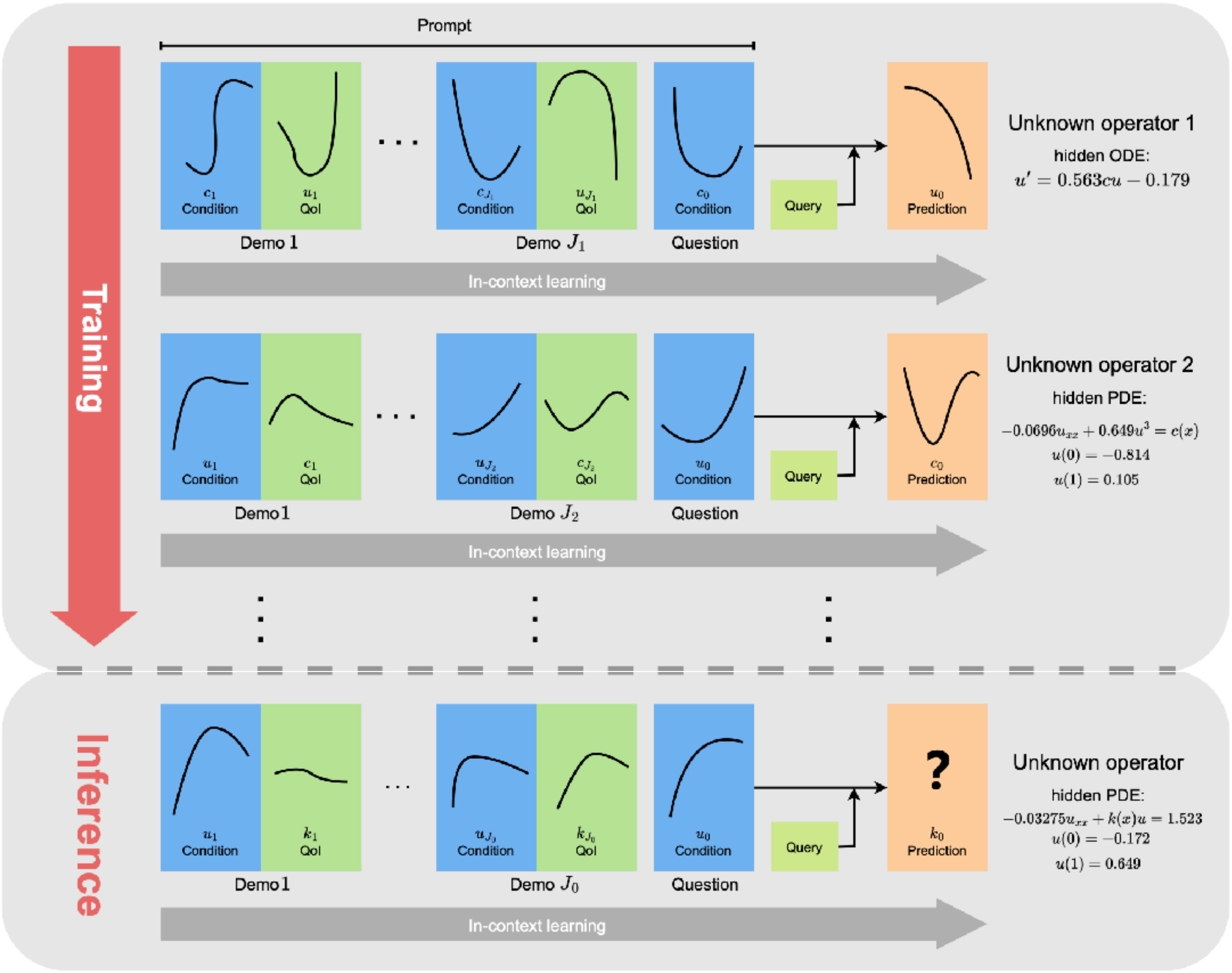
In-context operator networks

In-Context Operator Learning with Data Prompts for Differential Equation Problems, *PNAS,* L. Yang, S. Liu, T. Meng and S. Osher

Fine-Tune Language Models as Multi-Modal Differential Equation Solvers, Neural Networks, L. Yang, S. Liu, S. Osher

Differential equations	Parameters	Conditions	QoIs
$\frac{d}{dt}u(t) = a_1 c(t) + a_2$	a_1, a_2	$u(0), c(t), t \in [0,1]$	$u(t), t \in [0,1]$
for $t \in [0,1]$		$u(t), t \in [0,1]$	$c(t), t \in [0,1]$
$\frac{d}{dt}u(t) = a_1 c(t)u(t) + a_2$	a_1, a_2	$u(0), c(t), t \in [0,1]$	$u(t), t \in [0,1]$
for $t \in [0,1]$		$u(t), t \in [0,1]$	$c(t), t \in [0,1]$
$\frac{d}{dt}u(t) = a_1 u(t) + a_2 c(t) + a_3$	a_1, a_2, a_3	$u(0), c(t), t \in [0,1]$	$u(t), t \in [0,1]$
for $t \in [0,1]$		$u(t), t \in [0,1]$	$c(t), t \in [0,1]$
$u(t) = A\sin(\frac{2\pi}{T}t + \eta)e^{-kt}$	k	$u(t), t \in [0, 0.5)$	$u(t), t \in [0.5, 1]$
for $t \in [0,1]$		$u(t), t \in [0.5, 1]$	$u(t), t \in [0, 0.5)$
$\frac{d^2}{dx^2}u(x) = c(x)$	$u(0), u(1)$	$c(x), x \in [0,1]$	$u(x), x \in [0,1]$
for $x \in [0,1]$		$u(x), x \in [0,1]$	$c(x), x \in [0,1]$
$-\lambda a \frac{d^2}{dx^2}u(x) + k(x)u(x) = c$	$u(0), u(1), a, c$	$k(x), x \in [0,1]$	$u(x), x \in [0,1]$
for $x \in [0,1]$, $\lambda = 0.05$		$u(x), x \in [0,1]$	$k(x), x \in [0,1]$
$-\lambda a \frac{d^2}{dx^2}u(x) + ku(x)^3 = c(x)$	$u(0), u(1), k, a$	$c(x), x \in [0,1]$	$u(x), x \in [0,1]$
for $x \in [0,1]$, $\lambda = 0.1$		$u(x), x \in [0,1]$	$c(x), x \in [0,1]$
$\inf_{\rho,m} \iint c\frac{m^2}{2\rho}dxdt + \int g(x)\rho(1,x)dx$	$g(x), x \in [0,1]$	$\rho(t=0,x), x \in [0,1]$	$\rho(t=1,x), x \in [0,1]$
s.t. $\partial_t \rho(t,x) + \nabla_x \cdot m(t,x) = \mu \Delta_x \rho(t,x)$		$\rho(t=0,x), x \in [0,1]$	$\rho(t,x), t \in [0.5,1], x \in [0,1]$
for $t \in [0,1], x \in [0,1]$,		$\rho(t,x), t \in [0,0.5), x \in [0,1]$	$\rho(t,x), t \in [0.5,1], x \in [0,1]$
$c = 20, \mu = 0.02$,	$\rho(t=0,x)$	$g(x), x \in [0,1]$	$\rho(t=1,x), x \in [0,1]$
Periodic spatial boundary condition	$x \in [0,1]$		$\rho(t,x), t \in [0.5,1], x \in [0,1]$





What exactly is in-context operator learning?

