Machine learning tools for inference and experimental design in particle physics

Conor Sheehan (*Supevisor: André Freitas*)

conor.sheehan-2@manchester.ac.uk

Motivation

Two types of **statistical inference** in particle physics:

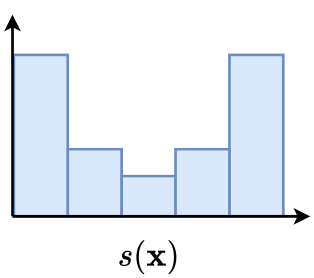
1. **Hypothesis testing:** allows us to claim discovery or rejection of a theory – e.g. Higgs boson discovery in 2012.
2. **Maximum likelihood estimation:** estimation of physical quantities – e.g. mass of the Higgs boson.

Complicating factors:

1. Observational data (detector readings) $\mathbf{x}$ are high-dimensional.
2. Theories have many free parameters θ.
3. Likelihood of data under theory $p(\mathbf{x}|\theta)$ is not known explicitly.

Simulation-based inference: accurately simulate the theory to draw samples from $p(\mathbf{x}|\theta)$, and use these to perform inference [2].

Traditional methods, e.g. histograms and kernel density estimates, require dimensionality reduction and therefore discard information.



Machine learning likelihoods

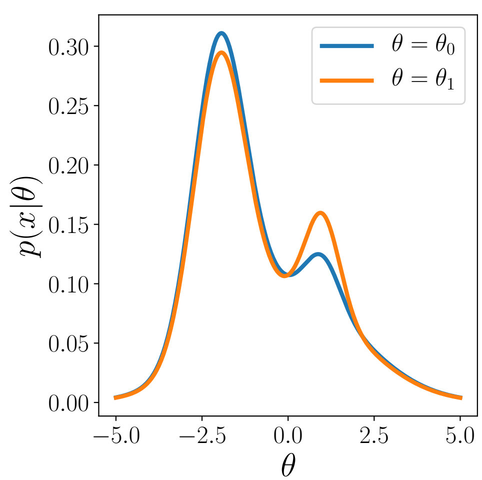
Neural density estimation:

- Approximate $p(\mathbf{x}|\theta)$ with a neural network.
- Train by maximising likelihood of samples drawn from simulator.
- Example architectures: mixture density networks [1] and normalising flows [4].

Ratio estimation:

- Train a classifier to distinguish between samples drawn from two different parameter points θ_0 and θ_1.
- Classifier's probabilistic predictions can be used to estimate the **likelihood ratio**:

$$r(\mathbf{x}) = \frac{p(\mathbf{x}|\theta_1)}{p(\mathbf{x}|\theta_0)}\,.$$

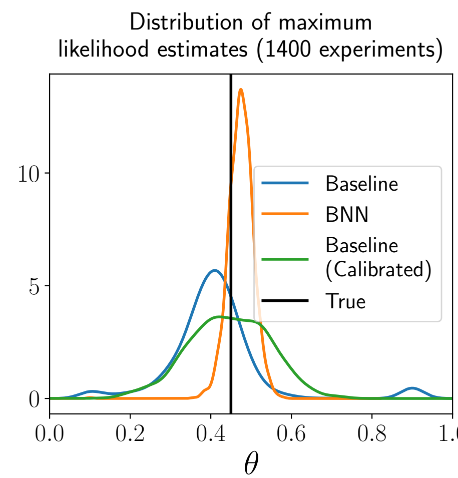


Bayesian neural networks for ratio estimation

Bayesian neural networks (BNNs): define probability distributions over neural network weights – allows expression of model uncertainty [3].

Two reasons BNNs should work well for ratio estimation:

1. **Calibration** due to inherent regularisation.
2. Model uncertainty can be used to perform **Bayesian optimisation** to find maximum likelihood estimates with fewer simulations.



References

[1] C. M. Bishop. Mixture density networks. 1994.

[2] K. Cranmer, J. Brehmer, and G. Louppe. The frontier of simulation-based inference. *Proceedings of the National Academy of Sciences*, 2020.

[3] Y. Gal. Uncertainty in deep learning. 2016.

[4] G. Papamakarios. Neural density estimation and likelihood-free inference.