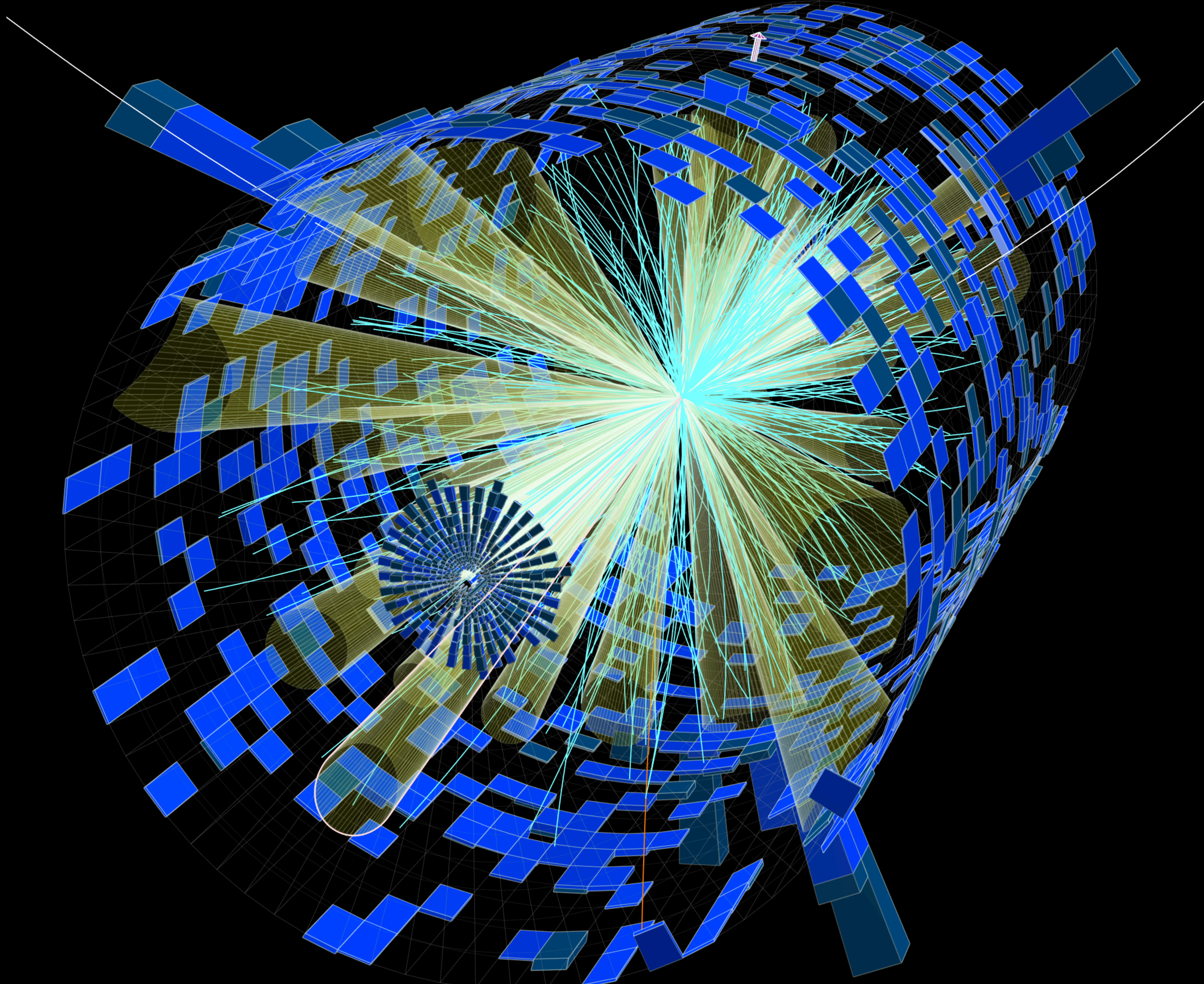
NYU Center for Data Science

Meta AI

Center for Cosmology and Particle Physics

SIMULATION-BASED INFERENCE

FOR GRAVITATIONAL WAVE ASTRONOMY



@KyleCranmer
New York University
Department of Physics
Center for Data Science
CILVR Lab

Collaborators + Many More


Johann Brehmer
NYU → Qualcom


Gilles Louppe
NYU → U. Liège


Juan Pavez
Santa Maria U.


Lukas Heinrich
NYU → CERN


Atılım Güneş Baydin
U. Oxford

NSF


Irina Espejo
NYU

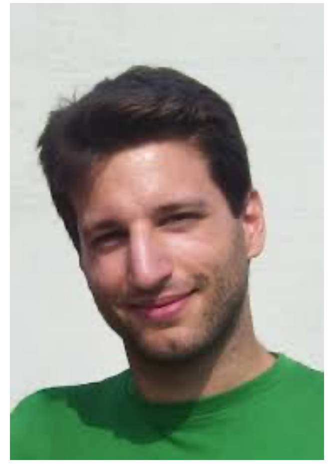

Felix Kling
SLAC

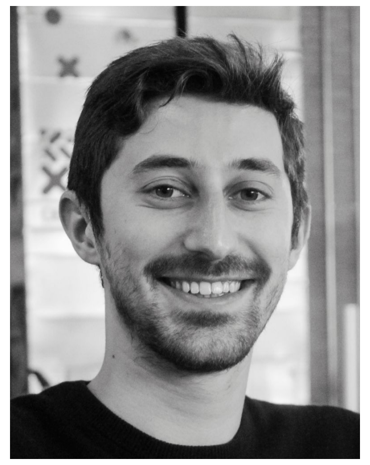

Sebastian Macaluso
NYU


Sid Mishra-Sharma
NYU → IAIFI


Joeri Hermans
NYU → U. Liège

MSDSE
Moore - Sloan
Data Science Environments


George Papamakarios
DeepMind

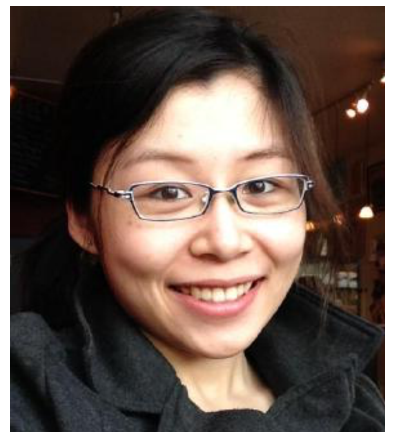

Michael Albergo
NYU


Danilo Rezende
DeepMind


Prabhat
NERSC/ LBNL


Wahid Bhimji
NERSC/ LBNL


Frank Wood
U. Victoria


Lei Shao
Intel


Andreas Munk
Oxford

Overview: Gravitational-wave (GW) observations offer a unique opportunity to study astrophysical and cosmological sources that are difficult to access through electromagnetic observations. **Inferring the sources' properties** from their GW signal is one of the key objectives of GW data analysis. The planned improvements in the sensitivity of the ground-based detectors and future space-based observatories, however, bring **unique computational and mathematical challenges to the inference problem** including long-duration signals, high signal-to-noise ratios, increased parameter dimensionality and overlapping signals. These challenges must be overcome to fully exploit the scientific potential of GW observations. The goal of this workshop is to connect statisticians, computer scientists and GW astrophysicists to discuss the **current state-of-the-art approaches to parameter estimation** in GW astrophysics, and to identify the open issues to enable **fast and reliable inference** for different GW sources, including modelled and un-modelled signals, for the current and planned GW observatories.

Questions to keep in the back of your mind

What's the product of inference?

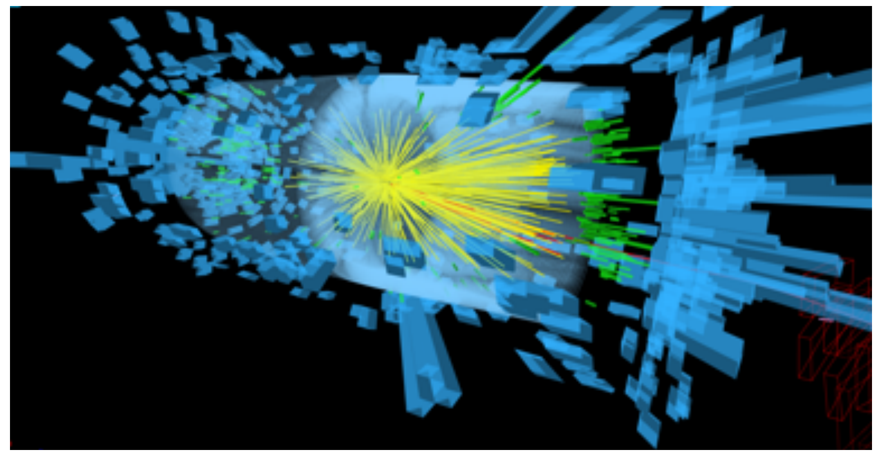
- Samples from posterior $\theta_i \sim p(\theta \mid x)$
- The posterior $p(\theta \mid x)$ itself
- The likelihood $p(x \mid \theta)$
- Confidence/credible intervals
- Expectations of various quantities with respect to posterior $\mathbb{E}_{p(\theta|x)}[f(\theta)]$
- A component to a larger decision making / planning system

How is important is speed (amortized inference)?

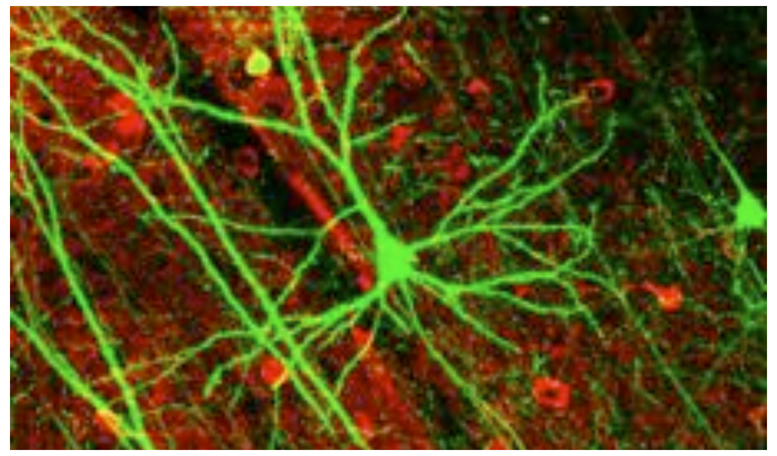
Are we after population-level inference or inference on individual objects?

What is the role of summary statistics / inductive bias / expert domain knowledge?

Science is replete with high-fidelity simulators



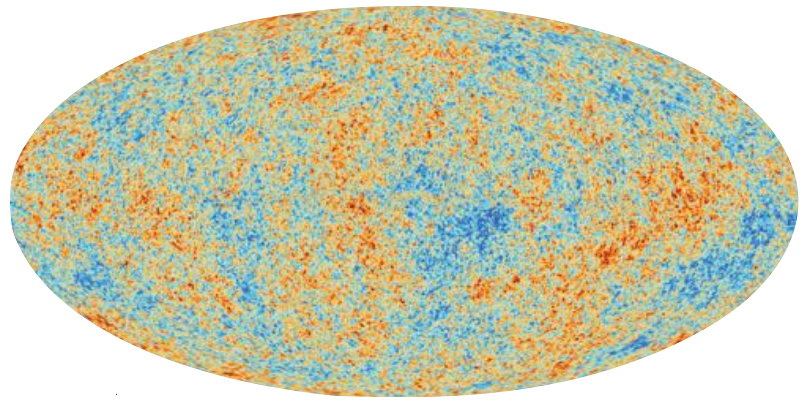
Particle colliders



Neuron activity

Epidemics

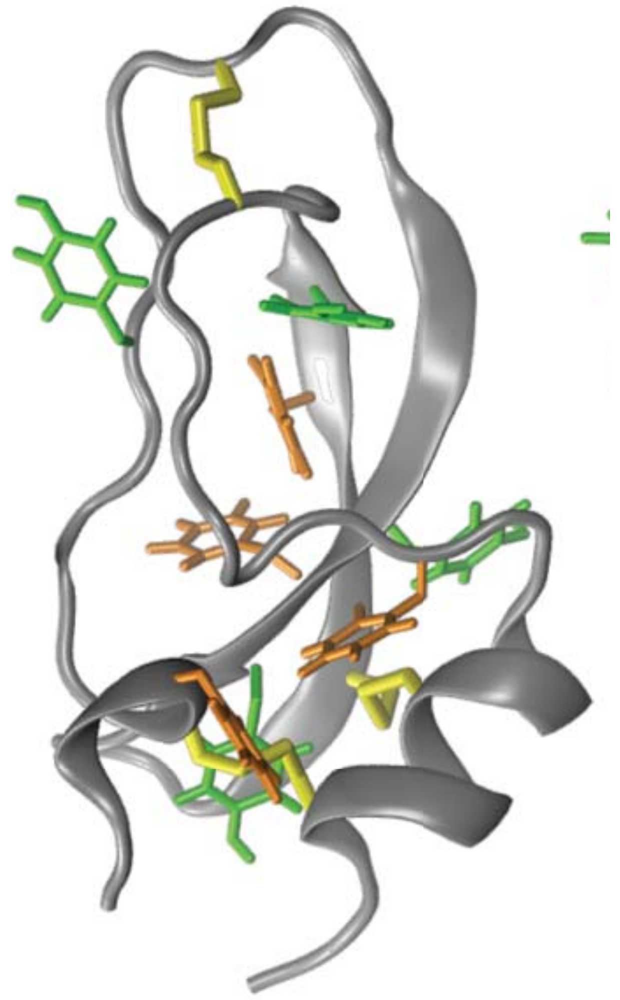
Gravitational lensing

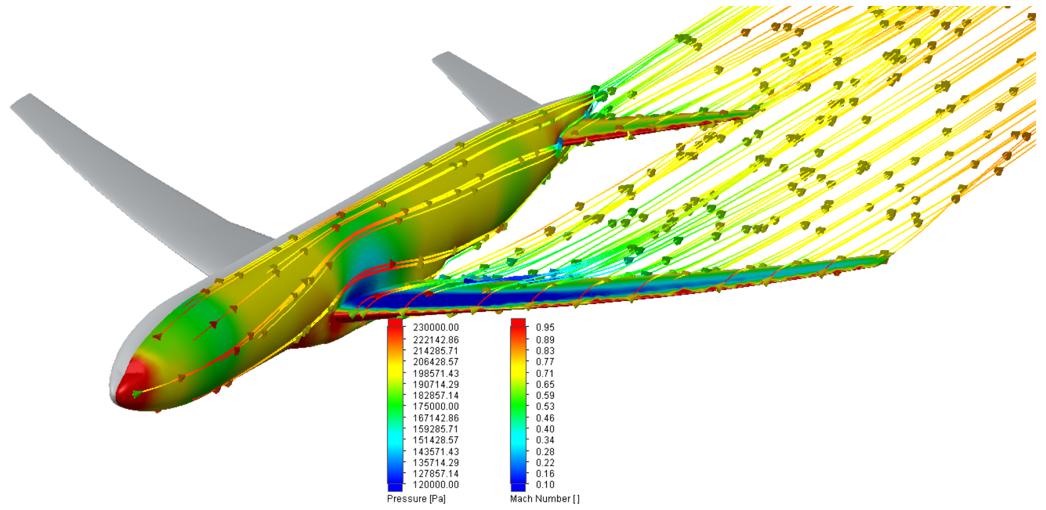


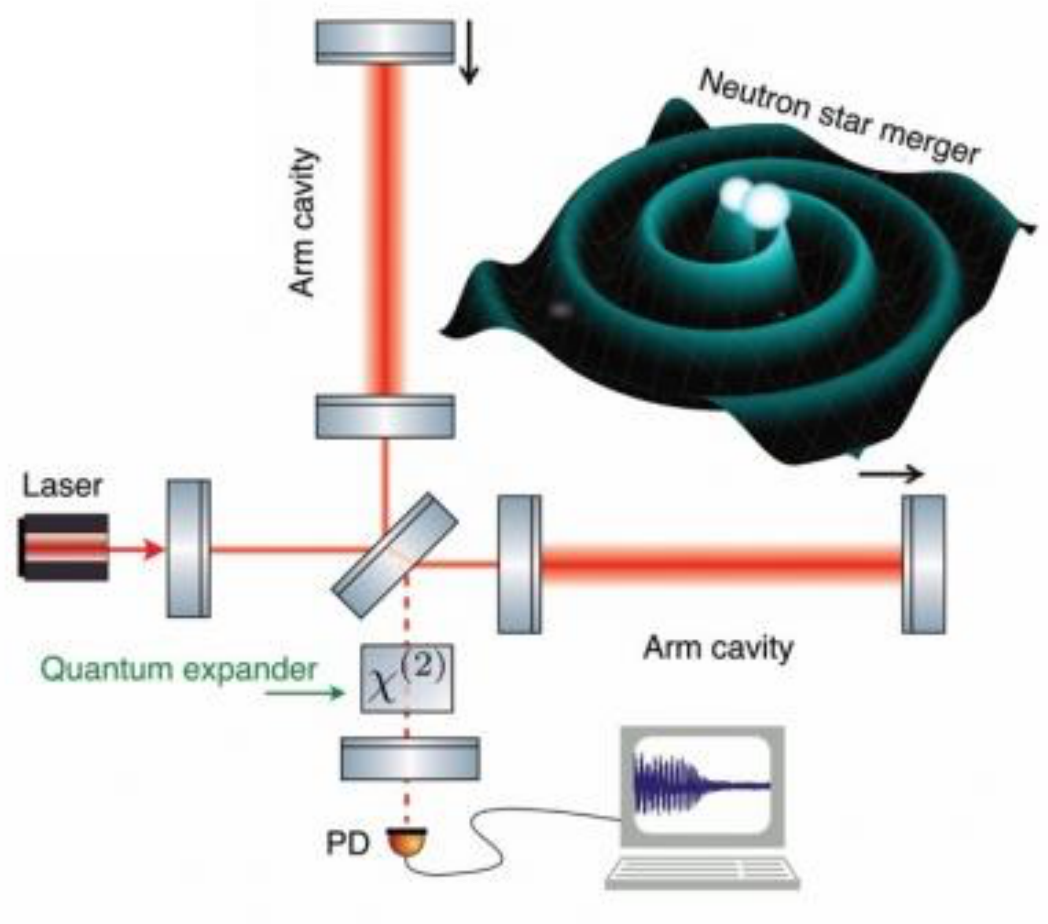
Evolution of the Universe

10^{-18} 10^{-15} 10^{-12} 10^{-9} 10^{-6} 10^{-3} 10^{0} 10^{3} 10^{6} 10^{9} 10^{12} 10^{15} 10^{18} 10^{21} 10^{24} 10^{27}

Length scale [m]

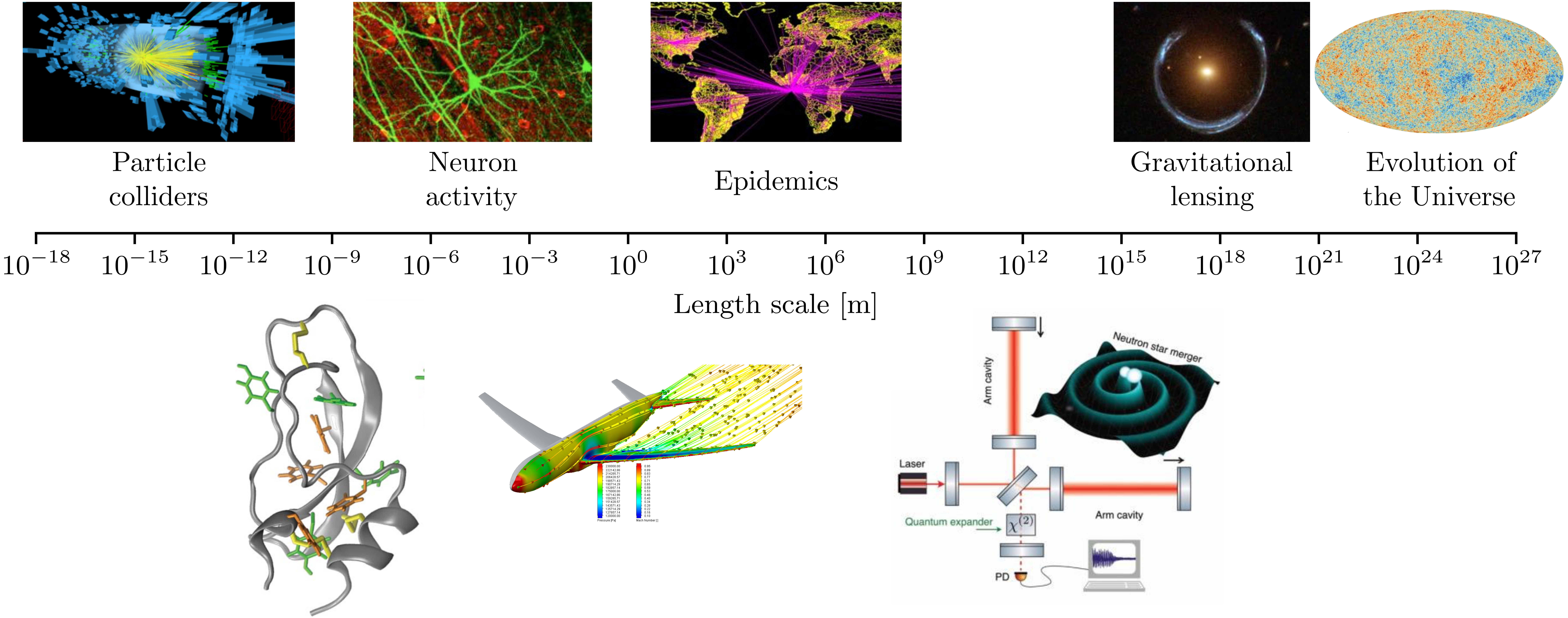






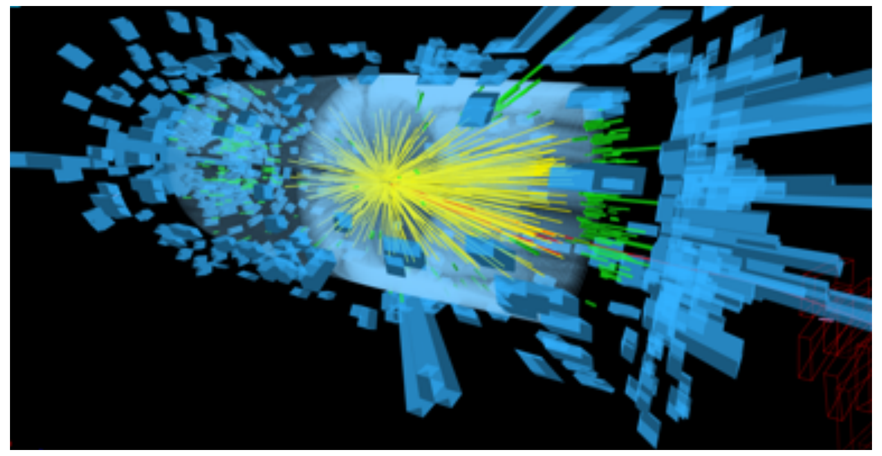
Simulators are causal, generative models of the data generating process

Science is replete with high-fidelity simulators

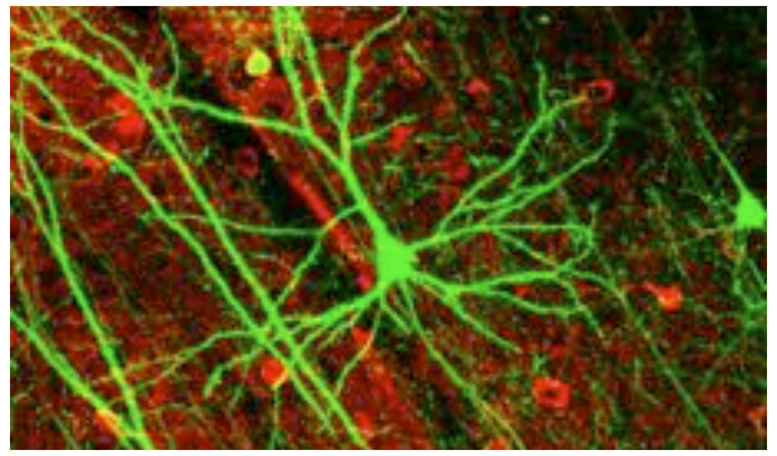


The expressiveness of programming languages facilitates the development of complex, high-fidelity simulations, and the power of modern computing provides the ability to generate synthetic data from them.

Science is replete with high-fidelity simulators



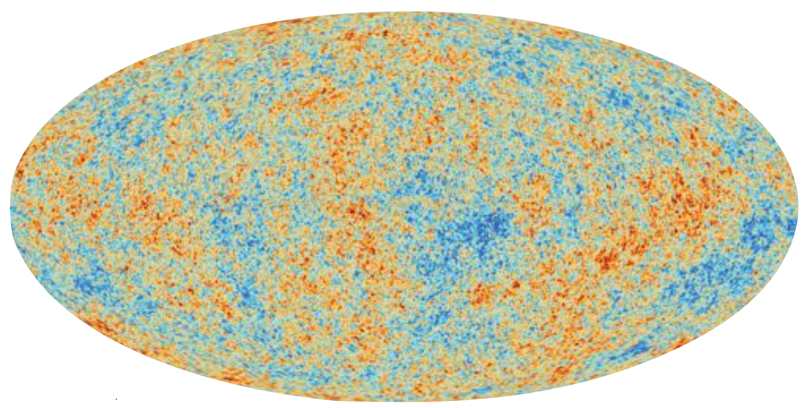
Particle colliders



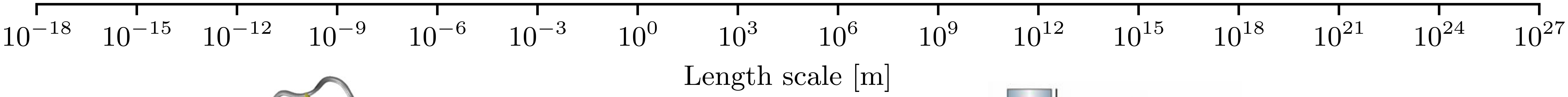
Neuron activity

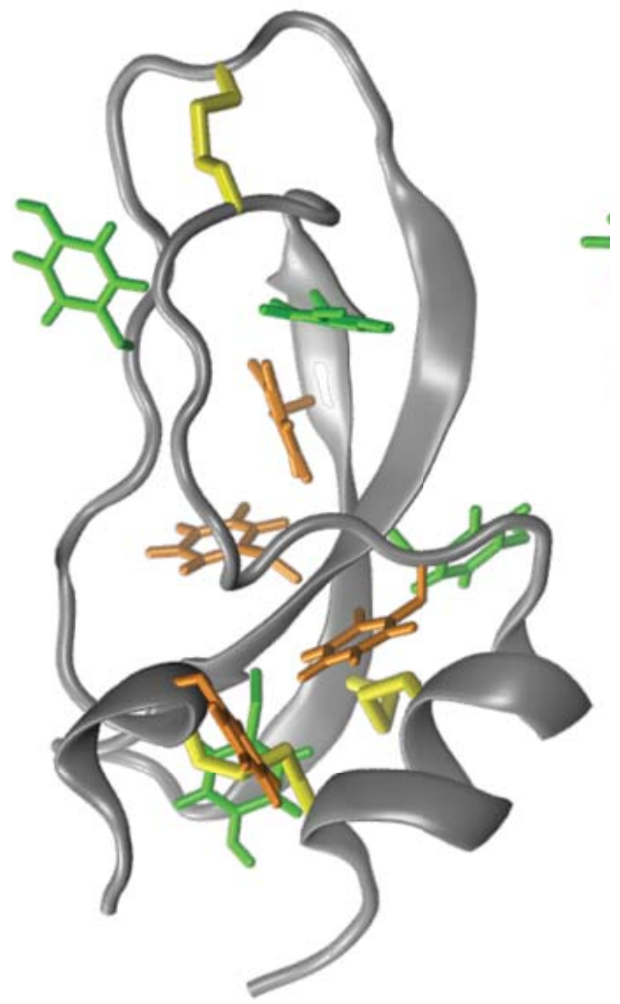
Epidemics

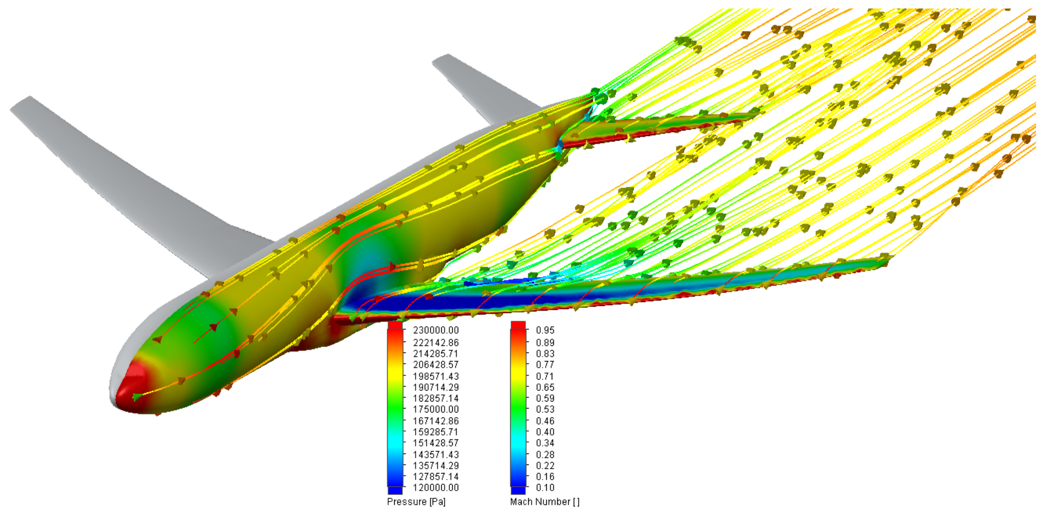
Gravitational lensing

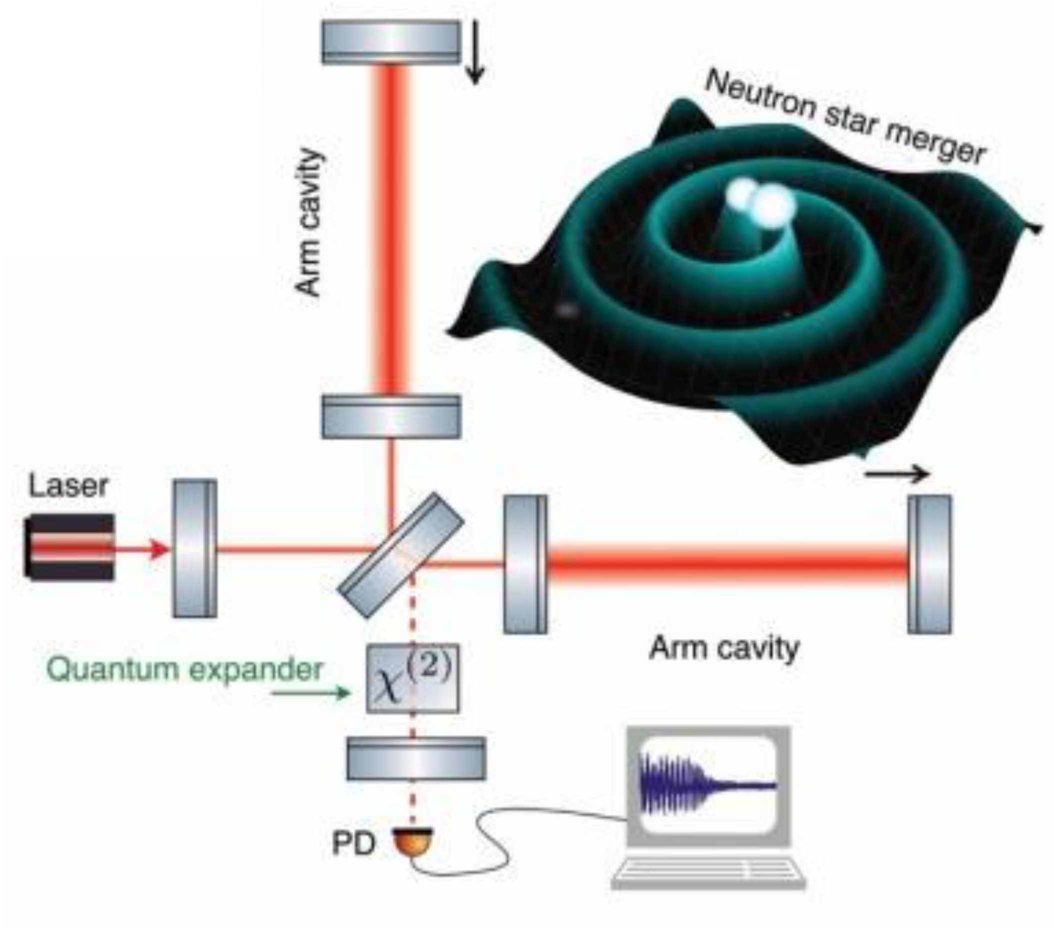


Evolution of the Universe



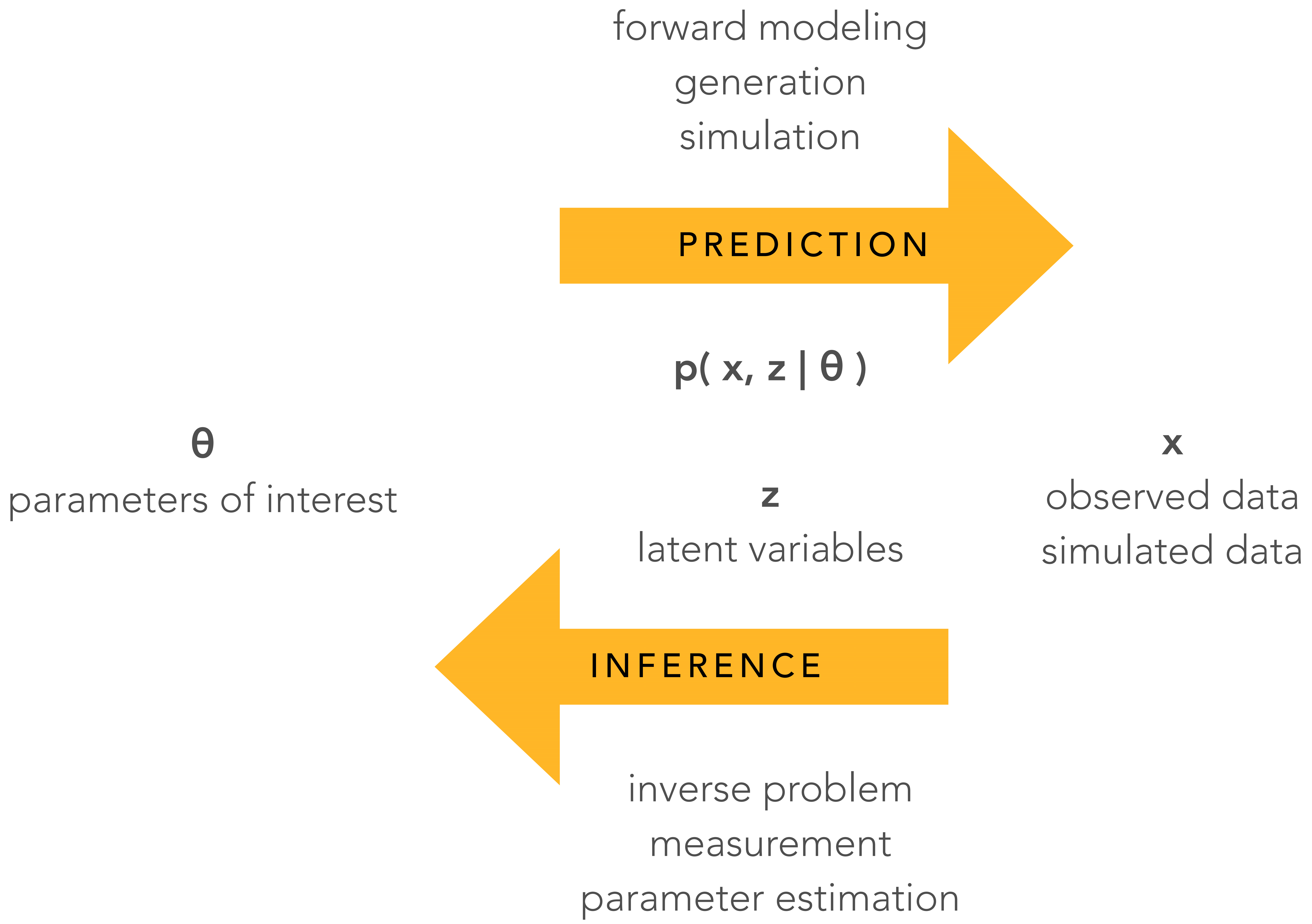






Unfortunately, these simulators are poorly suited for statistical inference.

