Simulation-based Inference

Inverting Simulators

Talk by Stefan Wezel

mlcolab @ Tübingen University Cluster of Excellence

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Overview

- The problem setting
- Traditional approaches and their issues
- Using Neural Nets to alleviate them
- A worked example
- Outlook

What and Why?

An Example

- Inverting simulators?
- What is a simulator?
  - Forward, generative model with parameters and stochasticity
  - Produces observations
  - In context of this talk computer program, but can be electrical circuit (Hodgkin–Huxley model)
- Used by scientists to model empirical observed data
- Used in particle physics, population genetics, epidemiology
- Encode knowledge about systems gathered over centuries

What and Why?

An Example

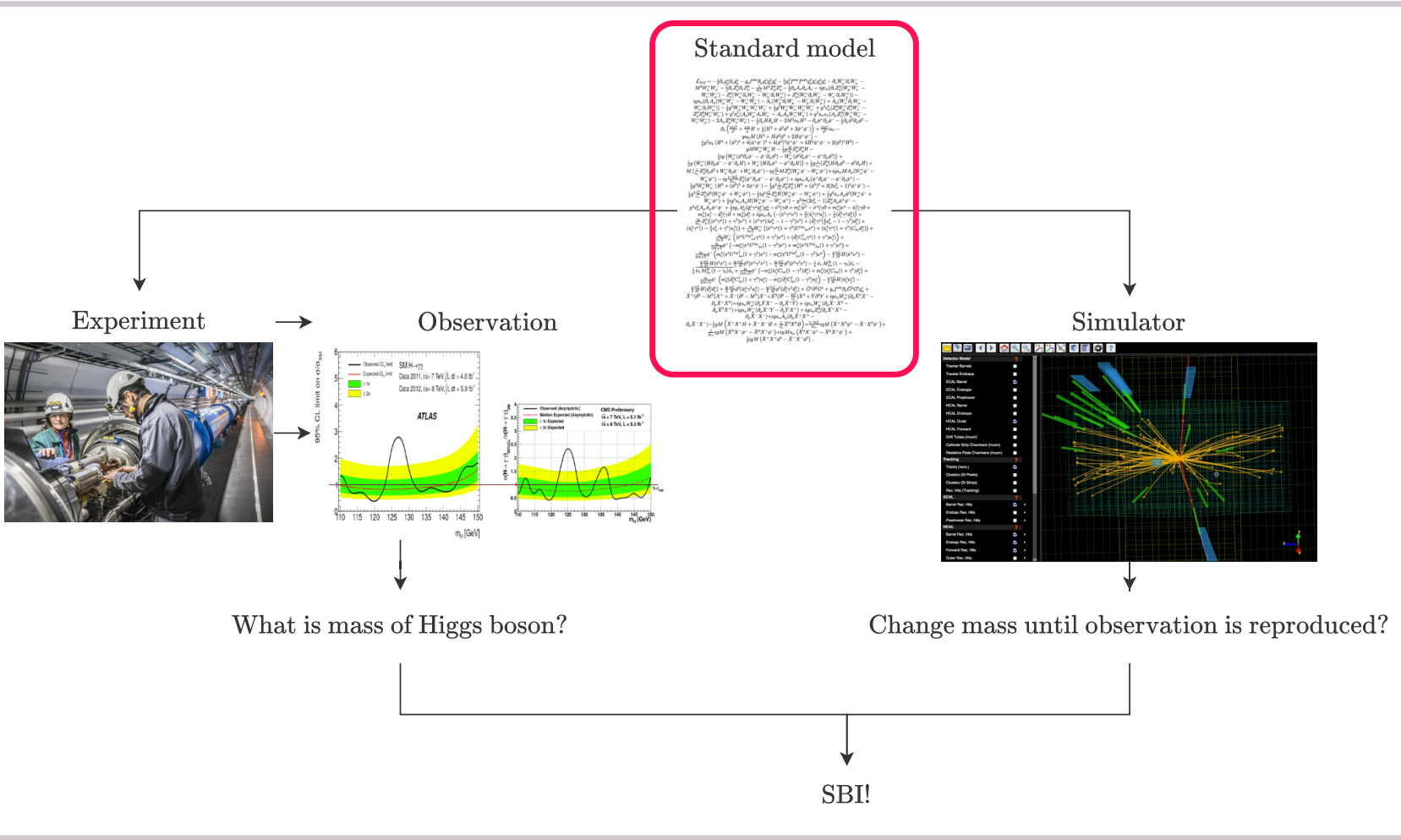
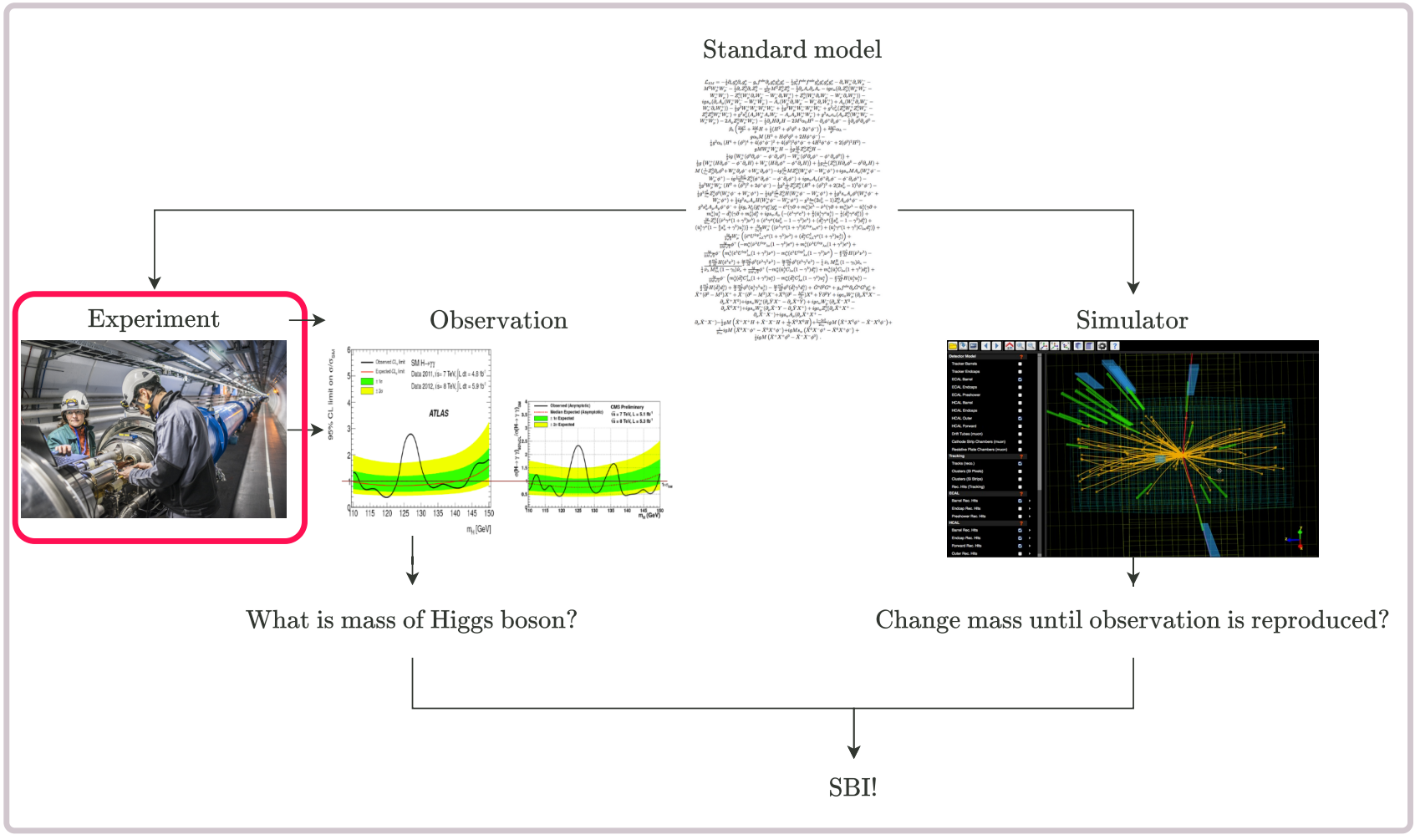


Figure derived from cern.ch, Achintya Rao and Tom McCauley, sciencealert.com

What and Why?