What is the fundamental math problem ICON solves?

- What are the tools we use to approach this problem?
  - A probabilistic formulation for operator learning: **random differential equations**
- What exactly *is* in-context operator learning in the probabilistic formulation?
  - In-context operator learning implicitly performs **Bayesian inference**
- What does the Bayesian interpretation provide us?
  - A motivated **generative** formulation of ICON provides **uncertainty quantification**

A probabilistic formulation for operator learning

Random differential equations describes the data generating process

Key idea: parameters, conditions, and QoIs are random variables

Fix a probability space $(\Omega, \mathfrak{F}, \mathbb{P})$

Model the family of ODEs/PDEs as RDEs.

Parameters: $\boldsymbol{\alpha}(\omega)$ **Conditions:** $y(\omega)$ **Quantities-of-interest:** $z(\omega)$

$$\begin{cases} \frac{d}{dt} z(t,\omega) = \alpha(t,\omega) z(t,\omega) \\ z(0,\omega) = z_0(\omega) = y(\omega) \end{cases}$$

RDEs induce probability measure which describes **data generating process** (data generating measure)

$$\mathcal{Q}(d\alpha, dy, dz)$$

In practice, requires discretization $0 = t_0 < t_1 < \cdots < t_N = T$

$$\{(\boldsymbol{\alpha}^{(i)}, y^{(i)}, z^{(i)})\}_{i=1}^{N} \sim \mathcal{Q}^N(d\alpha, dy, dz_1, \ldots, dz_N) = \mathcal{Q}_y(dy)\mathcal{Q}_\alpha(d\alpha)\prod_{n=0}^{N-1}\mathcal{K}(dz_{n+1} \,|\, z_n, \alpha)$$

$$\approx \mathcal{Q}(d\alpha, dy, dz)$$

Recall: Regression and conditional expectation

Least squares regression approximates conditional expectation

Let X and Y be random variables with joint distribution p_{XY}, and $h(X)$ be a predictor for Y. The predictor that minimizes the mean-squared error is the conditional expectation of Y given X.

$$\mathbb{E}[Y\,|\,X] = \arg\min_h \mathbb{E}_{p_{XY}} \|Y - h(X)\|_2^2$$

Joint: $p_{XY}(x, y)$

Marginal: $p_X(x) = \int p_{XY}(x, y)dy$

Conditional: $p_{Y|X}(y\,|\,x) = \dfrac{p_{XY}(x, y)}{p_X(x)}$

$$\mathbb{E}[Y\,|\,X = x] = \int y p_{Y|X}(y\,|\,x)dy$$

What does this mean for "traditional" operator learning?

Training data: $\{(\boldsymbol{\alpha}^{(i)}, y^{(i)}, z^{(i)})\}_{i=1}^N \sim \mathcal{Q}(\boldsymbol{\alpha}, y, z)$

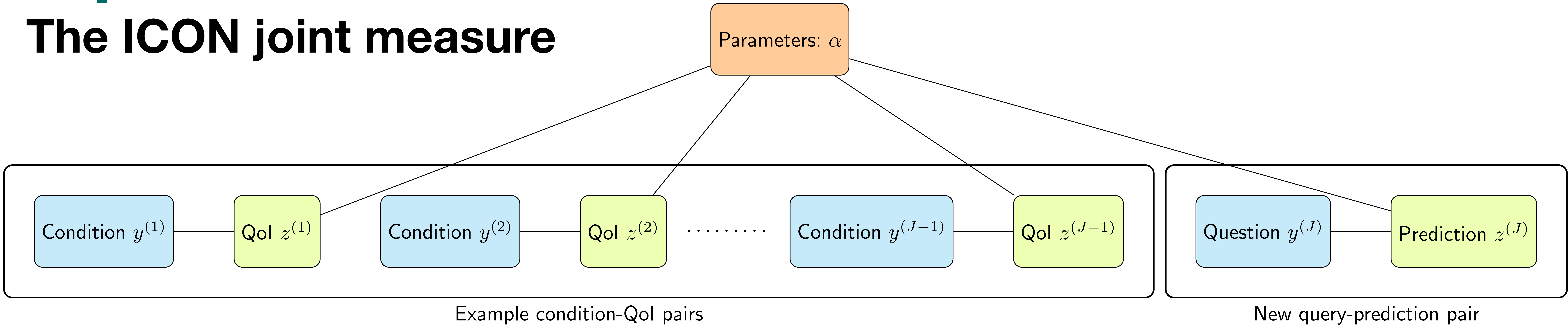
Objective: $\min_\theta \sum_{i=1}^N \|z^{(i)} - \mathcal{F}_\theta(y^{(i)}; \boldsymbol{\alpha}^{(i)})\|_2^2$

The optimal learned operator approximates conditional expectation

$$\mathbb{E}[z\,|\,y, \boldsymbol{\alpha}] \approx \mathcal{F}_{\theta^\star}(y^{(i)}; \boldsymbol{\alpha}^{(i)})$$

A probabilistic formulation for ICON

The ICON joint measure



Group according to $\boldsymbol{\alpha}$: $\left\{ \left\{ (\boldsymbol{\alpha}^{(i)}, y^{(i,j)}, z^{(i,j)}) \right\}_{j=1}^{J} \right\}_{i=1}^{N} \sim \mathcal{Q}(\boldsymbol{\alpha}, y, z) = \mathcal{Q}(z \,|\, y, \boldsymbol{\alpha}) \mathcal{Q}_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) \mathcal{Q}_y(y)$

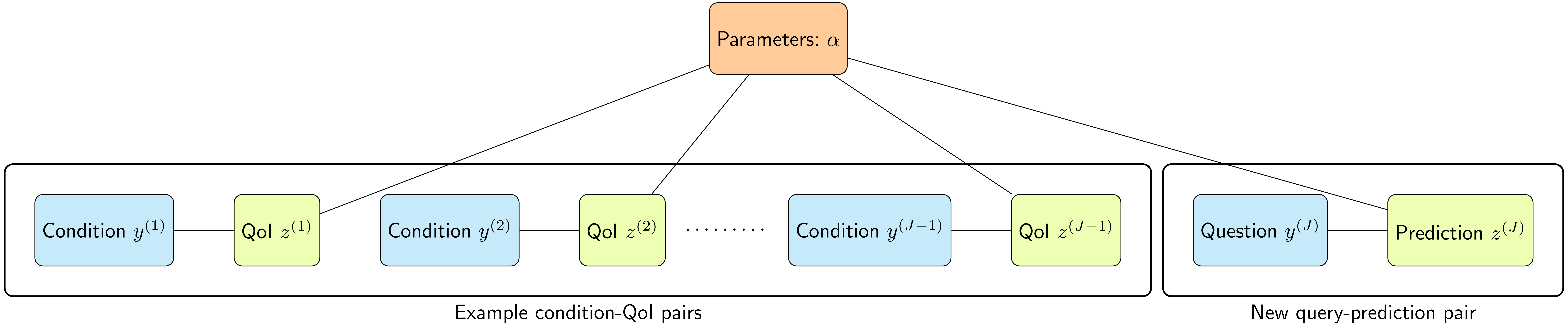
<u>Training data omits</u> $\boldsymbol{\alpha}$: $\left\{ \left\{ (y^{(i,j)}, z^{(i,j)}) \right\}_{j=1}^{J} \right\}_{i=1}^{N} \sim \mathcal{Q}\left(\{(y^{(j)}, z^{(j)})\}_{j=1}^{J} \right)$ **Subtly non-i.i.d!**

The joint measure of conditions-QoIs pairs

$$\mathcal{Q}\left(\{(y^{(j)}, z^{(j)})\}_{j=1}^{J} \right) = \int \mathcal{Q}_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) \prod_{j=1}^{J} \mathcal{Q}(z^{(j)} \,|\, y^{(j)}, \alpha) \mathcal{Q}_y(y^{(j)}) d\boldsymbol{\alpha}$$

What conditional expectation does ICON approximate?