Statistical Framing



Model misspecification

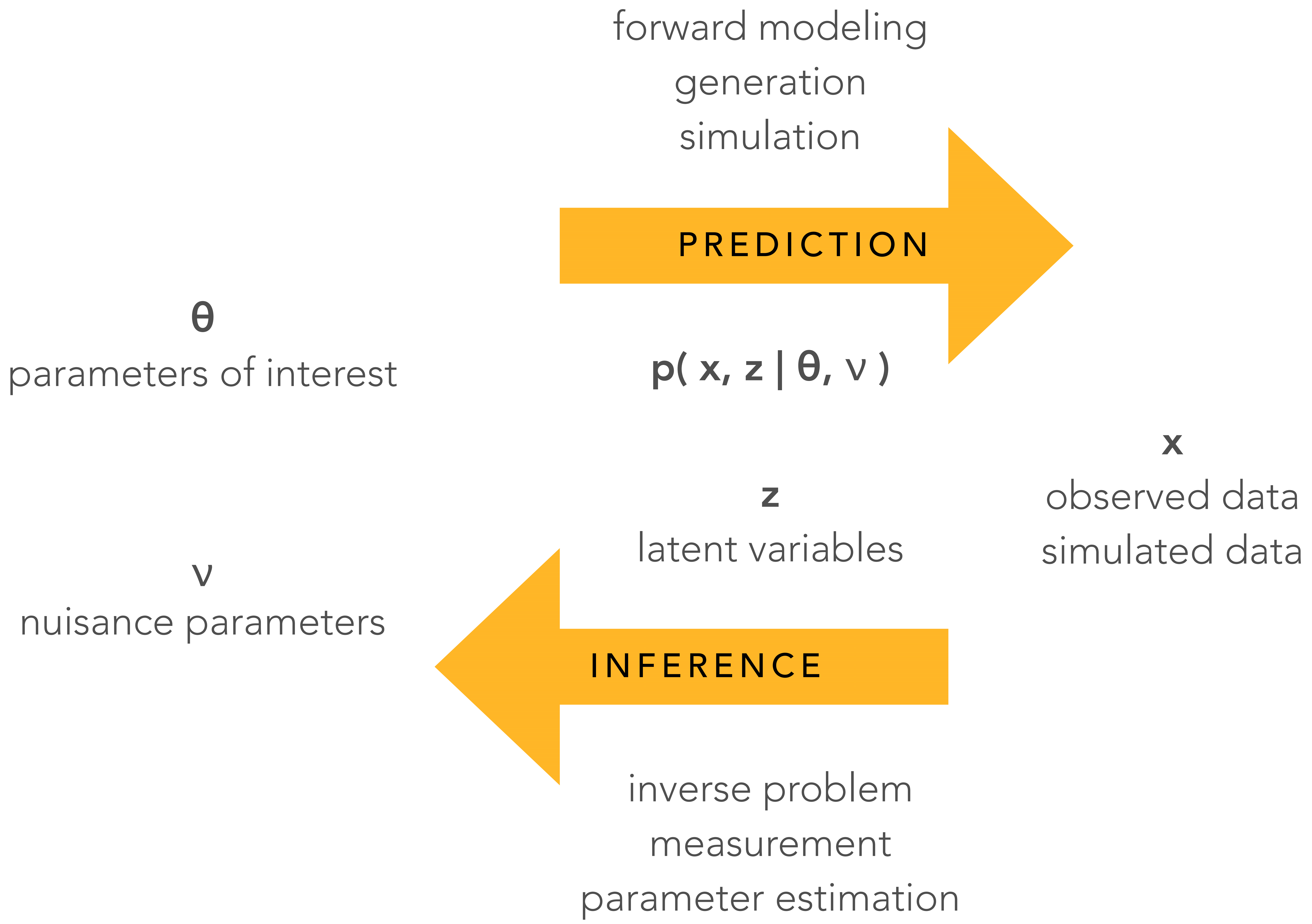
Inference is always done within the context of a model

- If the model is mis-specified it will affect inference
- Here the model **is** the simulator
  - the simulator may not be perfect, but
  - simulators usually include more effects than traditional prescribed models

To account for mis-modeling, simulators are often expanded to model residuals

- The simulator now also depends on **nuisance parameters** ν

Statistical Framing

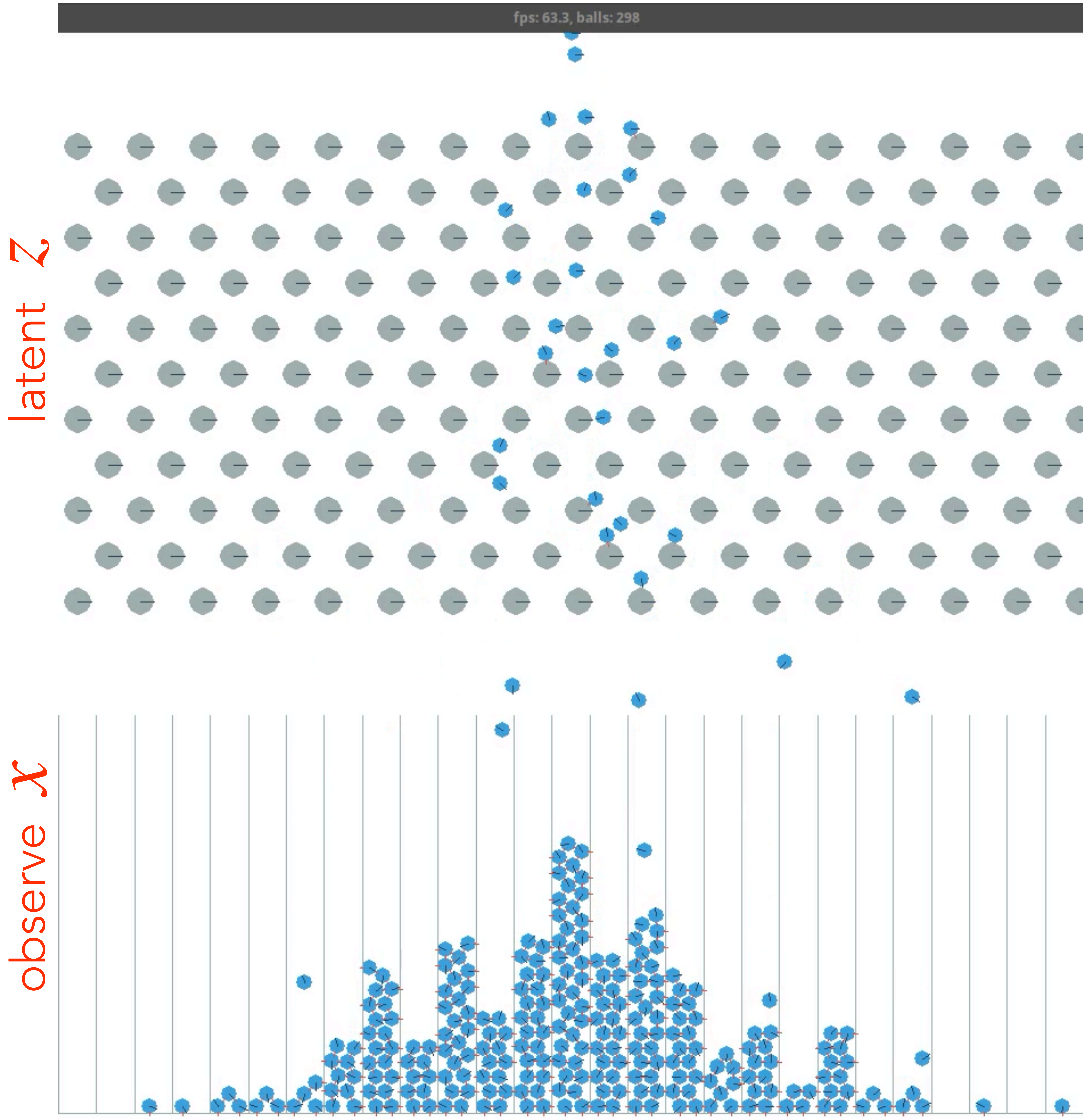


Properties of simulators

ANIMATION BY ATILIM GÜNEŞ BAYDIN

Two broad classes:

- Deterministic evolution of initial state
  - (eg. differential equations, fluid dynamics, N-body simulations, etc.)
- Stochastic evolution
  - (eg. Markov processes, molecular dynamics, Gibbs / Boltzmann distribution in statistical mechanics, stochastic differential equations, etc.)



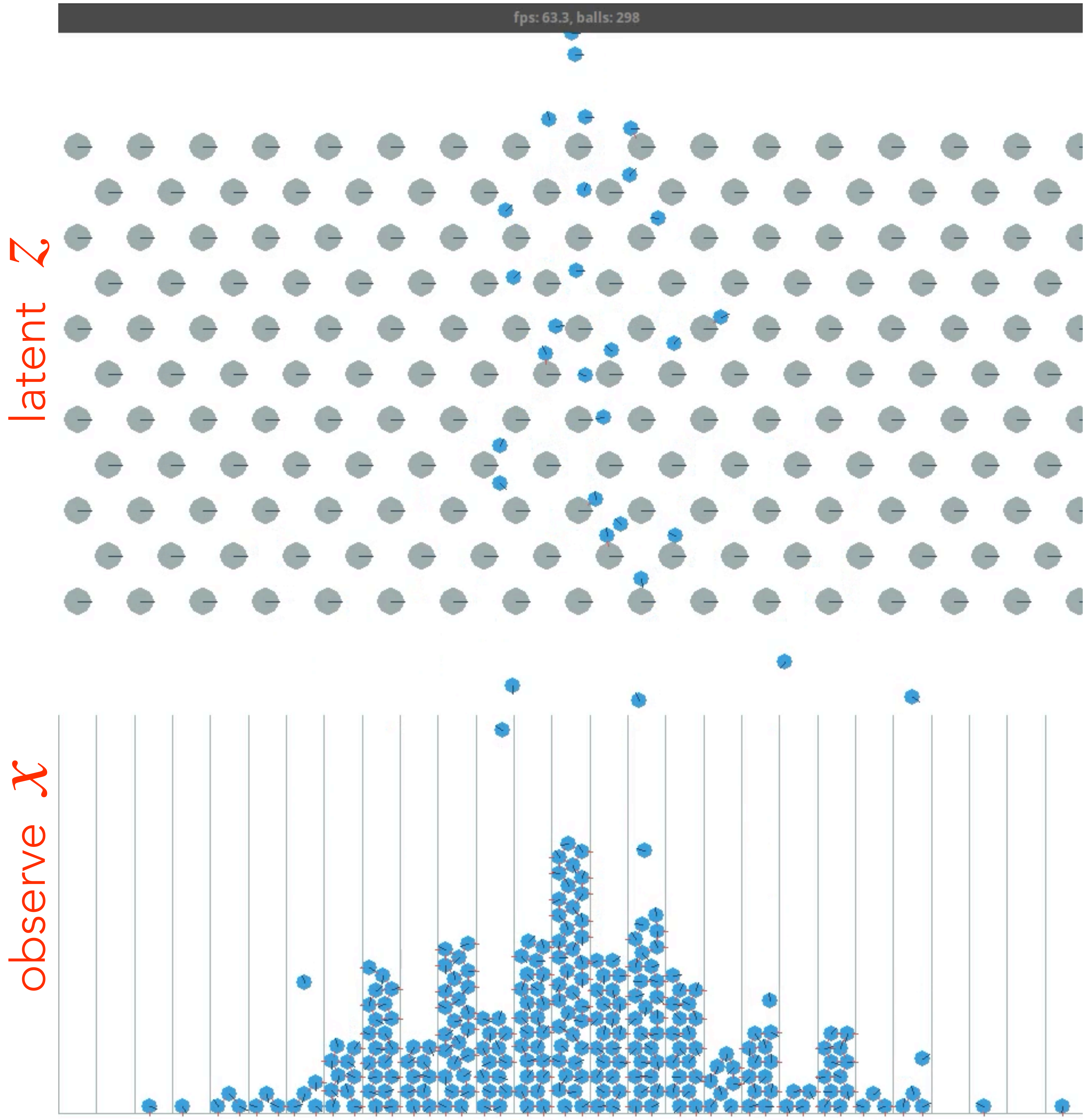
Integral over latent variables is typically **intractable** $p(x|\theta) = \int p(x, z \mid \theta)\mathrm{d}z$

Properties of simulators

Two broad classes:

- Deterministic evolution of initial state
  - (eg. differential equations, fluid dynamics, N-body simulations, etc.)
- Stochastic evolution
  - (eg. Markov processes, molecular dynamics, Gibbs / Boltzmann distribution in statistical mechanics, stochastic differential equations, etc.)

ANIMATION BY ATILIM GÜNEŞ BAYDIN



Integral over latent variables is typically **intractable** $p(x|\theta) = \int p(x, z \mid \theta) \mathrm{d}z$

A rose by any other name

This motivates a class of inference methods for a stochastic simulator where

- evaluating the **likelihood is intractable**, but
- it is **possible to sample** synthetic data $x \sim p(x \mid \theta)$

This setting is often referred to as **likelihood-free inference**, but I prefer the term **simulation-based inference** because usually one approximates the likelihood (or likelihood ratio) and then use established inference techniques

- applies to both Bayesian or Frequentist inference

Simulating particle physics processes

$$\mathcal{L}_{SM} = \underbrace{\frac{1}{4}\mathbf{W}_{\mu\nu}\cdot\mathbf{W}^{\mu\nu} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{4}G^{a}_{\mu\nu}G^{\mu\nu}_{a}}_{\text{kinetic energies and self-interactions of the gauge bosons}}$$

$$+ \underbrace{\bar{L}\gamma^{\mu}(i\partial_{\mu} - \frac{1}{2}g\tau\cdot\mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})L + \bar{R}\gamma^{\mu}(i\partial_{\mu} - \frac{1}{2}g'YB_{\mu})R}_{\text{kinetic energies and electroweak interactions of fermions}}$$

$$+ \underbrace{\frac{1}{2}\left|(i\partial_{\mu} - \frac{1}{2}g\tau\cdot\mathbf{W}_{\mu} - \frac{1}{2}g'YB_{\mu})\,\phi\right|^{2} - V(\phi)}_{W^{\pm},Z,\gamma,\text{and Higgs masses and couplings}}$$

$$+ \underbrace{g''(\bar{q}\gamma^{\mu}T_{a}q)\,G^{a}_{\mu}}_{\text{interactions between quarks and gluons}} + \underbrace{(G_{1}\bar{L}\phi R + G_{2}\bar{L}\phi_{c}R + h.c.)}_{\text{fermion masses and couplings to Higgs}}$$

Simulating particle physics processes

Simulating particle physics processes

Theory parameters

θ

Evolution

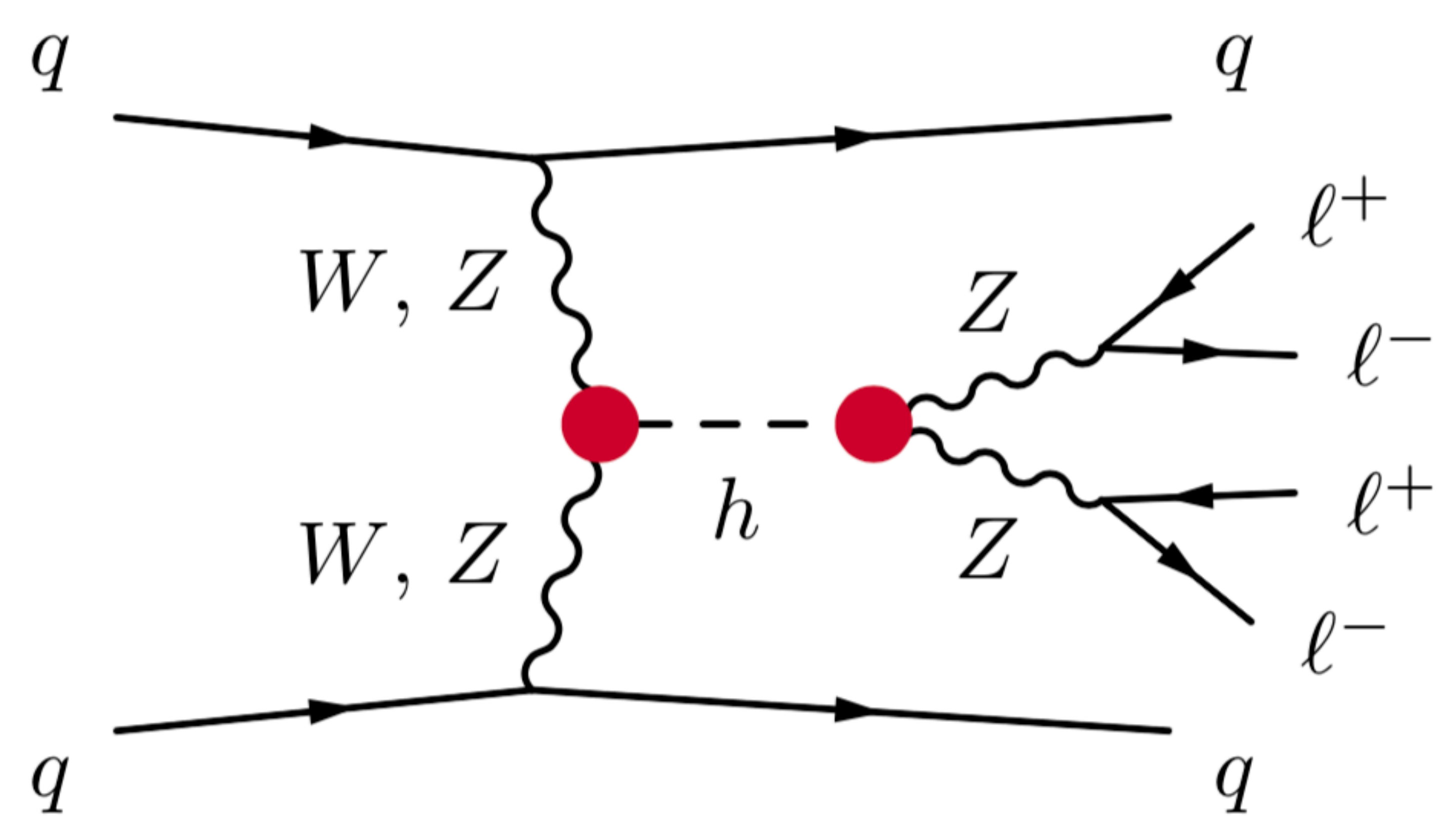
Simulating particle physics processes

Latent variables

Parton-level momenta

Theory parameters

$z_p \longleftarrow \theta$

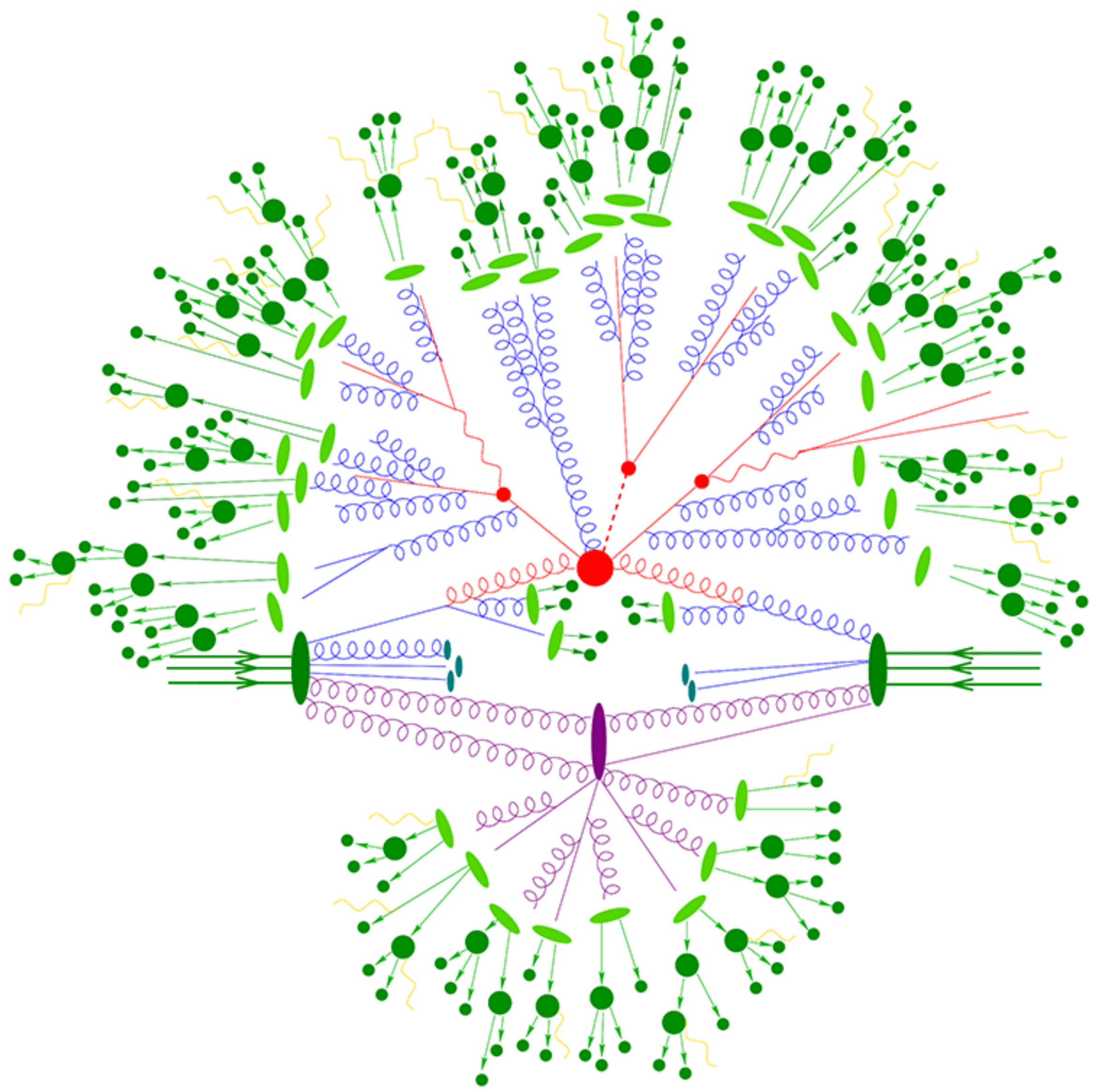


Evolution

Simulating particle physics processes

Latent variables

Shower splittings		Parton-level momenta		Theory parameters
z_s	←	z_p	←	θ



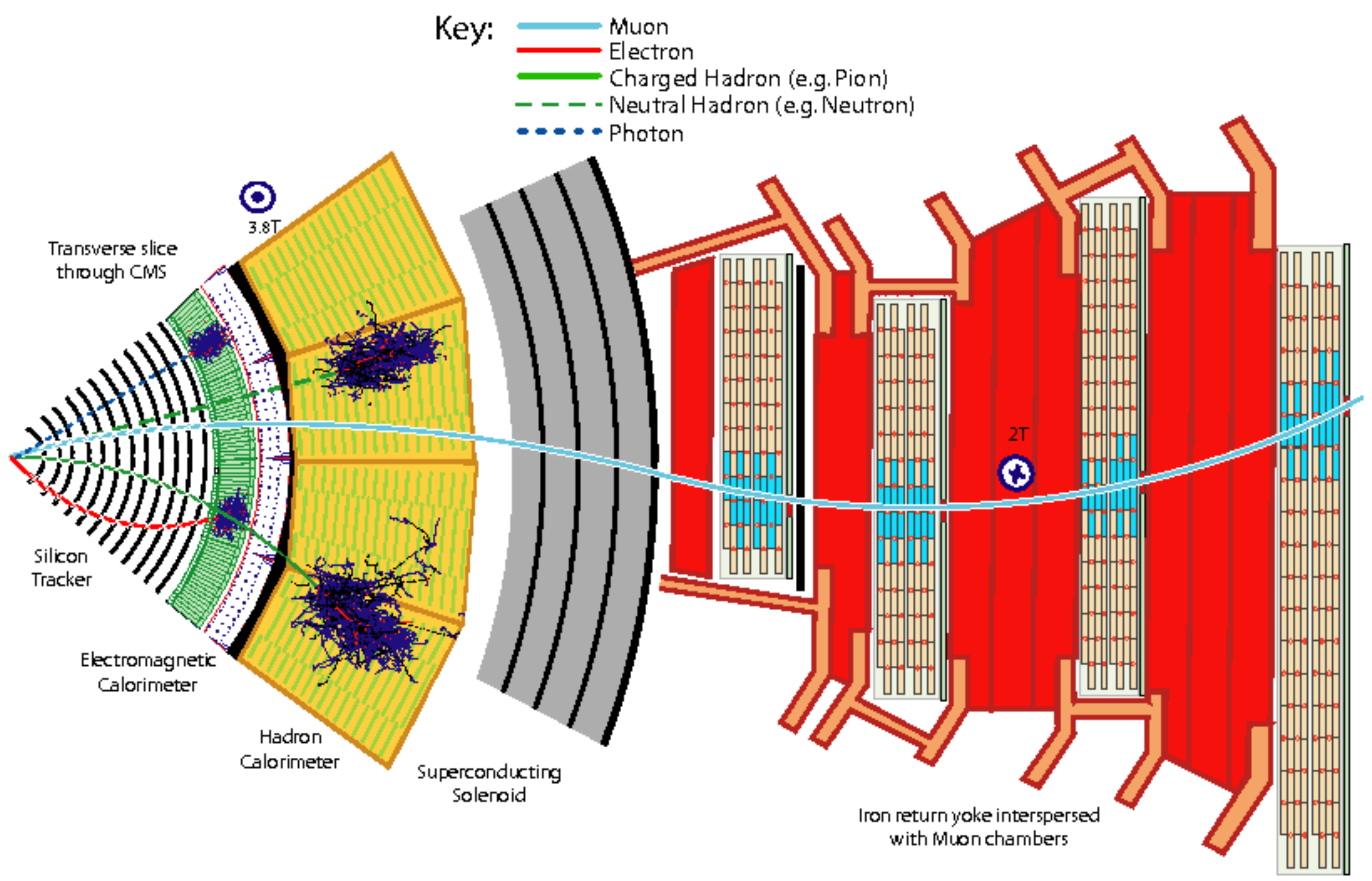
[F. Krauss]

← Evolution

Simulating particle physics processes

Latent variables

Detector interactions		Shower splittings		Parton-level momenta		Theory parameters
z_d	$\leftarrow$	z_s	$\leftarrow$	z_p	$\leftarrow$	θ



[CMS]

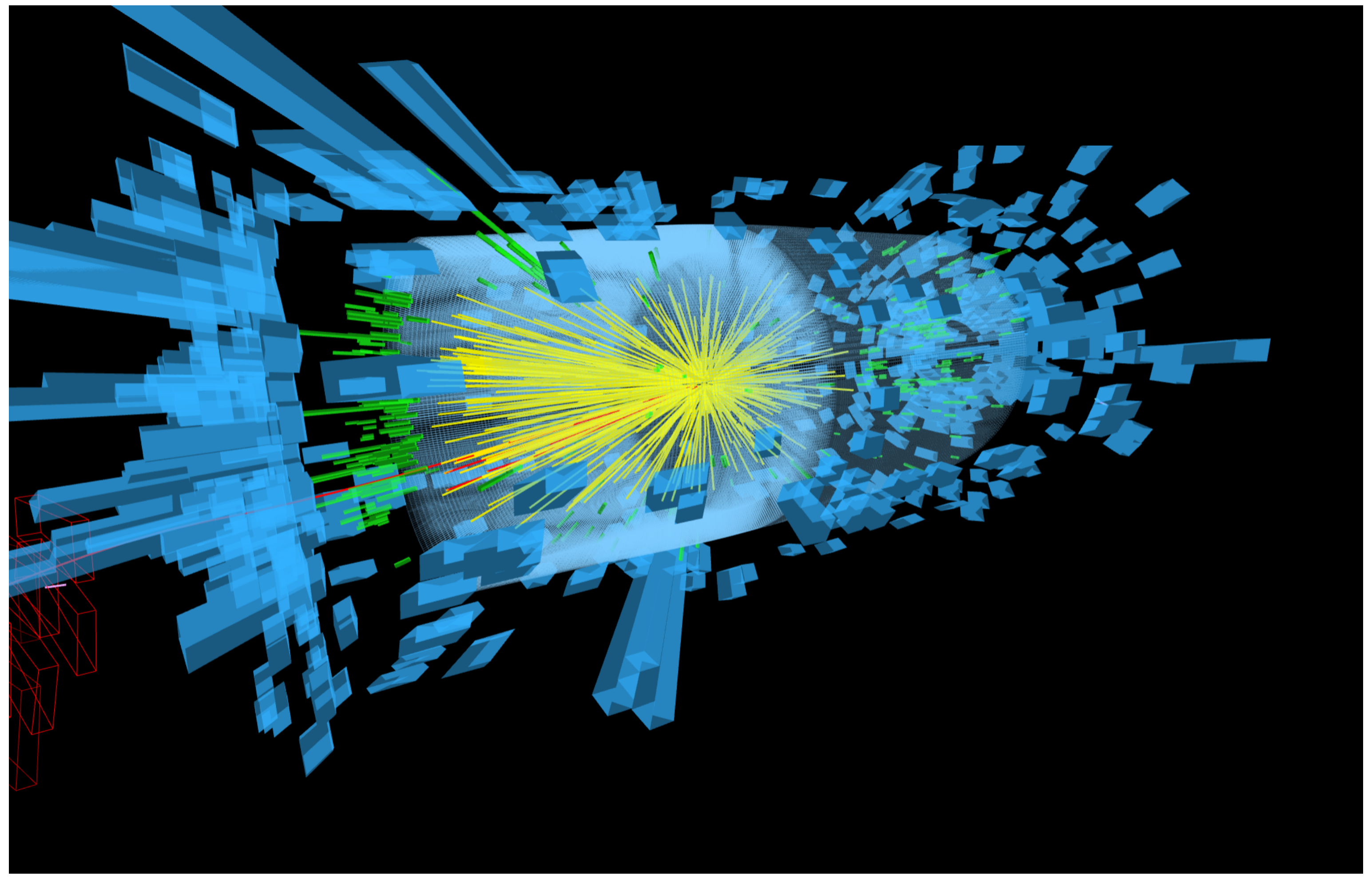
$\longleftarrow$

Evolution

Simulating particle physics processes

Latent variables

Observables	Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
x ←	z_d ←	z_s ←	z_p ←	θ



← Evolution

Simulating particle physics processes

Latent variables

Observables	Detector interactions	Shower splittings	Parton-level momenta	Theory parameters
x ←	z_d ←	z_s ←	z_p ←	θ

Sample from $p(x|z_d)$ $p(z_d|z_s)$ $p(z_s|z_p)$ $p(z_p|\theta)$

GEANT4 A SIMULATION TOOLKIT

MADGRAPH5_aMC@NLO

Prediction (simulation)

Simulating particle physics processes

Latent variables

Observables		Detector interactions		Shower splittings		Parton-level momenta		Theory parameters
x	$\longleftarrow$	z_d	$\longleftarrow$	z_s	$\longleftarrow$	z_p	$\longleftarrow$	θ

$$p(x|\theta) = \int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p \quad p(x|z_d) \quad p(z_d|z_s) \quad p(z_s|z_p) \quad p(z_p|\theta)$$

$\longrightarrow$ Inference

Simulating particle physics processes

Latent variables

Observables		Detector interactions		Shower splittings		Parton-level momenta		Theory parameters
x	$\leftarrow$	z_d	$\leftarrow$	z_s	$\leftarrow$	z_p	$\leftarrow$	θ

$$p(x|\theta) = \boxed{\int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p} \; p(x|z_d) \quad p(z_d|z_s) \quad p(z_s|z_p) \quad p(z_p|\theta)$$

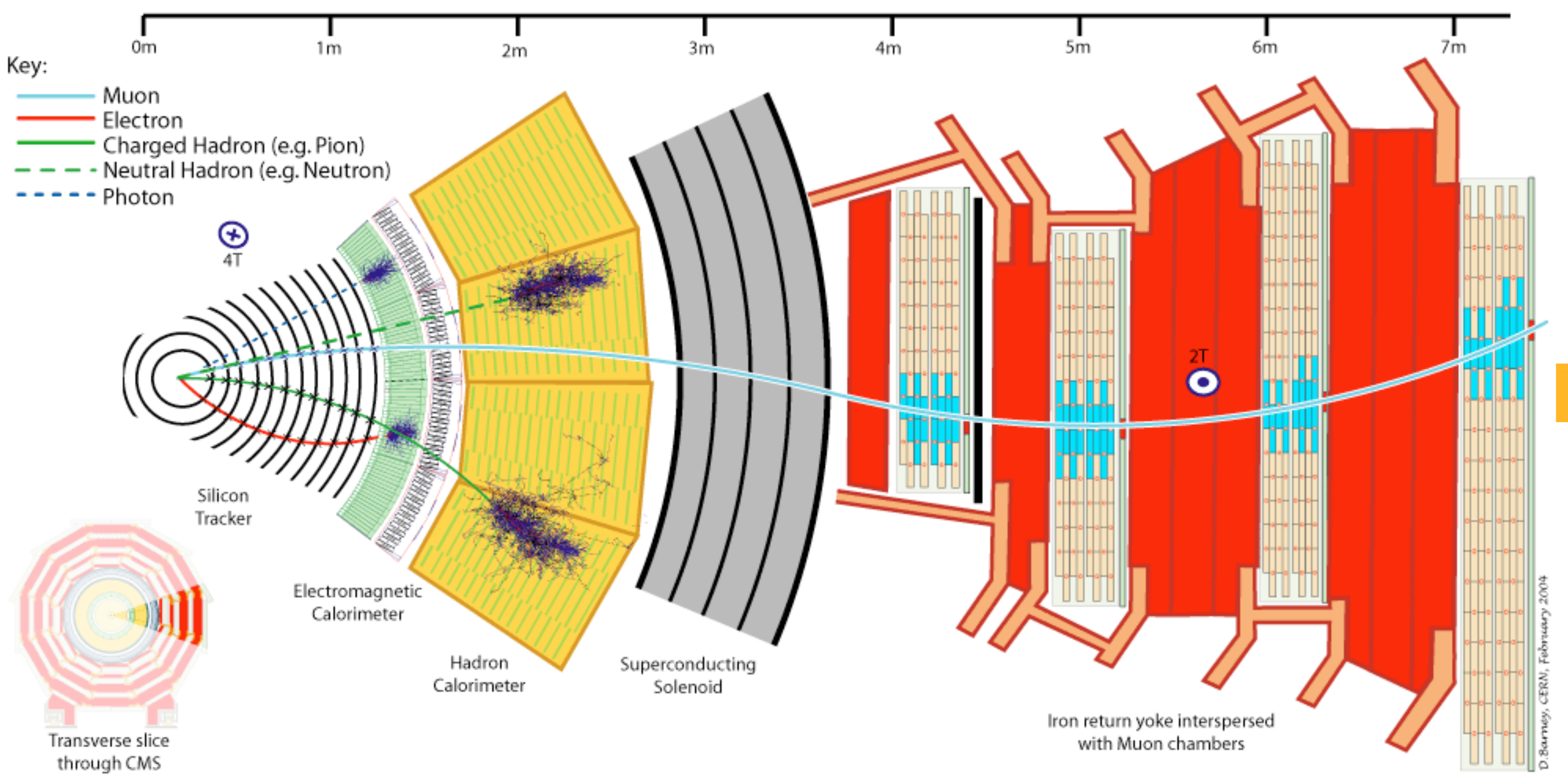
It's infeasible to calculate the integral over this enormous space!