An Example



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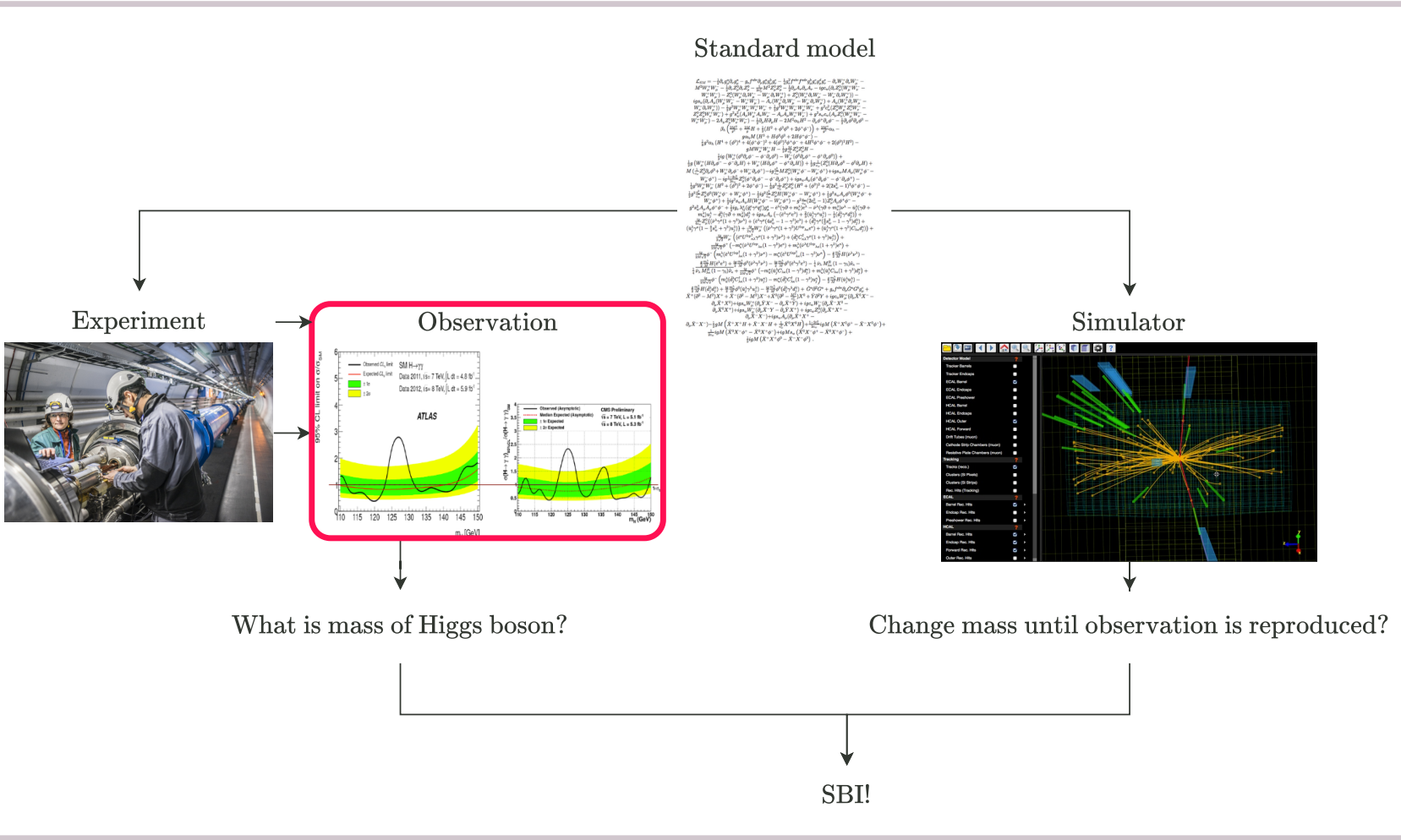

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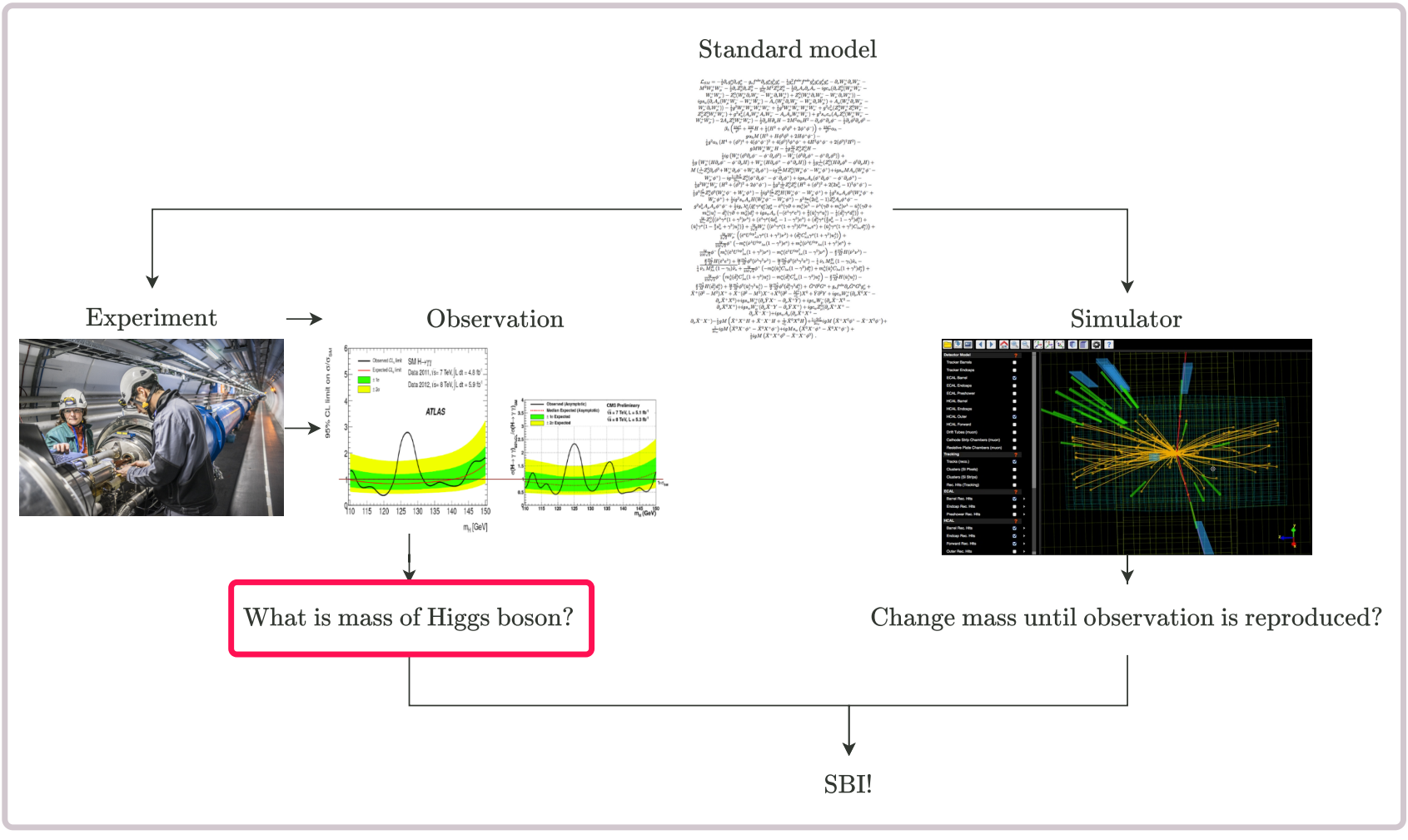

