Simulation-based Inference

Learning a Posterior by Inverting Simulators

Talk by Stefan Wezel

mlcolab @ Tübingen University

May 5, 2021

Overview

- Problem Setting
- Traditional Approaches and their Issues
- Using Neural Networks to alleviate them
- SBI in the Wild

What and Why?

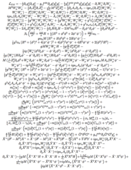
What is a simulator?

- 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 empirically observed data
- In particle physics, population genetics, epidemiology
- Encode knowledge about systems

What and Why?

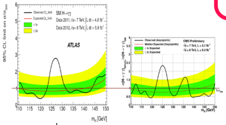
An Example

Standard model

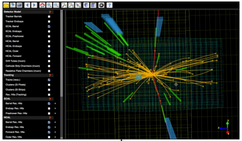


Experiment

Observation



Simulator

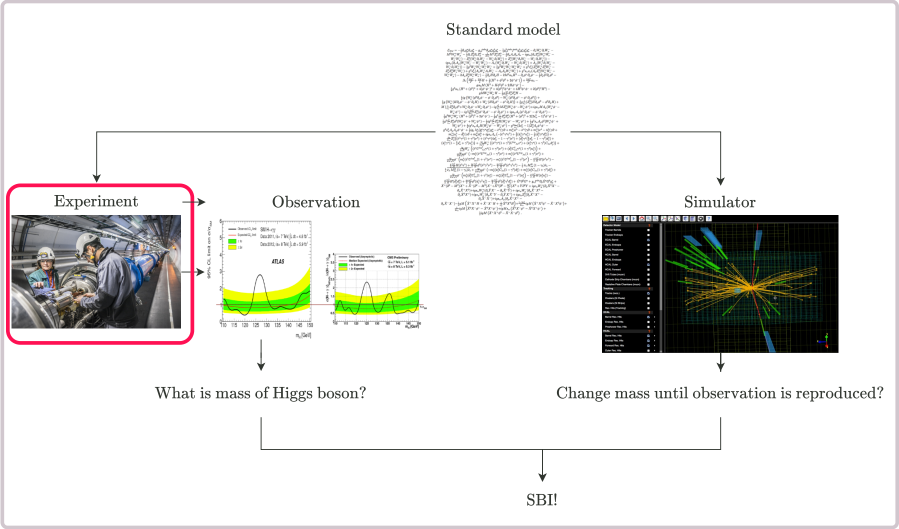


What is mass of Higgs boson?

Change mass until observation is reproduced?

SBI!

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



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What and Why?

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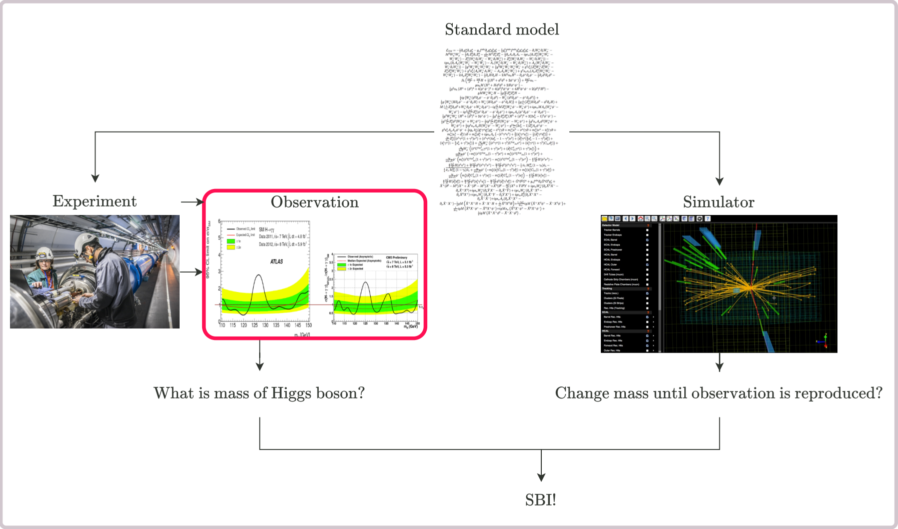