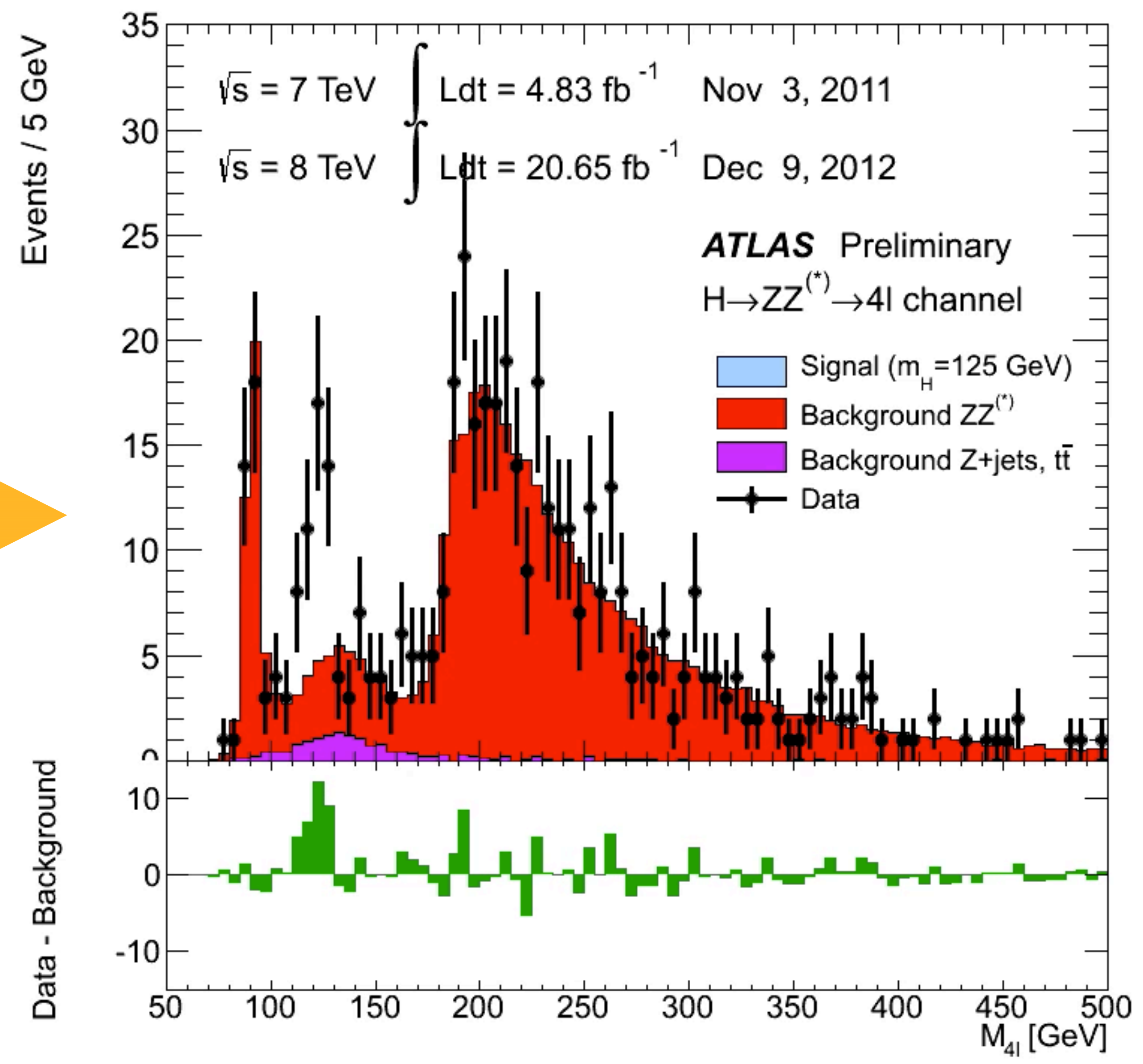
$\longrightarrow$ Inference

10^8 sensors → summary statistic

Most measurements and searches for new particles at the LHC are based on the distribution of a single **summary statistic**

- choosing a good summary statistic $s(x)$ (feature engineering) is a task for a skilled physicist and tailored to the goal of measurement or new particle search
- likelihood $p(s\,|\,\theta)$ **approximated** using histograms or kernel density estimation [Similar to Diggle & Gratton (1984)]

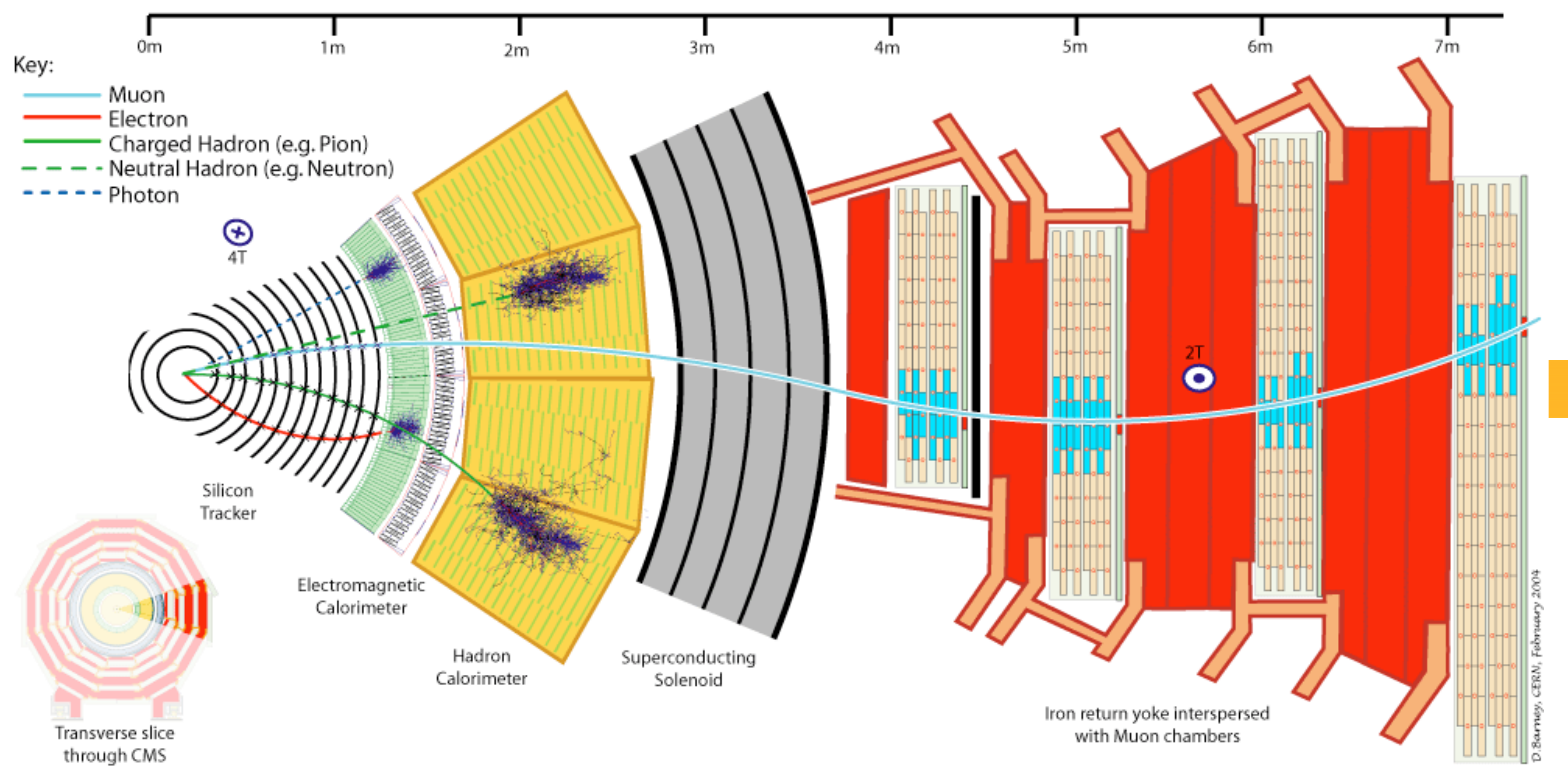


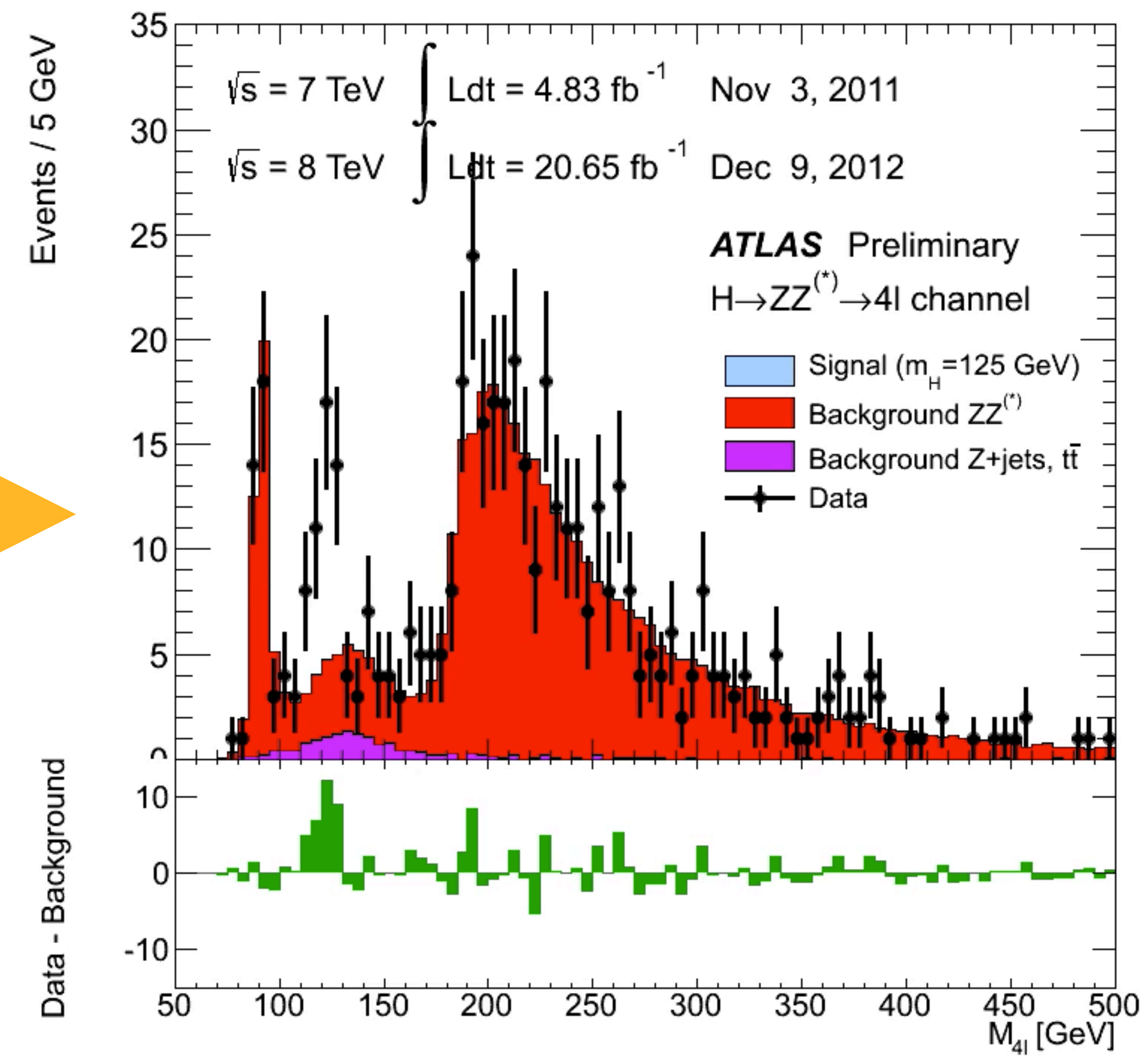


10^8 sensors → summary statistic

Most measurements and searches for new particles at the LHC are based on the distribution of a single **summary statistic**

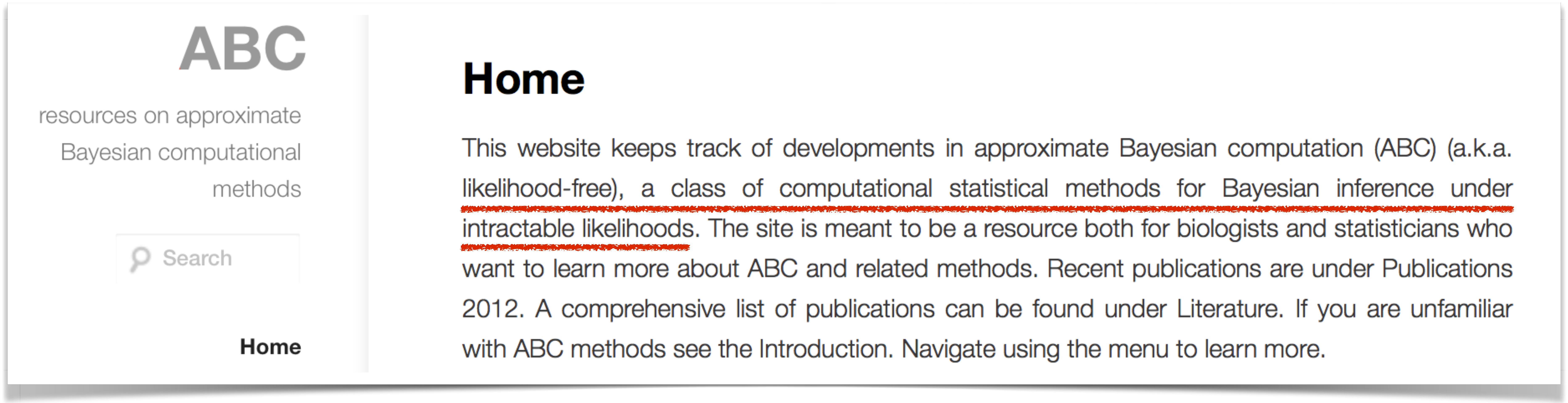
- choosing a good summary statistic $s(x)$ (feature engineering) is a task for a skilled physicist and tailored to the goal of measurement or new particle search
- likelihood $p(s \mid \theta)$ **approximated** using histograms or kernel density estimation [Similar to Diggle & Gratton (1984)]

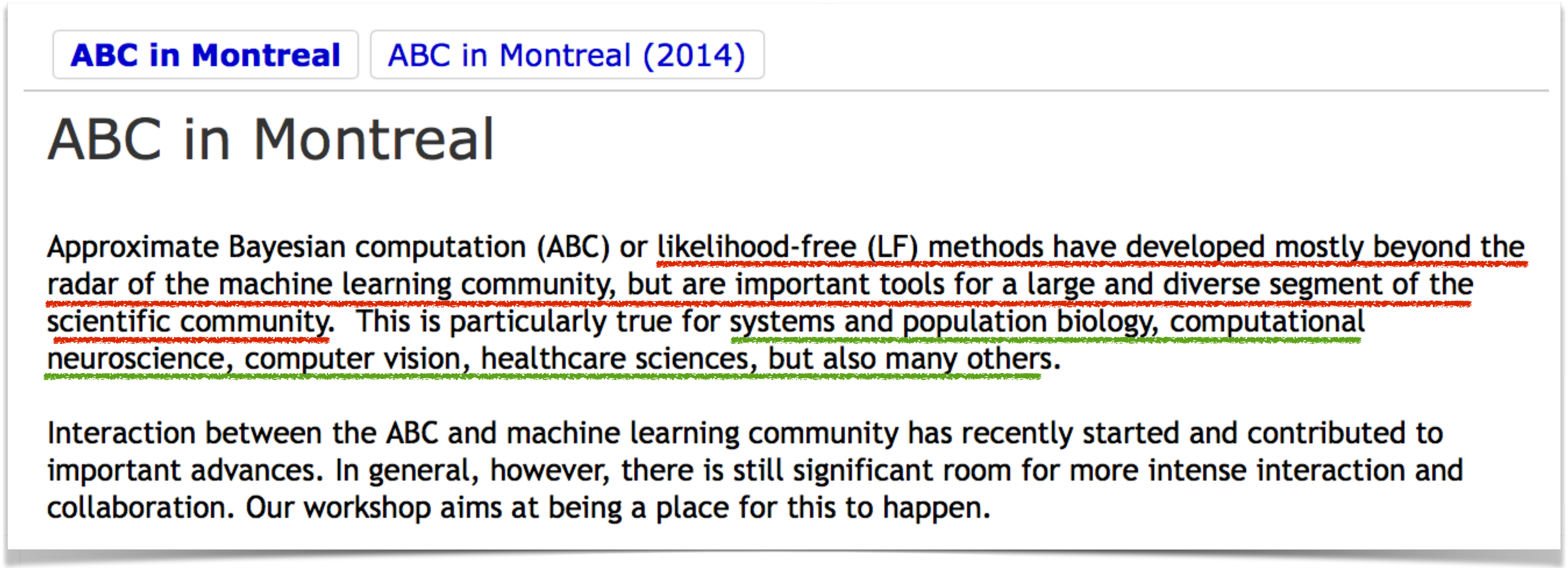




This doesn’t scale if summary is high dimensional!

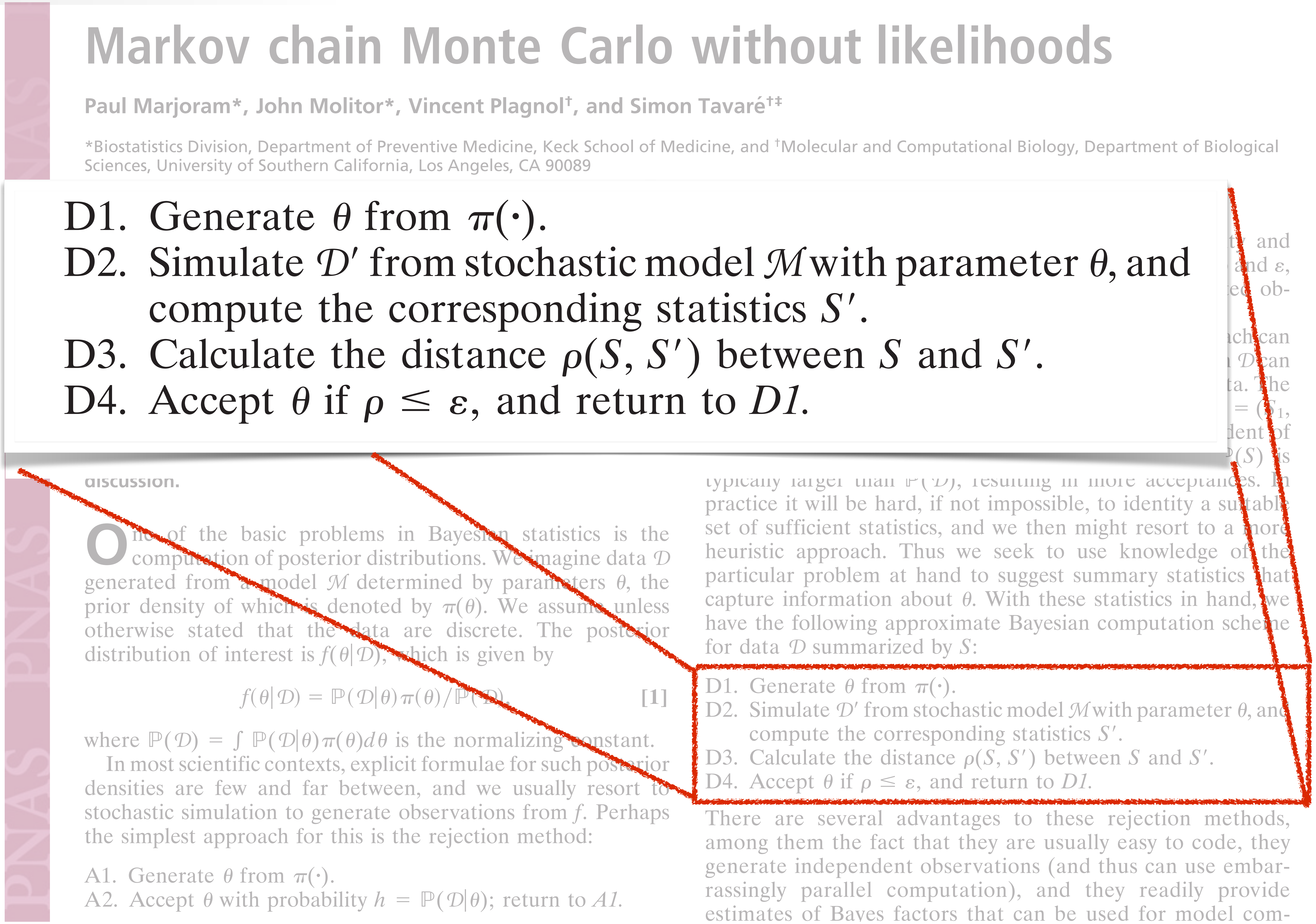
A common theme, a common language





ABC

D1. Generate θ from $\pi(\cdot)$.
D2. Simulate $\mathcal{D}'$ from stochastic model $\mathcal{M}$ with parameter θ, and compute the corresponding statistics S'.
D3. Calculate the distance $\rho(S, S')$ between S and S'.
D4. Accept θ if $\rho \leq \varepsilon$, and return to *D1*.



Markov chain Monte Carlo without likelihoods

Paul Marjoram*, John Molitor*, Vincent Plagnol†, and Simon Tavaré†‡

*Biostatistics Division, Department of Preventive Medicine, Keck School of Medicine, and †Molecular and Computational Biology, Department of Biological Sciences, University of Southern California, Los Angeles, CA 90089

discussion.

One of the basic problems in Bayesian statistics is the computation of posterior distributions. We imagine data $\mathcal{D}$ generated from a model $\mathcal{M}$ determined by parameters θ, the prior density of which is denoted by $\pi(\theta)$. We assume unless otherwise stated that the data are discrete. The posterior distribution of interest is $f(\theta|\mathcal{D})$, which is given by

$$f(\theta|\mathcal{D}) = \mathbb{P}(\mathcal{D}|\theta)\pi(\theta)/\mathbb{P}(\mathcal{D}). \quad [1]$$

where $\mathbb{P}(\mathcal{D}) = \int \mathbb{P}(\mathcal{D}|\theta)\pi(\theta)d\theta$ is the normalizing constant.

In most scientific contexts, explicit formulae for such posterior densities are few and far between, and we usually resort to stochastic simulation to generate observations from f. Perhaps the simplest approach for this is the rejection method:

A1. Generate θ from $\pi(\cdot)$.
A2. Accept θ with probability $h = \mathbb{P}(\mathcal{D}|\theta)$; return to *A1*.

typically larger than $\mathbb{P}(\mathcal{D})$, resulting in more acceptances. In practice it will be hard, if not impossible, to identity a suitable set of sufficient statistics, and we then might resort to a more heuristic approach. Thus we seek to use knowledge of the particular problem at hand to suggest summary statistics that capture information about θ. With these statistics in hand, we have the following approximate Bayesian computation scheme for data $\mathcal{D}$ summarized by S:

D1. Generate θ from $\pi(\cdot)$.
D2. Simulate $\mathcal{D}'$ from stochastic model $\mathcal{M}$ with parameter θ, and compute the corresponding statistics S'.
D3. Calculate the distance $\rho(S, S')$ between S and S'.
D4. Accept θ if $\rho \leq \varepsilon$, and return to *D1*.

There are several advantages to these rejection methods, among them the fact that they are usually easy to code, they generate independent observations (and thus can use embarrassingly parallel computation), and they readily provide estimates of Bayes factors that can be used for model com-

Markov chain Monte Carlo without likelihoods

Paul Marjoram*, John Molitor*, Vincent Plagnol†, and Simon Tavaré†‡

*Biostatistics Division, Department of Preventive Medicine, Keck School of Medicine, and †Molecular and Computational Biology, Department of Biological Sciences, University of Southern California, Los Angeles, CA 90089

Communicated by Michael S. Waterman, University of Southern California, Los Angeles, CA, October 24, 2003 (received for review June 20, 2003)

Many stochastic simulation approaches for generating observations from a posterior distribution depend on knowing a likelihood function. However, for many complex probability models, such likelihoods are either impossible or computationally prohibitive to obtain. Here we present a Markov chain Monte Carlo method for generating observations from a posterior distribution without the use of likelihoods. It can also be used in frequentist applications, in particular for maximum-likelihood estimation. The approach is illustrated by an example of ancestral inference in population genetics. A number of open problems are highlighted in the discussion.

One of the basic problems in Bayesian statistics is the computation of posterior distributions. We imagine data $\mathcal{D}$ generated from a model $\mathcal{M}$ determined by parameters θ, the prior density of which is denoted by $\pi(\theta)$. We assume unless otherwise stated that the data are discrete. The posterior distribution of interest is $f(\theta|\mathcal{D})$, which is given by

A1. Generate θ from $\pi(\cdot)$.
A2. Accept θ with probability $h = \mathbb{P}(\mathcal{D}|\theta)$; return to *A1*.

of ε therefore reflects a tension between computability and accuracy. The method is still honest in that, for a given ρ and ε, we are generating independent and identically distributed observations from $f(\theta|\rho(\mathcal{D}, \mathcal{D}') \leq \varepsilon)$.

When $\mathcal{D}$ is high-dimensional or continuous, this approach can be impractical as well, and then the comparison of $\mathcal{D}'$ with $\mathcal{D}$ can be made by using lower-dimensional summaries of the data. The motivation for this approach is that if the set of statistics $S = (S_1, \ldots, S_p)$ is sufficient for θ, in that $\mathbb{P}(\mathcal{D}|S, \theta)$ is independent of θ, then $f(\theta|\mathcal{D}) = f(\theta|S)$. The normalizing constant $\mathbb{P}(S)$ is typically larger than $\mathbb{P}(\mathcal{D})$, resulting in more acceptances. In practice it will be hard, if not impossible, to identity a suitable set of sufficient statistics, and we then might resort to a more heuristic approach. Thus we seek to use knowledge of the particular problem at hand to suggest summary statistics that capture information about θ. With these statistics in hand, we have the following approximate Bayesian computation scheme for data $\mathcal{D}$ summarized by S:

θ, and

...ods, ... they generate independent observations (and thus can use embarrassingly parallel computation), and they readily provide estimates of Bayes factors that can be used for model com-

practice it will be hard, if not impossible, to identity a suitable set of sufficient statistics, and we then might resort to a more heuristic approach.

Statistical Framing

forward modeling
generation
simulation

PREDICTION

$p(x, z \mid \theta)$

θ
parameters of interest

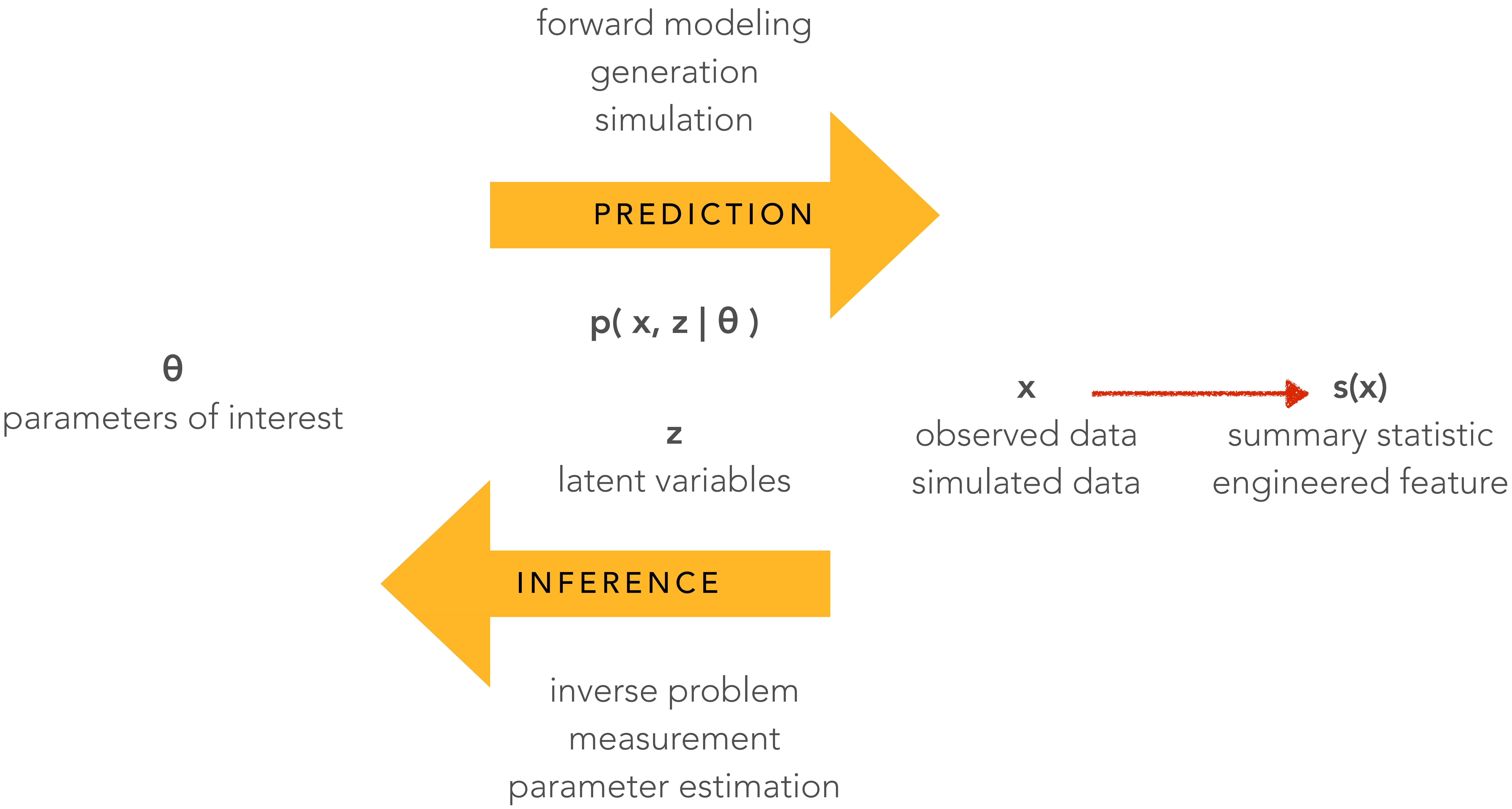
z
latent variables

x
observed data
simulated data

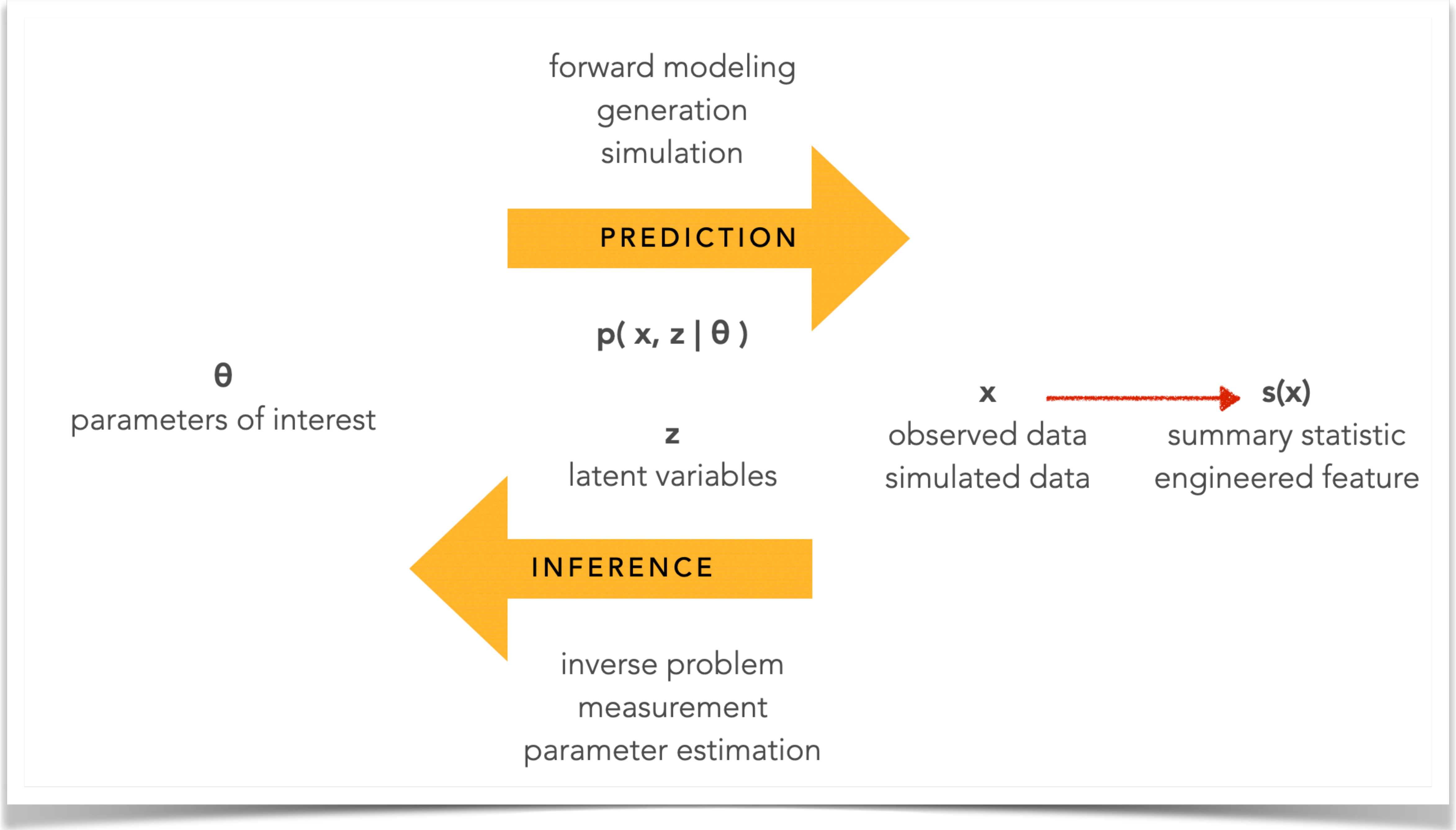
INFERENCE

inverse problem
measurement
parameter estimation

Statistical Framing



Forward modeling and inverse problems



$s \in \mathbb{R}^o$

summary statistic

$x \in X$

observed data

$z \in Z$

latent variables

$\theta \in R^p$

parameters of interest

1 10 100 1,000 10,000 100,000

Dimensionality

Published in Proceedings of the National Academy of Sciences

Gilles Louppe

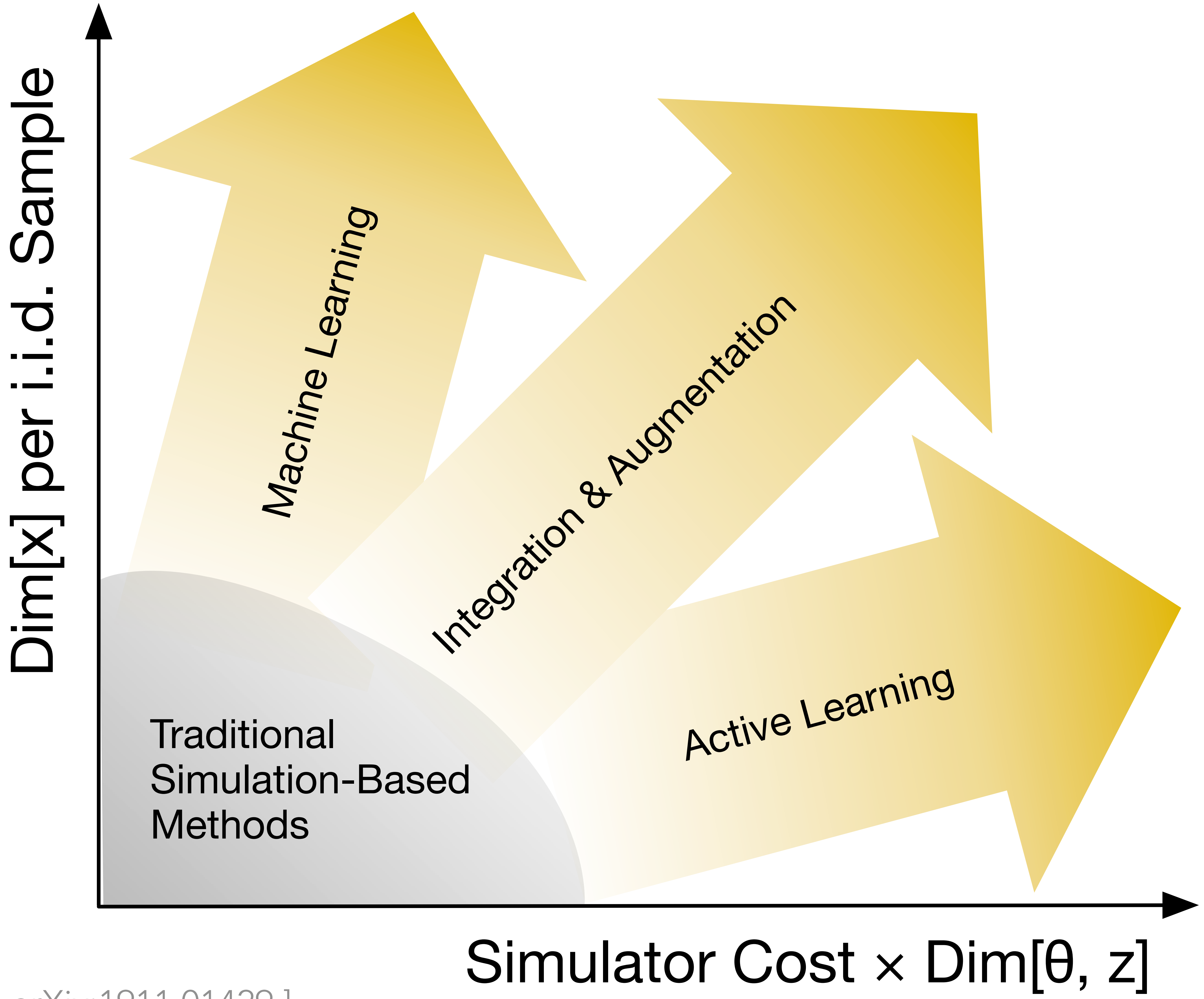
Johann Brehmer

The frontier of simulation-based inference

Kyle Cranmer[a,b,1], **Johann Brehmer**[a,b], **and Gilles Louppe**[c]

[a]Center for Cosmology and Particle Physics, New York University, USA; [b]Center for Data Science, New York University, USA; [c]Montefiore Institute, University of Liège, Belgium

April 3, 2020



[Cranmer, Brehmer, Louppe PNAS (2020), arXiv:1911.01429]

ICML 2017 Workshop on Implicit Models

Workshop Aims

Probabilistic models are an important tool in machine learning. They form the basis for models that generate realistic data, uncover hidden structure, and make predictions. Traditionally, probabilistic models in machine learning have focused on prescribed models. Prescribed models specify a joint density over observed and hidden variables that can be easily evaluated. The requirement of a tractable density simplifies their learning but limits their flexibility --- several real world phenomena are better described by simulators that do not admit a tractable density. Probabilistic models defined only via the simulations they produce are called implicit models.