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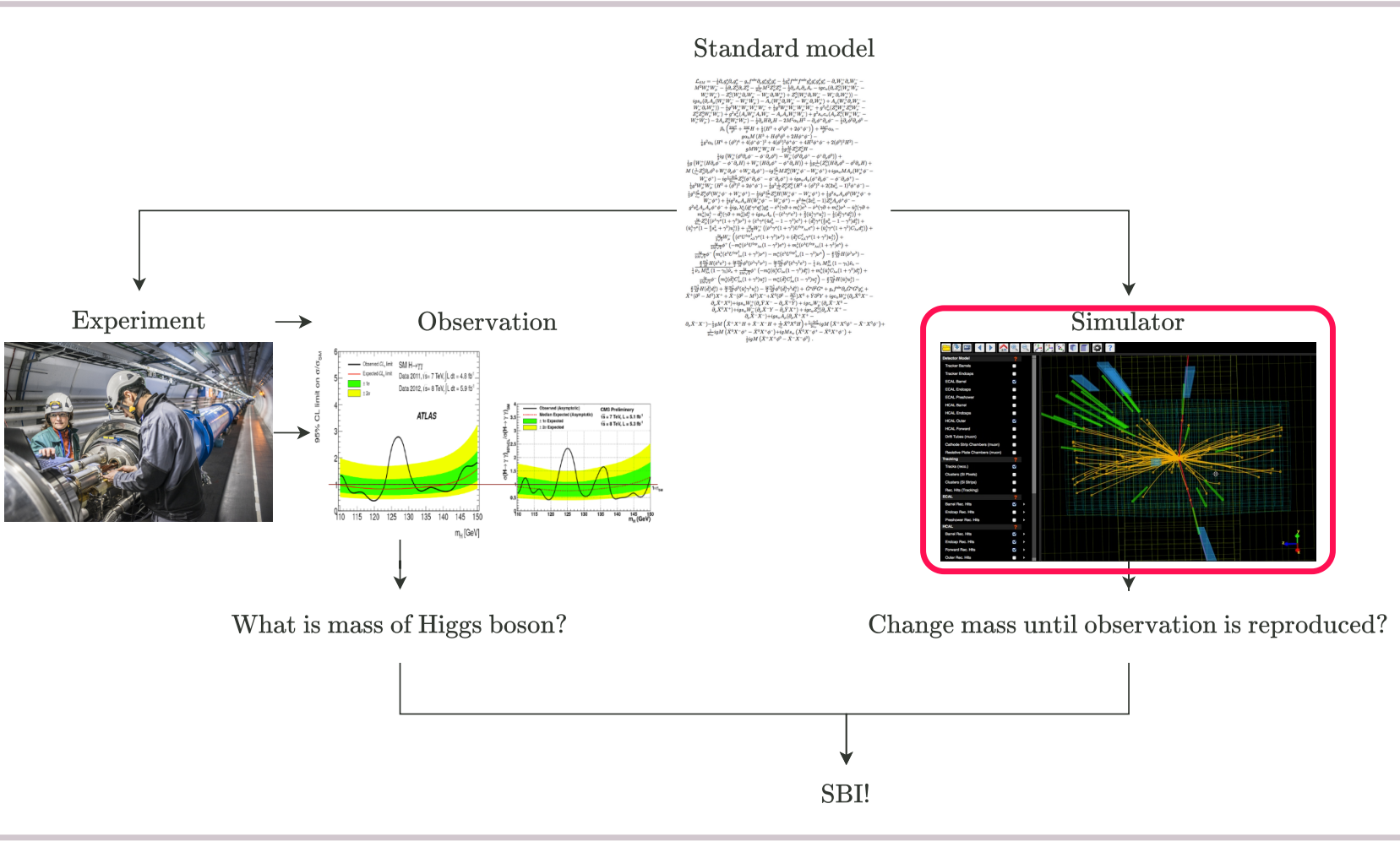

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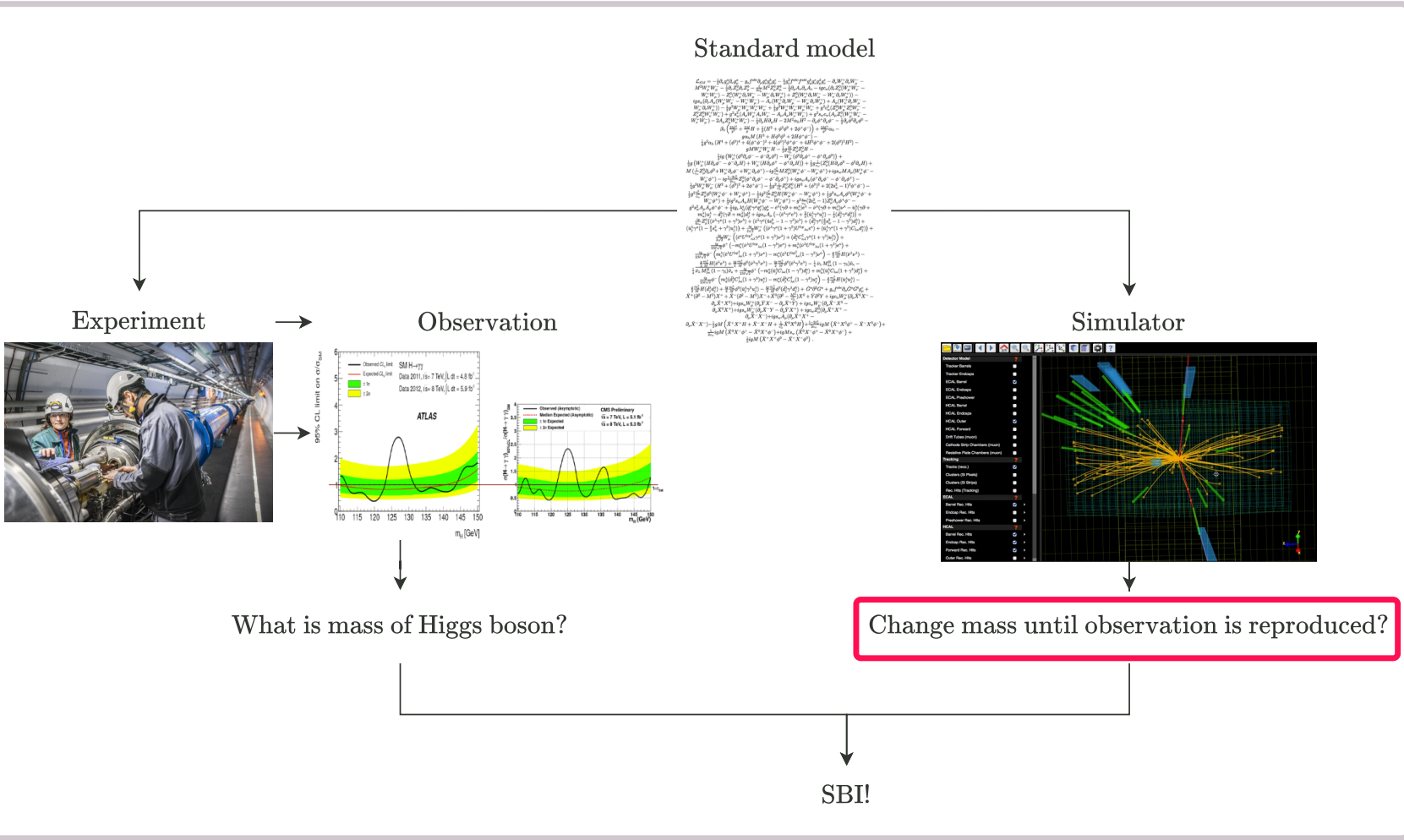

