Flow Matching Corrected Posterior Estimation (FMCPE)

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EDF workshop on Metamodels

About me

- PhD student at Inria Grenoble (3rd year)
- Statify/Thoth team
- Research focus: Simulation-based inference
- Supervisors: Pedro L. Rodrigues, Michael Arbel, Florence Forbes

About me

Introduction

Statistical Inference

Given observations x and unknown parameters θ, we use **Bayes' rule**:

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)}$$

- $p(\theta|x)$ - **Posterior**: what we want to compute
- $p(x|\theta)$ - **Likelihood**: probability of data given parameters
- $p(\theta)$ - **Prior**: initial beliefs about parameters
- $p(x)$ - **Evidence**: normalizing constant

Statistical Inference

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)}$$

Bayesian Inference

Input: Model likelihood $p(x|\theta)$

Methods: MCMC, Variational Inference

Output: Posterior $p(\theta|x)$

Simulation-Based Inference

Input: Simulator $S : \theta \mapsto x$

Methods: *(See next section)*

Output: Posterior $p(\theta|x)$

Key difference: SBI works when likelihood is intractable

Approximate Bayesian Computation (ABC)

Algorithm

Inputs: Simulator S, $\mathbf{y}_{\text{obs}}$, prior $p(\theta)$, distance ρ, threshold ϵ

For $i = 1, \ldots, n$:

1. Sample $\theta_i \sim p(\theta)$
2. Simulate $\mathbf{x}_i = S(\theta_i)$
3. Keep θ_i if $\rho(\mathbf{x}_i, \mathbf{y}_{\text{obs}}) < \epsilon$

Python Code

```python
# Inputs
S = simulator
y_obs = observed_data
prior = p_theta
rho = distance_function
epsilon = threshold

samples = []
for i in range(n):
    # 1. Sample from prior
    theta_i = prior.sample()
    # 2. Simulate
    x_i = S(theta_i)
    # 3. Keep if distance < epsilon
    if rho(x_i, y_obs) < epsilon:
        samples.append(theta_i)
```

Limitations:

- Poor scaling with dimension
- Requires summary statistics
- Not amortized

References: Beaumont et al. (2002), Sisson et al. (2018)

Neural Posterior Estimation (NPE)

Algorithm

Inputs: Simulator S, budget N_{train}, N_{epochs}, neural approximator q_ϕ, summary net h_ω

Generate training data:

Sample $\{(\theta_i, \mathbf{x}_i)\}_{i=1}^{N_{\text{train}}}$

For $e = 1, \ldots, N_{\text{epochs}}$:

Minimize KL divergence:

$$\mathcal{L}(\phi, \omega) = -\mathbb{E}[\log q_\phi(\theta | h_\omega(\mathbf{x}))]$$

Python Code

```python
# Inputs
S = simulator
N_train = budget
N_epochs = num_epochs
q_phi = neural_approximator
h_psi = summary_net

# Generate training data
thetas = prior.sample(N_train)
xs = S(thetas)

# Training loop
for epoch in range(N_epochs):
    # Minimize KL divergence
    loss = -q_phi.log_prob(thetas, h_psi(xs)).mean()
    loss.backward()
    optimizer.step()
```

Benefits: Amortized inference, no hand-crafted statistics needed

Limitations: Prone to overfitting, sensitive to distribution shift

References: Papamakarios & Murray (2016), Greenberg et al. (2019)

Challenges in SBI

- **Expensive simulations** - High computational cost
- **Exploit the simulator** - In certain cases where the simulator is not a black box, we can leverage information (e.g. its gradient) to improve inference.
- **Model misspecification** - Main focus of this work.

Model Misspecification

Types of Misspecification and Objective

Types of misspecification:

- **Simulator misspecification:** Model assumptions are wrong or incomplete (e.g., missing physics)
- **Prior misspecification:** Prior distribution does not reflect true parameter ranges
- **Observation noise:** Noise model in likelihood is misspecified

Approaches to address misspecification:

- **Robustness:** Ensemble methods or conservative posteriors
- **Detection:** Identify presence of misspecification
- **Correction:** Build new posterior accounting for discrepancy

→ In this work, we focus on correcting simulator misspecification.