Arguably starting with generative adversarial networks, research on implicit models in machine learning has exploded in recent years. This workshop's aim is to foster a discussion around the recent developments and future directions of implicit models.

Implicit models have many applications. They are used in ecology where models simulate animal populations over time; they are used in phylogeny, where simulations produce hypothetical ancestry trees; they are used in physics to generate particle simulations for high energy processes. Recently, implicit models have been used to improve the state-of-the-art in image and content generation. Part of the workshop's focus is to discuss the commonalities among applications of implicit models.

Of particular interest at this workshop is to unite fields that work on implicit models. For example:

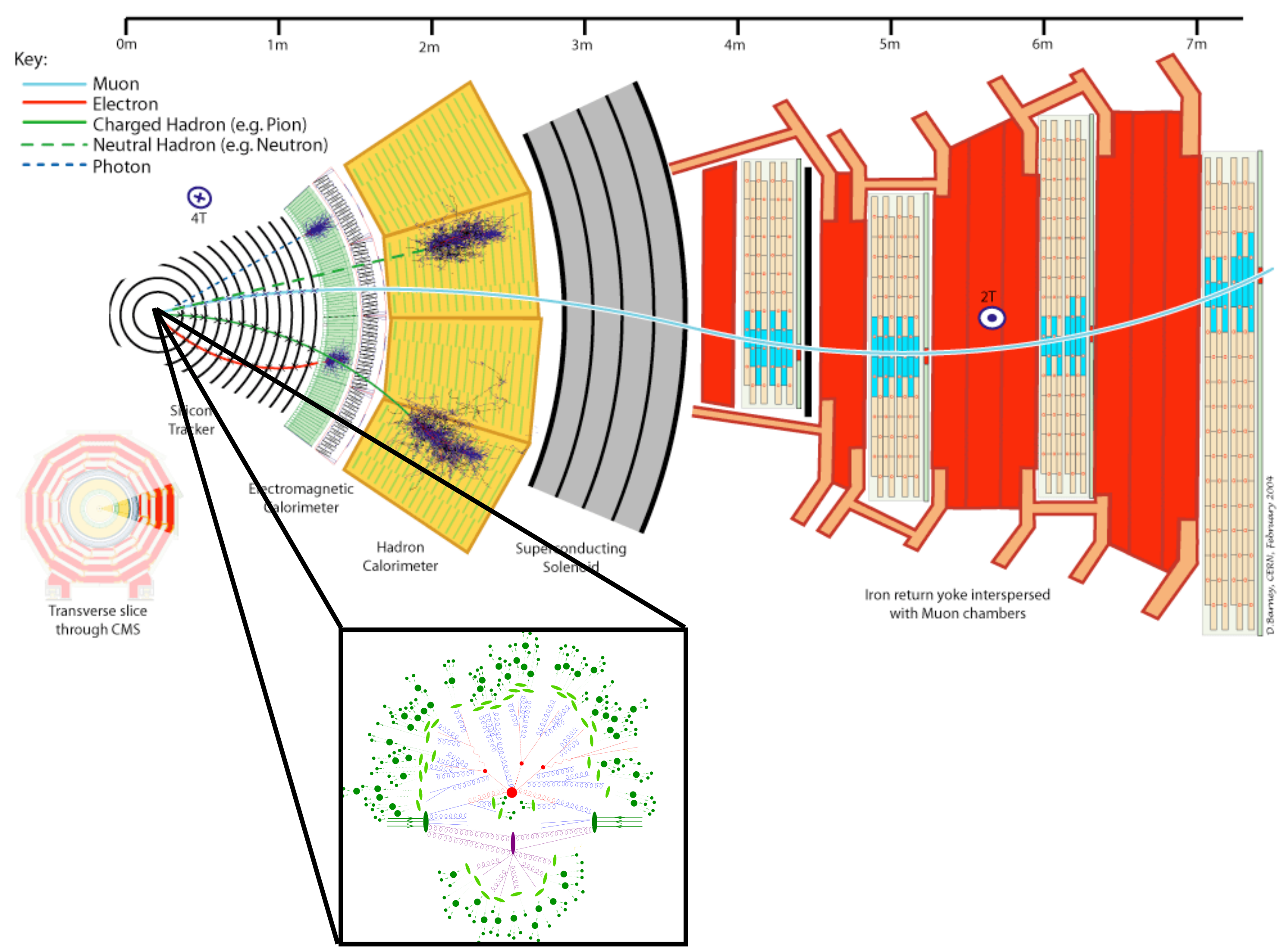
- **Generative adversarial networks** (a NIPS 2016 workshop) are implicit models with an adversarial training scheme.
- Recent advances in **variational inference** (a NIPS 2015 and 2016 workshop) have leveraged implicit models for more accurate approximations.
- **Approximate Bayesian computation** (a NIPS 2015 workshop) focuses on posterior inference for models with implicit likelihoods.
- Learning implicit models is deeply connected to **two sample testing, density ratio and density difference** estimation.

We hope to bring together these different views on implicit models, identifying their core challenges and combining their innovations.

Two approaches simulation-based inference

Use simulator

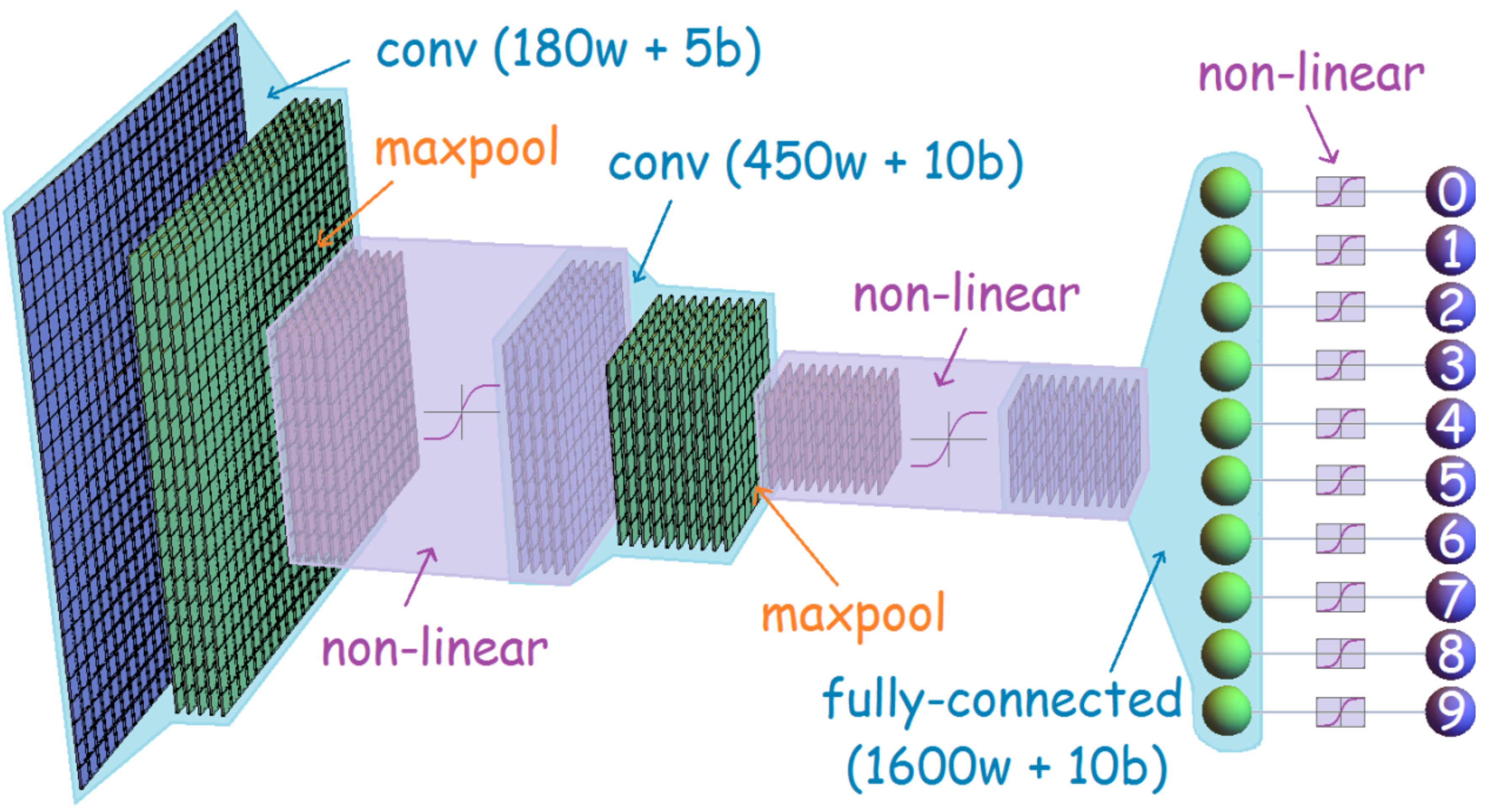
(much more efficiently)



- Approximate Bayesian Computation (ABC)
- Probabilistic Programming
- Adversarial Variational Optimization

Learn simulator

(with deep learning)



- Likelihood ratio trick (with classifiers)
- Conditional density estimate (with normalizing flows)
- Learned summary statistics

[image credit: A.P. Goucher]

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

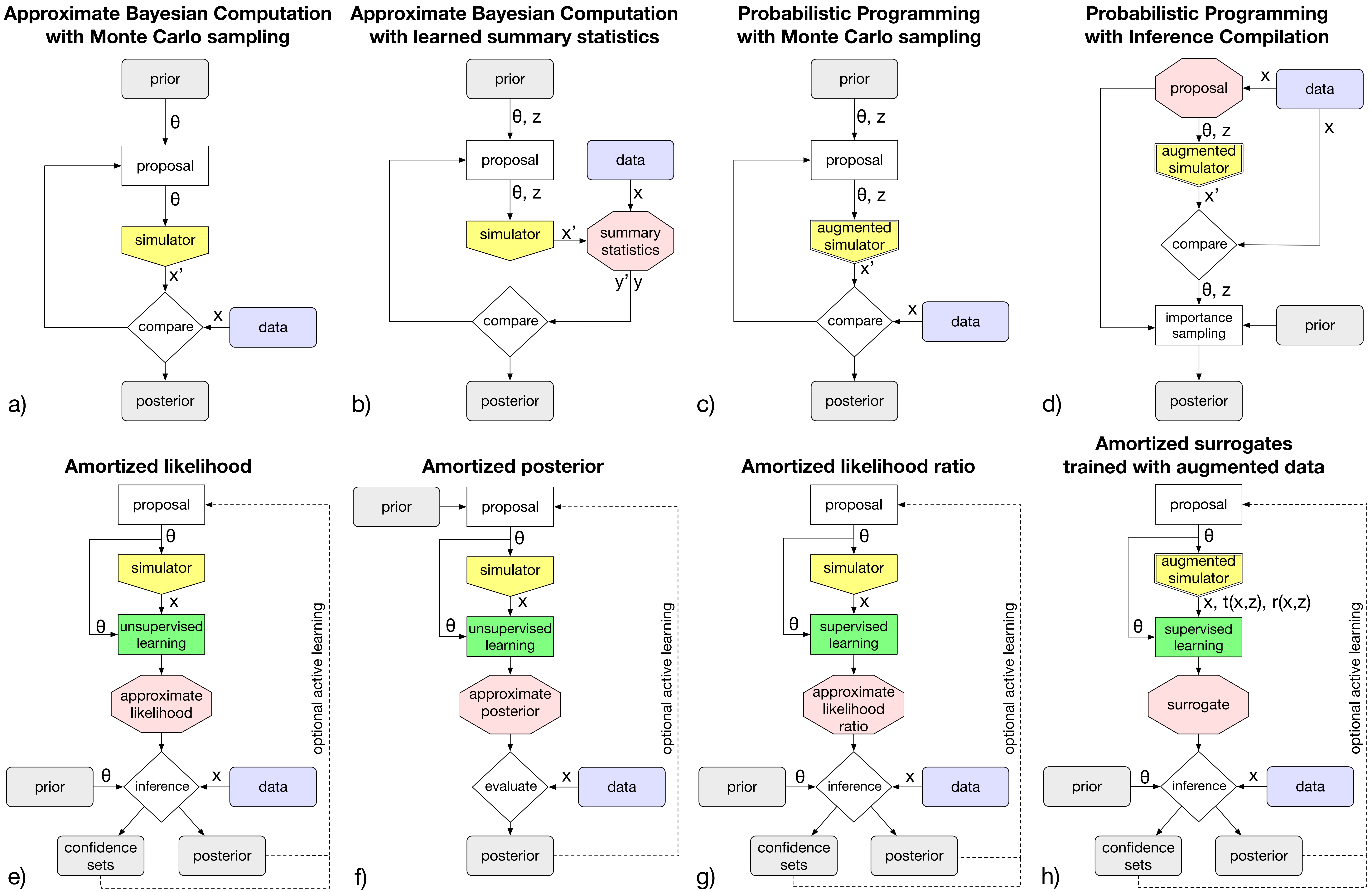


Fig. 3. Overview of different approaches to simulation-based inference.

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

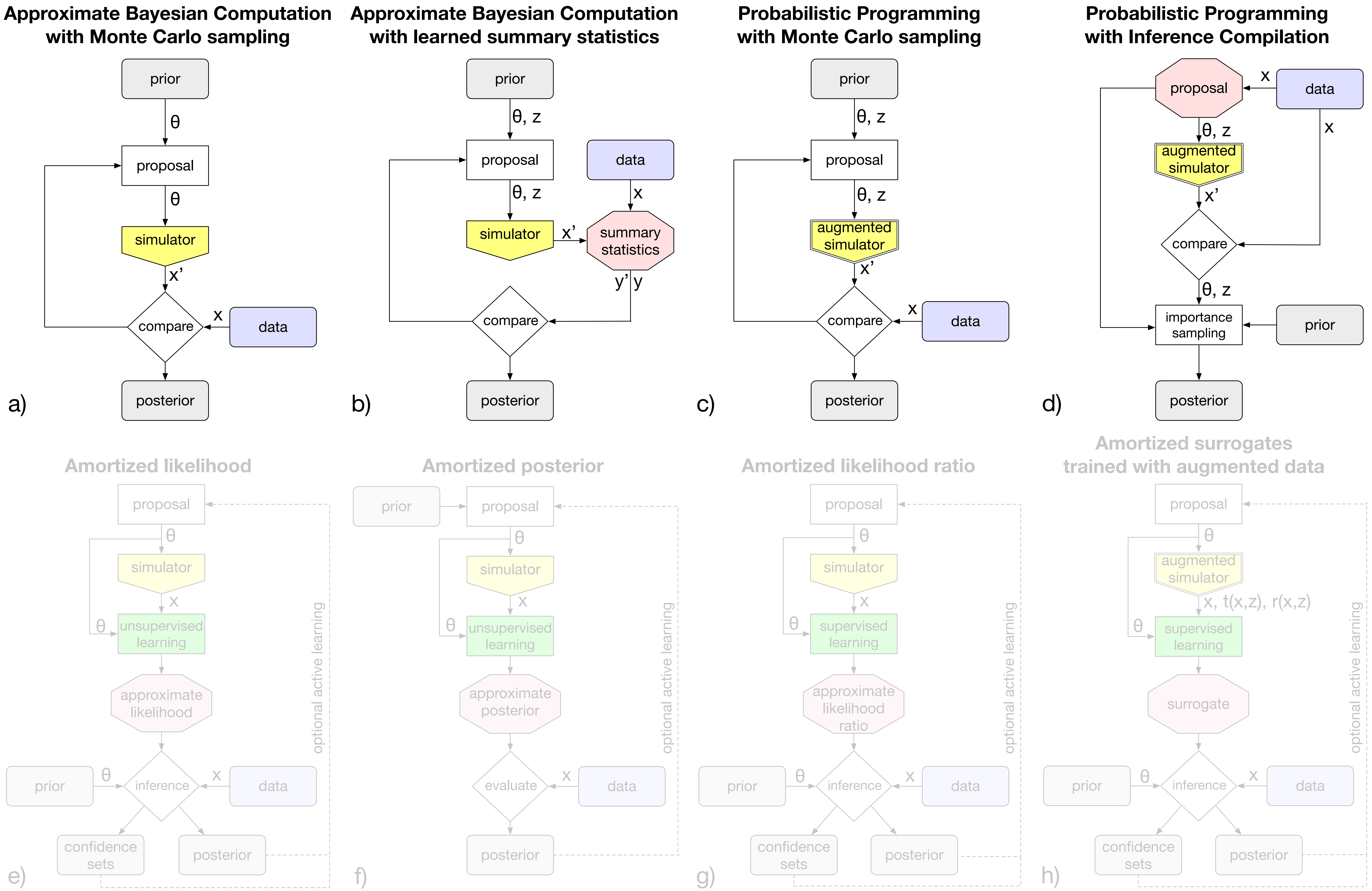


Fig. 3. Overview of different approaches to simulation-based inference.

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

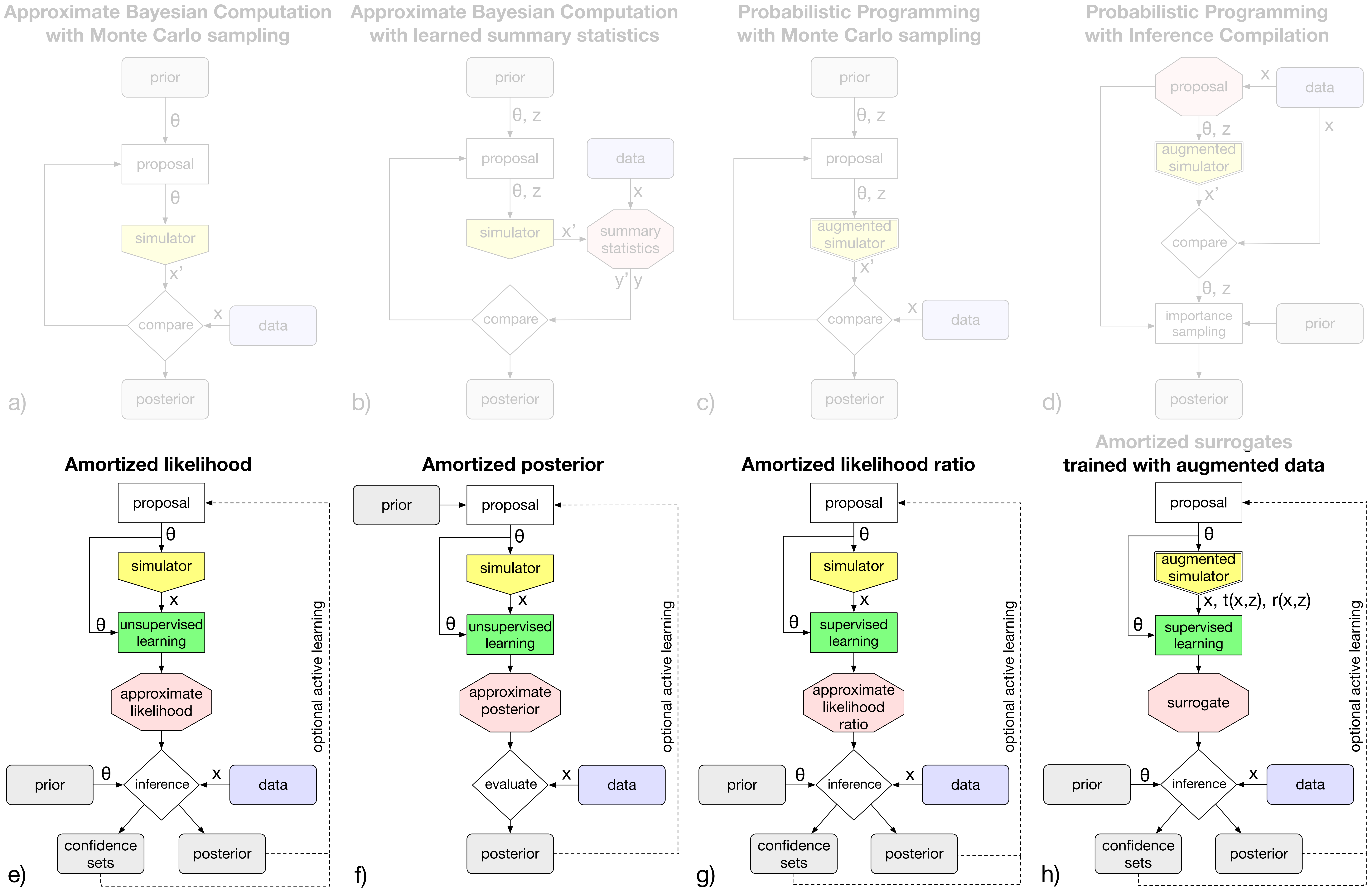


Fig. 3. Overview of different approaches to simulation-based inference.

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

Fig. 3. Overview of different approaches to simulation-based inference.

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

Fig. 3. Overview of different approaches to simulation-based inference.

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

Fig. 3. Overview of different approaches to simulation-based inference.

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

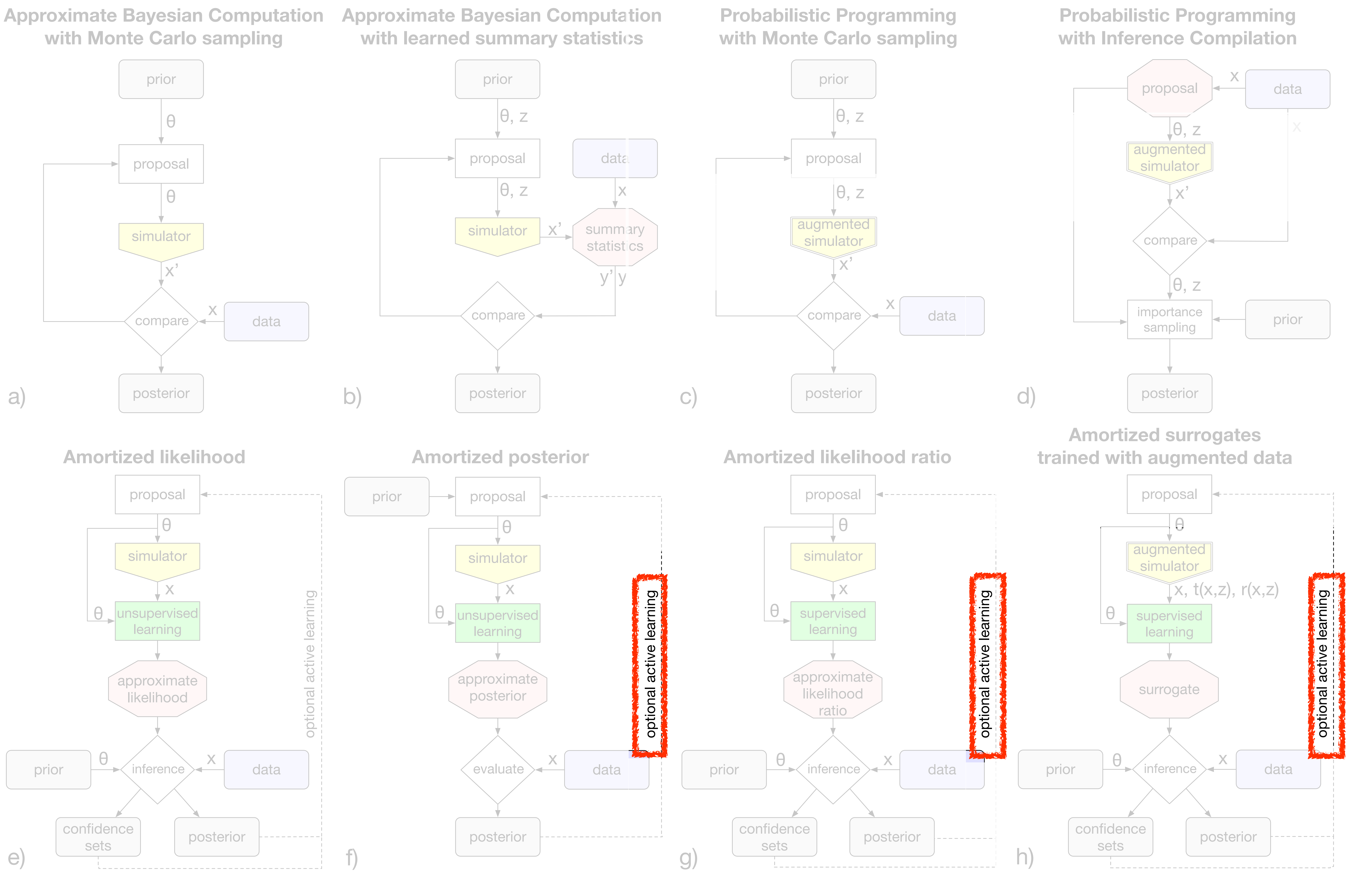


Fig. 3. Overview of different approaches to simulation-based inference.

Probabilistic Programming

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

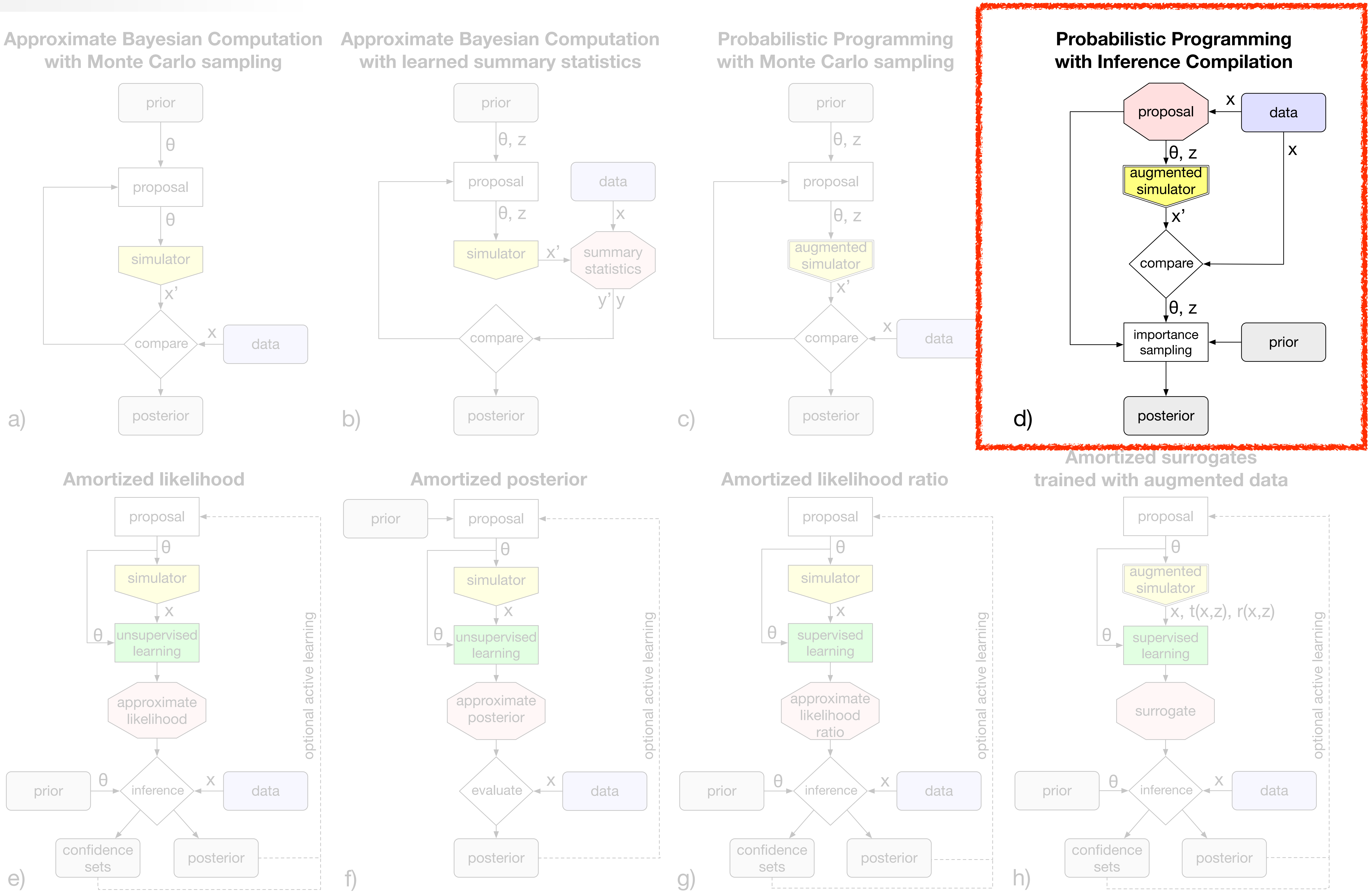
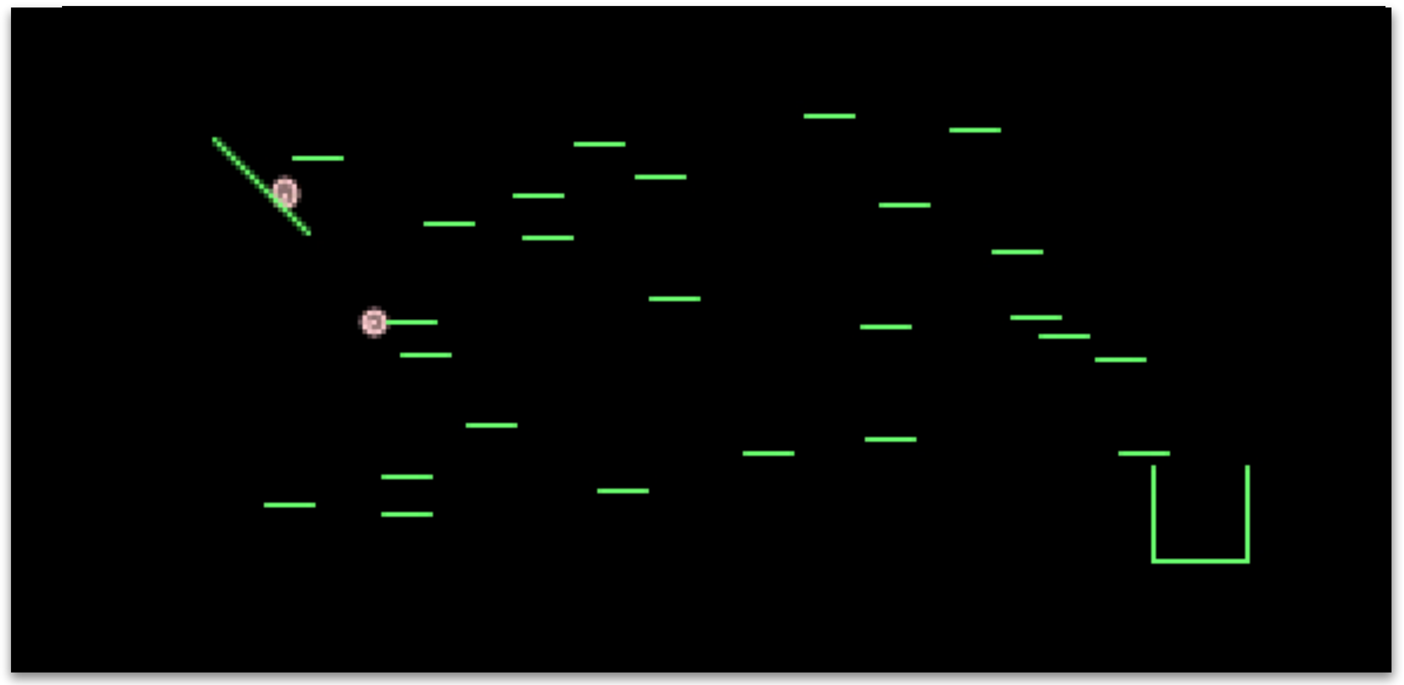
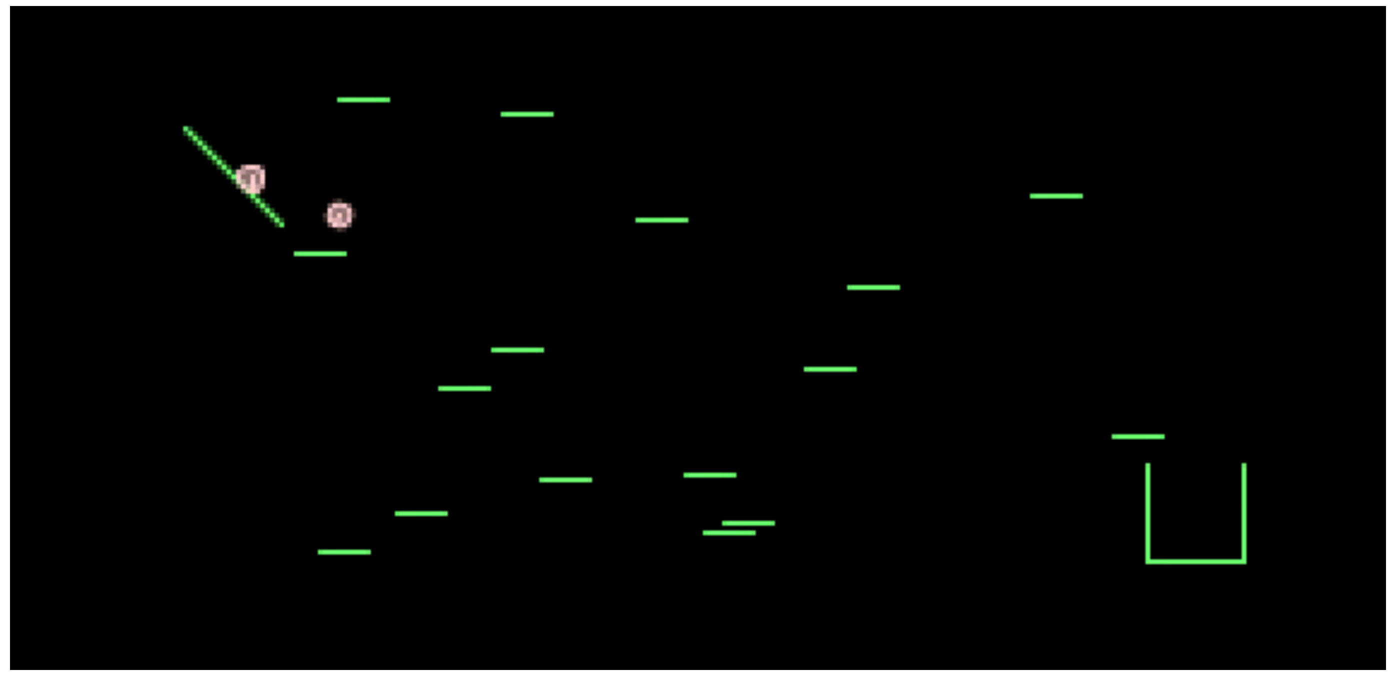


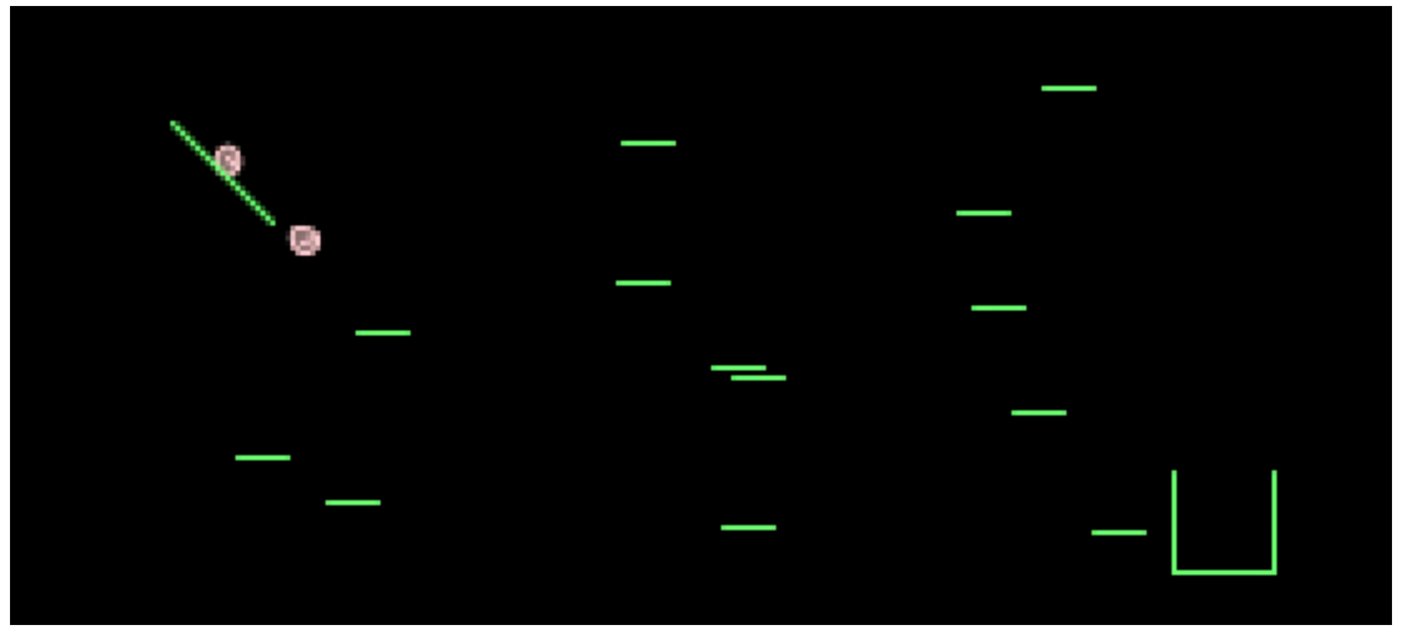
Fig. 3. Overview of different approaches to simulation-based inference.