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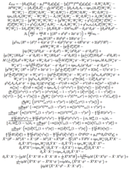

Experiment

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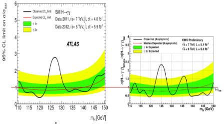

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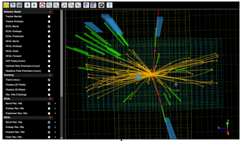

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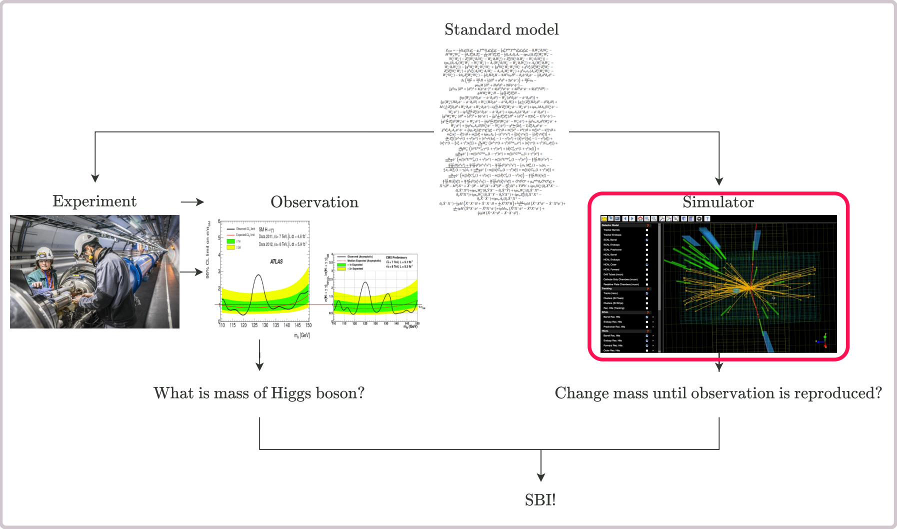

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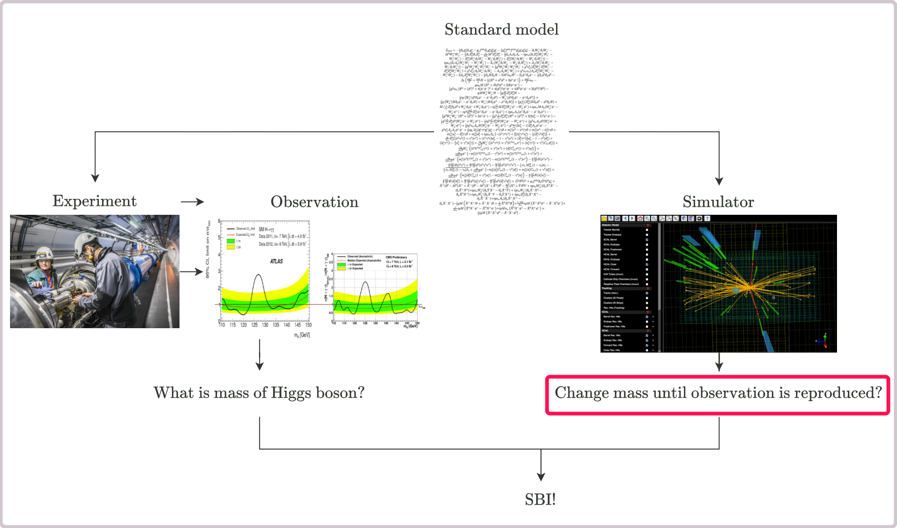