ICON estimates expectation of the posterior predictive



Training data: $\left\{ \{(y^{(i,j)}, z^{(i,j)})\}_{i=1}^{N} \right\}_{j=1}^{J} \sim \mathcal{Q}\left(\{(y^{(j)}, z^{(j)})\}_{j=1}^{J} \right)$ Training objective: $\min_{\theta} \sum_{i=1}^{N} \left\| z^{(J)} - \mathcal{T}_{\theta}\left(y^{(J)}; \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1} \right) \right\|_2^2$

<u>The conditional measure</u> of prediction conditioned on query and example condition-QoI pairs

$$\mathcal{Q}\left(z^{(J)} \middle| y^{(J)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1} \right)$$

Posterior predictive distribution

The in-context operator network approximates conditional expectation

$$\mathbb{E}\left[z^{(J)} \middle| y^{(J)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1} \right] \approx \mathcal{T}_{\theta^\star}\left(y^{(J)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1} \right)$$

Expectation of posterior predictive

What is the posterior predictive distribution?

What is the classical Bayesian approach to the ICON problem?

Model: $z'(t) = f(z(t); \alpha)$
$z(0) = y$

Task: Given $\{(y^{(j)}, z^{(j)})\}_{j=1}^{J}$ (from same α) and $y^{(J)}$, predict $z^{(J)}$

Step 1: Bayesian parameter estimation (compute the posterior distribution)

Bayes's Rule

$$\mathcal{Q}\left(\boldsymbol{\alpha} \,\middle|\, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1}\right) \propto \mathcal{Q}_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) \prod_{i=1}^{J-1} \mathcal{Q}\left(y^{(j)}, z^{(j)} \,\middle|\, \boldsymbol{\alpha}\right)$$

Posterior — Prior — Likelihood

Step 2: Compute the posterior predictive (Predictions under an inferred α)

$$\mathcal{Q}\left(z^{(J)} \,\middle|\, y^{(J)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1}\right) = \int \mathcal{Q}\left(z^{(J)} \,\middle|\, y^{(J)}, \boldsymbol{\alpha}\right) \mathcal{Q}\left(\boldsymbol{\alpha} \,\middle|\, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1}\right) d\boldsymbol{\alpha}$$

Posterior predictive — Prediction for a given $y^{(J)}$ and $\boldsymbol{\alpha}$ — Posterior on $\boldsymbol{\alpha}$

ICON implicitly performs Bayesian inference

Task: Given $\{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1}$ and new question $y^{(J)}$, predict $z^{(J)}$

Classical Bayesian approach

Step 1: Compute posterior distribution

$$Q\left(\alpha \middle| \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) \propto Q_0(\alpha) \prod_{j=1}^{J-1} Q\left(y^{(j)}, z^{(j)} \middle| \alpha\right)$$

Step 2: Compute posterior predictive distribution

$$Q\left(z^{(J)} \middle| y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) = \int Q\left(z^{(J)} \middle| y^{(J)}, \alpha\right) Q\left(\alpha \middle| \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) \mathrm{d}\alpha$$

In-context operator networks

Least squares regression

$$\mathcal{T}^\star\left(y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) = \arg\min_{\mathcal{T}} \mathbb{E}\left[\left\|z^{(J)} - \mathcal{T}\left(y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right)\right\|_2^2\right]$$

Expectation taken over Joint measure of condition-QoI pairs

Conditional expectation predicts $z^{(J)}$

$$\mathbb{E}\left[z^{(J)} \middle| y^{(J)}, \{y^{(j)}, z^{(j)}\}_{j=1}^{J-1}\right] = \mathcal{T}^\star\left(y^{(J)}, \{y^{(j)}, z^{(j)}\}_{j=1}^{J-1}\right)$$

ICON directly approximates mean of posterior predictive distribution

An explanation of in-context learning as implicit Bayesian inference, Xie et. al 2021

Ex: Reaction-diffusion equation

$$\begin{cases} -0.05y_1(\omega)u''(x,\omega) + \alpha(x,\omega)u(x,\omega) = y_2(\omega) \\ u(0,\omega) = y_3(\omega), u(1,\omega) = y_4(\omega) \end{cases}$$

$$z(x,\omega) = u(x,\omega) + \epsilon$$

$\epsilon \sim \mathcal{N}(0,\sigma_o^2)$, for each x

Parameters $\alpha(x,\omega)$

Conditions $\{y_i(\omega)\}_{i=1}^4$

QoI $z(x,\omega)$

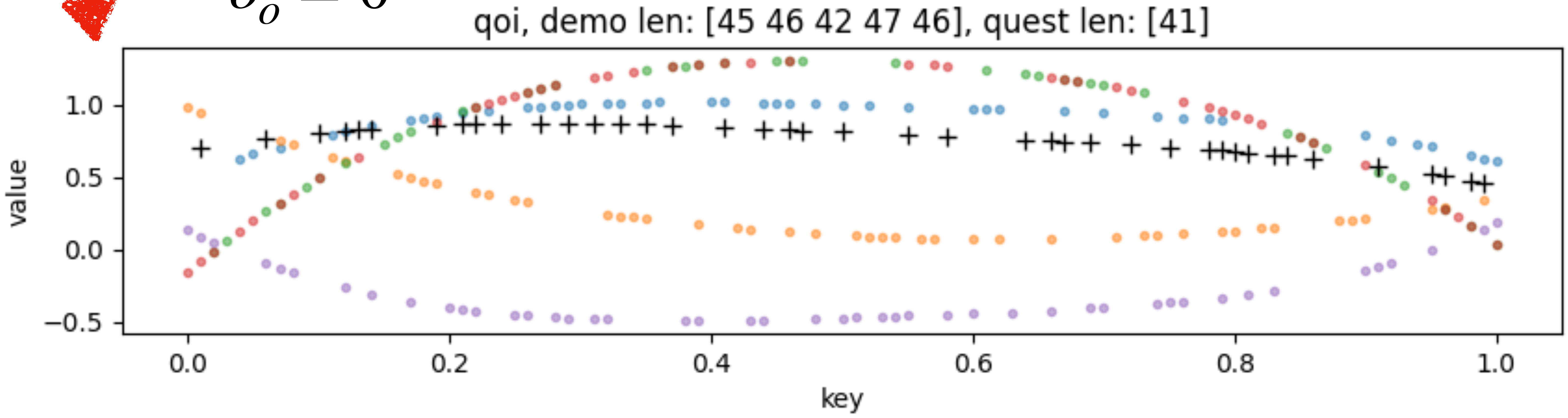
Noisy observations of the solution $u(x,\omega)$