Probabilistic Programming Example

```
(defquery arrange-bumpers []
    (let [number-of-bumpers (sample (poisson 20))
          bumpydist (uniform-continuous 0 10)
          bumpxdist (uniform-continuous -5 14)
          bumper-positions (repeatedly
                             number-of-bumpers
                             #(vector (sample bumpxdist)
                                      (sample bumpydist)))

          ;; code to simulate the world
          world (create-world bumper-positions)
          end-world (simulate-world world)
          balls (:balls end-world)

          ;; how many balls entered the box?
          num-balls-in-box (balls-in-box end-world)]

      {:balls balls
       :num-balls-in-box num-balls-in-box
       :bumper-positions bumper-positions}))
```





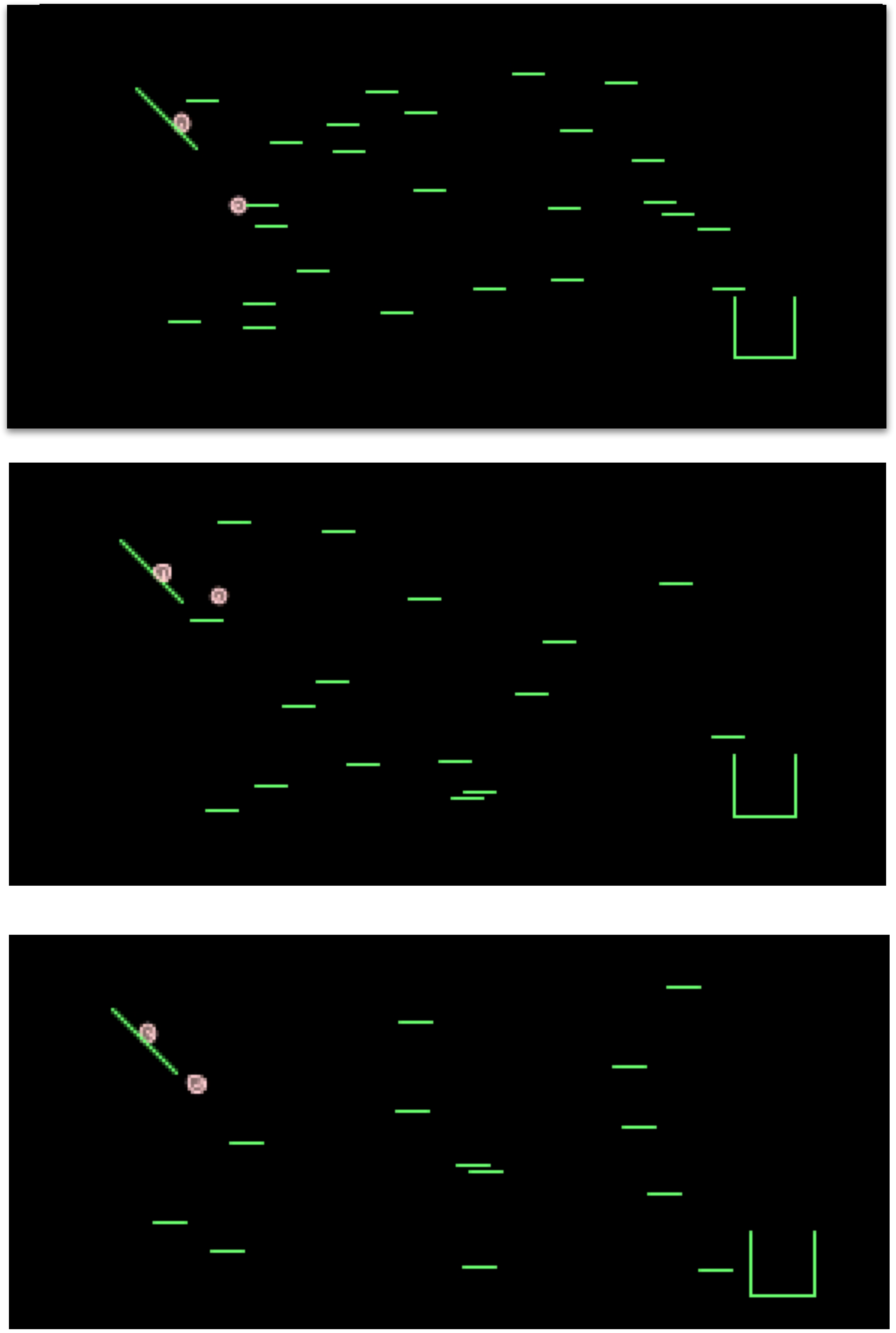


3 examples generated from simulator

[slides, Frank Wood]

Probabilistic Programming Example

```
(defquery arrange-bumpers []
    (let [number-of-bumpers (sample (poisson 20))
          bumpydist (uniform-continuous 0 10)
          bumpxdist (uniform-continuous -5 14)
          bumper-positions (repeatedly
                             number-of-bumpers
                             #(vector (sample bumpxdist)
                                      (sample bumpydist)))

          ;; code to simulate the world
          world (create-world bumper-positions)
          end-world (simulate-world world)
          balls (:balls end-world)

          ;; how many balls entered the box?
          num-balls-in-box (balls-in-box end-world)]

      {:balls balls
       :num-balls-in-box num-balls-in-box
       :bumper-positions bumper-positions}))
```

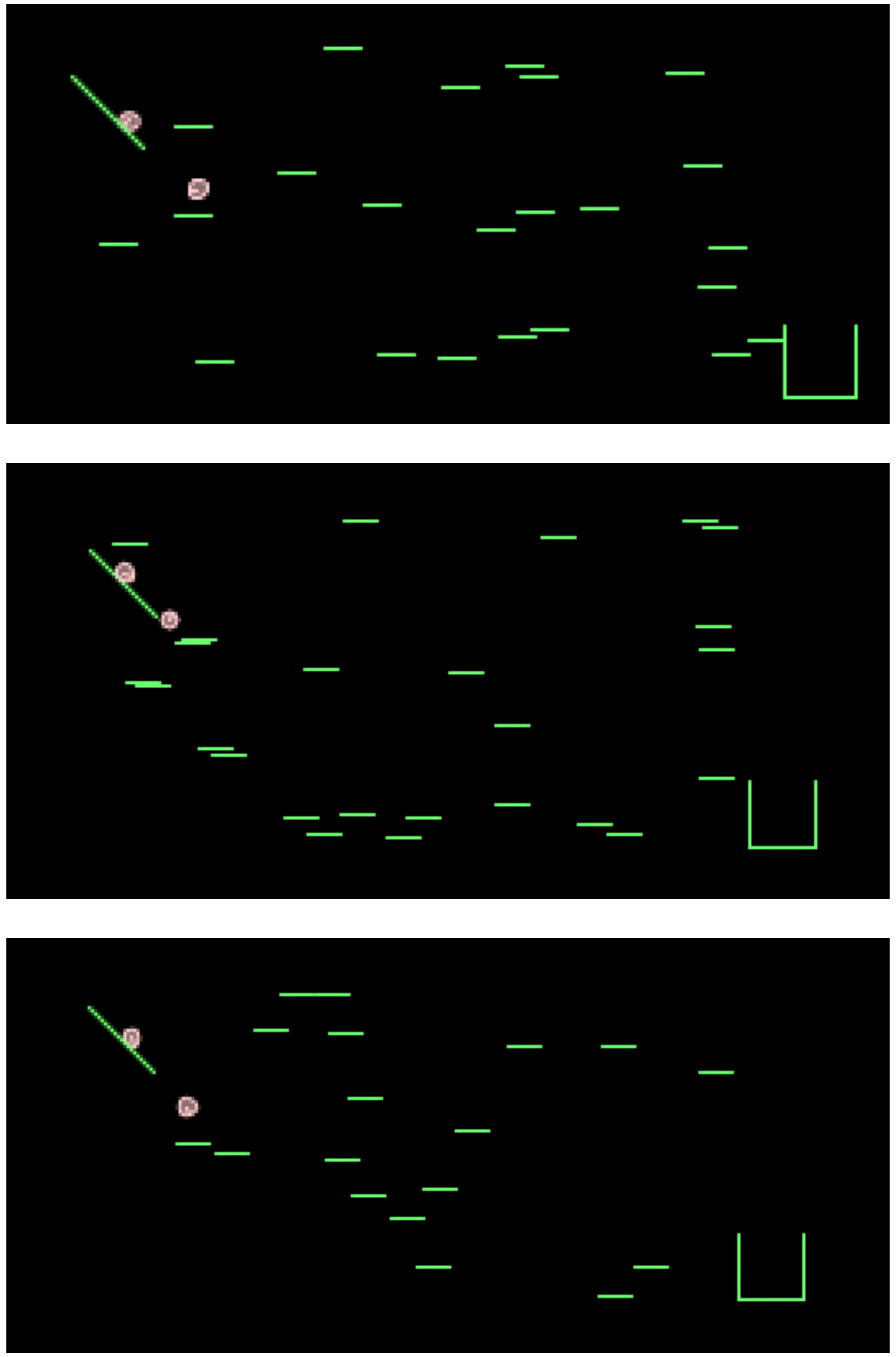


3 examples generated from simulator

[slides, Frank Wood]

Probabilistic Programming Example

```
(defquery arrange-bumpers []
   (let [number-of-bumpers (sample (poisson 20))
         bumpydist (uniform-continuous 0 10)
         bumpxdist (uniform-continuous -5 14)
         bumper-positions (repeatedly
                            number-of-bumpers
                            #(vector (sample bumpxdist)
                                     (sample bumpydist)))

         ;; code to simulate the world
         world (create-world bumper-positions)
         end-world (simulate-world world)
         balls (:balls end-world)

         ;; how many balls entered the box?
         num-balls-in-box (balls-in-box end-world)

         obs-dist (normal 4 0.1)]

     (observe obs-dist num-balls-in-box)
```

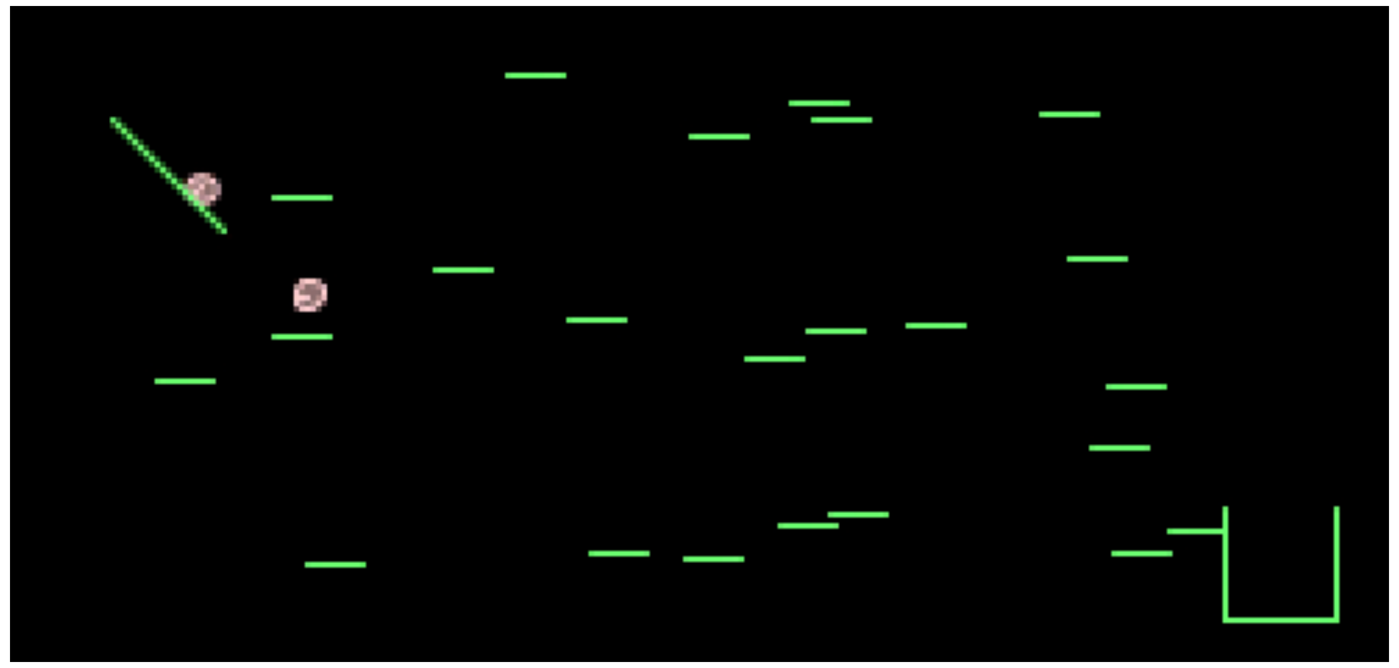


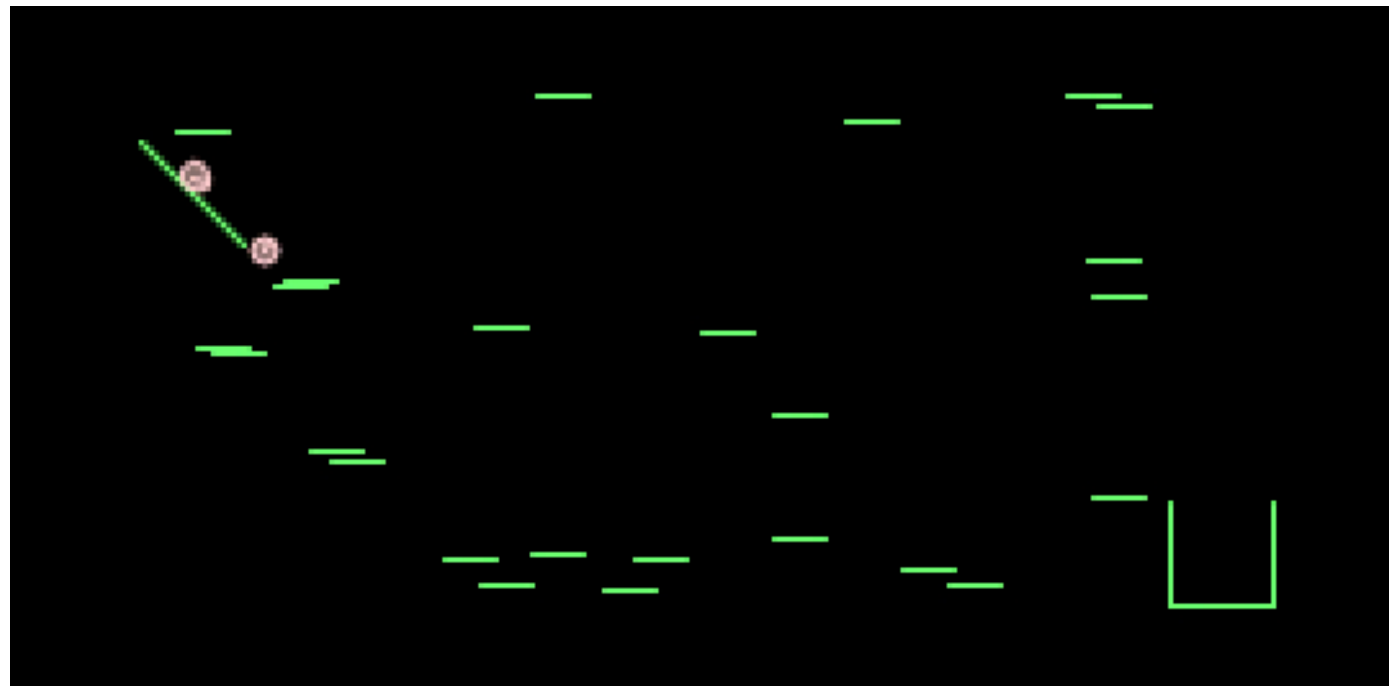
3 examples generated from simulator
conditioned on ~20% of balls land in box

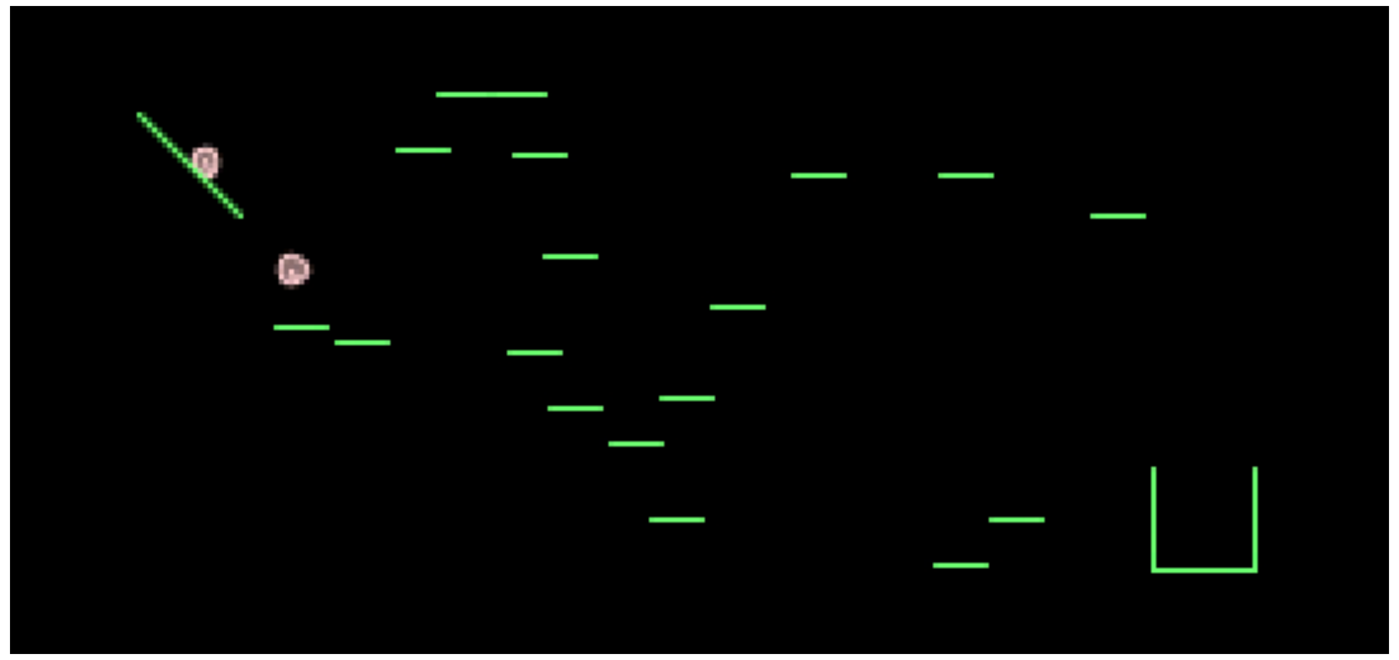
[slides, Frank Wood]

Probabilistic Programming Example

```
(defquery arrange-bumpers []
   (let [number-of-bumpers (sample (poisson 20))
         bumpydist (uniform-continuous 0 10)
         bumpxdist (uniform-continuous -5 14)
         bumper-positions (repeatedly
                            number-of-bumpers
                            #(vector (sample bumpxdist)
                                     (sample bumpydist)))

         ;; code to simulate the world
         world (create-world bumper-positions)
         end-world (simulate-world world)
         balls (:balls end-world)

         ;; how many balls entered the box?
         num-balls-in-box (balls-in-box end-world)

         obs-dist (normal 4 0.1)]

     (observe obs-dist num-balls-in-box)
```







3 examples generated from simulator
conditioned on ~20% of balls land in box

[slides, Frank Wood]

Structured latent space

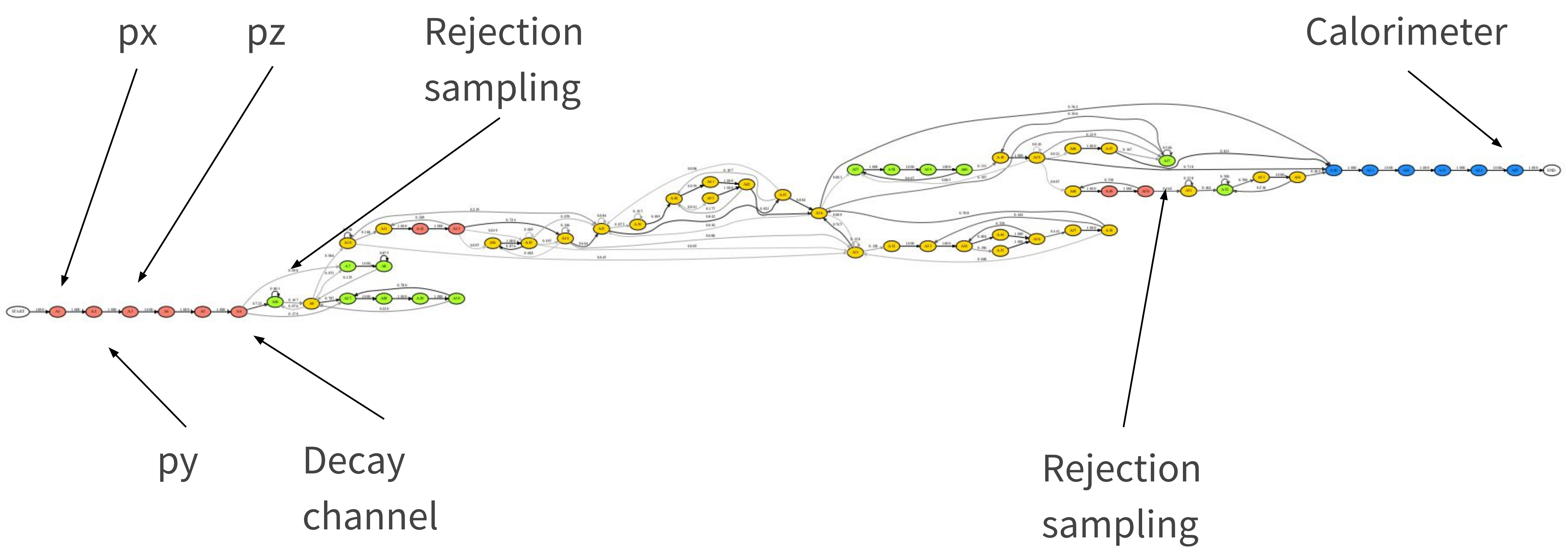
One can frame simulators as:

- first samples latent variables $z \sim p(z \mid \theta)$ and then run through some deterministic function $x = g(\theta, z)$
- with implicit likelihood $p(\mathbf{x} \mid \boldsymbol{\theta}) = \int \delta(\mathbf{x} - \mathbf{g}(\boldsymbol{\theta}, \mathbf{z}))\, p(\mathbf{z} \mid \boldsymbol{\theta})\, \mathrm{d}\mathbf{z}$

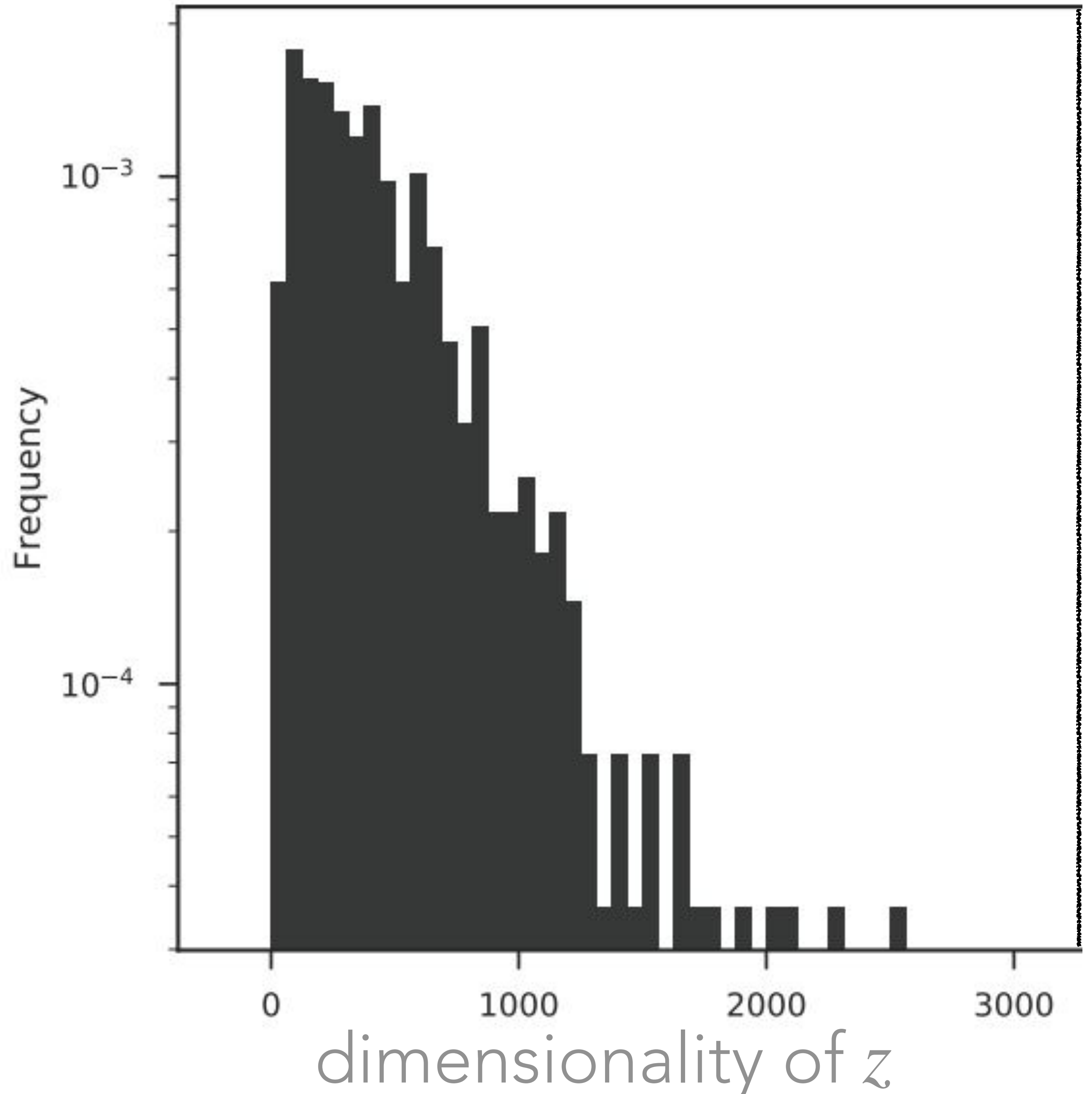
But

- $g(\theta, z)$ may be very weird… non-differentiable due to control flow
- and the latent space often very structured

Latent structure of 250 most frequent trace types in physics simulator

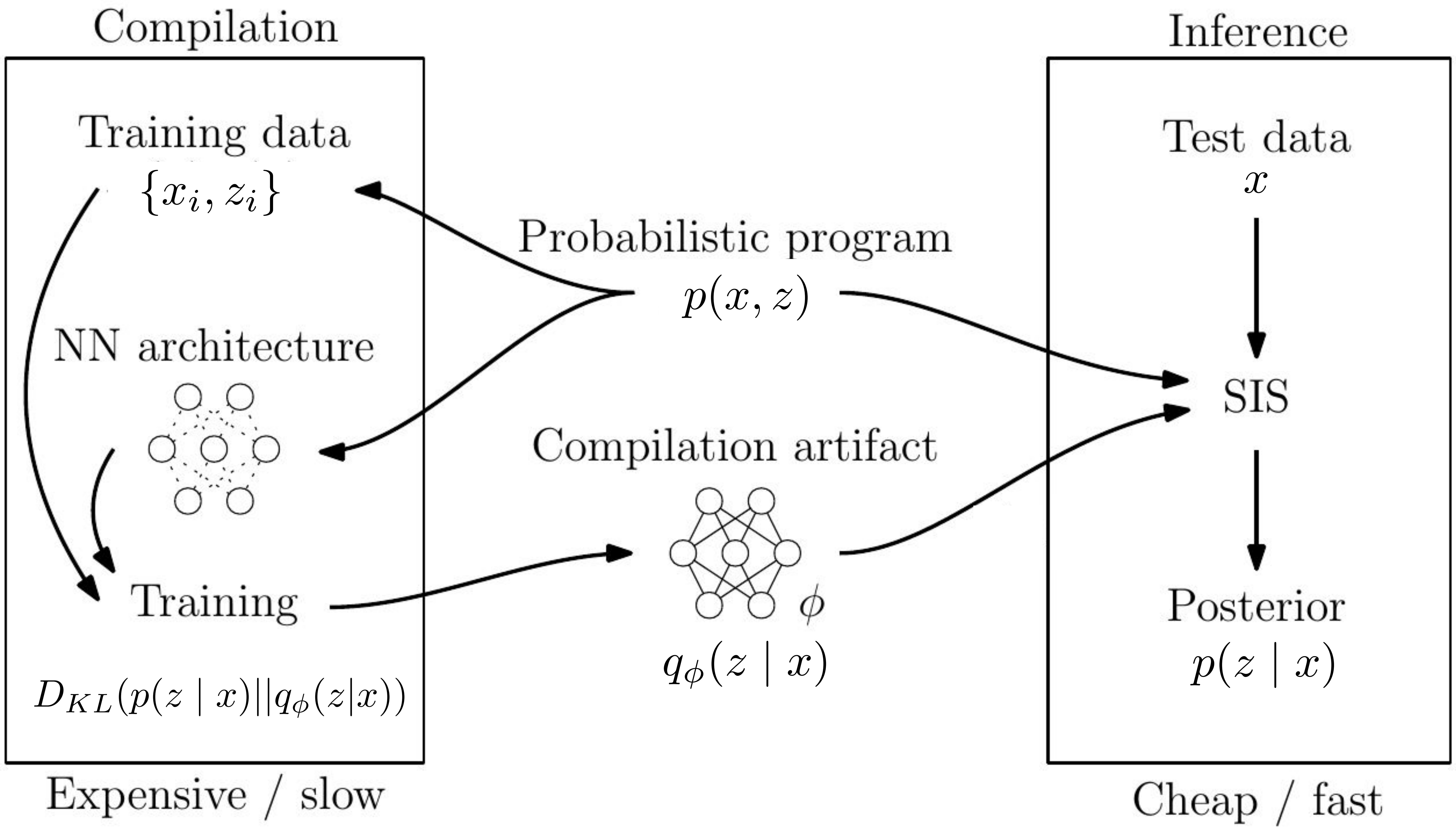



```
def stochastic_function():
    z1 = rand()
    if z1 < 0.5:
        z2t = rand()
        x = z1 + z2t
    else:
        z2f = rand()
        z3f = rand()
        x = z1 + z2f + z3f
    return x
```



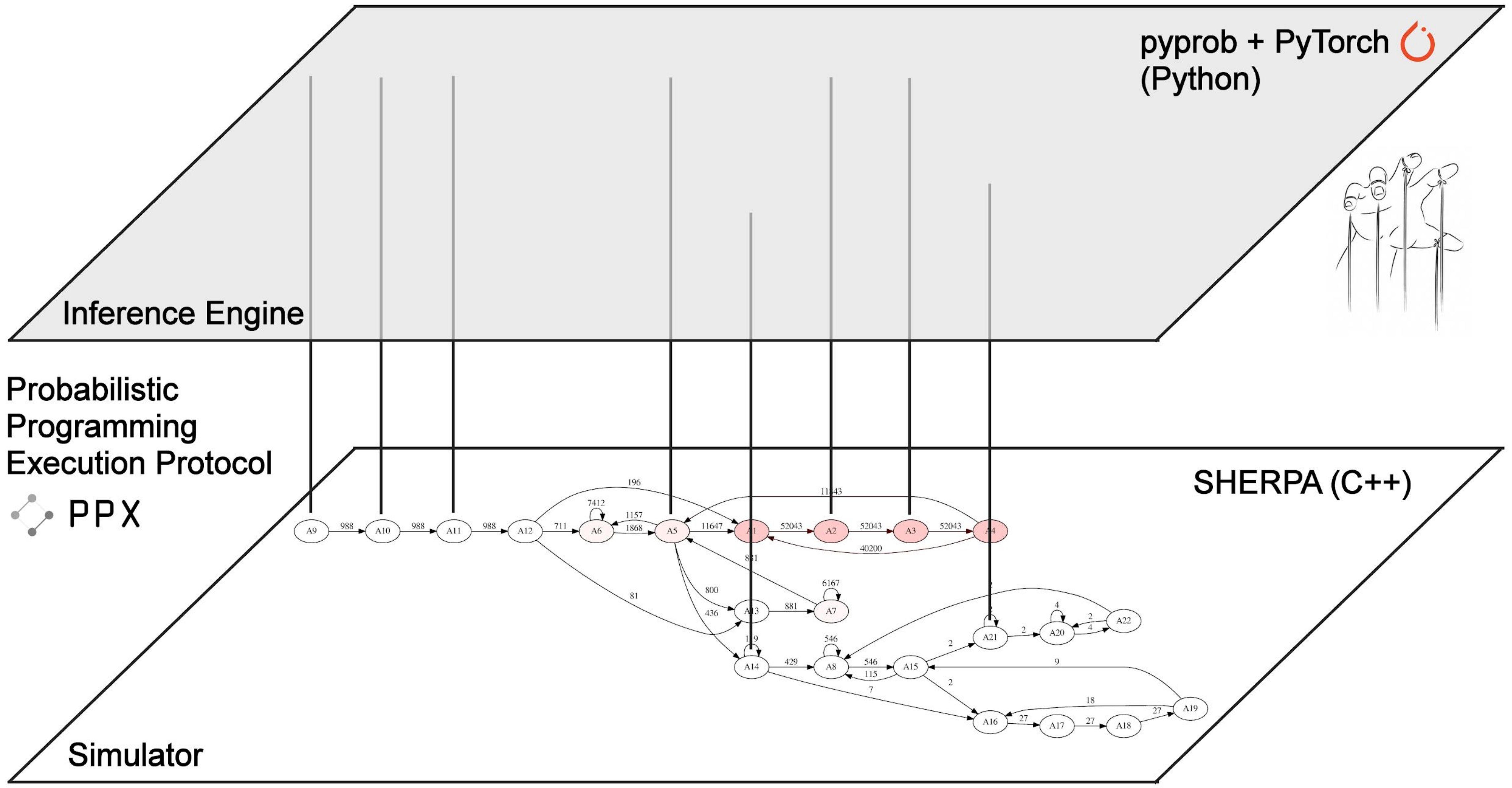
Inference Compilation

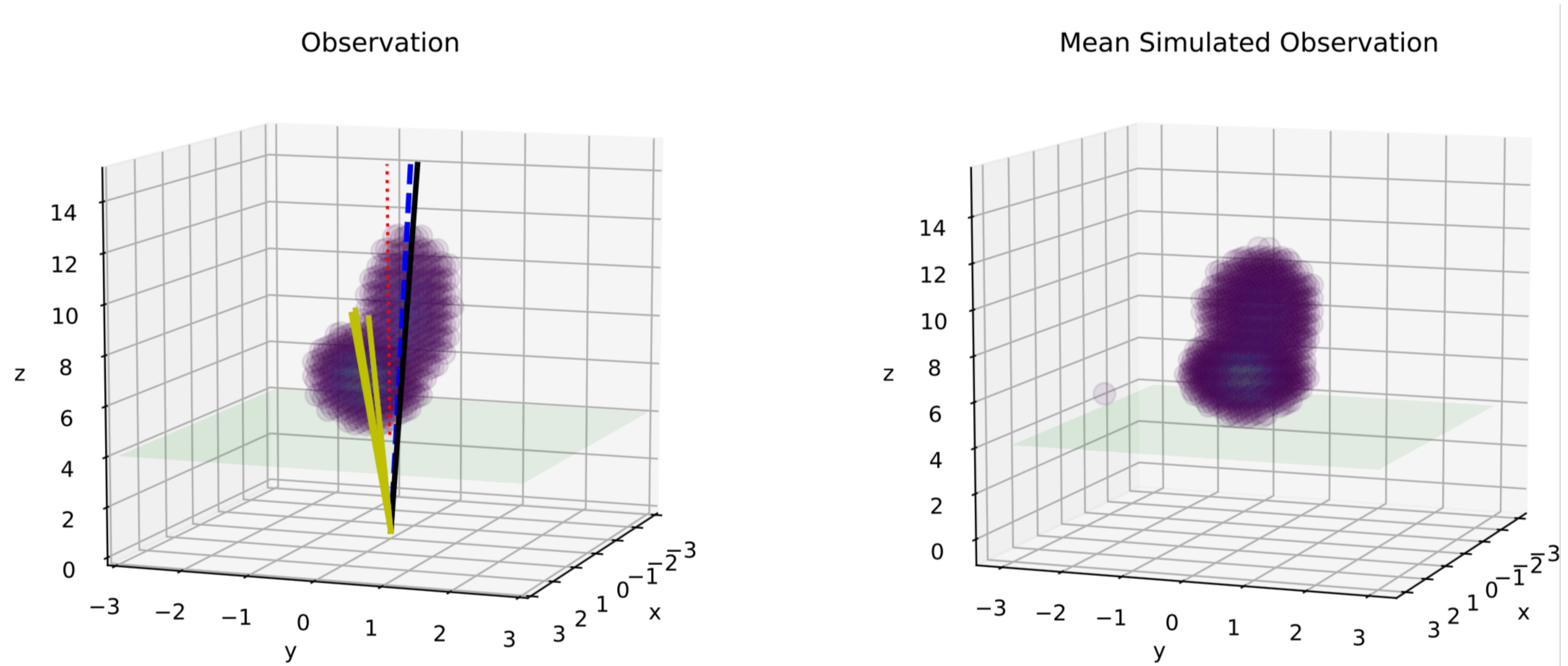
Hijack the random number generators and use NN's to learn $q_\phi(z \mid x)$ and then perform a *very* smart type of importance sampling over structured latent space of stack traces.