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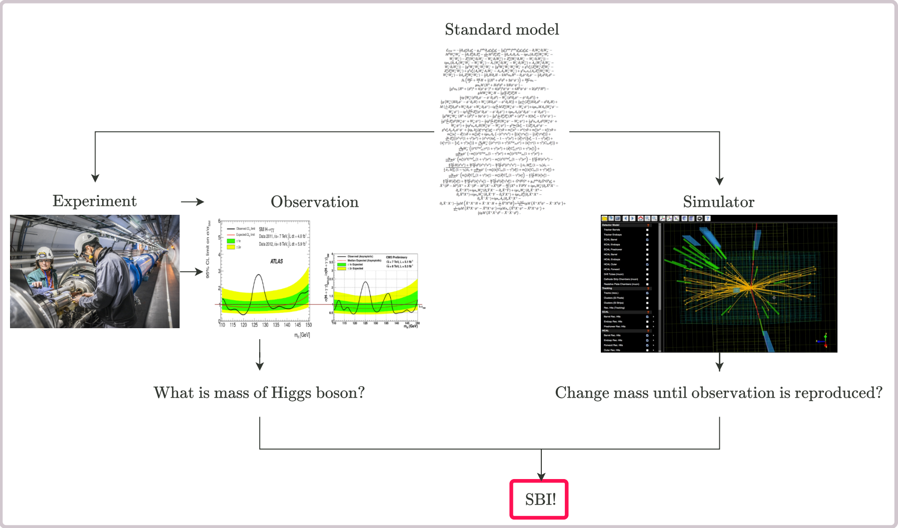

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- Simulator has parameters θ, nuisance parameter z
- Produces data x
  - Implicitly defines $p(x, z \mid \theta)$
- Given (real) observation x_0, we are interested in parameters that produced it

$$p(\theta \mid x = x_0) = \frac{p(x \mid \theta) p(\theta)}{p(x)} = \frac{\overbrace{\int p(x, z \mid \theta) \, \mathrm{d}z}^{\text{intractable}} \, p(\theta)}{\int p(x \mid \theta) p(\theta) \, \mathrm{d}\theta} \tag{1}$$

- Typical problem setting of scientists across domains
  - Sophisticated forward model that encapsulates prior knowledge
  - Inference means: What were parameters that produced observation?
- To find θ, invert simulator

- Broader term: Approximate Bayesian Computation (ABC)
- Rejection ABC
  - Change θ until something ϵ-close to x_0 is produced
  - Inefficient for small ϵ
  - No actual posterior but only point estimate
  - Approximates $p(\theta \mid || x - x_0 || < \epsilon)$
- Some improvements
  - Sampling ABC (perturb matched parameters) [6]
  - Sequential ABC (importance sampling) [1, 2]
- Point-estimate to posterior over parameters for ϵ-ball around observation