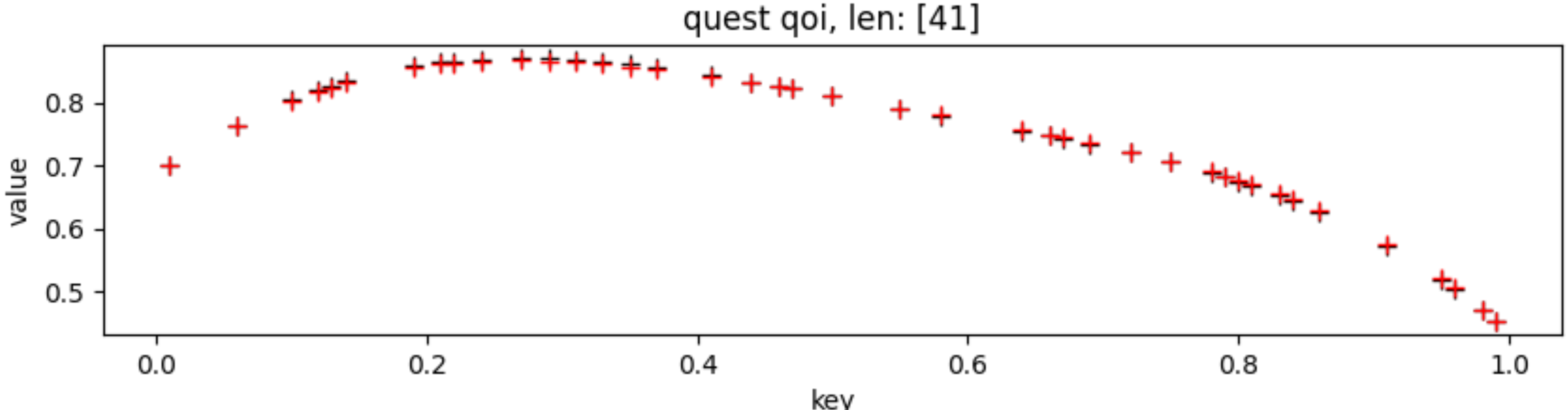
Data generating process

- $\alpha(x,\omega)$ rectified Gaussian process with squared exponential covariance
- $y_1 \sim \mathcal{U}[0.5,1.5], y_2 \sim \mathcal{U}[-2,2]$
  $y_3 \sim \mathcal{U}[-1,1], y_4 \sim \mathcal{U}[-1,1]$

QoI $z(x,\omega)$

$\sigma_o = 0$





- $J - 1 = 5$ Example condition-QoI pairs
- Colored lines: example solutions
- Truth (+) and prediction (+)
- **Learning from partial observations** (example pairs have different lengths)

Ex: Reaction-diffusion equation

$$\begin{cases} -0.05 y_1(\omega) u''(x,\omega) + \alpha(x,\omega) u(x,\omega) = y_2(\omega) \\ u(0,\omega) = y_3(\omega), u(1,\omega) = y_4(\omega) \end{cases}$$

$$z(x,\omega) = u(x,\omega) + \epsilon$$

$\epsilon \sim \mathcal{N}(0, \sigma_o^2)$, for each x

Parameters $\alpha(x,\omega)$

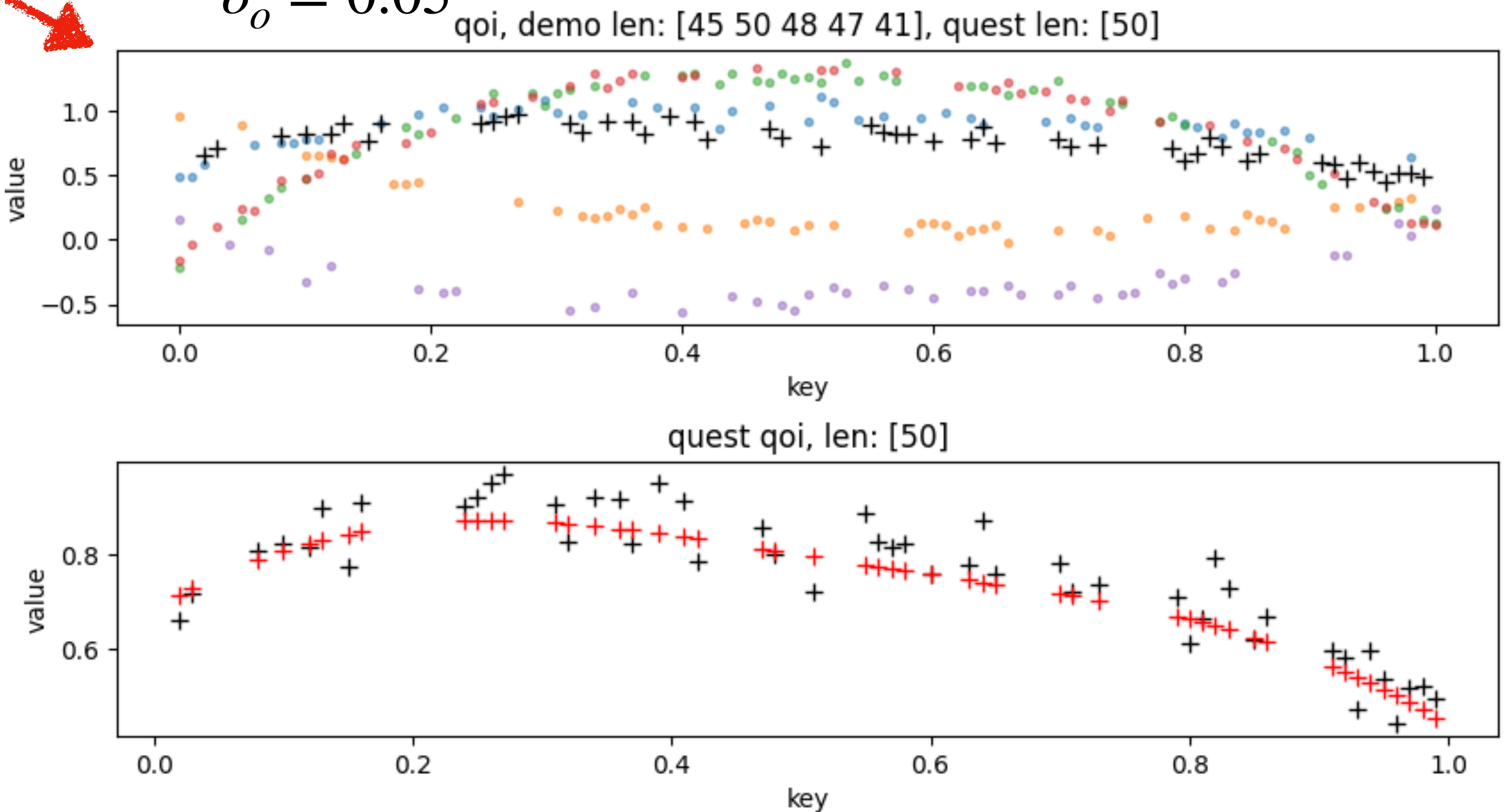
Conditions $\{y_i(\omega)\}_{i=1}^4$

QoI $z(x,\omega)$

QoI $z(x,\omega)$

Noisy observations of the solution $u(x,\omega)$

$\sigma_o = 0.05$



- $J - 1 = 5$ Example condition-QoI pairs
- Colored lines: example pairs
- Truth (+) and prediction (+)
- **ICON is de-noising**

$$\mathbb{E}\left[z^{(6)} \middle| y^{(6)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^5 \right]$$