Misspecification of the simulator

The data generating process $\mathbf{y} \sim p^*$

$$p^* \notin \{p(\cdot|\theta) \mid \theta \in \mathbf{\Theta}\}$$

Example: Damped Pendulum

High-fidelity model (ground truth):

$$\mathbf{y}(t) = e^{-\alpha t} A \cos(\omega_0 t) + \epsilon$$

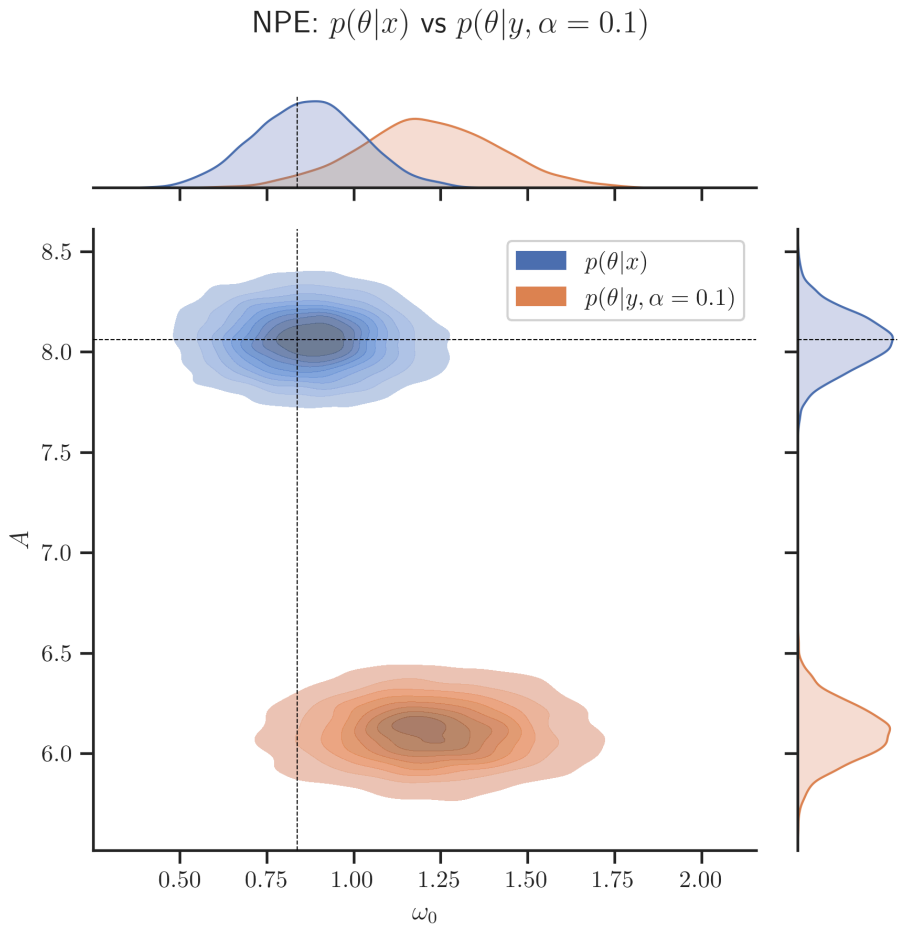
Parameters: $\theta = (\omega_0, A)$, damping $\alpha \sim \mathcal{U}(0, 1)$

Low-fidelity simulator (misspecified):

$$\mathbf{x}(t) = A \cos(\omega_0 t) + \epsilon$$

Missing damping term! $\alpha = 0$

$\rightarrow$ Even a small amount of misspecification can lead to highly biased posteriors !



Data setting

There are two main ways to approach model misspecification in SBI:

Case 1

1. Simulation data:
Access to simulated pairs $\{\theta_i, \mathbf{x}_i\}_{1:m}$

2. Observations:
Independent observations $\{\mathbf{y}_j\}_{1:n}$
($\mathbf{y}$ does not depend on θ)

3. Examples:
(Add examples here)

Case 2

1. Simulation data:
Access to simulated pairs $\{\theta_i, \mathbf{x}_i\}_{1:m}$

2. Calibration set:
Few paired observations $\{\theta_j, \mathbf{y}_j\}_{1:n}$
(Multi-fidelity simulation, expensive ground truth)

3. Examples:
(Add examples here)

→ In this work, we will focus on Case 2.

Existing Methods

MF-NPE

A first approach to correct the misspecification is to fine-tune the posterior estimator on the calibration set.