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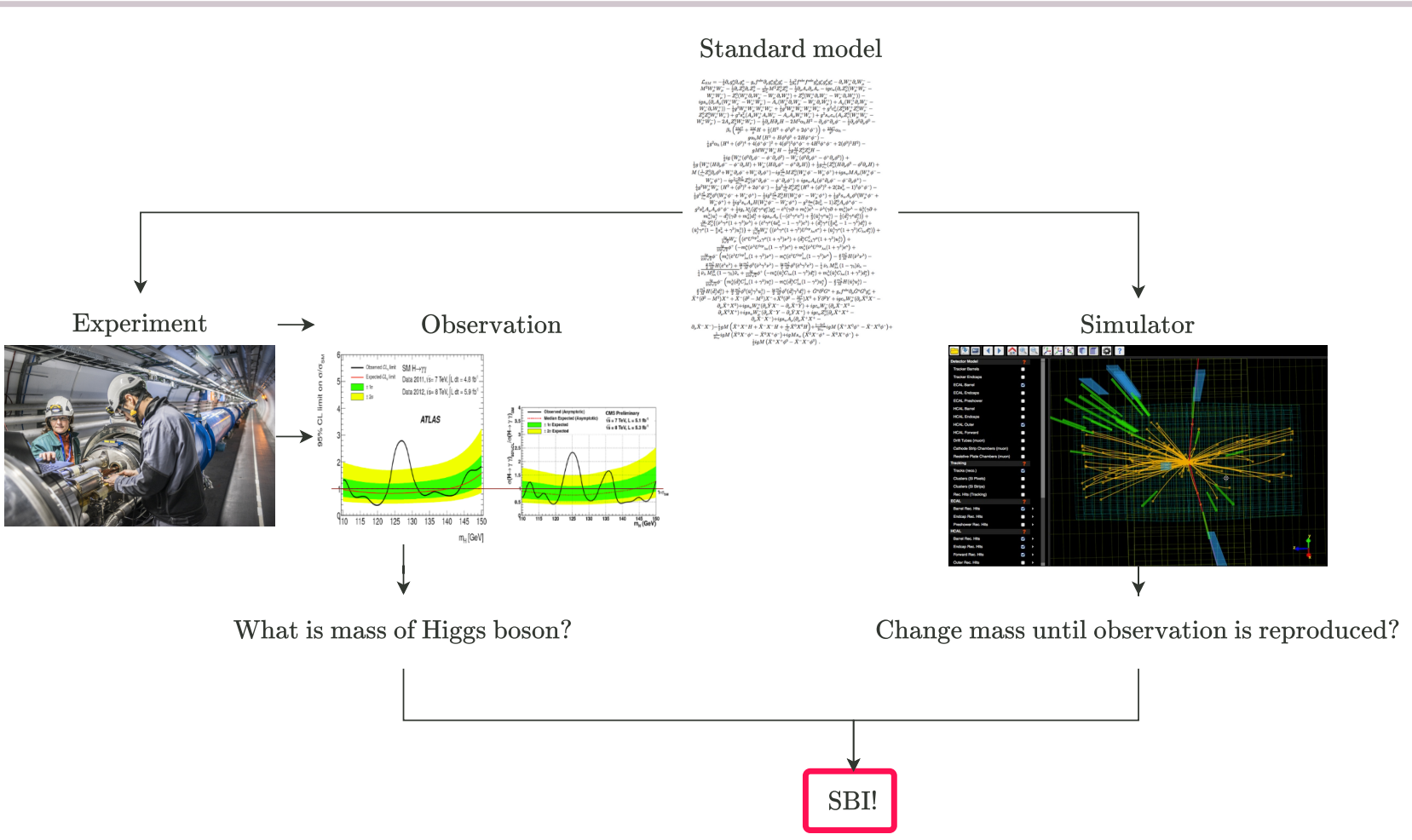

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- Before we go into SBI, let's take a minute to formalize our setting
- Simulator has parameters θ, nuisance parameter z and produces data $\hat{x}$
  - It implicitly defines $p(\hat{x}, z|\theta)$ (it yields samples from this distribution)
- Given a (real) observation x_0, we would be interested in the parameters that produced it

$$p(\theta|x = x_0) = \frac{p(x|\theta)p(\theta)}{p(x)} = \frac{\overbrace{\int p(x, z|\theta)dz}^{intractable}\, p(\theta)}{\underbrace{\int p(x|\theta)p(\theta)d\theta}_{intractable}}, \tag{1}$$

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

Simulation-based Inference

Traditional Approach

- Broader term: Approximate Bayesian Computation (ABC)
  - Rejection ABC
  - Sampling ABC (perturb initial parameters)
  - Sequential ABC (importance sampling)
- But gives only point estimates, not full posterior
- within ϵ
- [4] propose to use neural networks to parameterize GMM

for $n = 1..N$ do
  sample $\theta_n \sim \tilde{p}(\theta)$
  sample $x_n \sim p(x|\theta_n)$
end
train $q_\phi(\theta|x)$ on $\{\theta_n, x_n\}$
$\hat{p}(\theta|x = x_0) \leftarrow \frac{p(\theta)}{\tilde{p}(c)} q_\phi(\theta|x)$

Pseudocode derived from [4]

for $n = 1..N$ do

  sample $\theta_n \sim \tilde{p}(\theta)$

  sample $x_n \sim p(x|\theta_n)$

end

train $q_\phi(\theta|x)$ on $\{\theta_n, x_n\}$ (More in a second)

$\hat{p}(\theta|x = x_0) \leftarrow \frac{p(\theta)}{\tilde{p}(c)} q_\phi(\theta|x)$