Ex: Reaction-diffusion equation

$$\begin{cases} -0.05y_1(\omega)u''(x,\omega) + \alpha(\omega)u(x,\omega) = y_2(\omega) \\ u(0,\omega) = y_3(\omega), u(1,\omega) = y_4(\omega) \end{cases}$$

$$z(x,\omega) = u(x,\omega) + \epsilon$$

$\epsilon \sim \mathcal{N}(0,\sigma_o^2)$, for each x

Parameters $\alpha(\omega)$

Conditions $\{y_i(\omega)\}_{i=1}^4$

QoI $z(x,\omega)$

- **ICON learns from partial observations**
- **ICON is de-noising**

How? Implicitly performing Bayesian inference

Posterior $\mathcal{Q}\left(\boldsymbol{\alpha} \middle| \{(y^{(j)}, z^{(j)}\}_{j=1}^5\right)$

Posterior predictive $\mathcal{Q}\left(z^{(6)} \middle| y^{(6)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^5\right)$

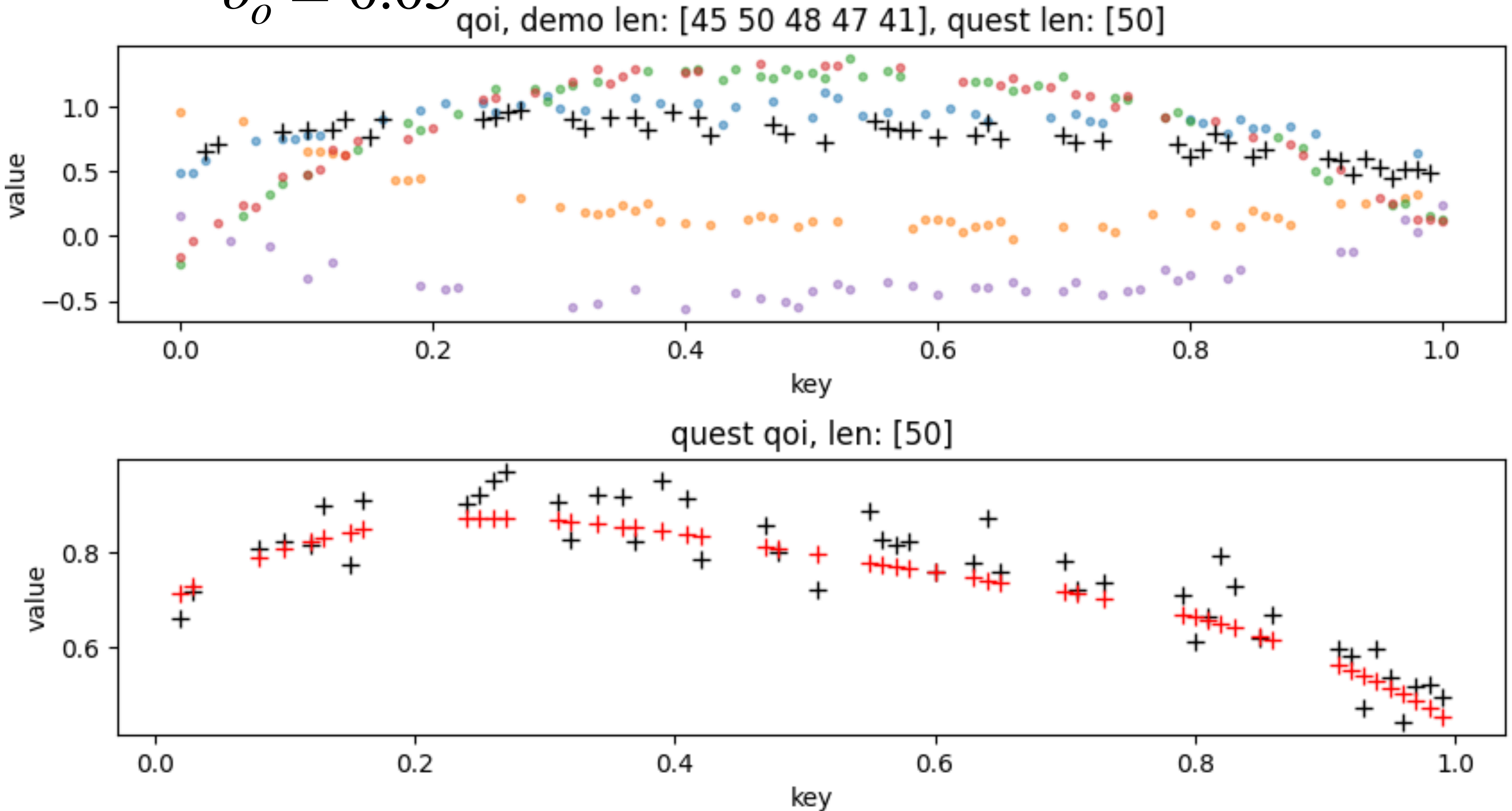
$$\mathbb{E}\left[z^{(6)} \middle| y^{(6)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^5\right]$$

$$= \mathbb{E}\left[u^{(6)} + \epsilon \middle| y^{(6)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^5\right]$$

$$= u^{(6)} \middle| y^{(6)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^5$$

Noisy observations of the solution $u(x,\omega)$

$\sigma_o = 0.05$



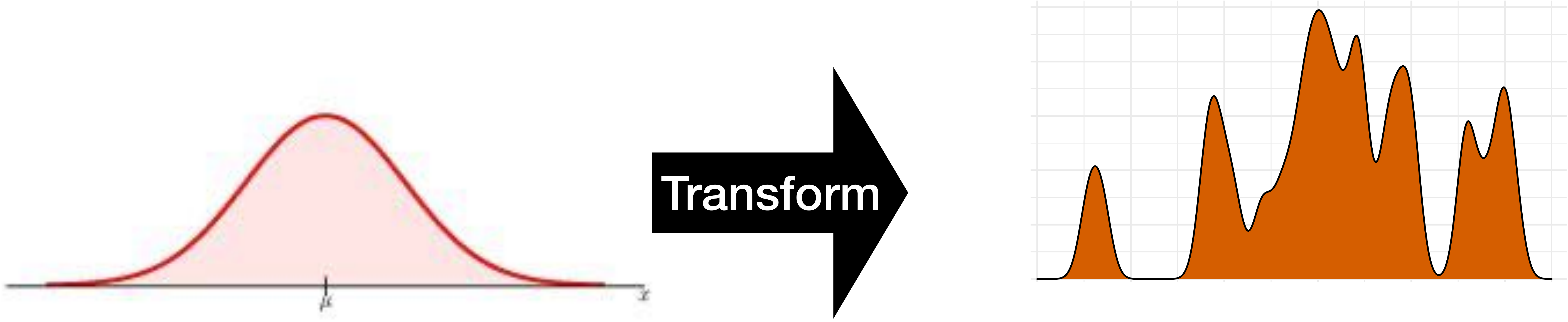
Can we sample from the posterior predictive?

A soupçon of generative modeling

Goal: Given data $\{Z_i\}_{i=1}^N \sim \mathbb{Q}$ from (unknown) **target distribution** $\mathbb{Q}$ **,** produce *new* samples from $\mathbb{Q}$

- Pick a **source distribution** p_X, easy to simulate (e.g. Gaussian).
- **Generative map:** Learn a **transport map** $\mathcal{G}$ such that:

$$\mathcal{G}_{\#}p_X \approx \mathbb{Q}, \textbf{ s.t. } X \sim p_X, \mathcal{G}(X) \sim \mathbb{Q}_\theta \approx \mathbb{Q}$$



source ρ (simple) **target** π (complex)

Can we sample from the posterior predictive?

