Simulation-based Inference

Inverting Simulators

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mlcolab @ Tübingen University Cluster of Excellence

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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?

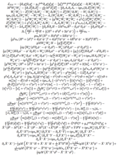
An Example

- Inverting simulators - so first let's find out what a simulator is
- Imagine you are a physicist
- You have also highly sophisticated experiments that can produce observations
- You have highly sophisticated models, theories that can produce observations like from your experiment, that were developed over centuries
- But what do we actually care about? How do you perform inference?
    - What were the parameters for your observation

What and Why?

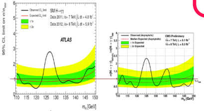
An Example

Standard model

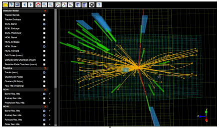


Experiment

Observation



Simulator



What is mass of Higgs boson?

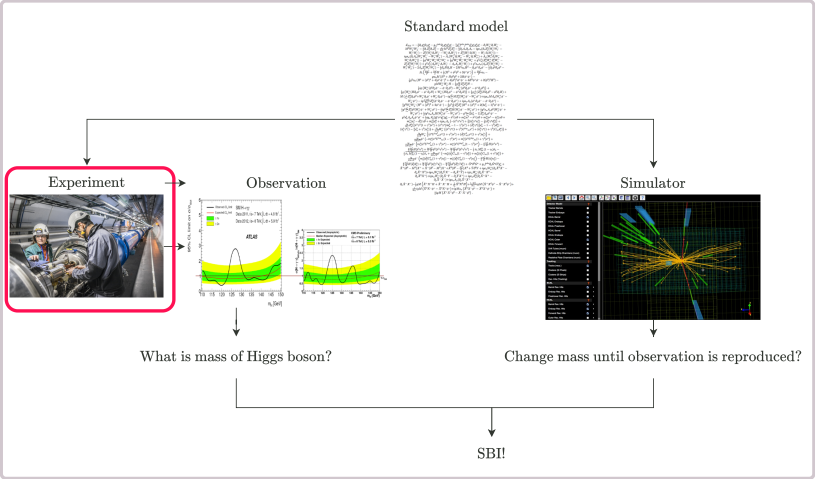
Change mass until observation is reproduced?

SBI!

Figure derived from cern.ch, Achintya Rao and Tom McCauley, sciencealert.com

What and Why?

An Example



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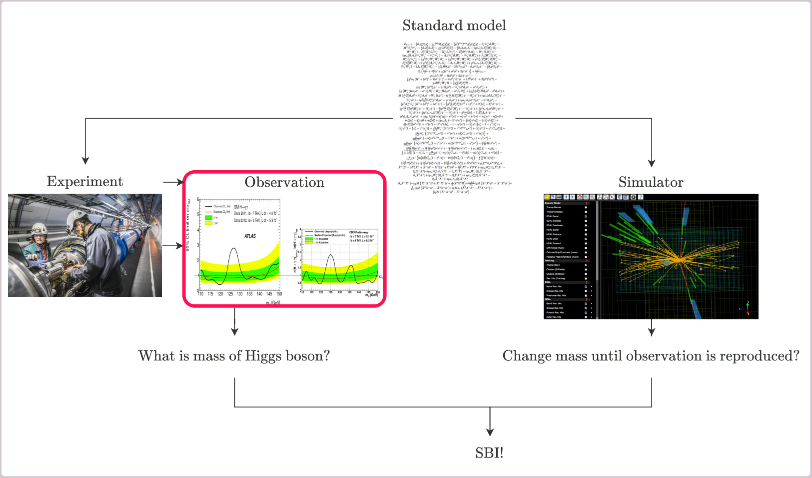

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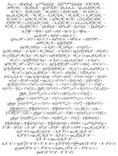
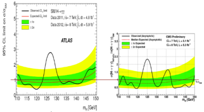
Standard model