G. Baydin, et al SC19 arXiv:1907.03382
G. Baydin, et al. NeurIPS 2019 arXiv:1807.07706

Previously had to use a special purpose probabilistic programming language. With **ppx** protocol, we decouple inference engine & control existing simulator.





- **Augment** real-world physics simulator
  (C++, 1M lines of code)
- 3DCNN-LSTM architecture for $q_\phi(z \mid x)$
  (Stack traces with Dim[z] ranging from 100 — 2,000)
- Inference is embarrassingly parallelizable unlike MCMC. 230x speedup

Atılım Güneş Baydin
Bradley Gram-Hansen

Lukas Heinrich

Kyle Cranmer

Frank Wood
Andreas Munk
Saeid Naderiparizi

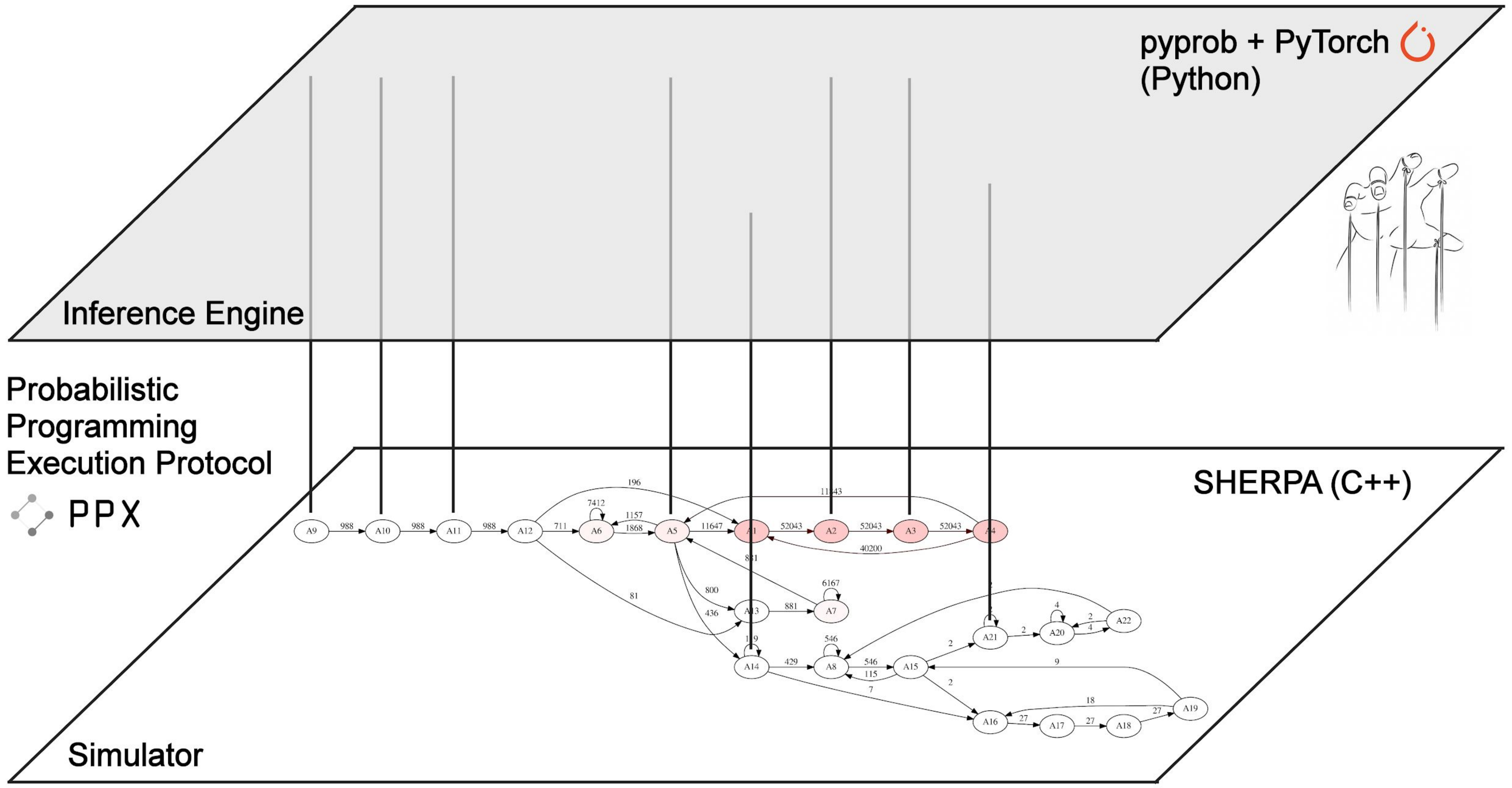
Wahid Bhimji
Jialin Liu
Prabhat

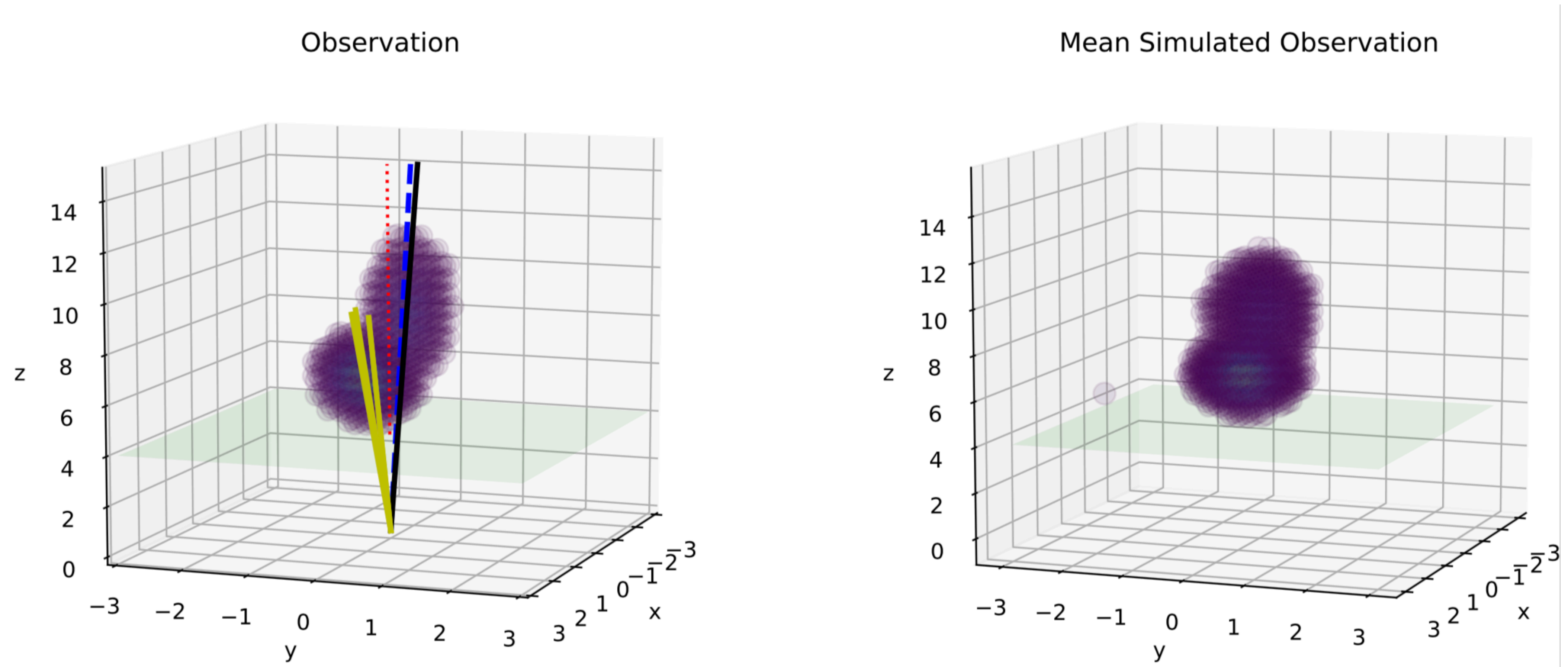
Gilles Louppe

Lei Shao
Larry Meadows

G. Baydin, et al SC19 arXiv:1907.03382
G. Baydin, et al. NeurIPS 2019 arXiv:1807.07706

Previously had to use a special purpose probabilistic programming language. With **ppx** protocol, we decouple inference engine & control existing simulator.





- **Augment** real-world physics simulator
  (C++, 1M lines of code)
- 3DCNN-LSTM architecture for $q_\phi(z \mid x)$
  (Stack traces with Dim[z] ranging from 100 — 2,000)
- Inference is embarrassingly parallelizable unlike MCMC. 230x speedup

University of Oxford: Atılım Güneş Baydin, Bradley Gram-Hansen

CERN: Lukas Heinrich

NYU: Kyle Cranmer

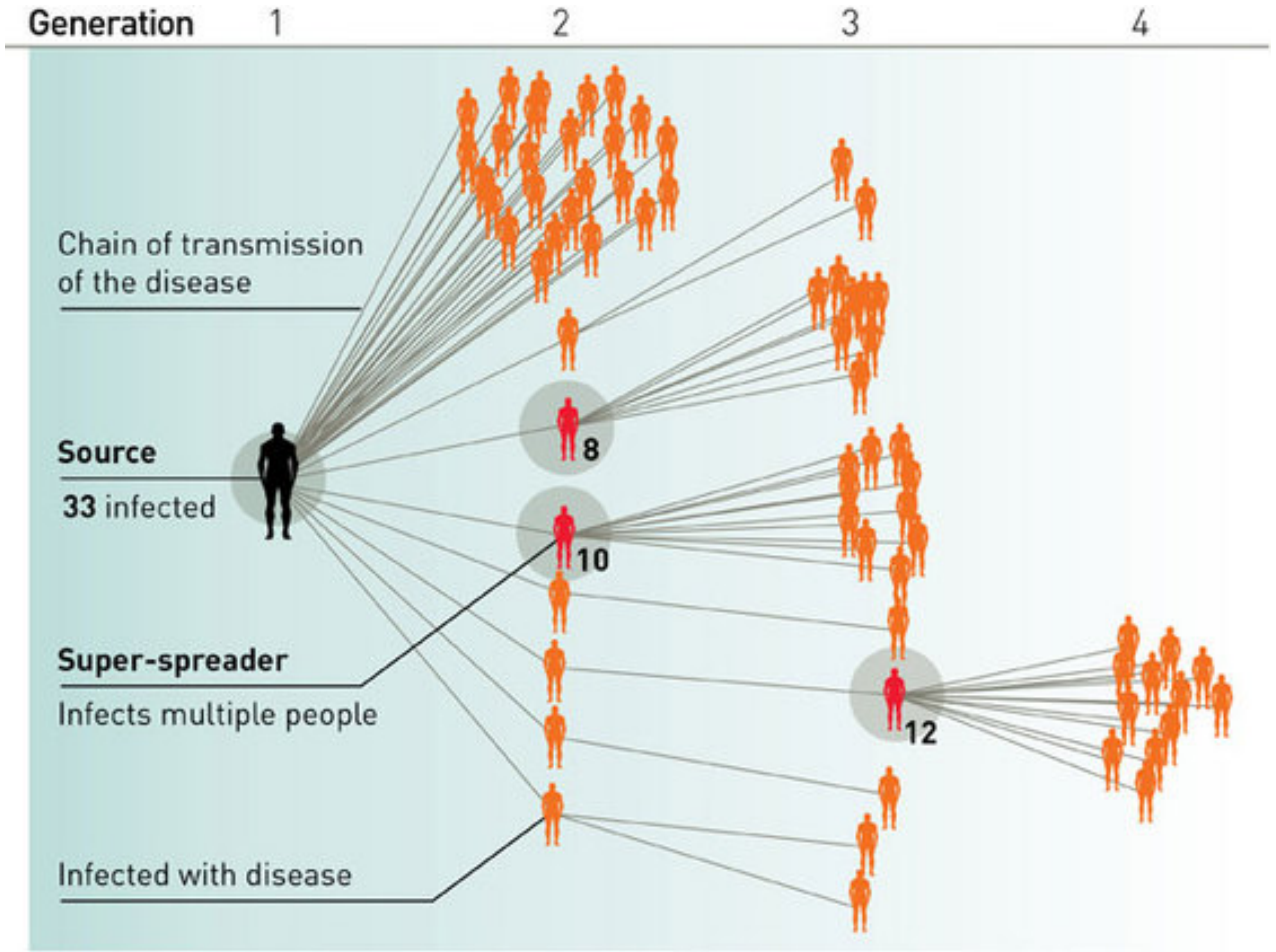
UBC: Frank Wood, Andreas Munk, Saeid Naderiparizi

Berkeley Lab: Wahid Bhimji, Jialin Liu, Prabhat

Liège université: Gilles Louppe

Intel: Lei Shao, Larry Meadows

Epidemiology & population Genetics



Simulation-Based Inference for Global Health Decisions

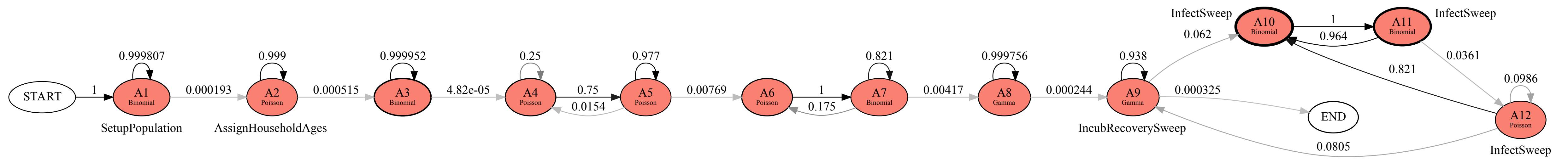


Figure 1: Latent probabilistic structure uncovered using `PyProb` from the Imperial College `CovidSim` simulator run on Malta, demonstrating the first step in working with this simulator as a probabilistic program. Uniform distributions are omitted for simplicity.

Simulation-Based Inference for Global Health Decisions

Christian Schroeder de Witt [1] Bradley Gram-Hansen [1] Nantas Nardelli [1]
Andrew Gambardella [1] Rob Zinkov [1] Puneet Dokania [1] N. Siddharth [1]
Ana Belen Espinosa-Gonzalez [2] Ara Darzi [2] Philip Torr [1] Atılım Güneş Baydin [1]

https://arxiv.org/abs/2005.07062

PLANNING AS INFERENCE IN EPIDEMIOLOGICAL DYNAMICS MODELS

A PREPRINT

Frank Wood[1,3,4], Andrew Warrington[2], Saeid Naderiparizi[1], Christian Weilbach[1], Vaden Masrani[1], William Harvey[1], Adam Ścibior[1], Boyan Beronov[1], and Ali Nasseri[1]

[1]Department of Computer Science, University of British Columbia
[2]Department of Engineering Science, University of Oxford
[3]MILA
[4]CIFAR AI Chair
{fwood,awarring,saeidnp,weilbach,vadmas,wsgh,ascibior,beronov}@cs.ubc.ca, ali.nasseri@ubc.ca

https://arxiv.org/abs/2003.13221

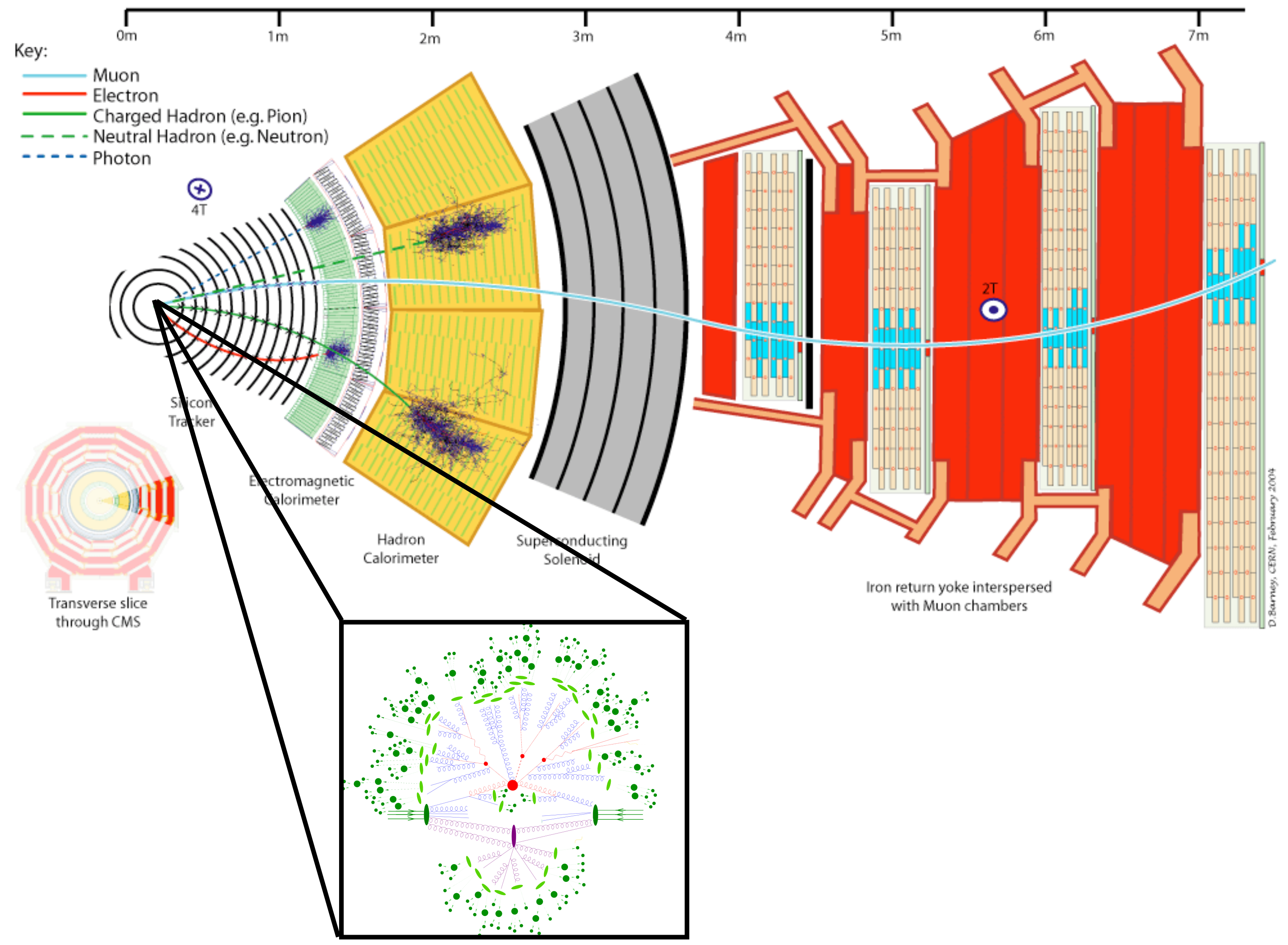
Hijacking Malaria Simulators with Probabilistic Programming

Bradley J. Gram-Hansen * 1 Christian Schröder de Witt * 1
Tom Rainforth [2] Philip H.S. Torr [1] Yee Whye Teh [2] Atılım Güneş Baydin [1]

https://arxiv.org/abs/1905.12432

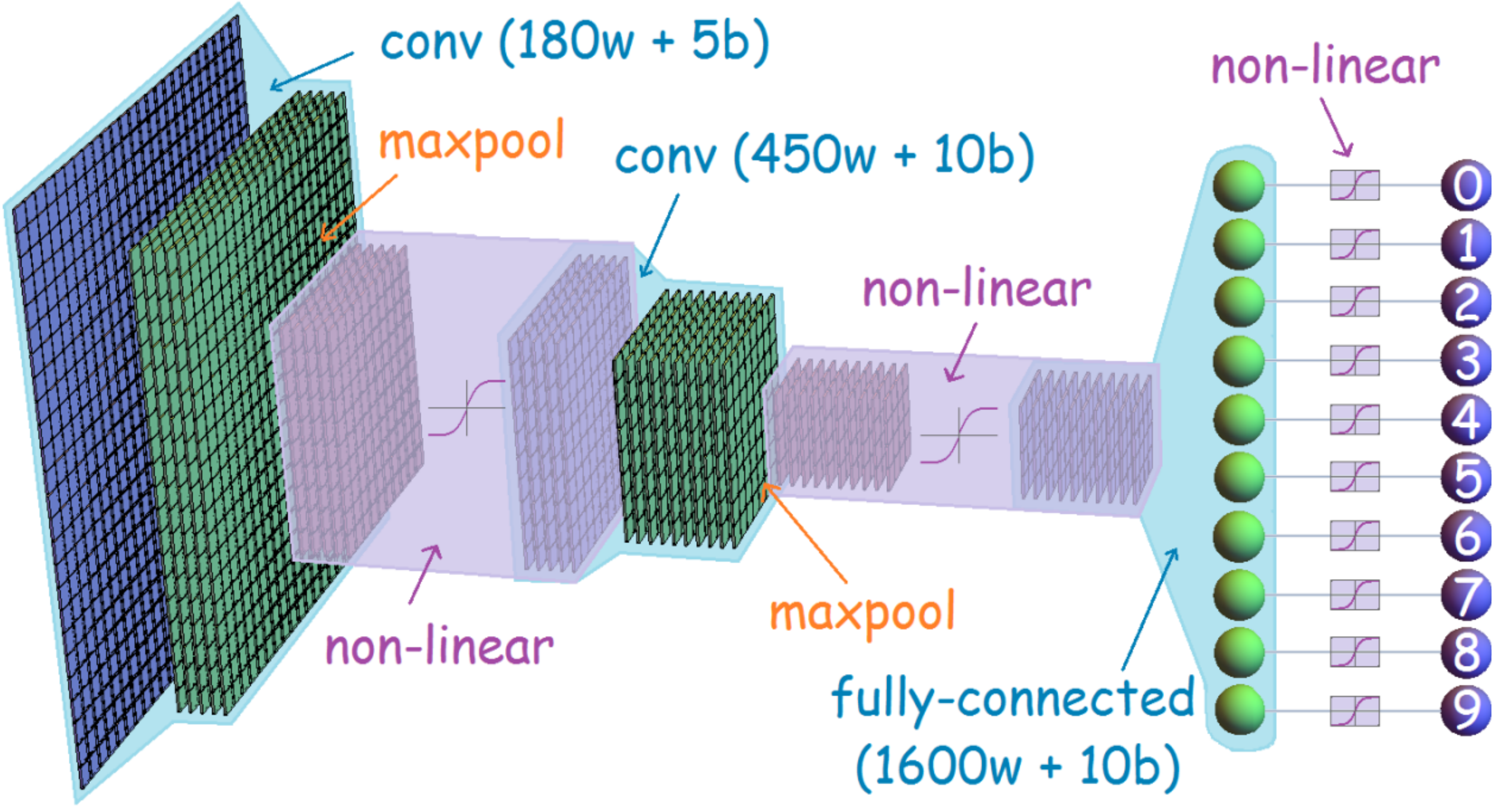
Two approaches simulation-based inference

Use simulator
(much more efficiently)



- Approximate Bayesian Computation (ABC)
- Probabilistic Programming
- Adversarial Variational Optimization

Learn simulator
(with deep learning)



- Likelihood ratio trick (with classifiers)
- Conditional density estimate (with normalizing flows)
- Learned summary statistics

[image credit: A.P. Goucher]

Different targets

Learn a likelihood ratio or density ratio with a classifier

- Neural Ratio Estimation [NRE]
- likelihood ratio to arbitrary reference $r(x;\theta) = \frac{p(x \mid \theta)}{p_{\text{ref}}(x)}$ or between $r(x;\theta_0,\theta_1) = \frac{p(x \mid \theta_0)}{p(x \mid \theta_1)}$
- likelihood / evidence = posterior / prior $r(x;\theta) = \frac{p(x \mid \theta)}{p(x)} = \frac{p(\theta \mid x)}{p(\theta)}$

Learn the likelihood $p(x \mid \theta)$ with a conditional density estimate

- Neural Likelihood Estimation [NLE]

Learn the posterior $p(\theta \mid x)$ with a conditional density estimate

- Neural Posterior Estimation [NPE]

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

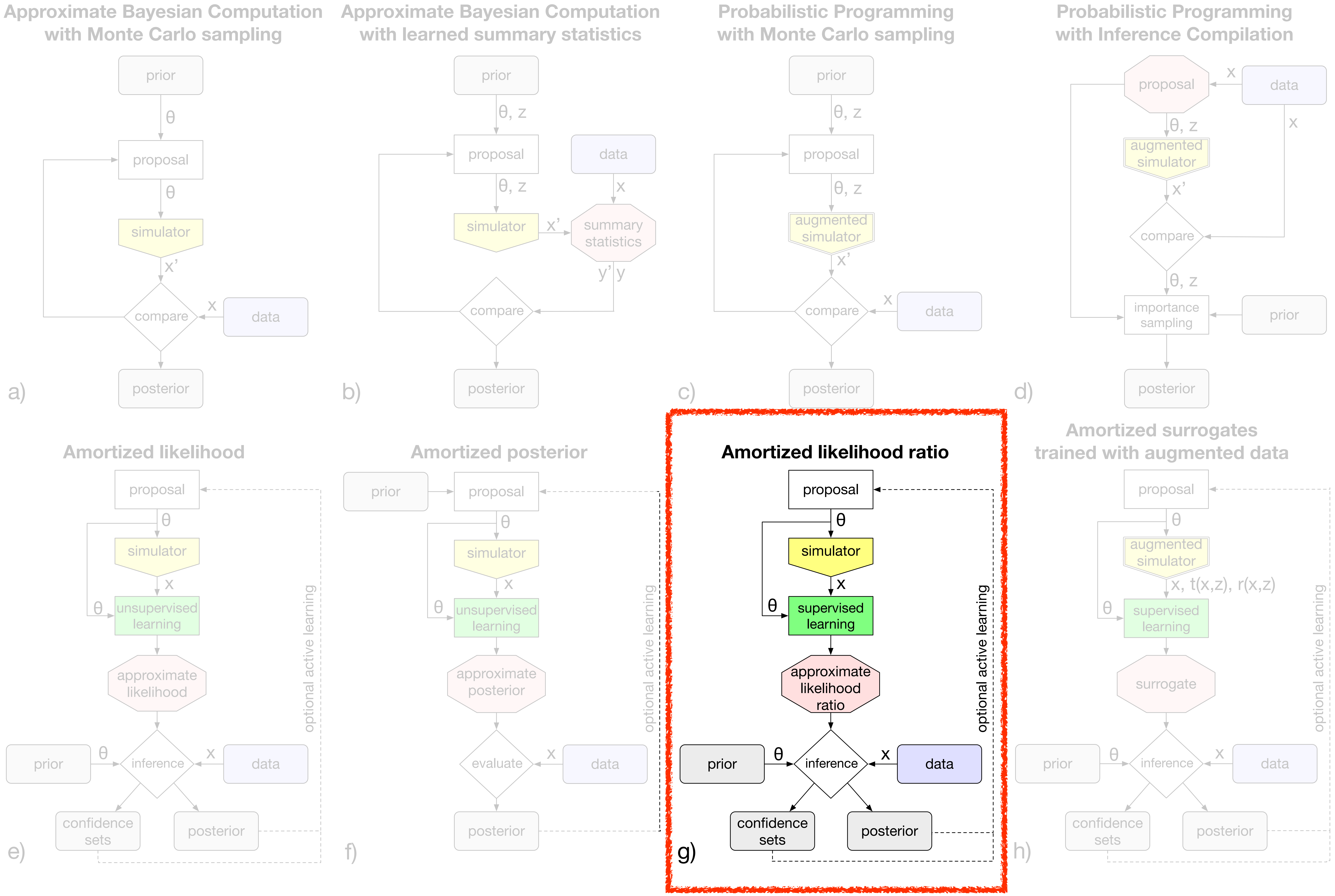


Fig. 3. Overview of different approaches to simulation-based inference.

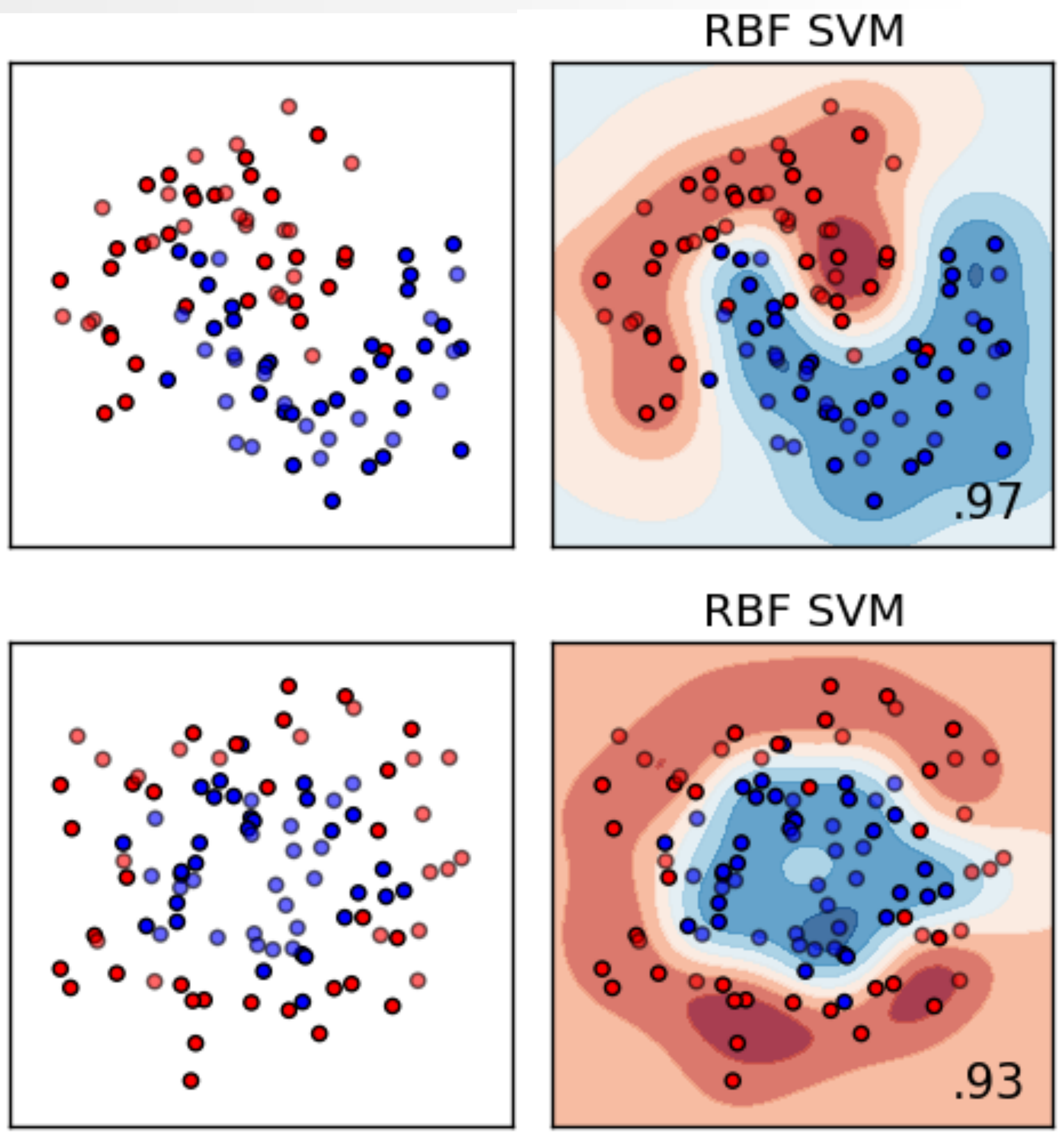
From the review

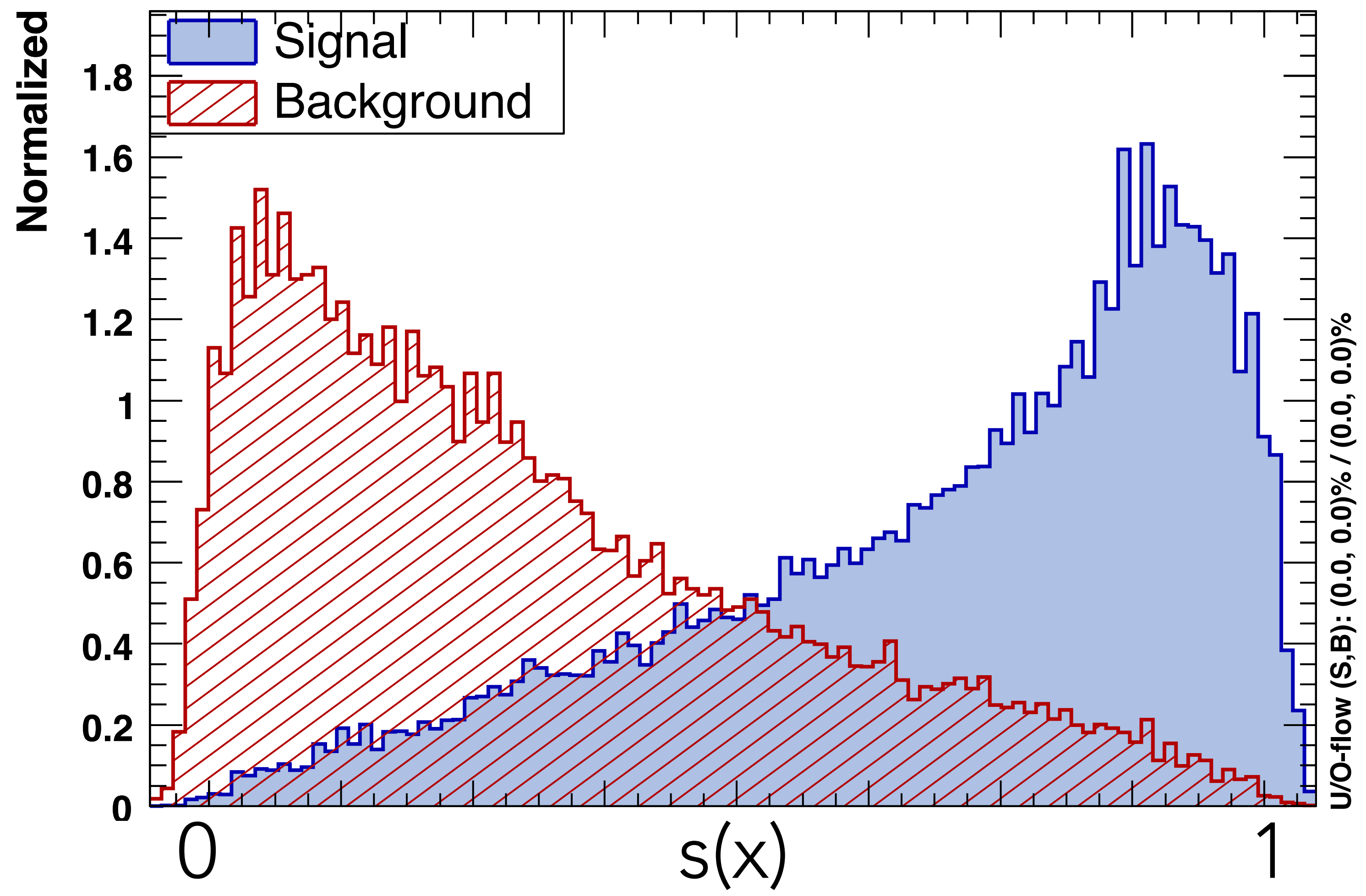
[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

Fig. 3. Overview of different approaches to simulation-based inference.