A generative ICON produces samples from the posterior predictive

Generative in-context operator network samples from the posterior predictive

Let p_X be a reference distribution. **Generative ICON** is a mapping such that

$$\mathcal{G}^\star\left(\cdot\,, y^{(J)}, \left\{(y^{(j)}, z^{(j)})\right\}_{j=1}^{J-1}\right)_\sharp p_X(x) = \mathcal{Q}\left(\cdot\,\middle|\, y^{(J)}, \left\{(y^{(j)}, z^{(j)})\right\}_{j=1}^{J-1}\right)$$

$$x \sim p_X \implies \mathcal{G}^\star\left(x, y^{(J)}, \left\{(y^{(j)}, z^{(j)})\right\}_{j=1}^{J-1}\right) = z^{(J)} \sim \mathcal{Q}\left(\cdot\,\middle|\, y^{(J)}, \left\{(y^{(j)}, z^{(j)})\right\}_{j=1}^{J-1}\right)$$

Original ICON is the average Generative ICON!

$$\mathcal{T}^\star\left(y^{(J)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1}\right) = \mathbb{E}\left[z^{(J)}\,\middle|\, y^{(J)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1}\right]$$

$$= \mathbb{E}_X\left[\mathcal{G}^\star\left(x, y^{(J)}, \left\{(y^{(j)}, z^{(j)})\right\}_{j=1}^{J-1}\right)\right] = \int \mathcal{G}^\star\left(x, y^{(J)}, \left\{(y^{(j)}, z^{(j)})\right\}_{j=1}^{J-1}\right) p_X(x)dx$$

The posterior predictive provides uncertainty quantification

Why we should sample from the posterior predictive

Original ICON

$$\mathcal{T}^\star\left(y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) = \mathbb{E}\left[z^{(J)} \middle| y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right]$$

- ICON **approximates mean** of posterior predictive distribution
- $\mathcal{T}^\star(\cdot,\cdot)$ is an operator learner

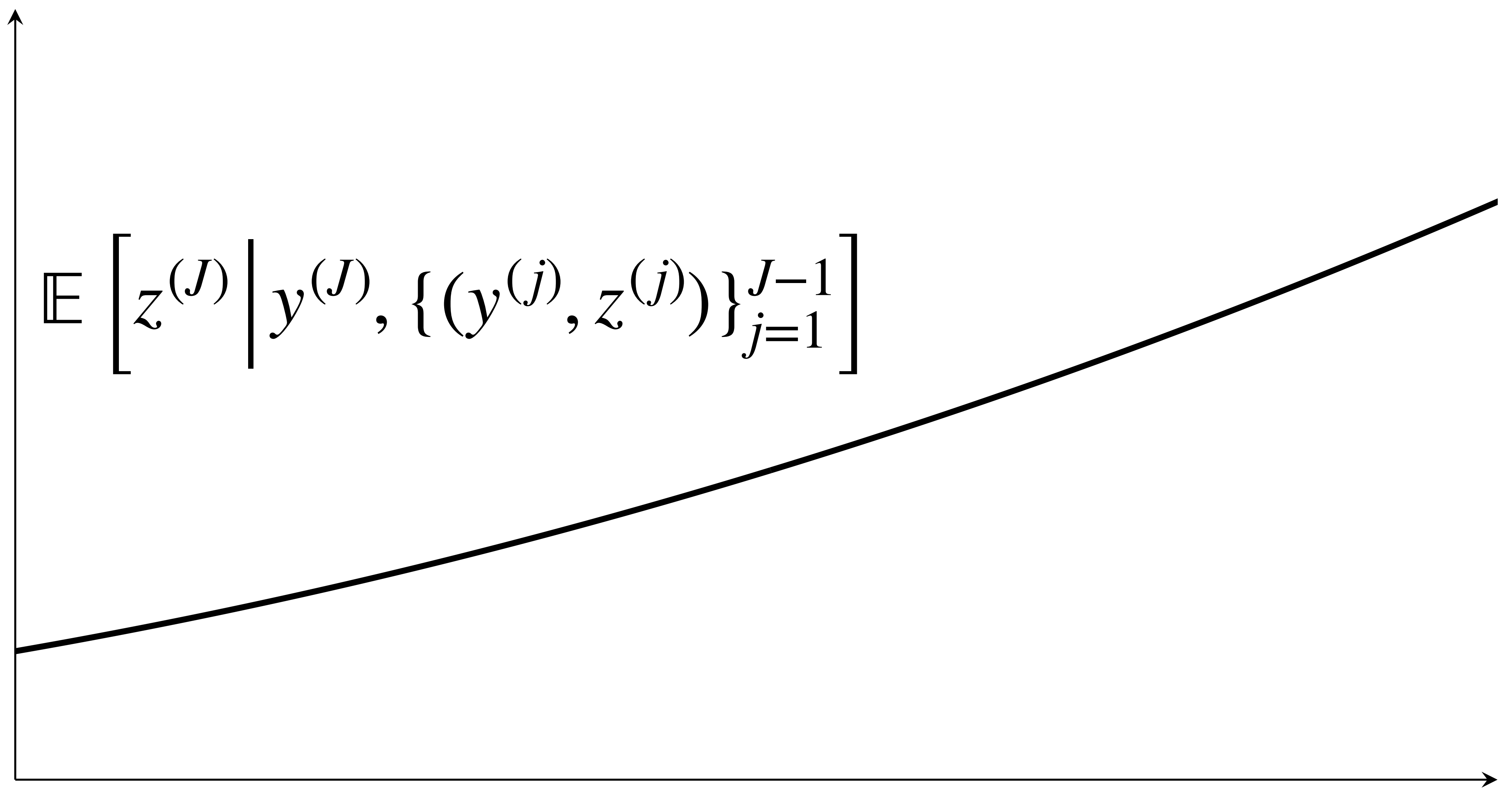
Theorem: Average generative ICON equals Original ICON