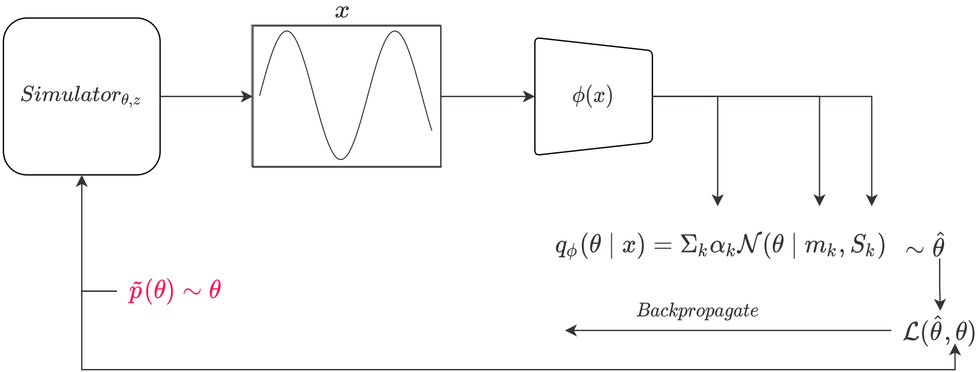
Simulation-based Inference

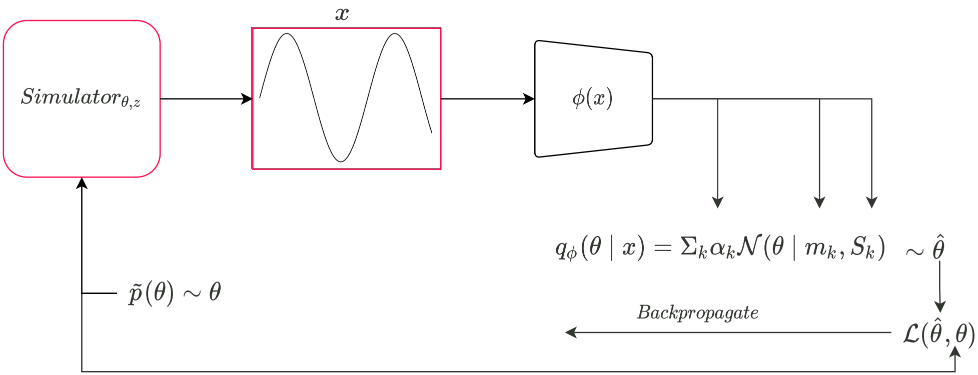
Predicting Parameter Posterior

- Papamakarios and Murray [7] learn approximation to actual posterior
- Use simulator to create training set
  - $\{x_j, \theta_j\}_{j \in N}$
- Train neural network to predict parameters of posterior over θs

Learning a Posterior

from Simulations

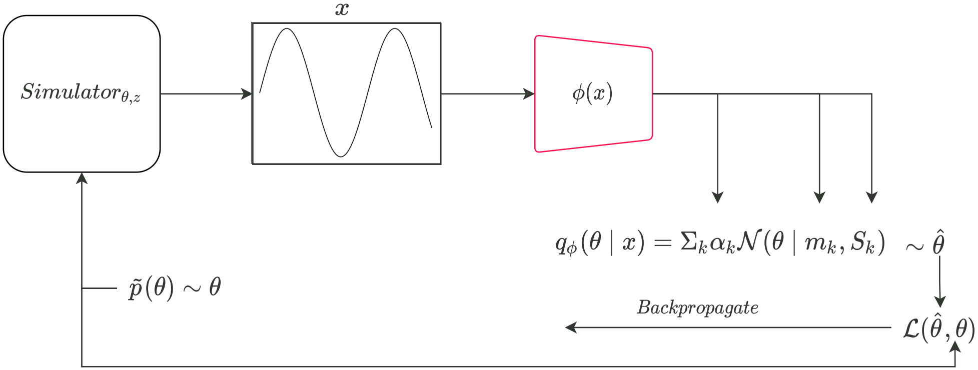




$Simulator_{\theta,z}$
x
$\phi(x)$
$q_\phi(\theta \mid x) = \Sigma_k \alpha_k \mathcal{N}(\theta \mid m_k, S_k) \sim \hat{\theta}$
$\tilde{p}(\theta) \sim \theta$
$Backpropagate$
$\mathcal{L}(\hat{\theta}, \theta)$

Learning a Posterior

from Simulations



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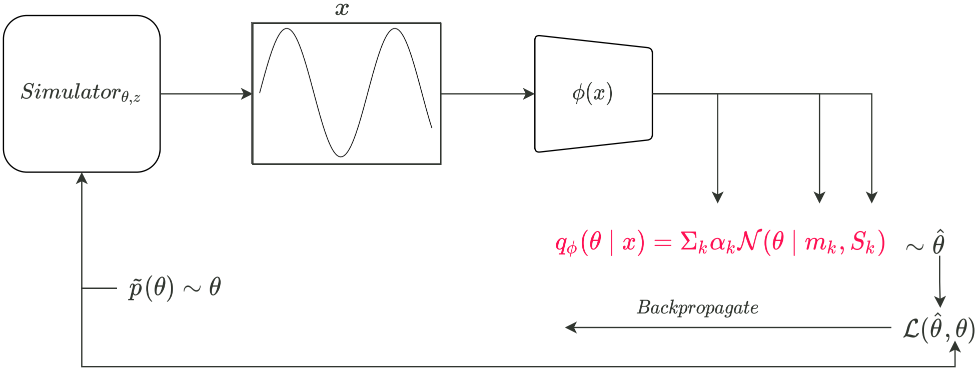