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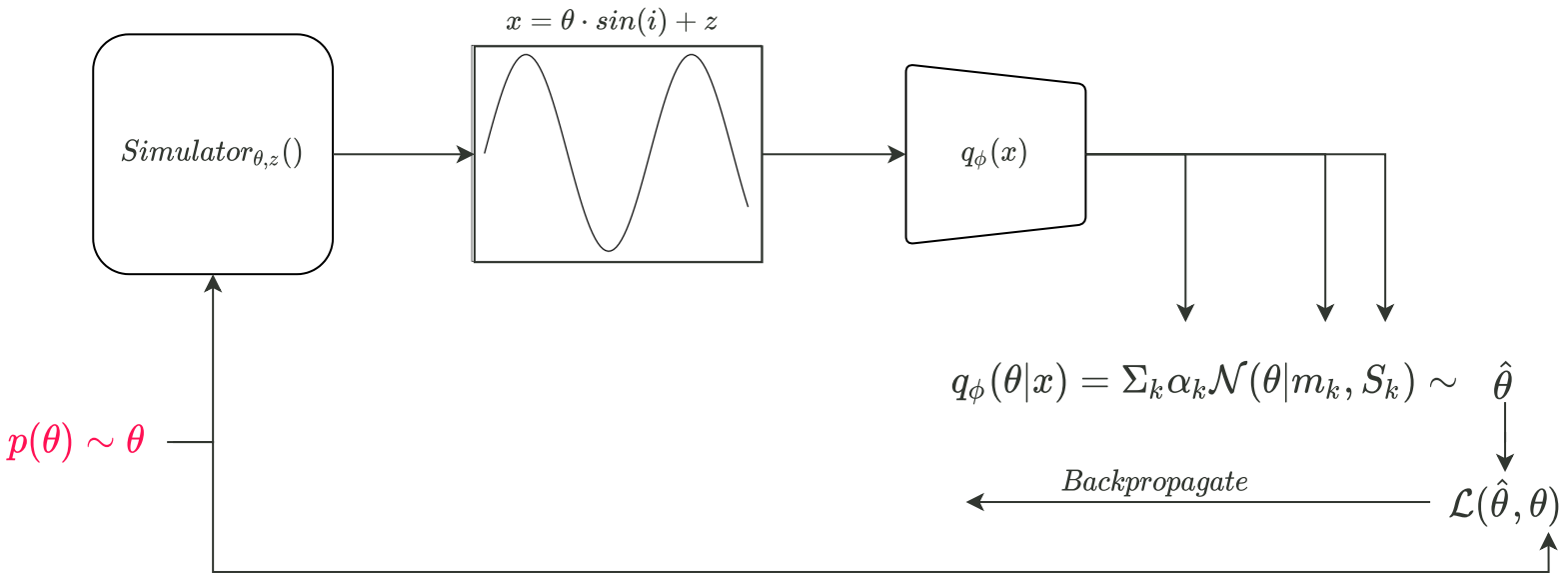
Learning a Posterior

from Simulations



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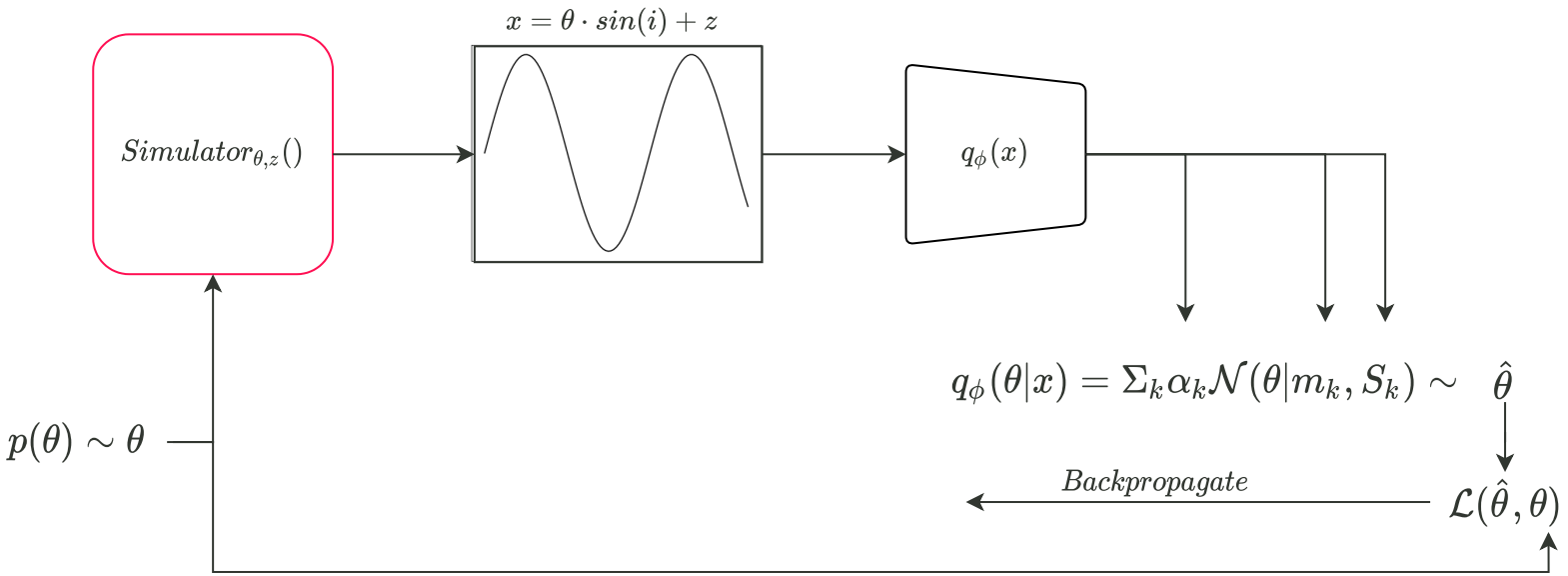

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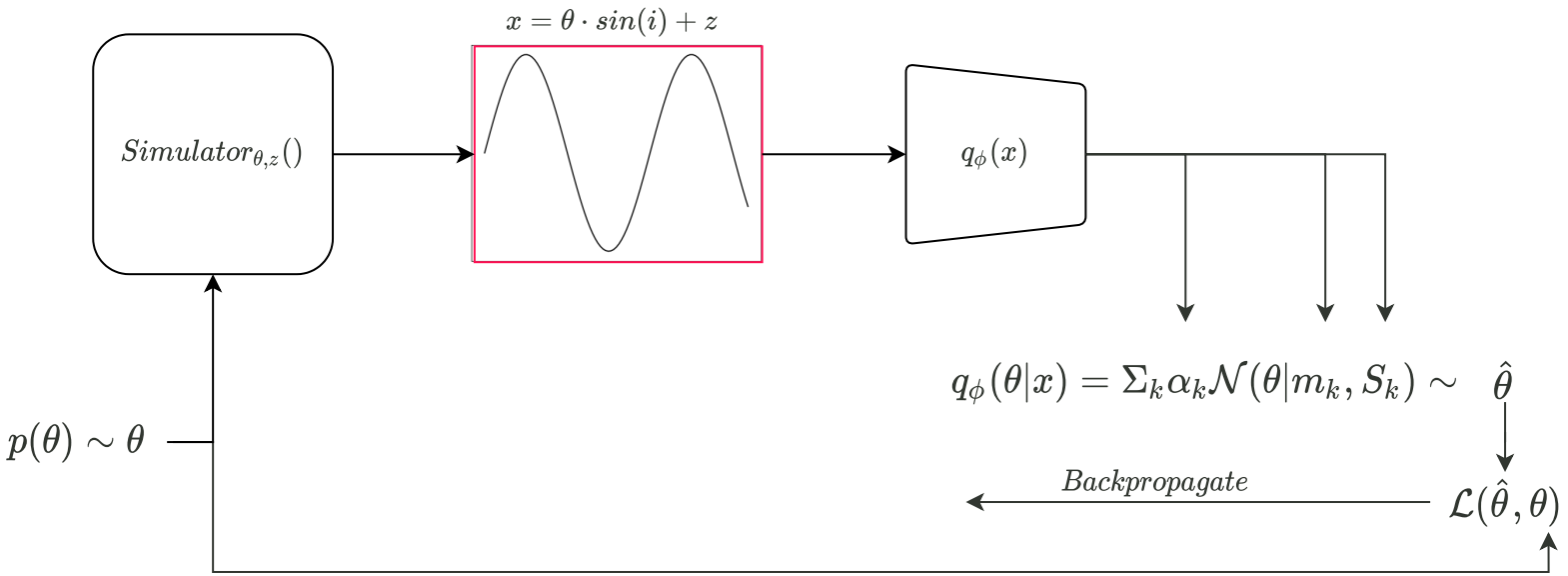