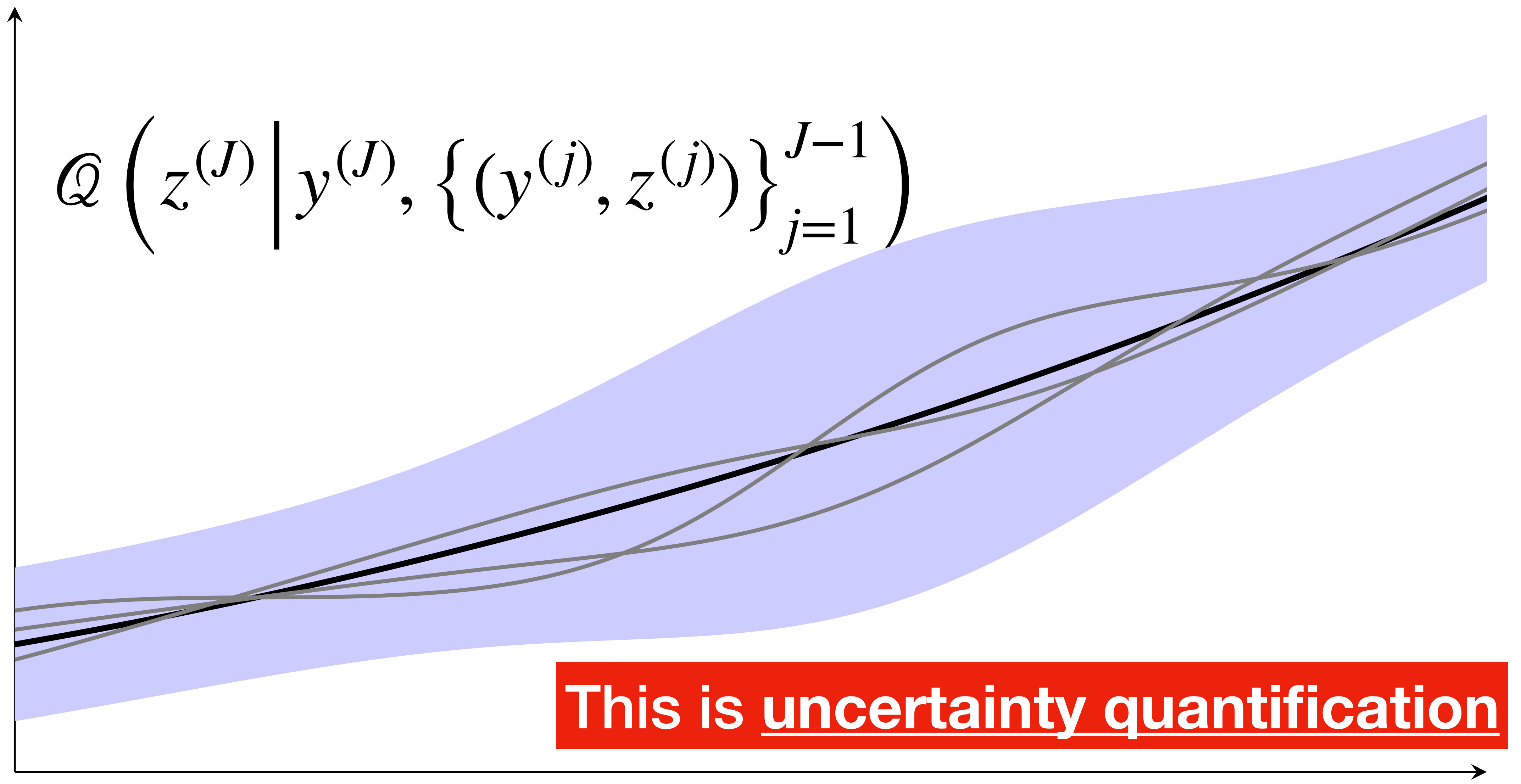
$$\mathcal{T}^\star\left(y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) = \int \mathcal{G}^\star\left(x, y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) p_X(x)\, dx$$

Generative ICON

$$\mathcal{G}^\star\left(\cdot, y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right)_\sharp p_X = Q\left(\cdot \middle| y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right)$$

- Generative ICON **generates** from the posterior predictive distribution
- $\mathcal{G}^\star(x,\cdot,\cdot)$ is a *sample* operator learner





Generative in-context operator networks

Conditional sampling from the posterior predictive distribution

Example: training via conditional Generative Adversarial Networks

$$\min_{\theta} \mathscr{D}\left(\mathcal{Q}\left(z^{(J)} \,|\, y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right), \mathcal{Q}_\theta\left(z^{(J)} \,|\, y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right)\right) = \min_{\theta} \mathbb{E}_{\mathcal{Q}_\theta}\left[f\left(\frac{d\mathcal{Q}}{d\mathcal{Q}_\theta}\right)\right]$$

$$= \min_{\theta} \max_{\phi} \mathbb{E}_{Q}[D_\phi(y^{(J)})] - \mathbb{E}_{Q_\theta}[(f^\star \circ D_\phi)(y^{(J)})]$$

Training data: $\left\{ \left\{(y^{(i,j)}, z^{(i,j)})\right\}_{i=1}^{N} \right\}_{j=1}^{J} \sim \mathcal{Q}\left(\{(y^{(j)}, z^{(j)})\}_{j=1}^{J}\right)$

$$\min_{\theta} \max_{\phi} \left\{ \frac{1}{M} \sum_{m=1}^{M} D_\phi\left(y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}, z^{(J)}\right) - \frac{1}{N} \sum_{n=1}^{N} f^\star\left(D_\phi\left(y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}, \mathscr{G}_\theta(x^{(n)}, y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1})\right)\right) \right\}$$

Example: Generative ICON for Poisson

$$\begin{cases} -u''(x,\omega) = y(x,\omega) \\ u(0,\omega) = \alpha_1(\omega), u(1,\omega) = \alpha_2(\omega) \end{cases}$$