Likelihood Ratio Trick

[Hastie et al., 2001; Sugiyama et al., 2012; Cranmer et. al., 2015]





- **binary classifier**: find function $s(x)$ that minimizes ***loss***:

$$L[s] = \mathbb{E}_{p(x|H_1)}[-\log s(x)] + \mathbb{E}_{p(x|H_0)}[-\log(1 - s(x))]$$

- i.e. approximate the optimal classifier

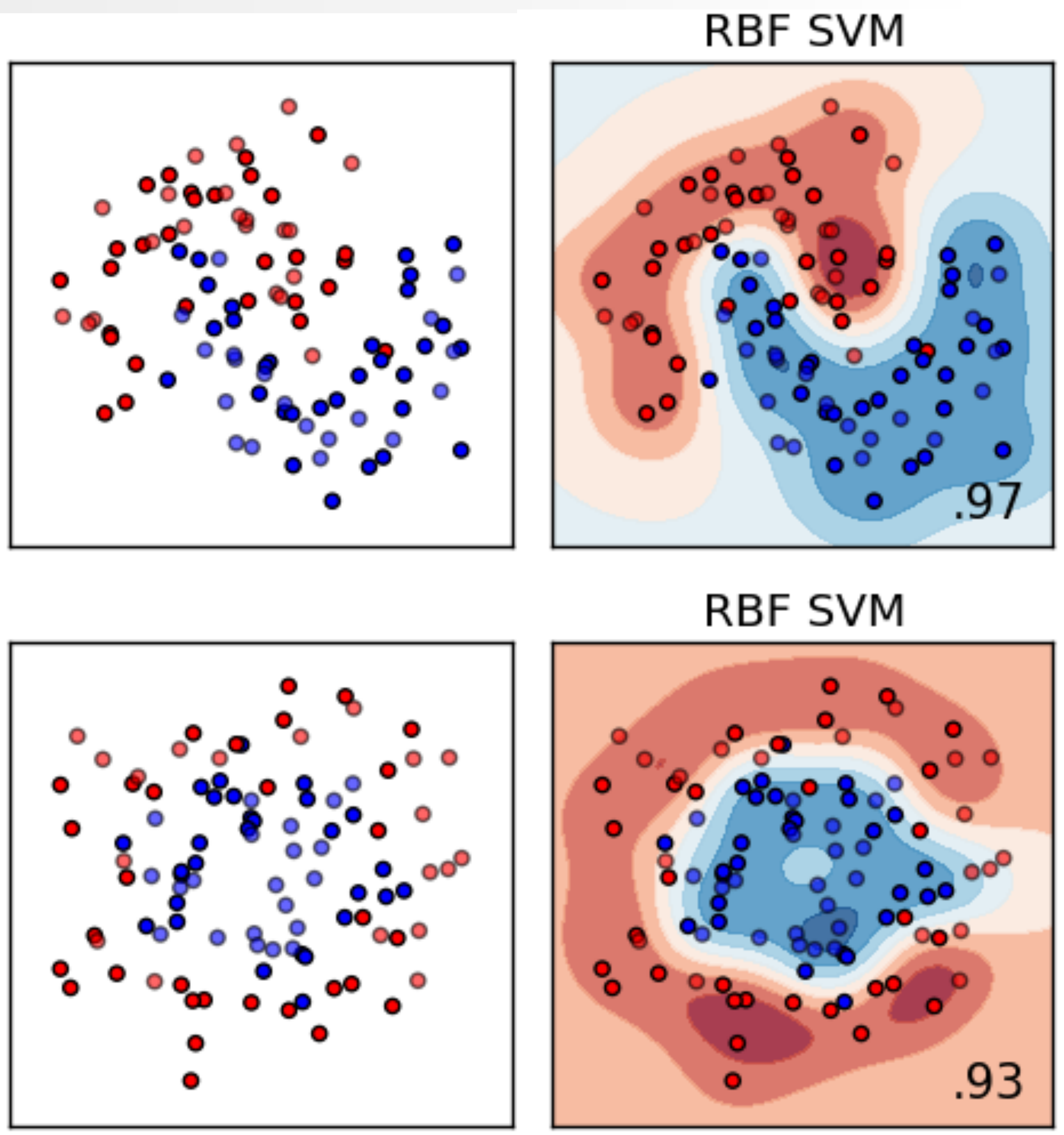
$$s(x) = \frac{p(x|H_1)}{p(x|H_0) + p(x|H_1)}$$

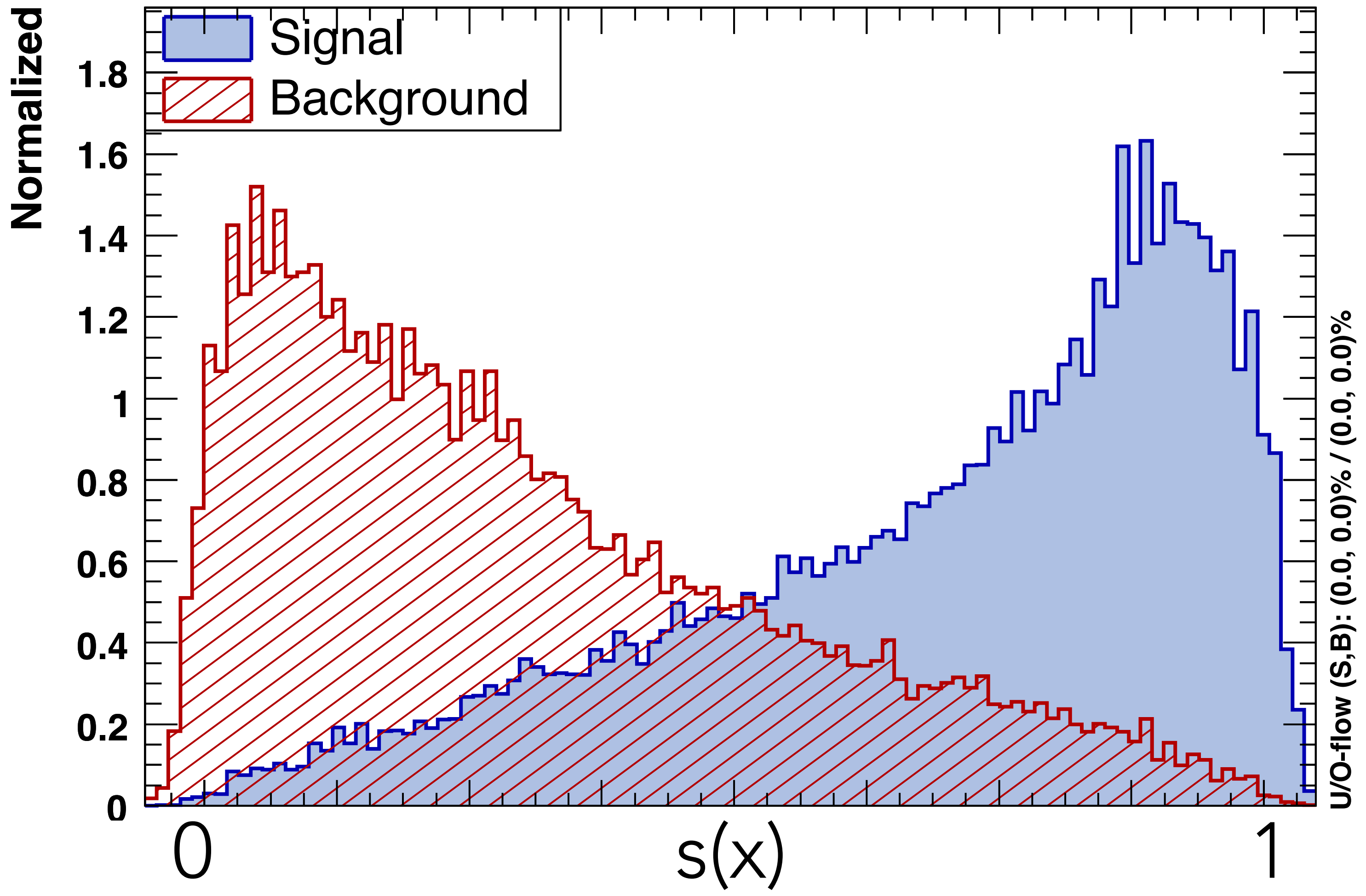
- which is 1-to-1 with the likelihood ratio

$$r(x) = \frac{p(x|H_1)}{p(x|H_0)} = 1 - \frac{1}{s(x)}$$

Likelihood Ratio Trick

[Hastie et al., 2001; Sugiyama et al., 2012; Cranmer et. al., 2015]





- **binary classifier**: find function $s(x)$ that minimizes ***loss***:

$$L[s] = \mathbb{E}_{p(x|H_1)}[-\log s(x)] + \mathbb{E}_{p(x|H_0)}[-\log(1 - s(x))]$$

$$\approx \frac{1}{N}\sum_{i=1}^{N} -y_i \log s(x_i) - (1 - y_i)\log(1 - s(x_i))$$

- i.e. approximate the optimal classifier

$$s(x) = \frac{p(x|H_1)}{p(x|H_0) + p(x|H_1)}$$

- which is 1-to-1 with the likelihood ratio

$$r(x) = \frac{p(x|H_1)}{p(x|H_0)} = 1 - \frac{1}{s(x)}$$

Parametrizing the Likelihood Ratio Trick

Can do the same thing for any two points θ_0 & θ_1 in parameter space $\boldsymbol{\Theta}$.

$$r(x;\theta_0,\theta_1) = \frac{p(x \mid \theta_0)}{p(x \mid \theta_1)} = 1 - \frac{1}{s(x;\theta_0,\theta_1)}$$

Or train to classify data from $p(x|\theta)$ versus some fixed reference $p_{\mathrm{ref}}(x)$

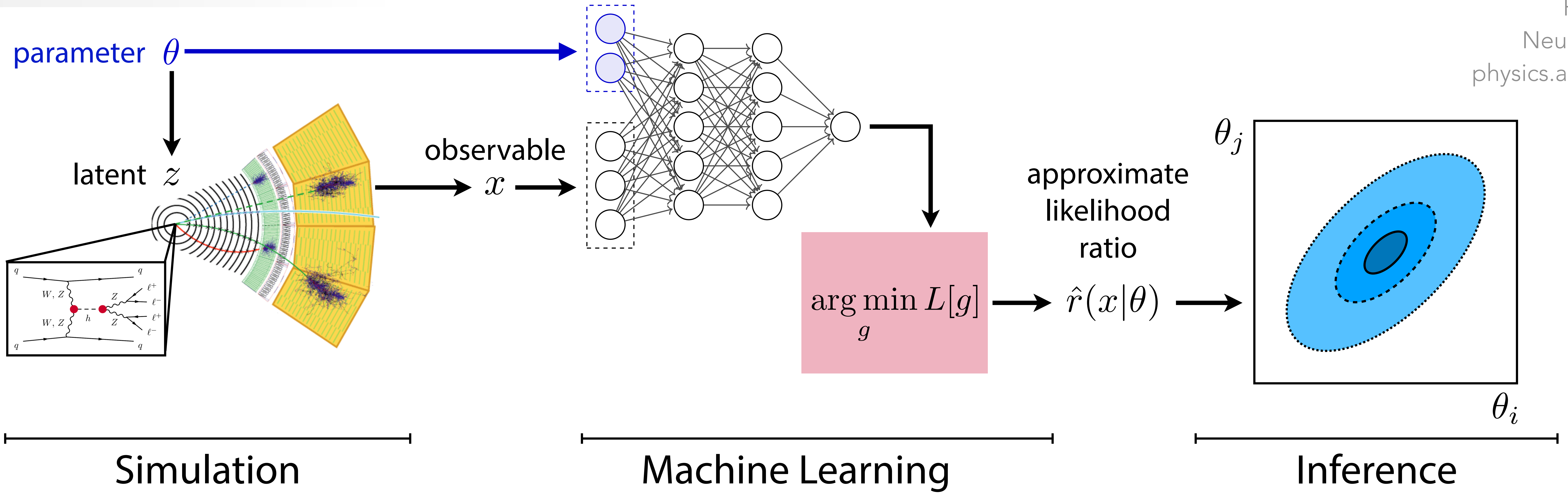
$$r(x;\theta) = \frac{p(x|\theta)}{p_{\mathrm{ref}}(x)} = 1 - \frac{1}{s(x;\theta)}$$

I call this a **parametrized classifier.**

K.C., G. Louppe, J. Pavez: Approximating Likelihood Ratios with Calibrated Discriminative Classifiers [arXiv:1506.02169]

Learning the likelihood ratio

Cranmer, Louppe, Pavez, arXiv:1506.02169
PNAS, arXiv:1805.12244
PRL, arXiv:1805.00013
PRD, arXiv:1805.00020
NeurIPS, arXiv:1808.00973
physics.aps.org/articles/v11/90



The **surrogate for the likelihood ratio** used for inference

A 2-stage process:

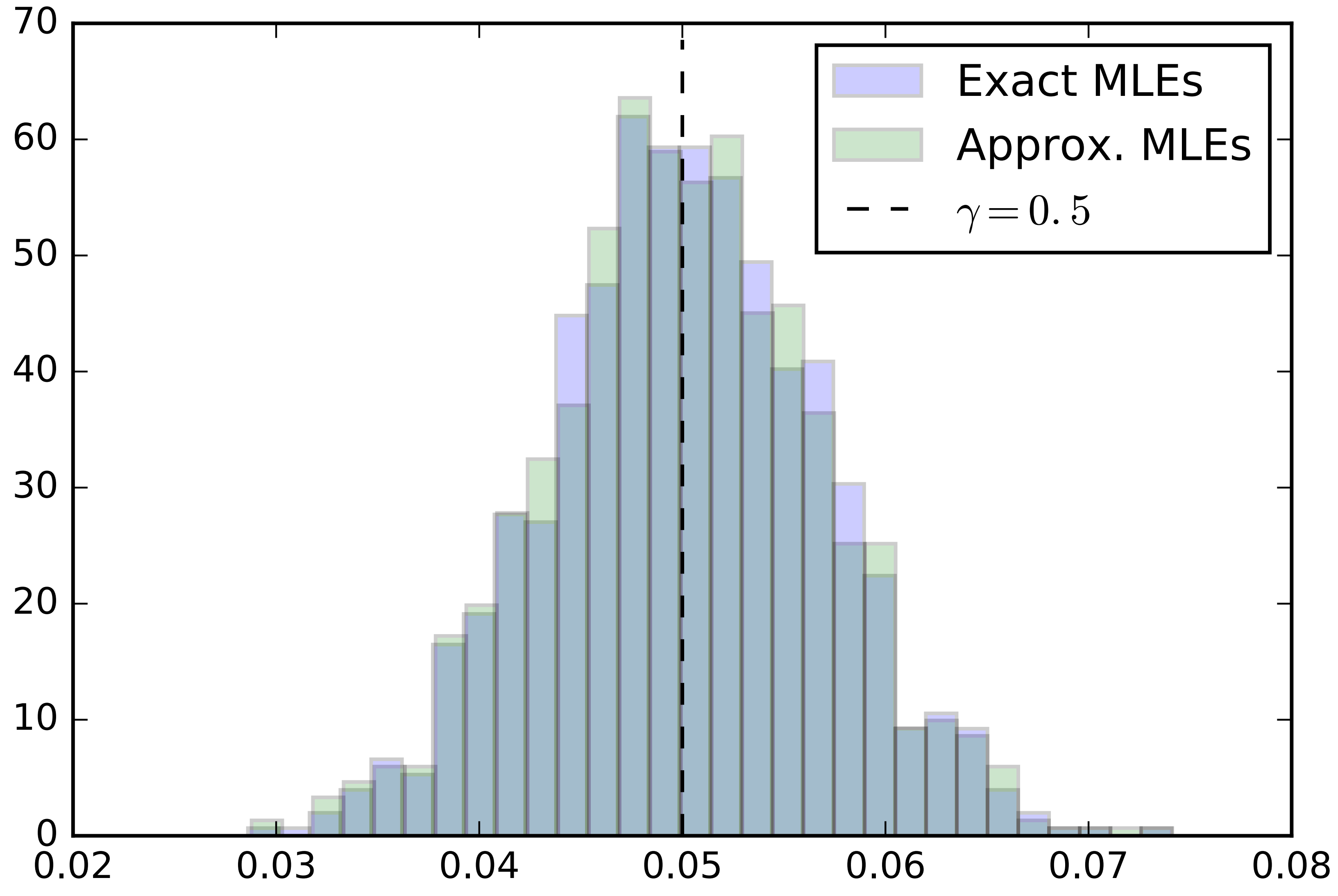
1. learning surrogate (**amortized**)
2. Inference on parameters of simulator (frequentist or Bayesian)

No Bayesian prior used for training, but one can use prior for inference.

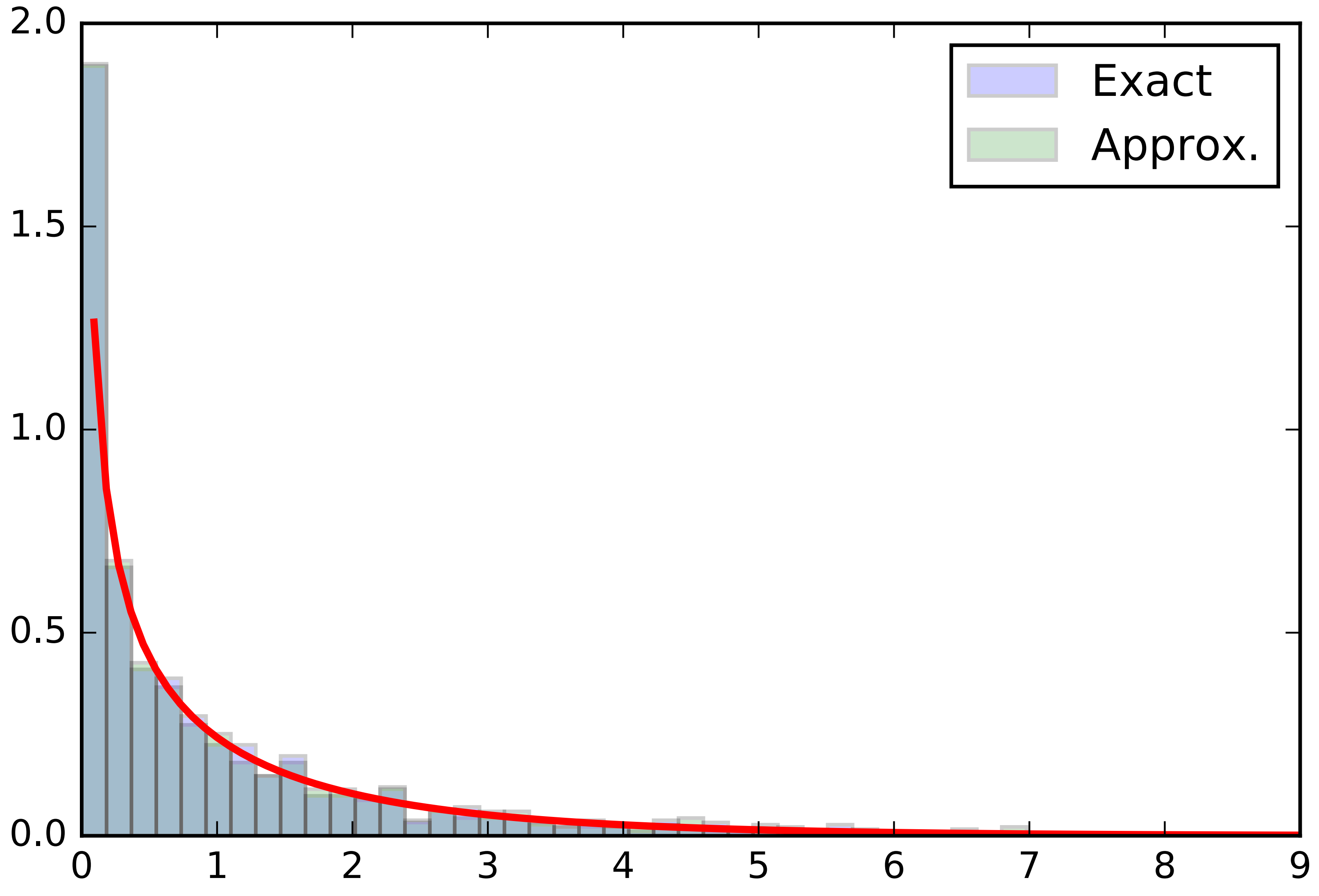
Amortized likelihood ratio

Once we've learned the likelihood ratio $r(x;\theta)$, we can apply it to any data x.

- unlike ABC, we pay biggest computational costs up front
- Great for calibrated frequentist confidence intervals with guaranteed coverage
- Here we repeat inference thousands of times & check asymptotic statistical theory



(a) Exact vs. approximated MLEs.



(b) $p(-2 \log \Lambda(\gamma = 0.05) \,|\, \gamma = 0.05)$

K.C., G. Louppe, J. Pavez: http://arxiv.org/abs/1506.02169

Calibrating the likelihood-ratio trick

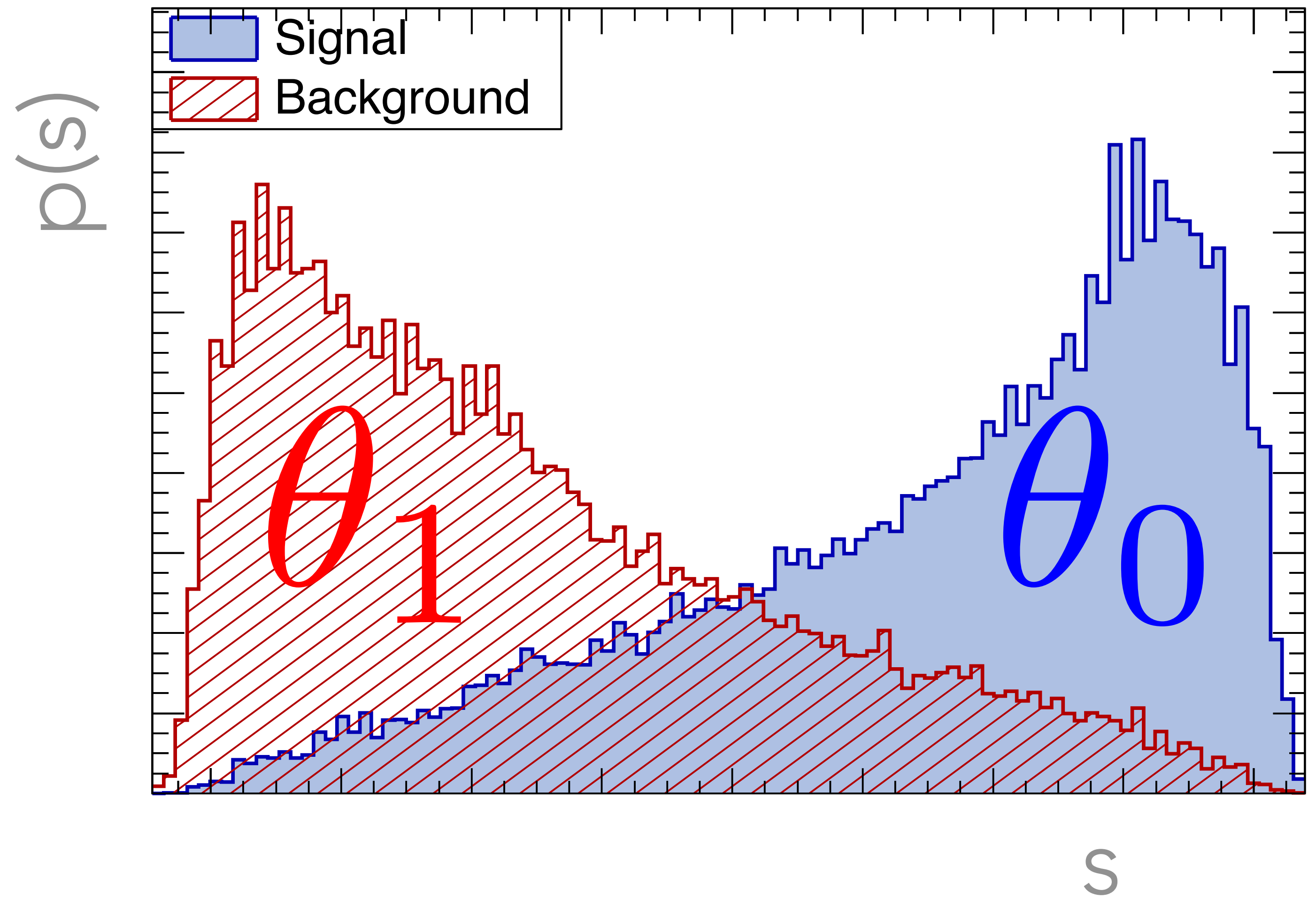
We can weaken the requirements for the likelihood ratio trick in case the classifier

If the scalar map s: X → ℝ has the same level sets as the likelihood ratio

$$s(x;\theta_0;\theta_1) = \text{monotonic}[\ p(x|\theta_0)/p(x|\theta_1)\ ]$$

We can show that an **equivalent test** can be made from 1-D projection

$$\frac{p(x|\theta_0)}{p(x|\theta_1)} = \frac{p(s(x;\theta_0,\theta_1)|\theta_0)}{p(s(x;\theta_0,\theta_1)|\theta_1)}$$



Estimating the density of $s(x;\theta_0,\theta_1)$ with data from the simulator calibrates the ratio.

Cranmer, Louppe, Pavez: Approximating Likelihood Ratios with Calibrated Discriminative Classifiers [arXiv:1506.02169]
[Dalmasso, Izbicki, Lee, ICML2020 arXiv:2002.10399]

Bayesian use of the likelihood ratio trick

Likelihood-free inference by ratio estimation

Owen Thomas[*], Ritabrata Dutta[†], Jukka Corander[*], Samuel Kaski[‡] and Michael U. Gutmann[§,¶]

Likelihood-free MCMC with Amortized Approximate Ratio Estimators

Joeri Hermans[1] Volodimir Begy[2] Gilles Louppe[1]

If reference distribution is marginal model

$$p_{\text{ref}}(x) = \int p(x \mid \theta) p(\theta) \, \mathrm{d}\theta$$

Then the learned ratio is proportional to the posterior

$$r(x;\theta) = \frac{p(x \mid \theta)}{p(x)} = \frac{p(\theta \mid x)}{p(\theta)}$$

and the prior is known

$$p(\theta \mid x) = p(\theta) r(x;\theta)$$

Use of likelihood ratio in MCMC

- Metropolis-Hastings

$$\rho = \min\left(1, \frac{p(\boldsymbol{\theta}')p(\mathbf{x} \mid \boldsymbol{\theta}')}{p(\boldsymbol{\theta}_t)p(\mathbf{x} \mid \boldsymbol{\theta}_t)} \frac{q(\boldsymbol{\theta}' \mid \boldsymbol{\theta}_t)}{q(\boldsymbol{\theta}_t \mid \boldsymbol{\theta}')}\right)$$

- Hamiltonian Monte Carlo

$$\nabla_{\boldsymbol{\theta}} U(\boldsymbol{\theta}) = -\frac{\nabla_{\boldsymbol{\theta}} r(\mathbf{x} \mid \boldsymbol{\theta})}{r(\mathbf{x} \mid \boldsymbol{\theta})}.$$

Thomas et. Al, Bayesian Analysis (2020) arXiv:1611.10242

Hermans, Begy, Louppe ICML 2020,arXiv:1903.04057

Bayesian use of the likelihood ratio trick

Likelihood-free inference by ratio estimation

Owen Thomas*, Ritabrata Dutta†, Jukka Corander*, Samuel Kaski‡ and Michael U. Gutmann§,¶

Likelihood-free MCMC with Amortized Approximate Ratio Estimators

Joeri Hermans [1] Volodimir Begy [2] Gilles Louppe [1]

If reference distribution is marginal model

$$p_{\text{ref}}(x) = \int p(x \mid \theta) p(\theta) \, \mathrm{d}\theta$$

Then the learned ratio is proportional to the posterior

$$r(x;\theta) = \frac{p(x \mid \theta)}{p(x)} = \frac{p(\theta \mid x)}{p(\theta)}$$

Posterior-to-evidence ratio

and the prior is known

$$p(\theta \mid x) = p(\theta) r(x;\theta)$$

Use of likelihood ratio in MCMC

- Metropolis-Hastings

$$\rho = \min\left(1, \frac{p(\boldsymbol{\theta}')p(\mathbf{x} \mid \boldsymbol{\theta}')}{p(\boldsymbol{\theta}_t)p(\mathbf{x} \mid \boldsymbol{\theta}_t)} \frac{q(\boldsymbol{\theta}' \mid \boldsymbol{\theta}_t)}{q(\boldsymbol{\theta}_t \mid \boldsymbol{\theta}')}\right)$$

- Hamiltonian Monte Carlo

$$\nabla_{\boldsymbol{\theta}} U(\boldsymbol{\theta}) = -\frac{\nabla_{\boldsymbol{\theta}} r(\mathbf{x} \mid \boldsymbol{\theta})}{r(\mathbf{x} \mid \boldsymbol{\theta})}.$$

Thomas et. Al, Bayesian Analysis (2020) arXiv:1611.10242

Hermans, Begy, Louppe ICML 2020,arXiv:1903.04057

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

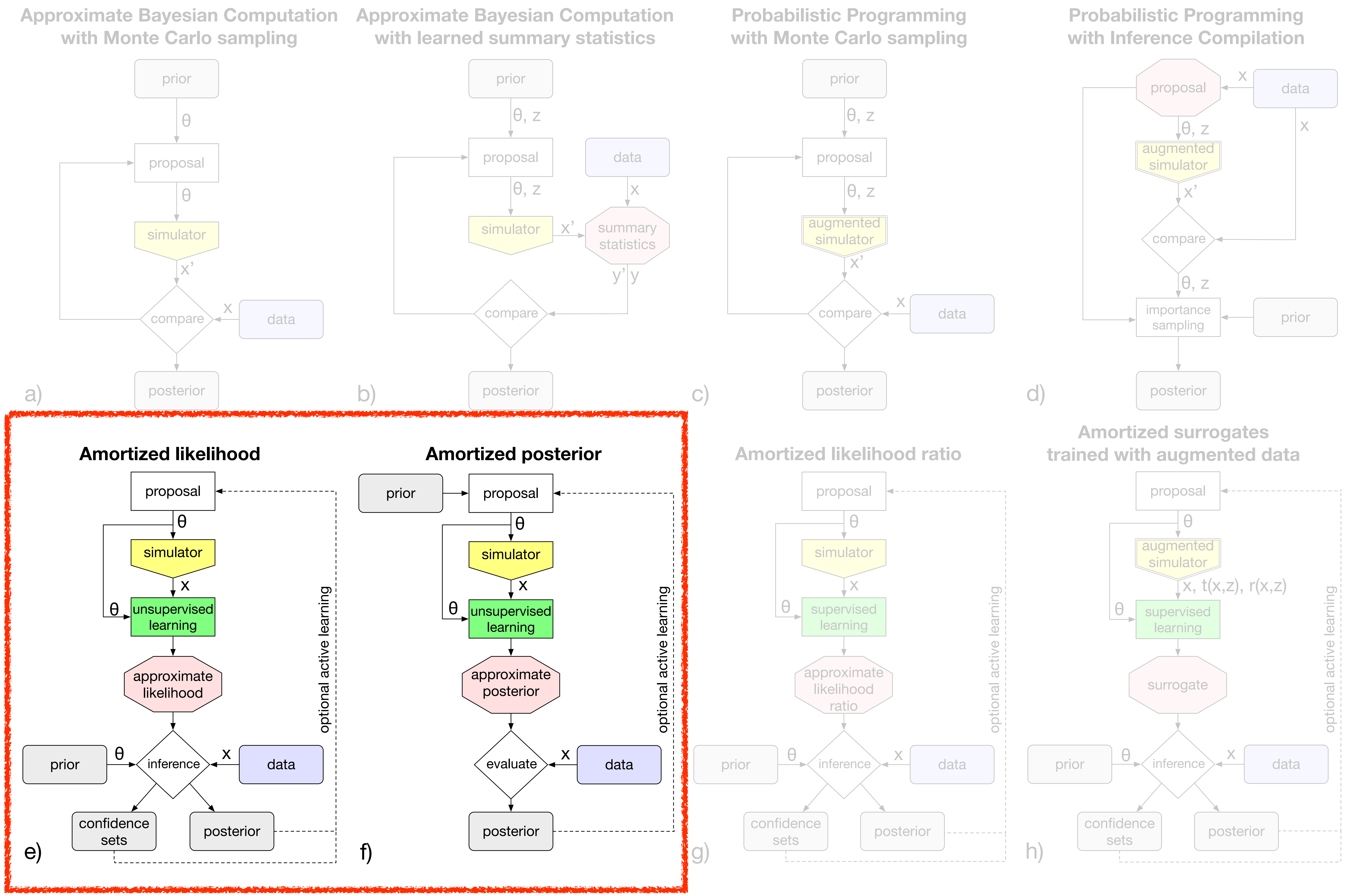


Fig. 3. Overview of different approaches to simulation-based inference.