Assuming we have data from a low-fidelity simulator $(\theta, \mathbf{x}) \sim p(\theta)p(\mathbf{x} \mid \theta)$, we train a neural density estimator using:

$$\mathcal{L}_{NPE}(\phi) = \mathbb{E}_{\theta,\mathbf{x}} \left[-\log q_\phi(\theta|\mathbf{x}) \right]$$

Then, using our small but precise calibration set $(\theta_i, \mathbf{y}_i) \sim p(\theta, \mathbf{y})$, we fine-tune the posterior estimator using the same loss:

$$\mathcal{L}_{NPE}(\phi) = \mathbb{E}_{\theta,\mathbf{y}} \left[-\log q_\phi(\theta|\mathbf{y}) \right]$$

Reference: Krouglova et al. (2025). Multifidelity Simulation-based Inference for Computationally Expensive Simulators. *arXiv:2502.08416*.

ROPE: Transporting $\mathbf{y}$ to $\mathbf{x}$

The ROPE method proposes to use optimal transport to match $p^*(\mathbf{y})$ and $p(\mathbf{x})$.

Input: Simulator $S(\theta, \epsilon)$, calibration data $\{(\theta^i, \mathbf{y}^i)\}_{i=1}^{N_c}$ and test set $\{\mathbf{y}^i\}_{i=1}^{N_o}$

Step 1: Train n.n. h_ω and density estimator q_ϕ

$$\mathcal{L}_{NPE}(\omega, \phi) = \mathbb{E}_{\theta,\mathbf{x}} \left[-\log q_\phi \left(\theta | h_\omega(\mathbf{x}) \right) \right]$$

Step 2: Fine-tune h_ω on calibration data $\{(\theta^i, \mathbf{y}^i)\}$ (Initialize $g = h$)

$$\mathcal{L}(\varphi) = \sum_{i=1}^{N_c} \| g_\varphi(\mathbf{y}^i) - \mathbb{E}_\epsilon [h_\omega \left(S(\theta^i, \epsilon) \right] \|^2$$

Step 3: Solve OT problem between $\mathbf{x}^j$ and $\mathbf{y}^i$ with cost:

$$C(\mathbf{x}^j, \mathbf{y}^i) = \| h_\omega(\mathbf{x}^j) - g_\psi(\mathbf{y}^i) \|^2$$

Output: Corrected posterior $\tilde{p}(\theta|\mathbf{y}) = \sum_{j}^{N_s} N_o P_{ij}^* q_\phi \left(\theta | h_\omega(\mathbf{x}^j) \right)$

Reference: Wehenkel et al. (2025). Addressing Misspecification in Simulation-based Inference through Data-driven Calibration. *ICML'25*.

Key takeaways of ROPE

- Two main components: The alignement of summary statistics using fine tuning and the transport between $\mathbf{x}$ and $\mathbf{y}$
- The correspondence between θ_i and $\mathbf{y}^i$ is only used to define the OT cost
- The "test" set is used for the computation of the optimal transport. The method can't be applied to new data
- The hypothesis $\mathbf{y} \perp \theta \mid \mathbf{x}$ is required to compute the posterior

Our Approach

Flow Matching Corrected Posterior Estimation

Main Idea: Learn to Correct the Posterior

The Challenge:

- We have a posterior $q_\phi(\theta|\mathbf{x})$ trained on cheap simulations $\mathbf{x}$
- We have a small **calibration set** $\mathcal{D}_{\text{cal}} = (\theta_i, \mathbf{y}_i)$ from the true process
- Goal: Estimate $p(\theta|\mathbf{y})$ by leveraging the calibration set and $q_\phi(\theta|\mathbf{x})$

Two step approach:

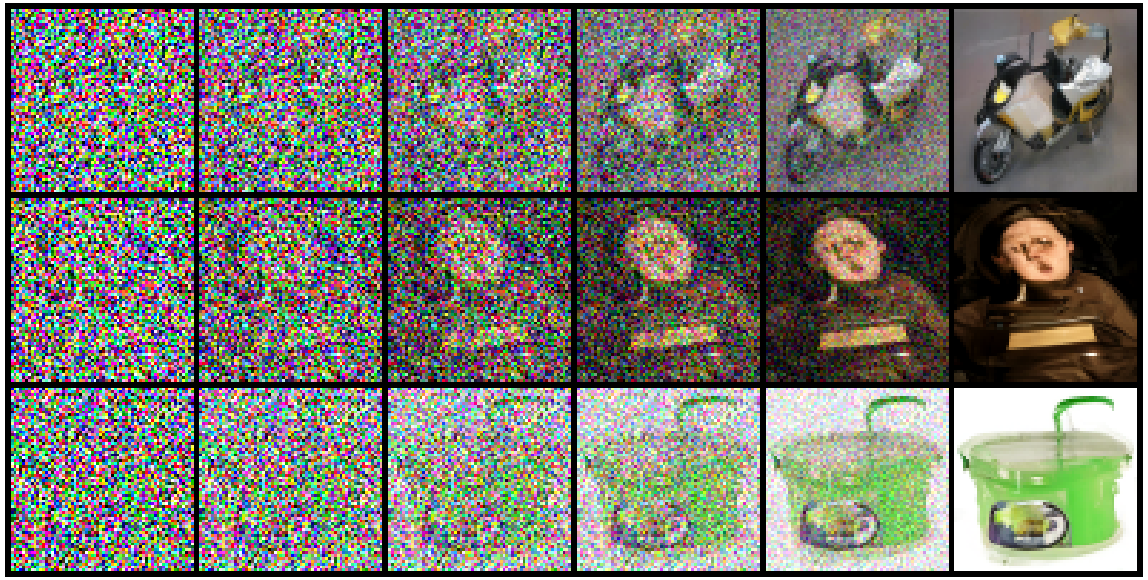
1. Design a **source distribution** $\pi(\theta|\mathbf{y})$ which acts as a first guess for the target $p(\theta|\mathbf{y})$
2. Use **Flow Matching** to move samples from the source $\pi(\theta|\mathbf{y})$ to $p(\theta|\mathbf{y})$

Key Advantages:

- Leverages abundant simulations AND expensive calibration data efficiently
- No independence assumption $\mathbf{y} \perp \theta|\mathbf{x}$ required (as opposed to RoPE).
- Can be plugged-in on top of any SBI methods that provides $\pi(\theta|\mathbf{x})$

Flow Matching: Key Idea

Flow Matching learns to transport samples between distributions



Three key elements:

1. **Base distribution** we can sample from (e.g., Gaussian) $\rightarrow q_0(x)$
2. **Target distribution** (arbitrary, potentially complex) $\rightarrow q_1(x)$
3. **Transport mechanism** to move samples $q_0(x)$ from $q_1(x) \rightarrow p_t(x)$

References:

Lipman et al. (2023). Flow Matching for Generative Modeling. *ICLR'23*.

Liu et al. (2023). Flow Straight and Fast: Learning to Generate and Transfer Data with Rectified Flow. *ICLR'23*.

Flow Matching

Objective: Match 2 distributions q_0, q_1 via an ODE, i.e. learn a probability path $p_t(\mathbf{x})$ with $p_0 = q_0$ and $p_1 = q_1$

$$\frac{\mathrm{d}\psi_t(\mathbf{x})}{\mathrm{d}t} = u_t(\psi_t(\mathbf{x})) \qquad \psi_0(\mathbf{x}) = \mathbf{x}$$

Relationship between flow and probability path:

$$\mathbf{x}_t = \psi_t(\mathbf{x}_0) \text{ with } \mathbf{x}_0 \sim q_0 \quad \Rightarrow \quad \mathbf{x}_t \sim p_t$$

Boundary conditions:

$$\psi_0 = \mathrm{Id} \quad \text{and} \quad \psi_1 \# q_0 = q_1$$

How: We can regress the vector field with a neural network

$$\mathcal{L}_{FM}(\phi) = \mathbb{E}_{t\sim\mathcal{U}[0,1]}\mathbb{E}_{\mathbf{x}\sim p_t}\left[\|u_\phi(t,\mathbf{x}) - u(t,\mathbf{x})\|^2\right]$$

→ We don't know $u_t(\mathbf{x})$!

Conditional Flow Matching

Key Idea: Since we have access to samples from q_1, we can condition the vector field on the target point $\mathbf{x}_1 \sim q_1$

$$p_t(\mathbf{x}_t) = \int q_1(\mathbf{x}_1) p_{t|1}(\mathbf{x}_t|\mathbf{x}_1) \mathrm{d}\mathbf{x}_1 \qquad p_{0|1}(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(0, I)$$

$$\Rightarrow p_{t|1}(\mathbf{x}_t|\mathbf{x}_1) = \mathcal{N}\left(t\mathbf{x}_1, (1-t)^2 I\right)$$

The induced $u_t(\mathbf{x}|\mathbf{x}_1)$ is available in closed form e.g.

$$u_t(\mathbf{x}|\mathbf{x}_1) = \frac{\mathbf{x}_1 - \mathbf{x}}{1-t}$$

The loss becomes

$$\mathcal{L}_{CFM}(\phi) = \mathbb{E}_{t\sim\mathcal{U}[0,1], \mathbf{x}_1\sim q_1, \mathbf{x}_t\sim p_t(\mathbf{x}|\mathbf{x}_1)} \left[\|u_\phi(t, \mathbf{x}) - u_t(\mathbf{x}|\mathbf{x}_1)\|^2\right]$$