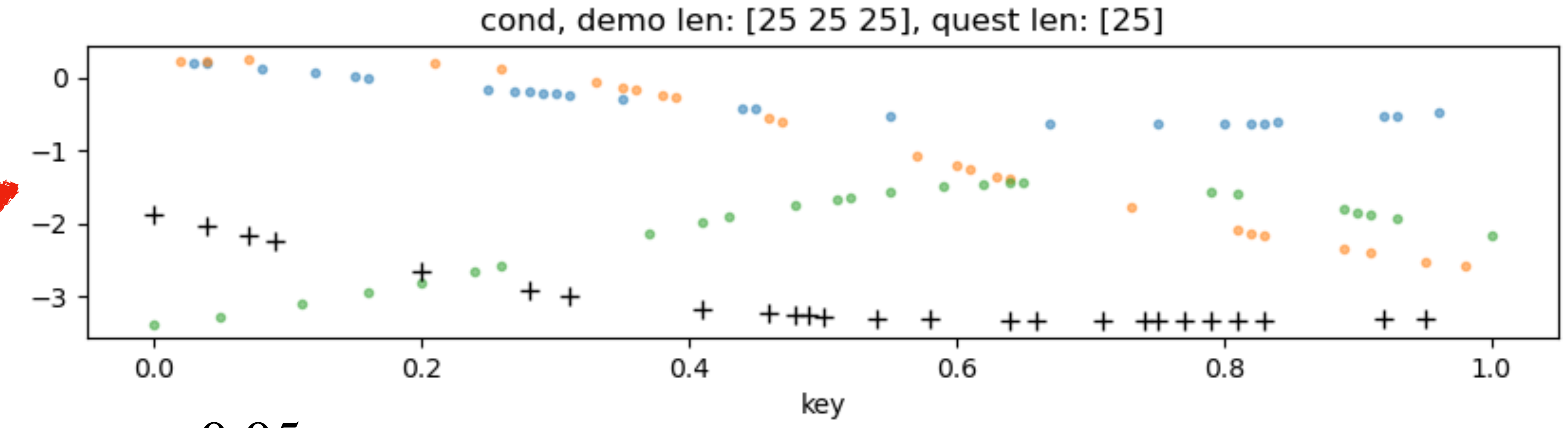
$z(x,\omega) = u(x,\omega) + \epsilon$

$\epsilon \sim \mathcal{N}(0,\sigma_o^2)$, for each x

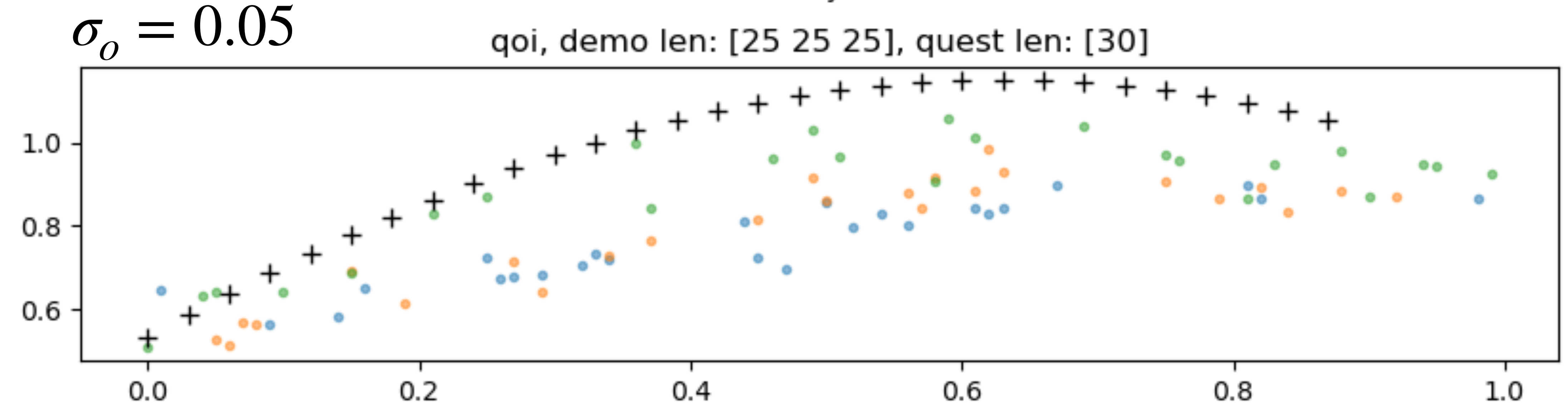
Parameters $\alpha_1(\omega)\ \alpha_2(\omega)$

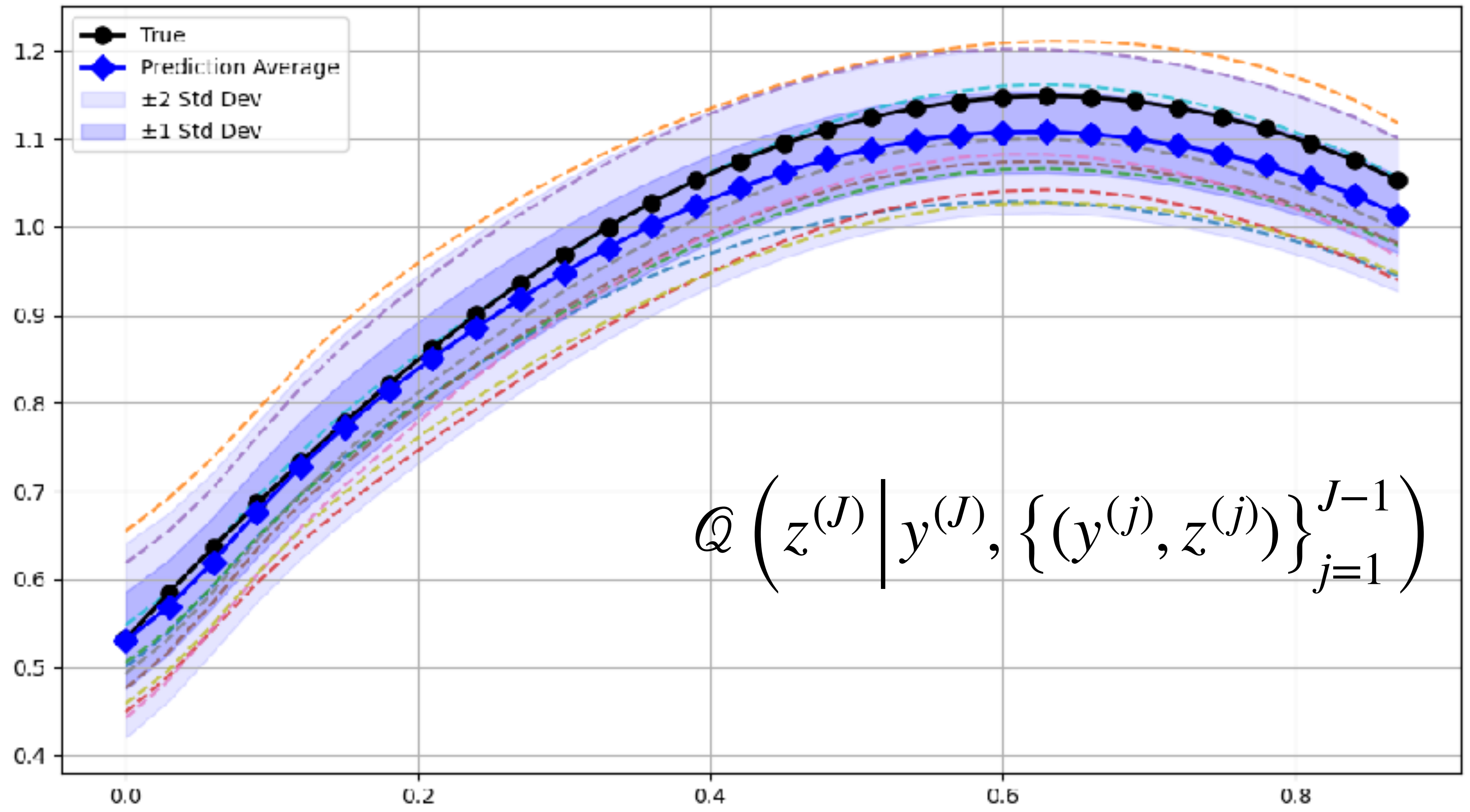
Conditions $y(x,\omega)$

QoI $z(x,\omega)$



$\sigma_o = 0.05$





Data generating process

- $y(x,\omega)$ Gaussian process with squared exponential covariance
- $\alpha_1 \sim \mathcal{U}[0,1]$, $\alpha_2 \sim \mathcal{U}[0,1]$
- $J - 1 = 3$ Example condition-QoI pairs
- Colored lines: example pairs
- Truth (+)
- Uncertainty bands computed from generated samples from $\mathcal{Q}\left(z^{(J)} \middle| y^{(J)}, \{(y^{(j)}, z^{(j)})\}_{j=1}^{J-1}\right)$

Conclusion and outlook

In-context operator learning implicitly performs Bayesian inference for differential equations

- **Random differential equations** provides a framework for probabilistic operator learning
- ICON directly approximates mean of the **Bayesian posterior predictive distribution**
- **Generative ICON** samples from the posterior predictive: a form of **uncertainty quantification**

Original ICON

$$\mathcal{T}^\star\left(y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) = \mathbb{E}\left[z^{(J)} \middle| y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right]$$

- ICON **approximates mean** of posterior predictive distribution
- $\mathcal{T}^\star(\cdot,\cdot)$ is an operator learner

Theorem: Average generative ICON equals Original ICON

$$\mathcal{T}^\star\left(y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) = \int \mathcal{G}^\star\left(x, y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right) p_X(x)\, dx$$

Generative ICON

$$\mathcal{G}^\star\left(\cdot, y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right)_\sharp p_X = Q\left(\cdot \middle| y^{(J)}, \left\{y^{(j)}, z^{(j)}\right\}_{j=1}^{J-1}\right)$$

- Generative ICON **generates** from the posterior predictive distribution
- $\mathcal{G}^\star(x,\cdot,\cdot)$ is a *sample* operator learner

Outlook

- Motivation to find Bayesian structure in other multi-task operator learners?
  - **PROSE [Liu et al.], BCAT [Liu et. al], POSEIDON [Herde et al.] and more…**
- Using other types of generative models beyond GANs

Thank you!