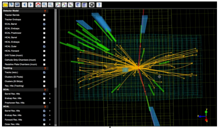


Experiment

Observation



Simulator



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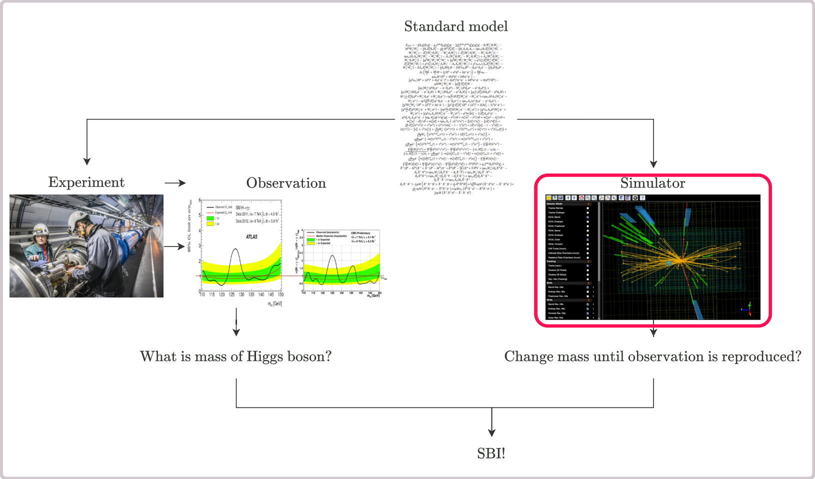

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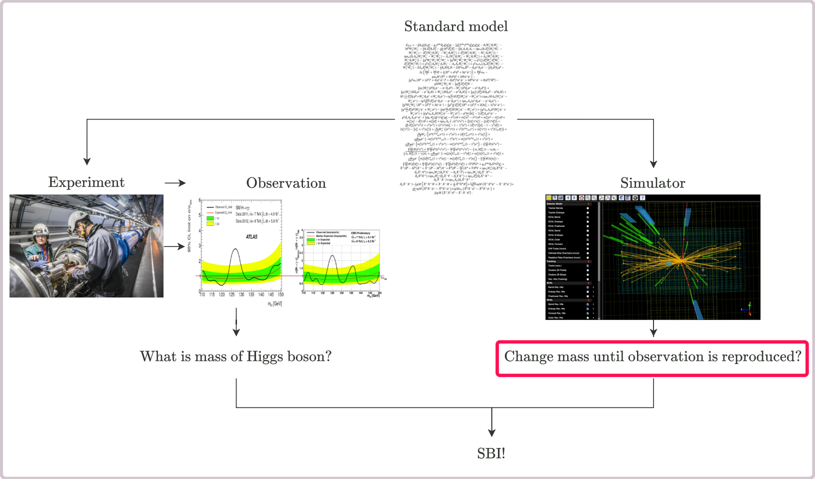
What and Why?

An Example



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What and Why?

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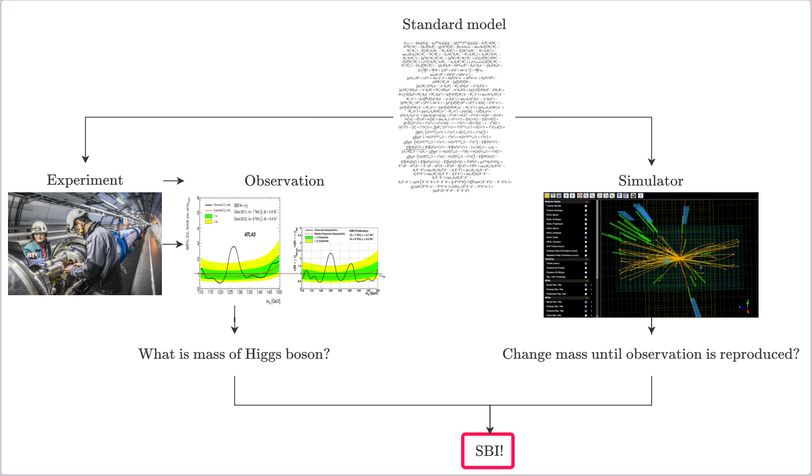

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What and Why?

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

What and Why?

Simulation-based Inference to the rescue

- 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
- Some improvements are MCMC ABC and Sequential ABC but they only improve sample efficiency but still produce merely point estimate

Learning a Posterior

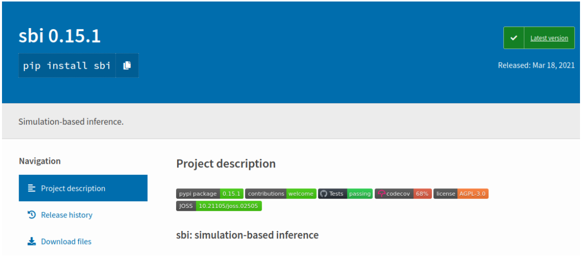
Bayesian Neural Nets to the Rescue

- 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

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- 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?