→ Same gradient as $\mathcal{L}_{FM}$

FMCPE: Three Main Components

1. **Parameter space flow:** Transport samples from source $\pi(\theta|y)$ to target $p(\theta|y)$

2. **Source distribution construction:** Design $\pi(\theta|y)$ using NPE and learnable kernel

$$\pi(\theta|y) = \int p(\theta|x)q(x|y)dx$$

3. **Joint optimization:** Learn both flows together for improved robustness

Component 1: Parameter Space Flow

Goal: Map samples from source $\pi(\theta|y)$ to corrected posterior $p(\theta|y)$

Flow definition:

$$\frac{d\theta_t}{dt} = u_\Theta(t, \theta_t, y)$$

Training objective: Conditional Flow Matching loss

$$\mathcal{L}_\Theta = \mathbb{E}\left[\|u_\Theta(t, \theta_t, y) - (\theta_1 - \theta_0)\|^2\right]$$

where $\theta_1 \sim p(\theta|y)$ (from calibration) and $\theta_0 \sim \pi(\theta|y)$ (from source)

Component 2: Source Distribution

Key insight: Use simulation-trained NPE $p(\theta|x)$ with learned correction

Source construction:

$$\pi(\theta|y) = \int p(\theta|x)q(x|y)dx$$

- $p(\theta|x)$: Pretrained NPE on cheap simulations (frozen)
- $q(x|y)$: Learnable kernel mapping y to simulator space

Why this works: Bridges the gap between calibration data y and simulations x

Component 3: Learning q(x|y)

Approach: Use Flow Matching to learn $q(x|y)$

Flow in simulation space:

$$\frac{dx_t}{dt} = u_X(t, x_t, y)$$

Training data generation: For each calibration pair (θ_i, y_i):

1. Generate $x_1 = S(\theta_i)$ using the simulator
2. Sample base $x_0 \sim \mathcal{N}(y, \sigma^2 I)$
3. Train flow to match $x_0 \to x_1$

Result: $q(x|y)$ learns to transport from observed space to simulator space

Joint Training Algorithm

Key idea: Train both flows u_X and u_Θ simultaneously

Training loop:

For each minibatch:

1. Sample (θ_1, y) from calibration set $\mathcal{D}_{\text{cal}}$
2. Generate $x_1 = S(\theta_1)$ using simulator
3. Sample base points: $x_0 \sim \mathcal{N}(y, \sigma^2 I)$
4. Map x_0 to simulator space: $\tilde{x} = T_X(x_0; y)$ using current u_X
5. Sample from source: $\theta_0 \sim p(\theta|\tilde{x})$ using pretrained NPE
6. Compute flow matching losses for both flows:

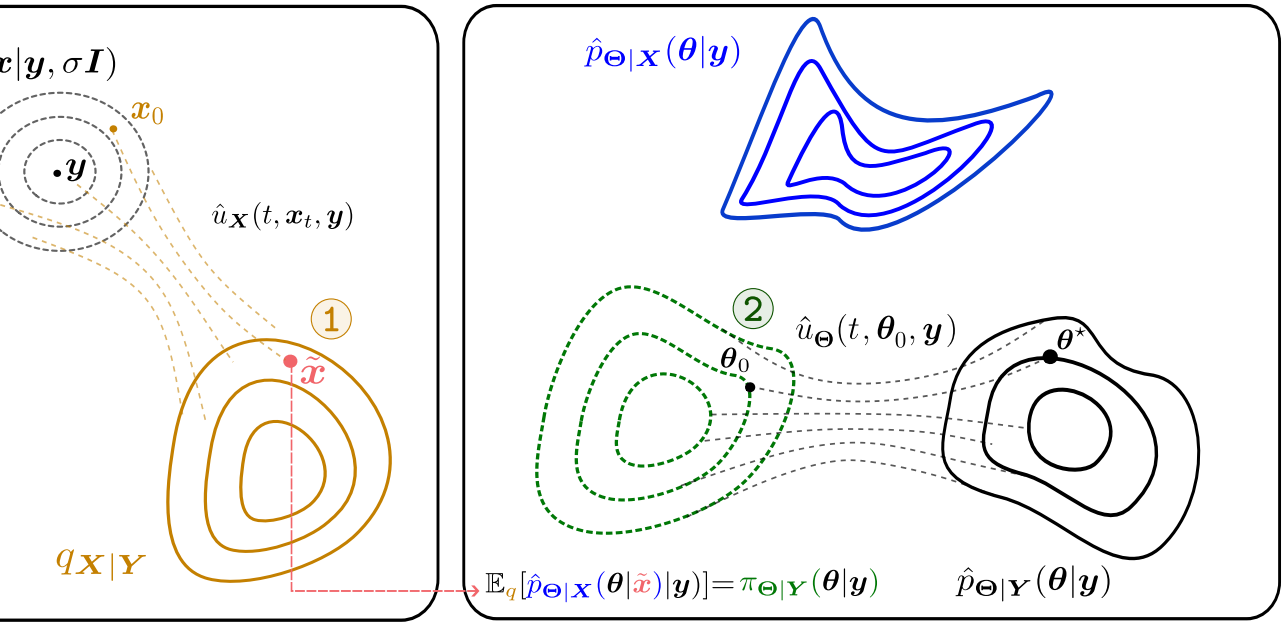
$$\ell_X = \|u_X(t, x_t, y) - (x_1 - x_0)\|^2$$