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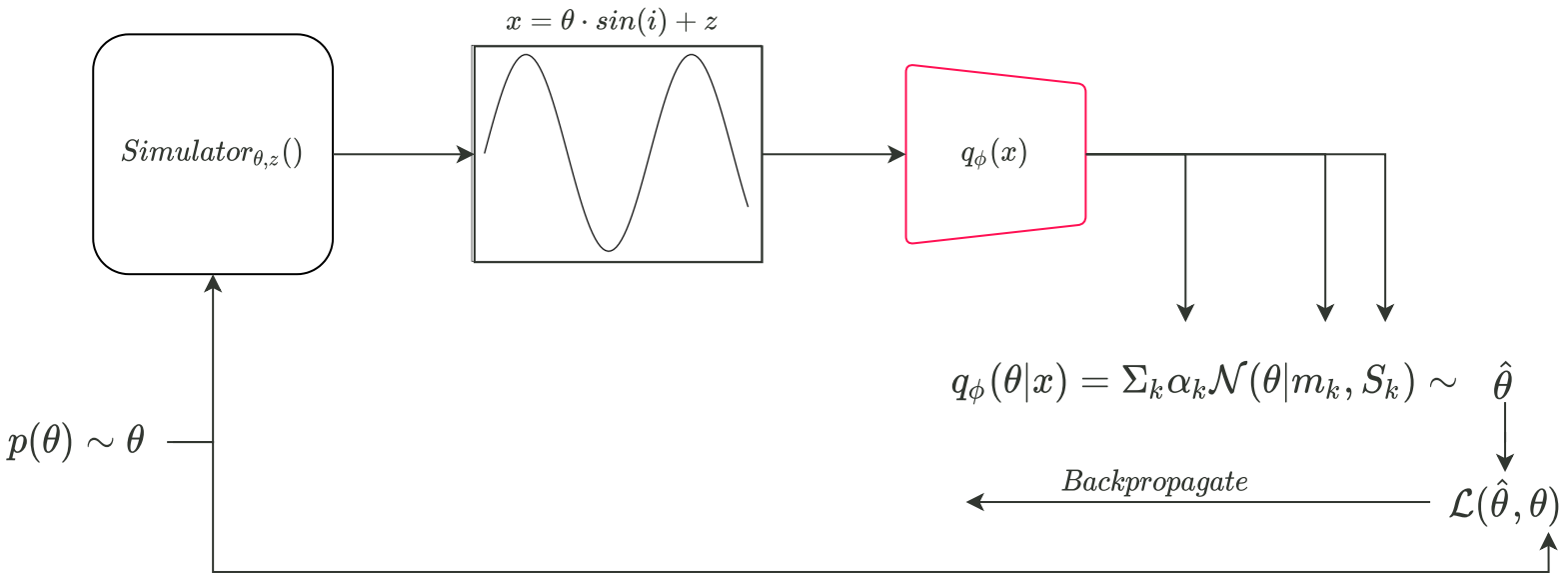

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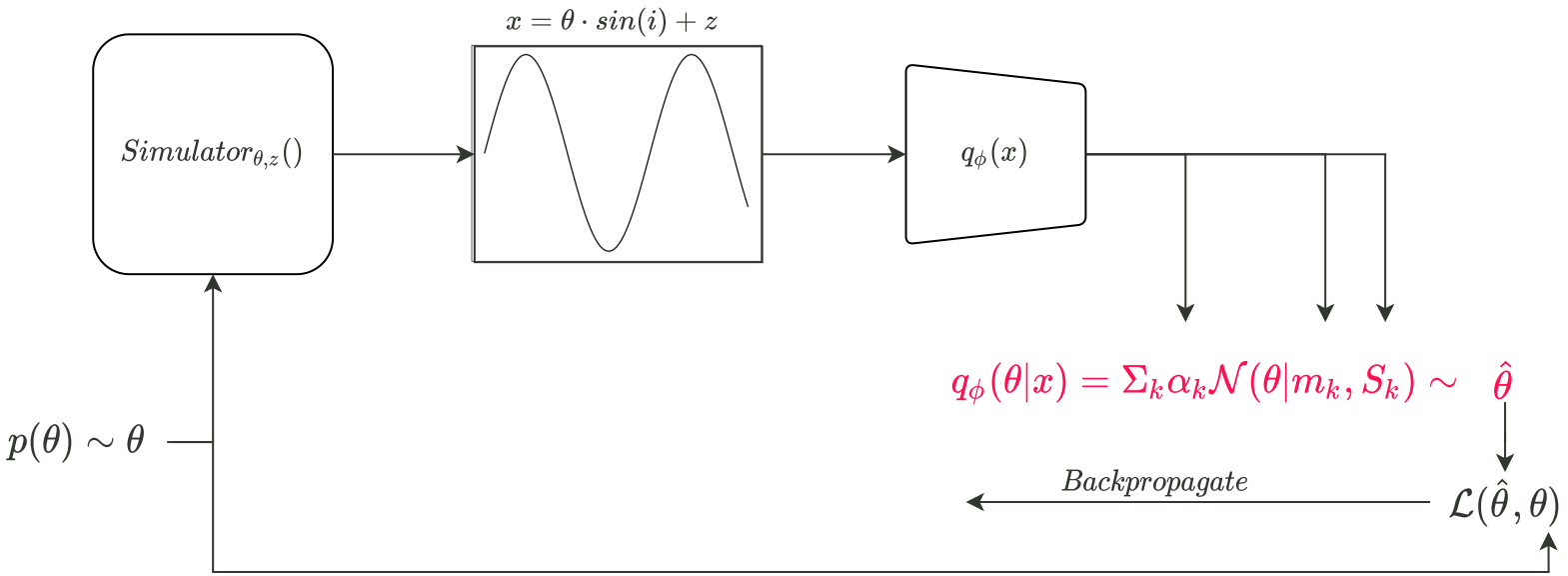

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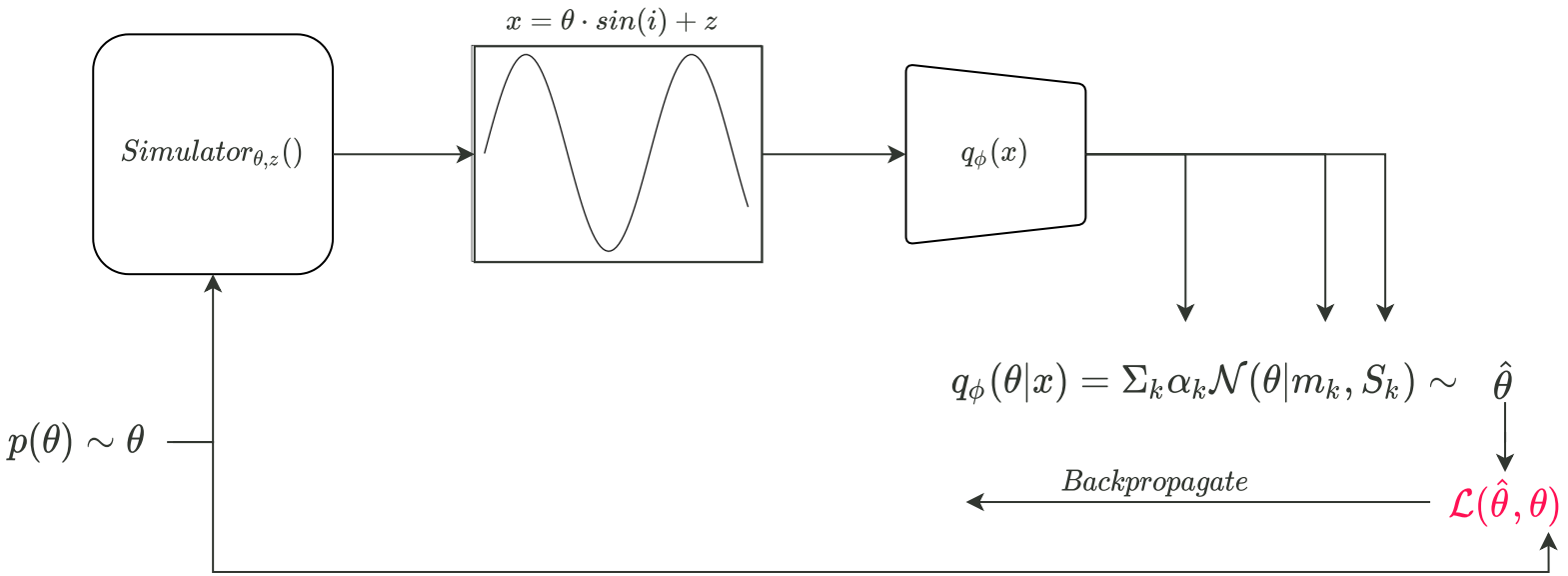