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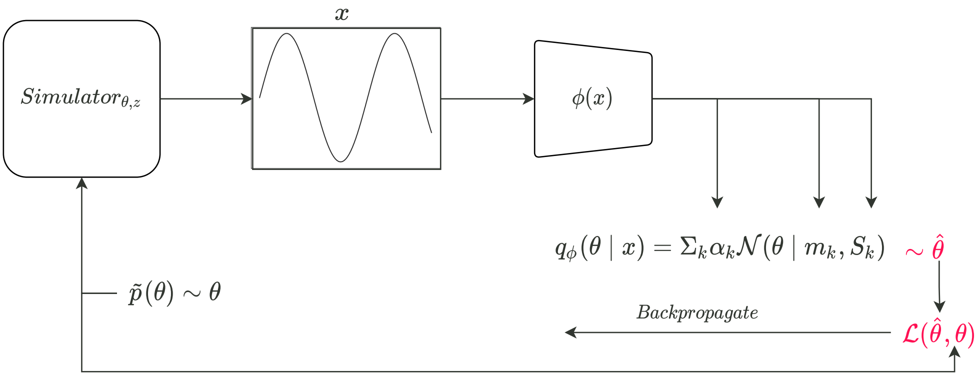

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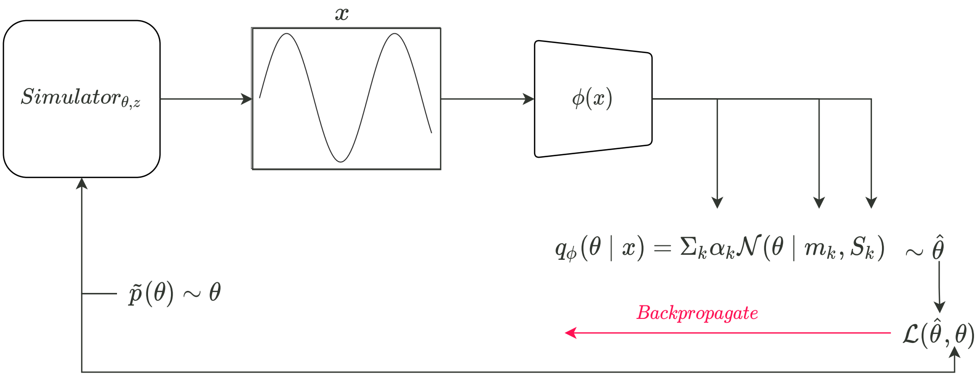
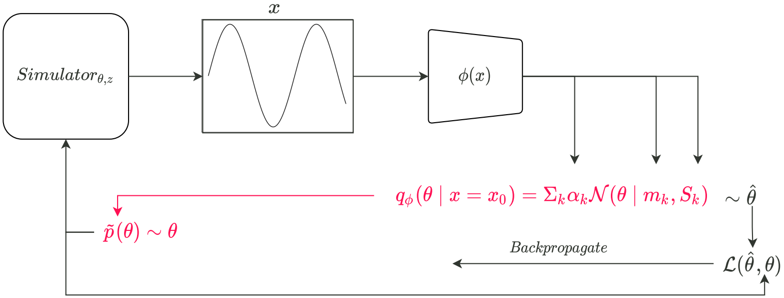


Updating the Prior

With the Posterior

- What if we only care about single observation?
- Iteratively replace prior with posterior
- Faster convergence



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

repeat

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

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

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

  end

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

  $\tilde{p}(\theta) \leftarrow q_\phi(\theta \mid x)$

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

Pseudocode derived from [7]