$$\ell_\Theta = \|u_\Theta(\tau, \theta_\tau, y) - (\theta_1 - \theta_0)\|^2$$

7. Update both u_X and u_Θ using $\mathcal{L} = \ell_X + \ell_\Theta$

→ Joint training ensures consistency between source and parameter flows

FMCPE Overview



③ $\hat{\mathcal{L}}_{\boldsymbol{X}} = \sum_{j=1}^{N_{\text{cal}}} \|\hat{u}^k_{\boldsymbol{X}}(t^j, \boldsymbol{x}^j_0, \boldsymbol{y}^j) - (\boldsymbol{x}^j_1 - \boldsymbol{x}^j_0)\|$

④ $\hat{u}^{k+1}_{\boldsymbol{X}} \leftarrow \texttt{GDstep}(\hat{u}^k_{\boldsymbol{X}})$

③ $\hat{\mathcal{L}}_{\boldsymbol{\Theta}} = \sum_{j=1}^{N_{\text{cal}}} \|\hat{u}^k_{\boldsymbol{\Theta}}(t^j, \boldsymbol{\theta}^j_0, \boldsymbol{y}^j) - (\boldsymbol{\theta}^j_1 - \boldsymbol{\theta}^j_0)\|$

④ $\hat{u}^{k+1}_{\boldsymbol{\Theta}} \leftarrow \texttt{GDstep}(\hat{u}^k_{\boldsymbol{\Theta}})$

Algorithm 1: Iterative update of $\hat{u}_{\boldsymbol{\Theta}}$ and $\hat{u}_{\boldsymbol{X}}$

Input: Calibration set $\mathcal{D}_{\text{cal}} = \{(\boldsymbol{\theta}^j, \boldsymbol{y}^j)\}_{1 \le N_{\text{cal}}}$, pre-trained $p_{\boldsymbol{\Theta}|\boldsymbol{X}}$

for $k = 1$ *to* K do

`/*` ① `Sample from noise model`

Sample $\tilde{\boldsymbol{x}}$ from $q_{\boldsymbol{X}|\boldsymbol{Y}}(\boldsymbol{x}|\boldsymbol{y})$:

$$\boldsymbol{x}_0 \sim \mathcal{N}(\boldsymbol{y}, \sigma^2 \boldsymbol{I}), \qquad \tilde{\boldsymbol{x}} = \boldsymbol{x}_0 + \int \underbrace{\hat{u}^k_{\boldsymbol{X}}(t, \boldsymbol{x}_0, \boldsymbol{y})}_{\text{Weights at step } k} \, dt$$

`/*` ② `Sample from proposal`

Sample $\boldsymbol{\theta}_0$ from $\pi^k_{\boldsymbol{\Theta}|\boldsymbol{Y}}$:

$$\boldsymbol{\theta}_0 \sim \pi^k_{\boldsymbol{\Theta}|\boldsymbol{Y}}(\boldsymbol{\theta}|\boldsymbol{y}) = \mathbb{E}_{q^k_{\boldsymbol{X}|\boldsymbol{Y}}}\left[\hat{p}_{\boldsymbol{\Theta}|\boldsymbol{X}}(\boldsymbol{\theta}|\tilde{\boldsymbol{x}})\right]$$

