Simulation-based Inference

Inverting Simulators

Talk by Stefan Wezel

mlcolab @ Tübingen University Cluster of Excellence

April 29, 2021

Overview

- The problem setting
- Traditional approaches and their issues
- Using Bayesian Neural Nets to alleviate them
- A worked example
- A more interesting, real-world example
- Outlook

What and Why?

An Example

- Imagine you are a astronomer
- You observe planetary movements
- and find that two parameters determine the movement (mass and velocity) (and some noise)
- So you build a mechanistic model that can simulate observations
- But what do we actually care about?
    - What was the mass and velocity of that planet

What and Why?

Formalizing our Example

- Mechanistic model (simulator) has parameters θ and produces data $\hat{x}$
  - It implicitly defines $p(\hat{x}|\theta)$ (it yields samples from this distribution)
- Given a (real) observation x_0, we would be interested in the parameters that produced it
  - $p(\theta|x_0)$ -> posterior over parameters
  - In simple cases, we could apply Bayes' rule and compute it analytically
  - What is simple? If we know Likelihood
  - But often we would not

- This is exactly a problem setting that scientists often deal with
    - They have a sophistic model (the simulator) that encapsulates a lot of prior knowledge
    - But inference in this setting often boils down to: What were parameters that produced this observation
- Simulation-based Inference inference tries to solve this problem
- by inverting the simulator

- Broader term: Approximate Bayesian Computation (ABC)
    - Rejection ABC
    - Sampling ABC (perturbe intitial params)
    - Sequential ABC

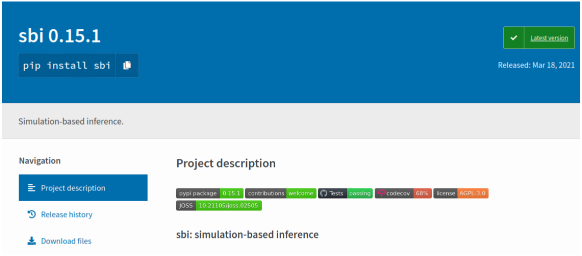
    - But gives only point estimates, not full posterior
    - within ϵ

- Create n training samples
- learn posterior over parameters by parametrizing GMM with DNN

How to use SBI?

Some advertisement

- Now that you are pretty excited about SBI and its applications
- mlcolab and mackelab is developing a python (and eventually Julia) library (that I've used earlier)
- If you are interested: try it out and give us your feedback
- link to colab
- link to github



References

[1] G. Papamakarios and I. Murray. Fast epsilon-free inference of simulation models with bayesian conditional density estimation. arXiv preprint arXiv:1605.06376, 2016.

How

Approximate Bayesian Computation

- Finding parameters/posterior over parameters with
  - Rejection ABC
  - Markov Chain Monte Carlo ABC
  - Sequential Monte Carlo ABC
  - ...
- Problems
  -

What

is Simulation-based Inference?

- If we know generating factors, we can build a simulator
- But we want to constrain simulator output on observations from real world
- Thus we need realistic values for simulator parameters
- -> inverse problem
- SBI solvers this inverse problem using Bayesian inference

How

does Simulation-based Inference work?