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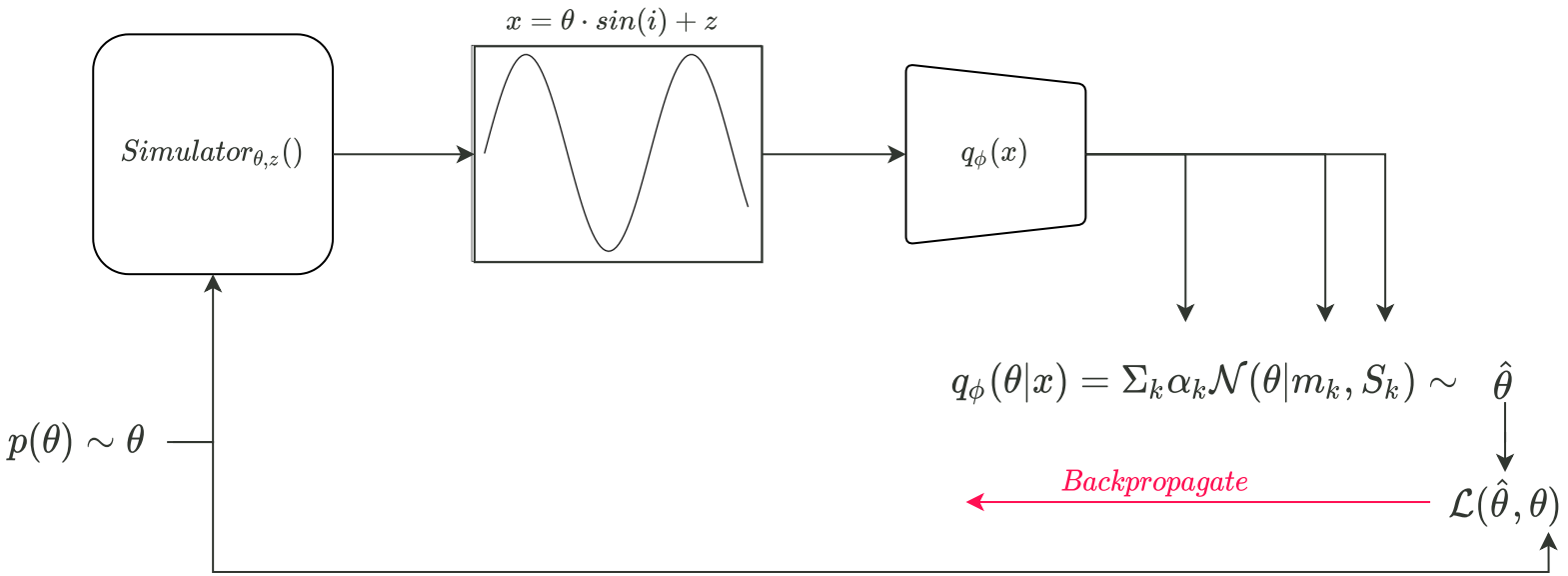
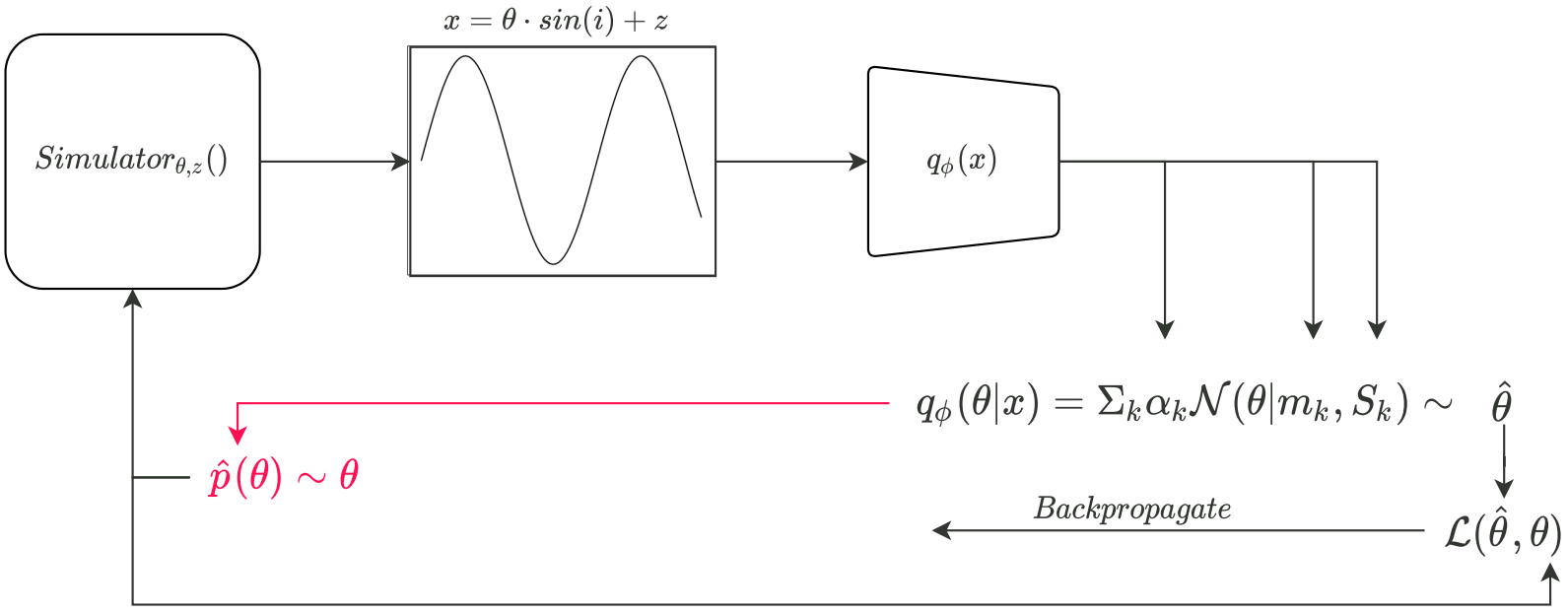


Learning a Prior

Proposing a New Prior



Learning a Prior

Starting from an Initial Prior

$\tilde{p}(\theta) \leftarrow p(\theta)$

repeat

  for $n = 1..N$ **do**

    sample $\theta_n \sim \tilde{p}(\theta)$

    sample $x_n \sim p(x|\theta_n)$

  end

  train $q_\phi(\theta|x)$ on $\{x_n, \theta_n\}$

  $\hat{p}(\theta|x = x_0) \leftarrow \frac{p(\theta)}{\tilde{p}(c)} q_\phi(\theta|x)$

until $\tilde{p}(\theta)$ has converged;