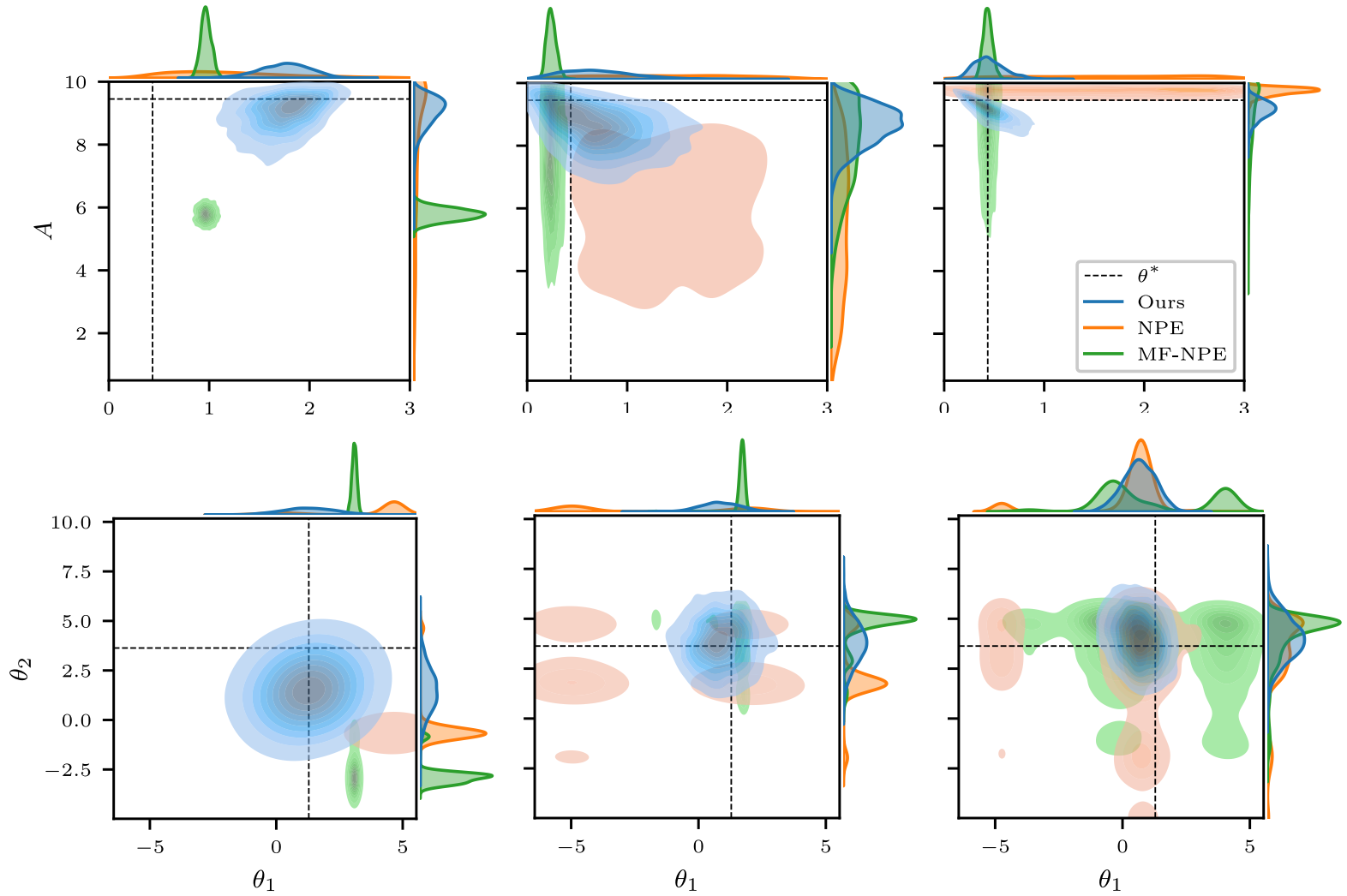
`/*` ③ `Compute losses with` $\boldsymbol{x}^j_1 = S(\boldsymbol{\theta}^j) \quad \boldsymbol{\theta}^j_1 = \boldsymbol{\theta}^j$

$$\hat{\mathcal{L}}_{\boldsymbol{\Theta}} = \sum_{j=1}^{N_{\text{cal}}} \|\hat{u}^k_{\boldsymbol{\Theta}}(t^j, \boldsymbol{\theta}^j_0, \boldsymbol{y}^j) - (\boldsymbol{\theta}^j_1 - \boldsymbol{\theta}^j_0)\| \quad \hat{\mathcal{L}}_{\boldsymbol{X}} = \sum_{j=1}^{N_{\text{cal}}} \|\hat{u}^k_{\boldsymbol{X}}(t^j, \boldsymbol{x}^j_0, \boldsymbol{y}^j) - (\boldsymbol{x}^j_1 - \boldsymbol{x}^j_0)\|$$

