Learning to infer:
Normalising flows for statistical inference

Project for the course
Machine Learning for Physics and Astronomy

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Outline

Introduction

Bayesian foundations and the SBI solution

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

- Prior: $p(\theta)$
- Likelihood: $p(x|\theta)$
- Posterior: $p(\theta|x)$
- Marginal: $p(x)$

Computing the likelihood can be challenging in many real-world applications $\rightarrow$ Bayesian inference becomes difficult or impossible

But... SBI bypasses the need for an explicit likelihood

What is SBI?

- SBI = Simulation-Based Inference
- It is a class of techniques used to estimate posterior distributions
- Used when the likelihood function is unknown or too complex to compute
- Neural networks learn to approximate posterior from simulated (parameter, data) pairs

How does SBI work?

The process works as follows:

1. Sample θ from the prior distribution
2. Simulate data x from the model using θ
3. Train a neural network to learn how θ and x relate
4. Input the observed data x_{obs} into the network to obtain the posterior $p(\theta|x_{\text{obs}})$

Techniques and tools

(S)NPE: (Sequential) Neural Posterior Estimation

1. Sample parameters from prior
2. Generate data with simulator
3. Train neural density estimator on (θ, x) pairs
4. Infer posterior using trained network

Once trained, it can quickly produce posterior estimates for new observations without retraining, making the inference process highly efficient and reusable.

Normalizing flows

Normalizing flows are a class of neural density estimation models that transform a simple base distribution (e.g., a multivariate Gaussian) into a complex target distribution using a sequence of invertible and differentiable transformations.

- Used for flexible density estimation
- Learn invertible mappings from simple to complex distributions
- Efficient sampling + likelihood evaluation