Pseudocode derived from [4]

$\tilde{p}(\theta) \leftarrow p(\theta)$

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until $\tilde{p}(\theta)$ has converged;

Pseudocode derived from [4]

Learning a Prior

Replacing the Initial Prior

$\tilde{p}(\theta) \leftarrow p(\theta)$

repeat

  for $n = 1..N$ **do**

    sample $\theta_n \sim \tilde{p}(\theta)$

    sample $x_n \sim p(x|\theta_n)$

  end

  train $q_\phi(\theta|x)$ on $\{x_n, \theta_n\}$

  $\hat{p}(\theta|x = x_0) \leftarrow \frac{p(\theta)}{\tilde{p}(c)} q_\phi(\theta|x)$

until $\tilde{p}(\theta)$ has converged;

Pseudocode derived from [4]

Refining SBI

Lueckman et al

- Include importance reweighting in loss
  - No analytical step necessary
  - Enables complex proposal priors
- posterior over network weights, that can be used to init network in next iteration
- Handle bad simulations to improve convergence (i.e. diverging firing rate)
  - training classifier to predict if sample fails
- (Extract Features with RNN)

Applying SBI

to Hodgkin–Huxley

- Hodgkin-Huxley model [2] describes dynamics of neuron's membrane
- Parameters (concentration of sodium, potassium, ...)
- Numerical simulators available (NEURON software [1])

- ...

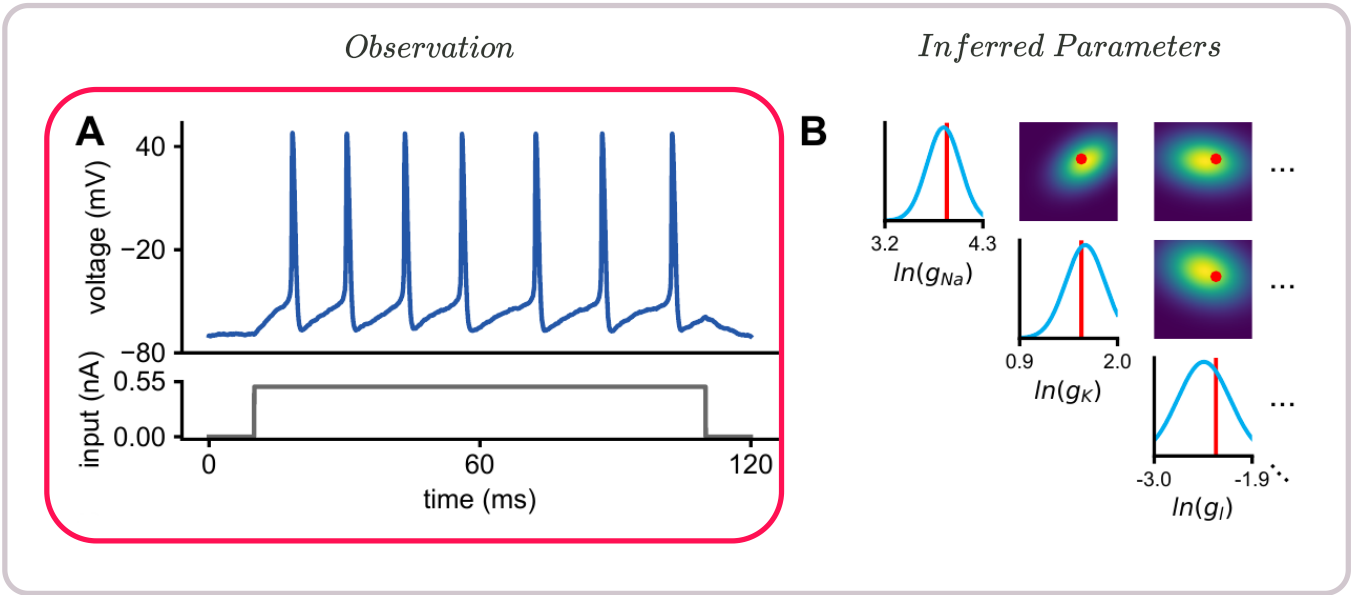

Figure derived from [3]

- ...

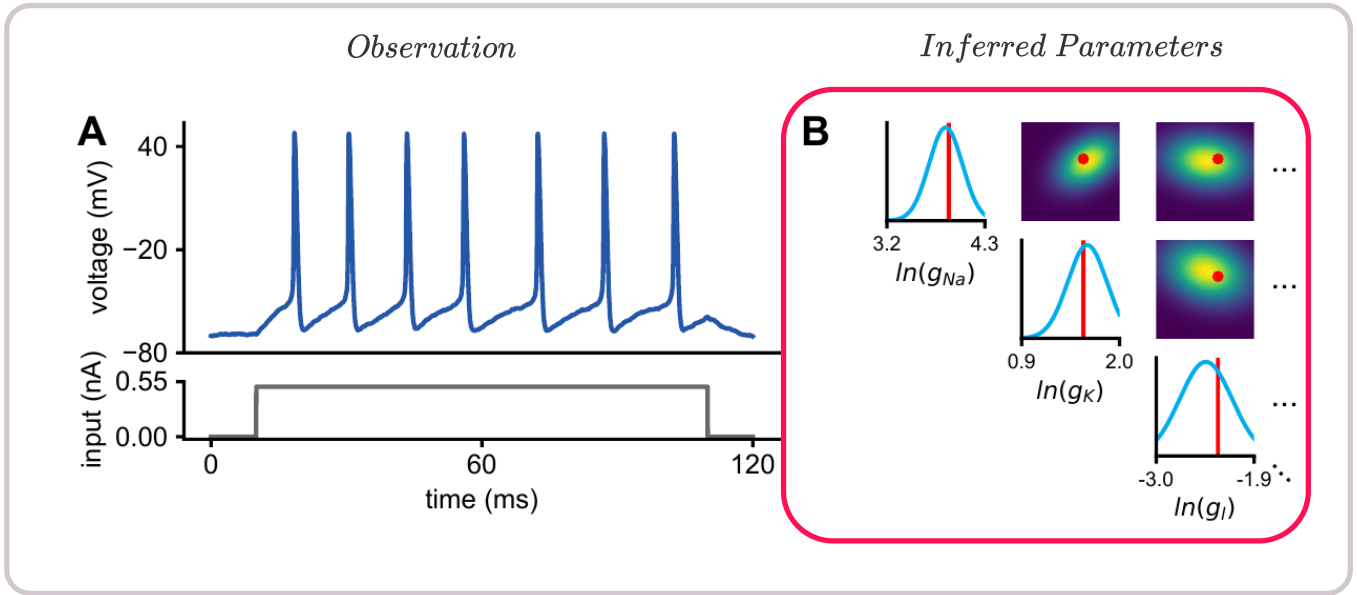

Figure derived from [3]

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] N. T. Carnevale and M. L. Hines. The NEURON book. Cambridge University Press, 2006.

[2] A. L. Hodgkin and A. F. Huxley. A quantitative description of membrane current and its application to conduction and excitation in nerve. The Journal of physiology, 117(4):500–544, 1952.

[3] J.-M. Lueckmann, P. J. Goncalves, G. Bassetto, K. Öcal, M. Nonnenmacher, and J. H. Macke. Flexible statistical inference for mechanistic models of neural dynamics. arXiv preprint arXiv:1711.01861, 2017.

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