`/*` ④ `Gradient update`

$$\hat{u}^{k+1}_{\boldsymbol{\Theta}} \leftarrow \texttt{GDstep}(\hat{u}^k_{\boldsymbol{\Theta}}), \qquad \hat{u}^{k+1}_{\boldsymbol{X}} \leftarrow \texttt{GDstep}(\hat{u}^k_{\boldsymbol{X}})$$

Results



(a) $N_{\text{cal}} = 10$ (b) $N_{\text{cal}} = 50$ (c) $N_{\text{cal}} = 200$

SBI Hackathon - Grenoble

January 21-23, 2026 | Grenoble

Join us for a hands-on hackathon on the `sbi` package - a simple and powerful tool for simulation-based inference!

🔗 https://github.com/SBI-Grenoble/sbi-hackathon-2026

Example: Training an NPE model in just a few lines:

```python
import torch
from sbi.inference import NPE

# define shifted Gaussian simulator
def simulator(θ): return θ + torch.randn_like(θ)

# draw parameters from Gaussian prior
θ = torch.randn(1000, 2)
# simulate data
x = simulator(θ)

# choose sbi method and train
inference = NPE()
inference.append_simulations(θ, x).train()

# do inference given observed data
x_o = torch.ones(2)
posterior = inference.build_posterior()
samples = posterior.sample((1000,), x=x_o)
```

Thank You!

Questions?

Appendix

Common hypothesis

In most settings, the error is assumed to be independent of θ:

$$\mathbf{y} \perp \theta \mid \mathbf{x}$$

This is a necessary condition to express $p\left(\theta|\mathbf{y}\right)$ using $p\left(\theta|\mathbf{x}\right)$ and $p\left(\mathbf{x}|\mathbf{y}\right)$:

$$p\left(\theta|\mathbf{y}\right) = \int_{\mathcal{X}} p\left(\theta|\mathbf{x}\right) p(\mathbf{x}|\mathbf{y}) \mathrm{d}\mathbf{x}$$

In practice, this is not always true for various physical systems. The low-fidelity simulator might not depend on some of the parameters, using a lower dimensional θ.

NPE Loss Derivation from KL Divergence

We want to minimize the KL divergence for all $\mathbf{x}$:

$$\mathbb{E}_{p(\mathbf{x})}\left[\mathrm{KL}(p(\theta|\mathbf{x}) \,||\, q_\phi(\theta|\mathbf{x}))\right]$$

$$= \mathbb{E}_{p(\mathbf{x})}\mathbb{E}_{p(\theta|\mathbf{x})}\left[\log \frac{p(\theta|\mathbf{x})}{q_\phi(\theta|\mathbf{x})}\right]$$

Expanding the logarithm:

$$= \mathbb{E}_{p(\mathbf{x})}\mathbb{E}_{p(\theta|\mathbf{x})}\left[\log p(\theta|\mathbf{x})\right]$$

$$-\mathbb{E}_{p(\mathbf{x})}\mathbb{E}_{p(\theta|\mathbf{x})}\left[\log q_\phi(\theta|\mathbf{x})\right]$$

First term does not depend on ϕ:

$$\min_\phi \mathbb{E}_{p(\mathbf{x})}\left[\mathrm{KL}(p \,||\, q_\phi)\right]$$

Equivalent to maximizing:

$$\max_\phi \mathbb{E}_{p(\mathbf{x})}\mathbb{E}_{p(\theta|\mathbf{x})}\left[\log q_\phi(\theta|\mathbf{x})\right]$$

Using joint distribution $p(\theta, \mathbf{x}) = p(\mathbf{x}|\theta)p(\theta)$:

$$= \max_\phi \mathbb{E}_{p(\theta,\mathbf{x})}\left[\log q_\phi(\theta|\mathbf{x})\right]$$

Approximate with samples:

$$\mathcal{L}(\phi, \omega) = -\frac{1}{N}\sum_{i=1}^{N} \log q_\phi(\theta_i | h_\omega(\mathbf{x}_i))$$

where $(\theta_i, \mathbf{x}_i) \sim p(\theta)p(\mathbf{x}|\theta)$