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Applying SBI

to Hodgkin–Huxley

- Lueckmann et al. [5] apply SBI to neuroscience setting
  - Diverging simulations
  - Summary statistics challenging
- They propose
  - Train classifier to predict whether parameters fail
  - Extract features with RNN
  - Posterior over network weights
- Apply Hodgkin-Huxley model [4]
  - Numerical simulators available (NEURON software [3])
  - Dynamics of neuron’s membrane
  - Parameters (concentration of sodium, potassium, …)

Applying SBI

Results

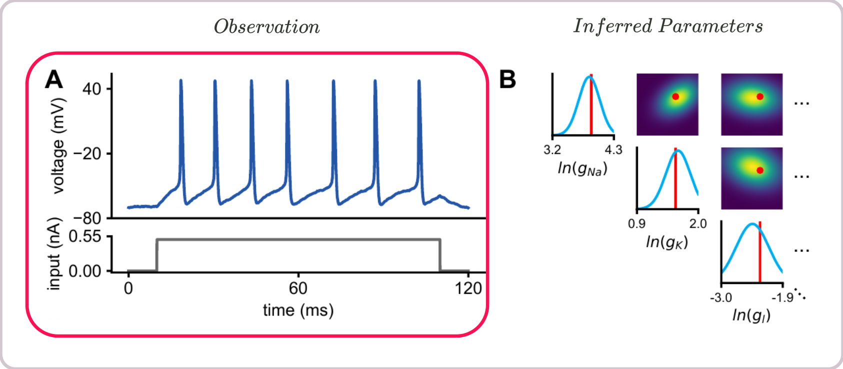

Figure derived from [5]

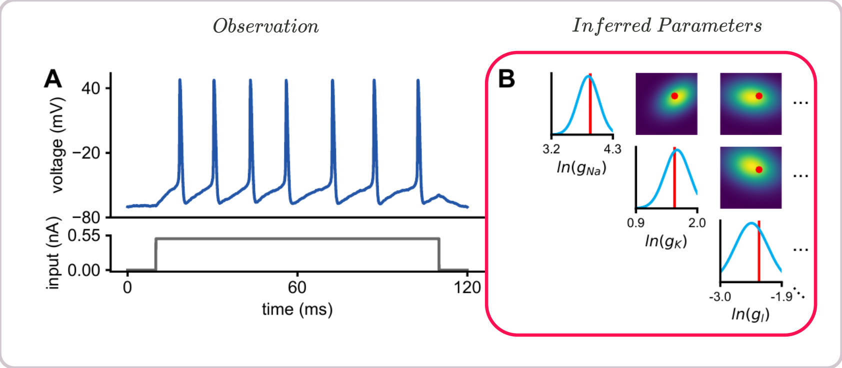

Figure derived from [5]

How to use SBI?

Some advertisement

- mlcolab and mackelab is developing sbi python library [8]
- If you are interested: try it out and give us your feedback
- `colab.research.google.com/drive/1L1T45hruoScyu3hN4WkDW6f0De4UemjI?usp=sharing`
- `github.com/mackelab/sbi`
- `pip install sbi` (ignore error message)

Questions for you

- Do you know a setting where SBI could be applied?
- What are downsides of SBI?
- Can't we just use a variational autoencoder?

References

[1] M. A. Beaumont, J.-M. Cornuet, J.-M. Marin, and C. P. Robert. Adaptive approximate bayesian computation. Biometrika, 96(4):983–990, 2009.

[2] F. V. Bonassi, M. West, et al. Sequential monte carlo with adaptive weights for approximate bayesian computation. Bayesian Analysis, 10(1):171–187, 2015.

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

[4] 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.

[5] 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.

[6] P. Marjoram, J. Molitor, V. Plagnol, and S. Tavaré. Markov chain monte carlo without likelihoods. Proceedings of the National Academy of Sciences, 100(26):15324–15328, 2003.

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

[8] A. Tejero-Cantero, J. Boelts, M. Deistler, J.-M. Lueckmann, C. Durkan, P. J. Gonçalves, D. S. Greenberg, and J. H. Macke. Sbi: a toolkit for simulation-based inference. Journal of Open Source Software, 5(52):2505, 2020.

- Example (if there is time)