From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

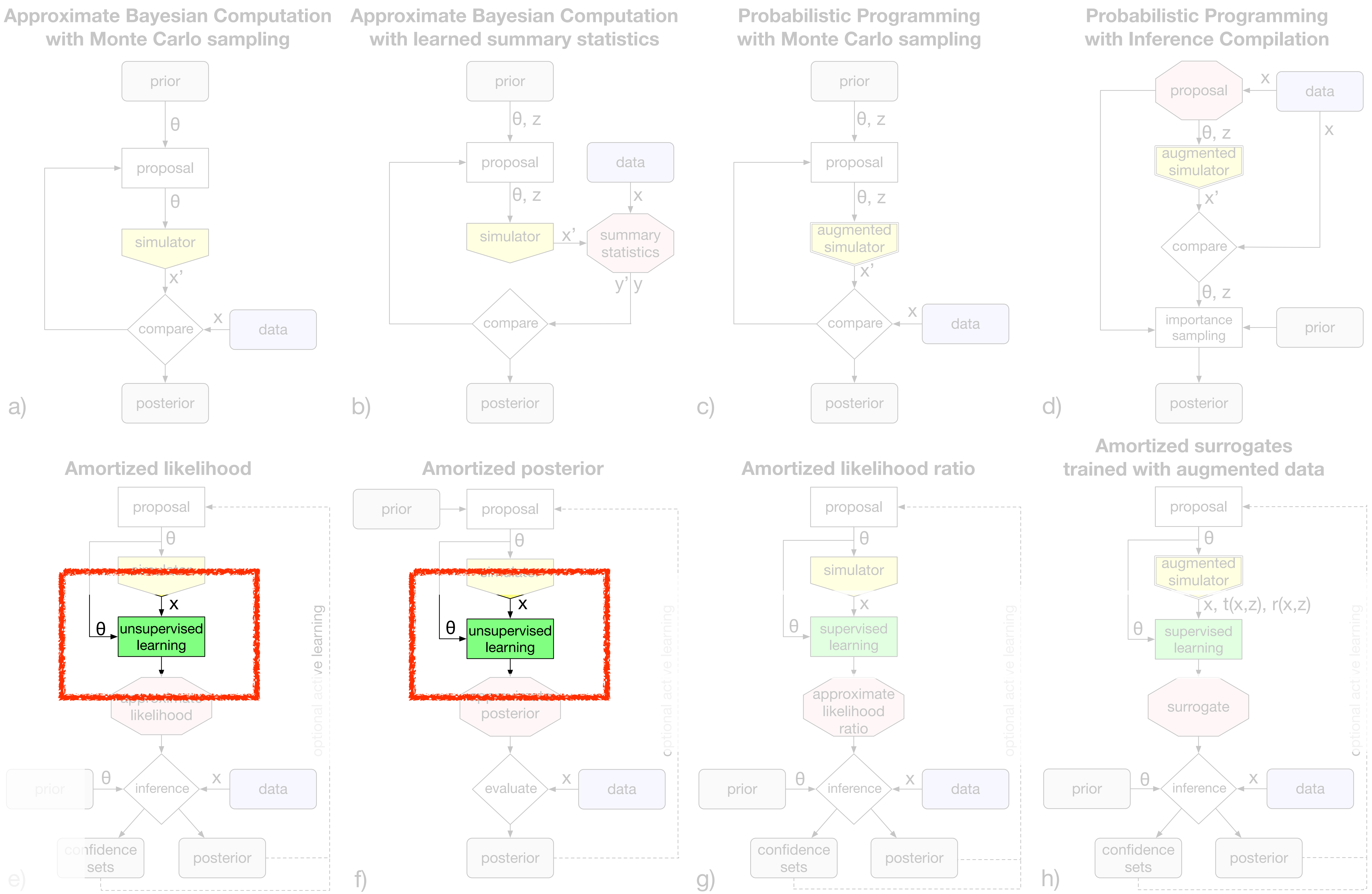
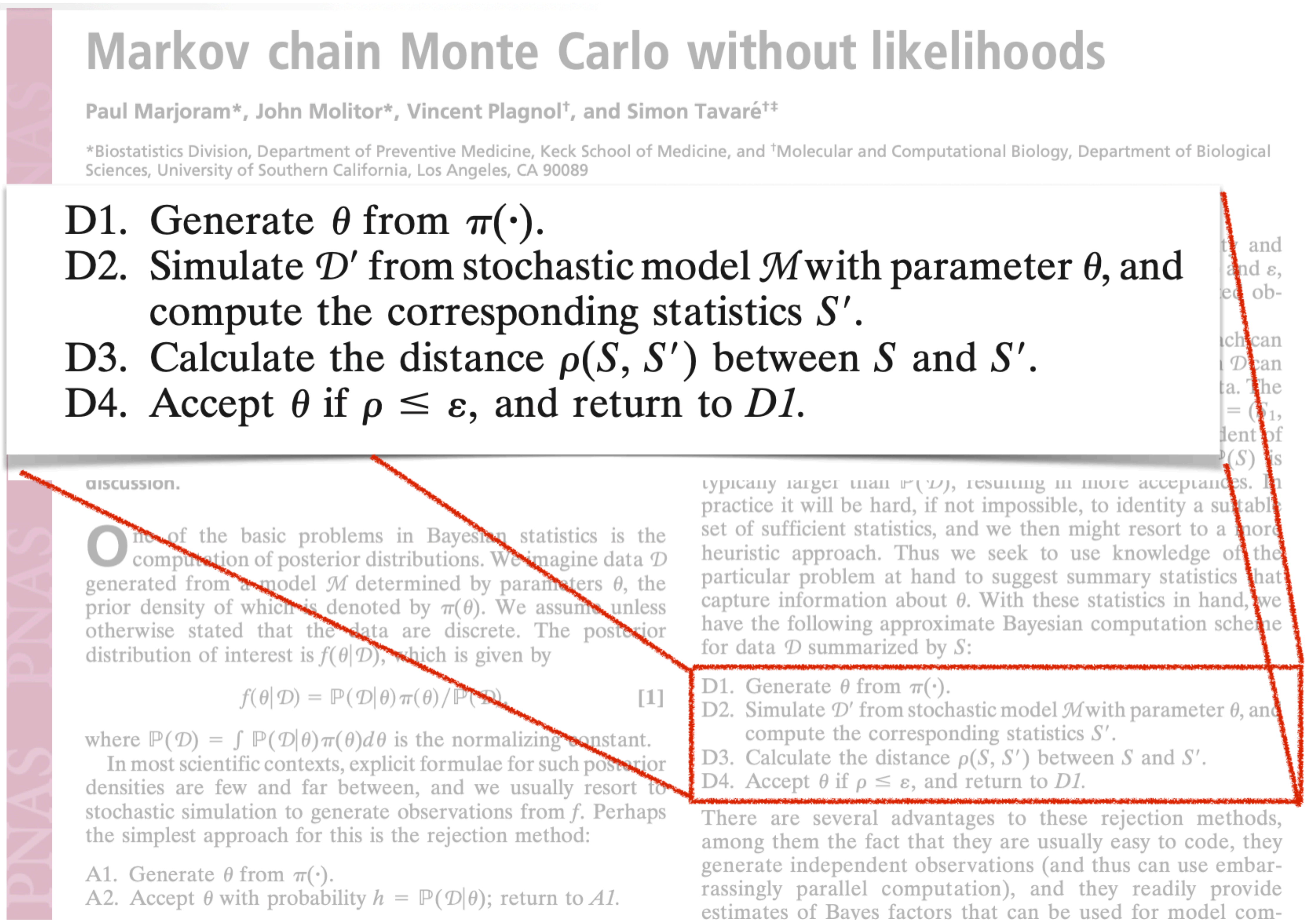


Fig. 3. Overview of different approaches to simulation-based inference.

Conditional Density Estimation

In traditional approaches to Simulation-Based Inference, one estimates the likelihood directly:

- For rejection ABC, the acceptance probability $\mathbb{P}(\rho(S, S') < \epsilon)$ estimates the likelihood
- In Diggle & Gratton (1984) and particle physics, histogram or kernel density estimate $p(S \mid \theta)$



Markov chain Monte Carlo without likelihoods

Paul Marjoram*, John Molitor*, Vincent Plagnol†, and Simon Tavaré†‡

*Biostatistics Division, Department of Preventive Medicine, Keck School of Medicine, and †Molecular and Computational Biology, Department of Biological Sciences, University of Southern California, Los Angeles, CA 90089

D1. Generate θ from $\pi(\cdot)$.
D2. Simulate $\mathcal{D}'$ from stochastic model $\mathcal{M}$ with parameter θ, and compute the corresponding statistics S'.
D3. Calculate the distance $\rho(S, S')$ between S and S'.
D4. Accept θ if $\rho \leq \varepsilon$, and return to *D1*.

One of the basic problems in Bayesian statistics is the computation of posterior distributions. We imagine data $\mathcal{D}$ generated from a model $\mathcal{M}$ determined by parameters θ, the prior density of which is denoted by $\pi(\theta)$. We assume unless otherwise stated that the data are discrete. The posterior distribution of interest is $f(\theta|\mathcal{D})$, which is given by

$$f(\theta|\mathcal{D}) = \mathbb{P}(\mathcal{D}|\theta)\pi(\theta)/\mathbb{P}(\mathcal{D}) \quad [1]$$

where $\mathbb{P}(\mathcal{D}) = \int \mathbb{P}(\mathcal{D}|\theta)\pi(\theta)d\theta$ is the normalizing constant.

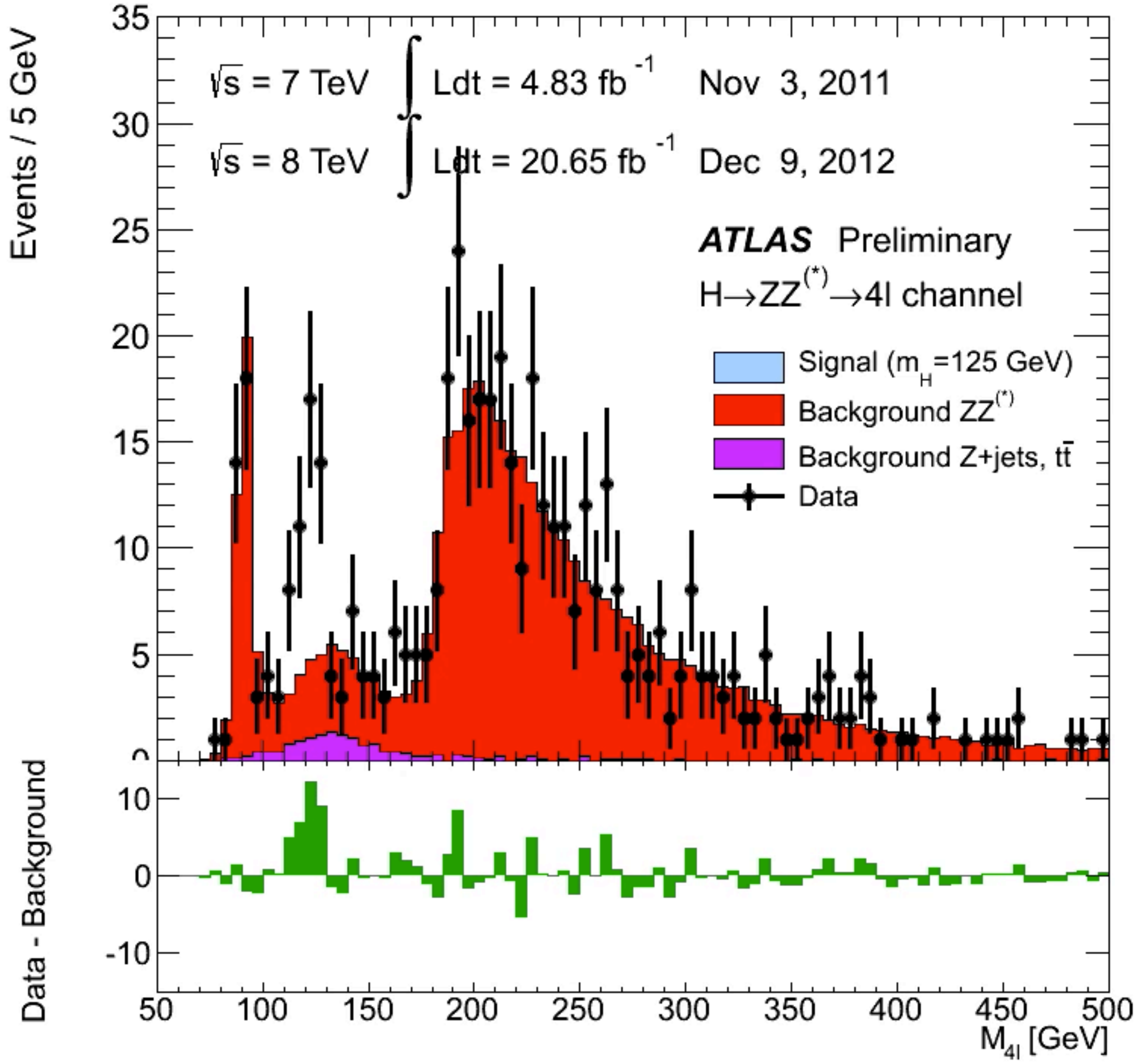
In most scientific contexts, explicit formulae for such posterior densities are few and far between, and we usually resort to stochastic simulation to generate observations from f. Perhaps the simplest approach for this is the rejection method:

A1. Generate θ from $\pi(\cdot)$.
A2. Accept θ with probability $h = \mathbb{P}(\mathcal{D}|\theta)$; return to *A1*.

... practice it will be hard, if not impossible, to identify a suitable set of sufficient statistics, and we then might resort to a more heuristic approach. Thus we seek to use knowledge of the particular problem at hand to suggest summary statistics that capture information about θ. With these statistics in hand, we have the following approximate Bayesian computation scheme for data $\mathcal{D}$ summarized by S:

D1. Generate θ from $\pi(\cdot)$.
D2. Simulate $\mathcal{D}'$ from stochastic model $\mathcal{M}$ with parameter θ, and compute the corresponding statistics S'.
D3. Calculate the distance $\rho(S, S')$ between S and S'.
D4. Accept θ if $\rho \leq \varepsilon$, and return to *D1*.

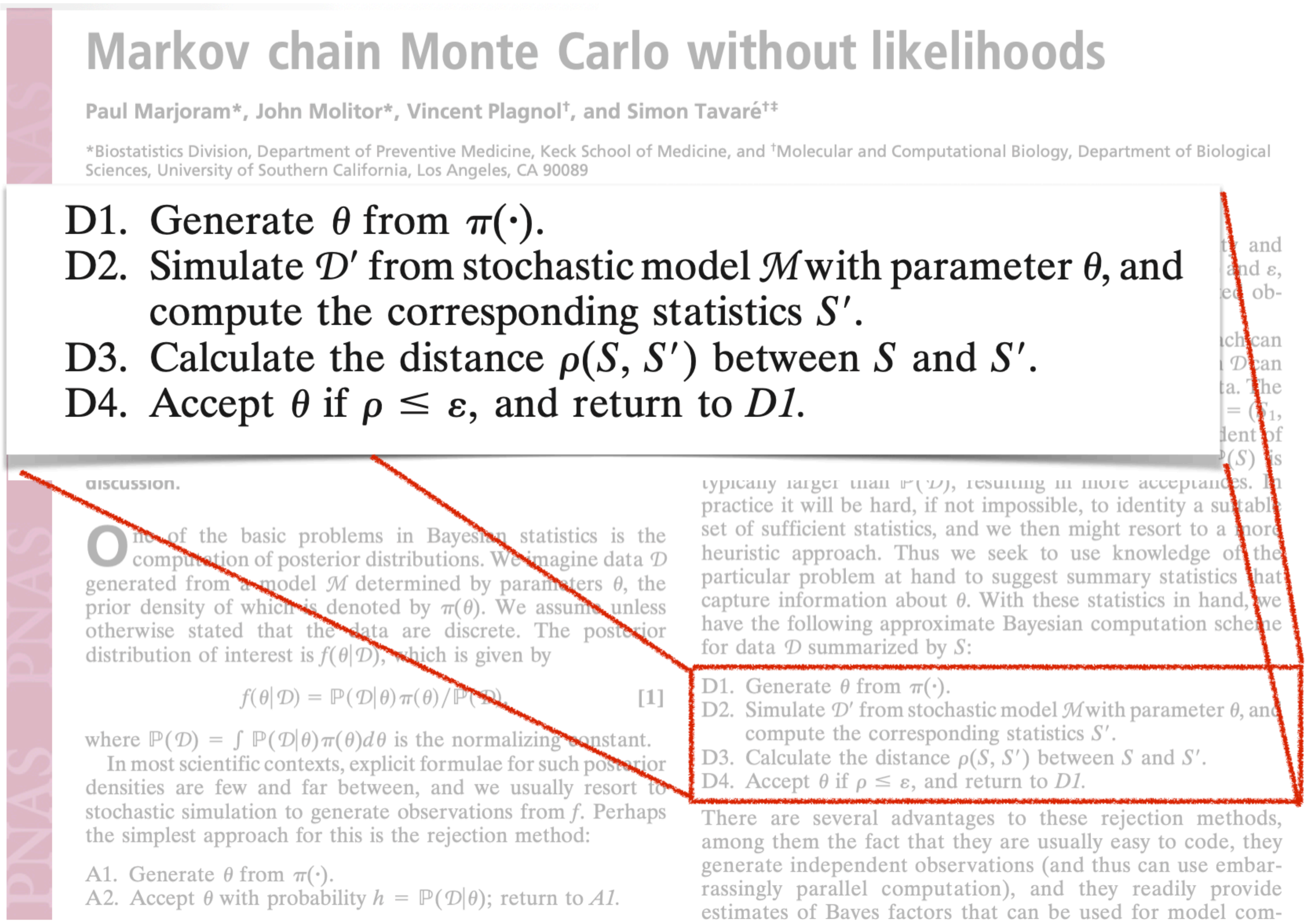
There are several advantages to these rejection methods, among them the fact that they are usually easy to code, they generate independent observations (and thus can use embarrassingly parallel computation), and they readily provide estimates of Bayes factors that can be used for model com-



Conditional Density Estimation

In traditional approaches to Simulation-Based Inference, one estimates the likelihood directly:

- For rejection ABC, the acceptance probability $\mathbb{P}(\rho(S, S') < \epsilon)$ estimates the likelihood
- In Diggle & Gratton (1984) and particle physics, histogram or kernel density estimate $p(S \mid \theta)$



Markov chain Monte Carlo without likelihoods

Paul Marjoram*, John Molitor*, Vincent Plagnol†, and Simon Tavaré†‡

*Biostatistics Division, Department of Preventive Medicine, Keck School of Medicine, and †Molecular and Computational Biology, Department of Biological Sciences, University of Southern California, Los Angeles, CA 90089

D1. Generate θ from $\pi(\cdot)$.
D2. Simulate $\mathcal{D}'$ from stochastic model $\mathcal{M}$ with parameter θ, and compute the corresponding statistics S'.
D3. Calculate the distance $\rho(S, S')$ between S and S'.
D4. Accept θ if $\rho \leq \varepsilon$, and return to *D1.*

discussion.

One of the basic problems in Bayesian statistics is the computation of posterior distributions. We imagine data $\mathcal{D}$ generated from a model $\mathcal{M}$ determined by parameters θ, the prior density of which is denoted by $\pi(\theta)$. We assume, unless otherwise stated, that the data are discrete. The posterior distribution of interest is $f(\theta|\mathcal{D})$, which is given by

$$f(\theta|\mathcal{D}) = \mathbb{P}(\mathcal{D}|\theta)\pi(\theta)/\mathbb{P}(\mathcal{D}) \quad [1]$$

where $\mathbb{P}(\mathcal{D}) = \int \mathbb{P}(\mathcal{D}|\theta)\pi(\theta)d\theta$ is the normalizing constant.

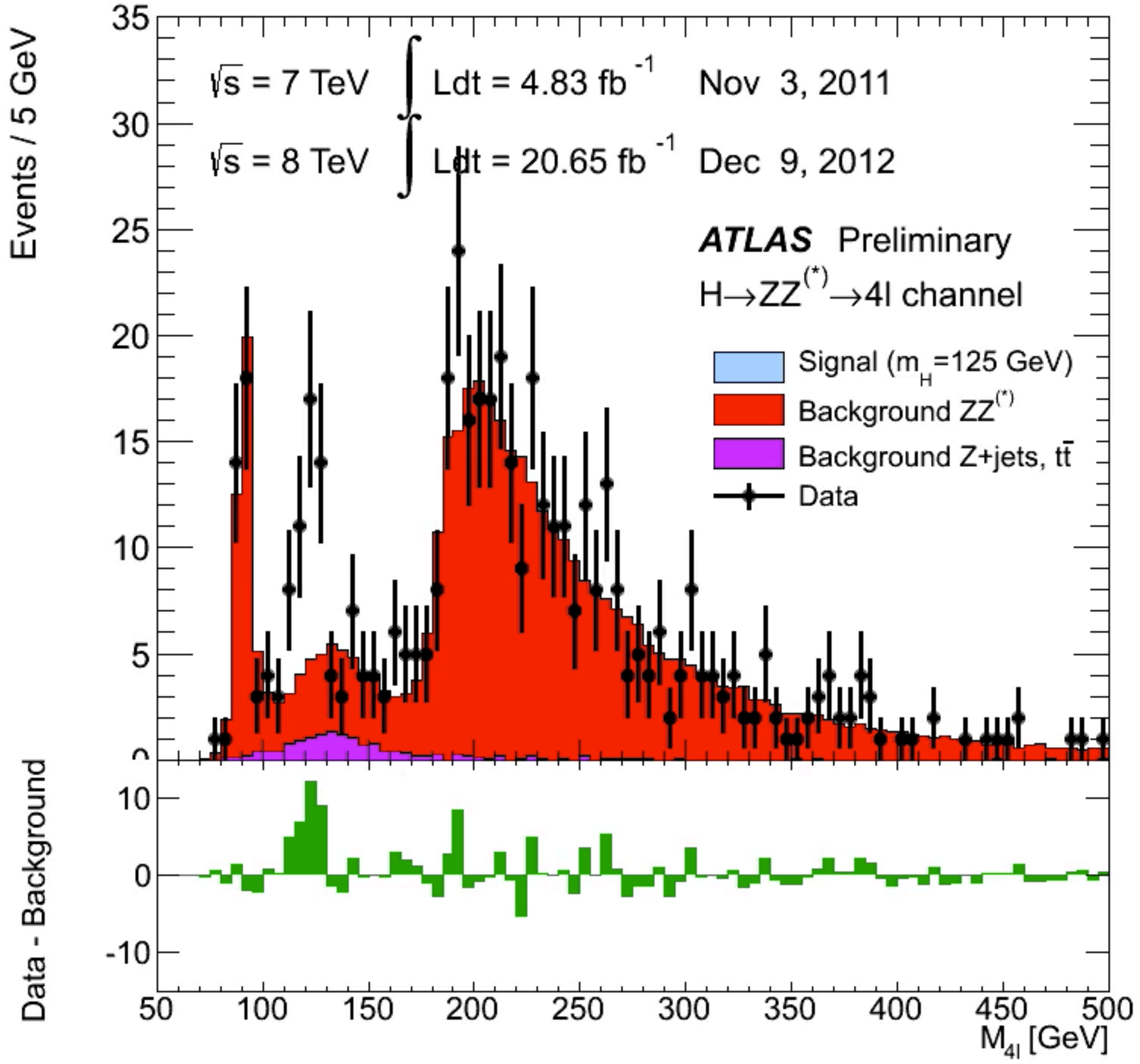
In most scientific contexts, explicit formulae for such posterior densities are few and far between, and we usually resort to stochastic simulation to generate observations from f. Perhaps the simplest approach for this is the rejection method:

A1. Generate θ from $\pi(\cdot)$.
A2. Accept θ with probability $h = \mathbb{P}(\mathcal{D}|\theta)$; return to *A1.*

typically larger than $\mathbb{P}(\mathcal{D})$, resulting in more acceptances. In practice it will be hard, if not impossible, to identify a suitable set of sufficient statistics, and we then might resort to a more heuristic approach. Thus we seek to use knowledge of the particular problem at hand to suggest summary statistics that capture information about θ. With these statistics in hand, we have the following approximate Bayesian computation scheme for data $\mathcal{D}$ summarized by S:

D1. Generate θ from $\pi(\cdot)$.
D2. Simulate $\mathcal{D}'$ from stochastic model $\mathcal{M}$ with parameter θ, and compute the corresponding statistics S'.
D3. Calculate the distance $\rho(S, S')$ between S and S'.
D4. Accept θ if $\rho \leq \varepsilon$, and return to *D1.*

There are several advantages to these rejection methods, among them the fact that they are usually easy to code, they generate independent observations (and thus can use embarrassingly parallel computation), and they readily provide estimates of Bayes factors that can be used for model com-



Neural likelihood

Cranmer, Louppe (2016). DOI:10.5281/zenodo.198541
Papamakarios, Sterratt, Murray AISTATS 2019 [arXiv:1805.07226]

Based on (θ_n, x_n) pairs with $x_n \sim p(x \mid \theta_n)$ estimate likelihood with a conditional density estimator $q_\phi(x \mid \theta)$

- Can sample $\theta_n \sim \tilde{p}(\theta)$ from any proposal distribution with appropriate support
- Leveraging advances in normalizing flows and neural density estimation

Unifying generative models and exact likelihood-free inference with conditional bijections

By *Kyle Cranmer*, *Gilles Louppe* J. Brief Ideas 2016

Sequential Neural Likelihood: Fast Likelihood-free Inference with Autoregressive Flows

George Papamakarios University of Edinburgh
David C. Sterratt University of Edinburgh
Iain Murray University of Edinburgh

AISTATS 2019

Neural posterior

Papamakarios, Murray NeurIPS 2016 arXiv:1605.06376

Based on (θ_n, x_n) pairs with $\theta_n \sim p(\theta)$ and $x_n \sim p(x \mid \theta_n)$ estimate posterior with a conditional density estimator $q_\phi(\theta \mid x)$

- Originally used a Mixture Density Network (MDN) to model $q_\phi(\theta \mid x)$
- More recently using advances in normalizing flows
- Posterior samples can be drawn directly from the model!
- Can also sample $\theta_n \sim \tilde{p}(\theta)$ and learn $q_\phi(\boldsymbol{\theta} \mid \mathbf{x}) \propto \frac{\tilde{p}(\boldsymbol{\theta})}{p(\boldsymbol{\theta})} p(\boldsymbol{\theta} \mid \mathbf{x})$

Fast ϵ-free Inference of Simulation Models with Bayesian Conditional Density Estimation

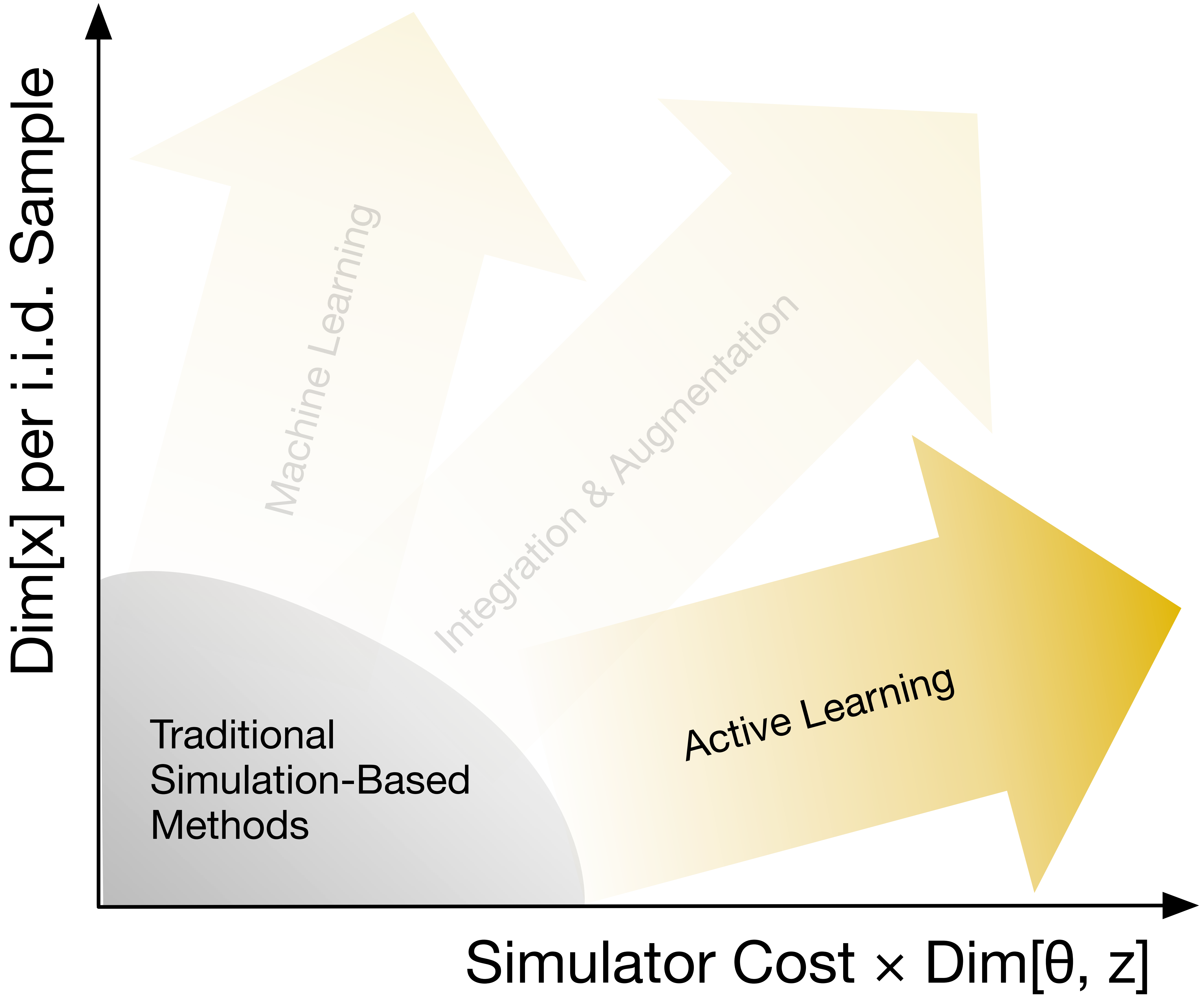
George Papamakarios
School of Informatics
University of Edinburgh
g.papamakarios@ed.ac.uk

Iain Murray
School of Informatics
University of Edinburgh
i.murray@ed.ac.uk

Active learning and sequential methods

Can we learn more efficiently for a fixed simulation budget ?

- What if we are smart about where we run the simulator?



From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

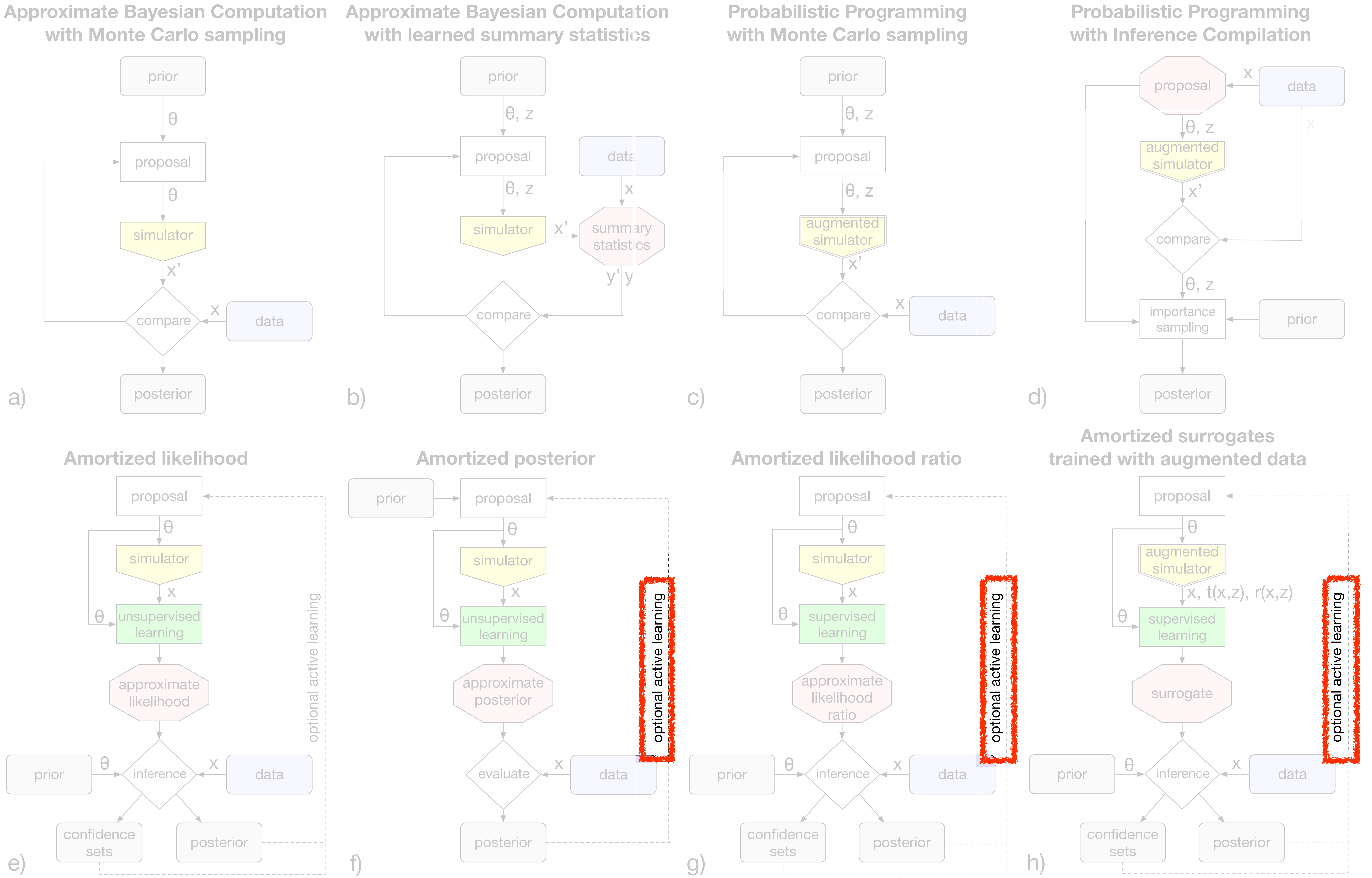


Fig. 3. Overview of different approaches to simulation-based inference.

Sequential Methods

When the posterior concentrates significantly compared to the prior, then we don't really need to estimate the likelihood accurately everywhere

- Instead, want to estimate likelihood or posterior only in the **relevant regions** of parameter / data space
- Motivates active learning / sequential techniques
- **Iteratively** estimate posterior $\tilde{p}(\theta \mid x_0)$, sample $\theta_n \sim \tilde{p}(\theta \mid x_0)$, $x_n \sim p(x \mid \theta_n)$, and then **refine**

Sequential Neural Likelihood Estimation [SNLE]

Sequential Neural Posterior Estimation [SNPE]

Sequential Neural Ratio Estimation [SNRE]

- Various sequential strategies

Sequential Neural Likelihood:
Fast Likelihood-free Inference with Autoregressive Flows

George Papamakarios, University of Edinburgh; David C. Sterratt, University of Edinburgh; Iain Murray, University of Edinburgh

Automatic Posterior Transformation for Likelihood-free Inference

David S. Greenberg [1] Marcel Nonnenmacher [1] Jakob H. Macke [1]

Likelihood-free MCMC with Amortized Approximate Ratio Estimators

Joeri Hermans [1] Volodimir Begy [2] Gilles Louppe [1]

On Contrastive Learning for Likelihood-free Inference

Conor Durkan [1] Iain Murray [1] George Papamakarios [2]

$$\tilde{p}(\theta|x) = p(\theta|x)\frac{\tilde{p}(\theta)\, p(x)}{p(\theta)\, \tilde{p}(x)}$$

Sequential Neural Posterior Estimation (SNPE, Papamakarios & Murray, 2016; Lueckmann et al., 2017; Greenberg et al., 2019),

Sequential Methods

When the posterior concentrates significantly compared to the prior, then we don't really need to estimate the likelihood accurately everywhere

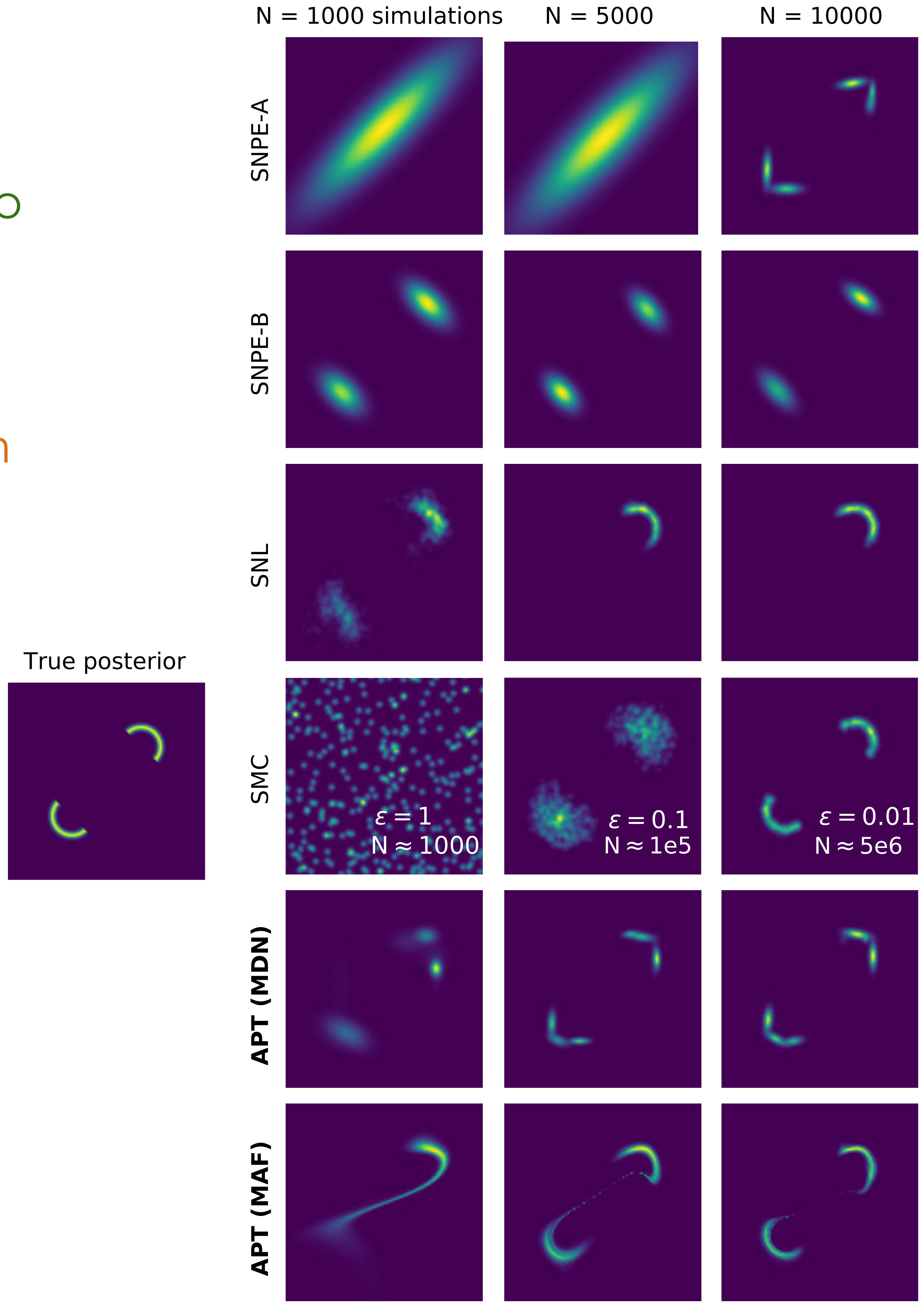
- Instead, want to estimate likelihood or posterior only in the **relevant regions** of parameter / data space
- Motivates active learning / sequential techniques
- **Iteratively** estimate posterior $\tilde{p}(\theta \mid x_0)$, sample $\theta_n \sim \tilde{p}(\theta \mid x_0)$, $x_n \sim p(x \mid \theta_n)$, and then **refine**

Sequential Neural Likelihood Estimation [SNLE]

Sequential Neural Posterior Estimation [SNPE]

Sequential Neural Ratio Estimation [SNRE]

- Various sequential strategies



Software

sbi: A toolkit for simulation-based inference

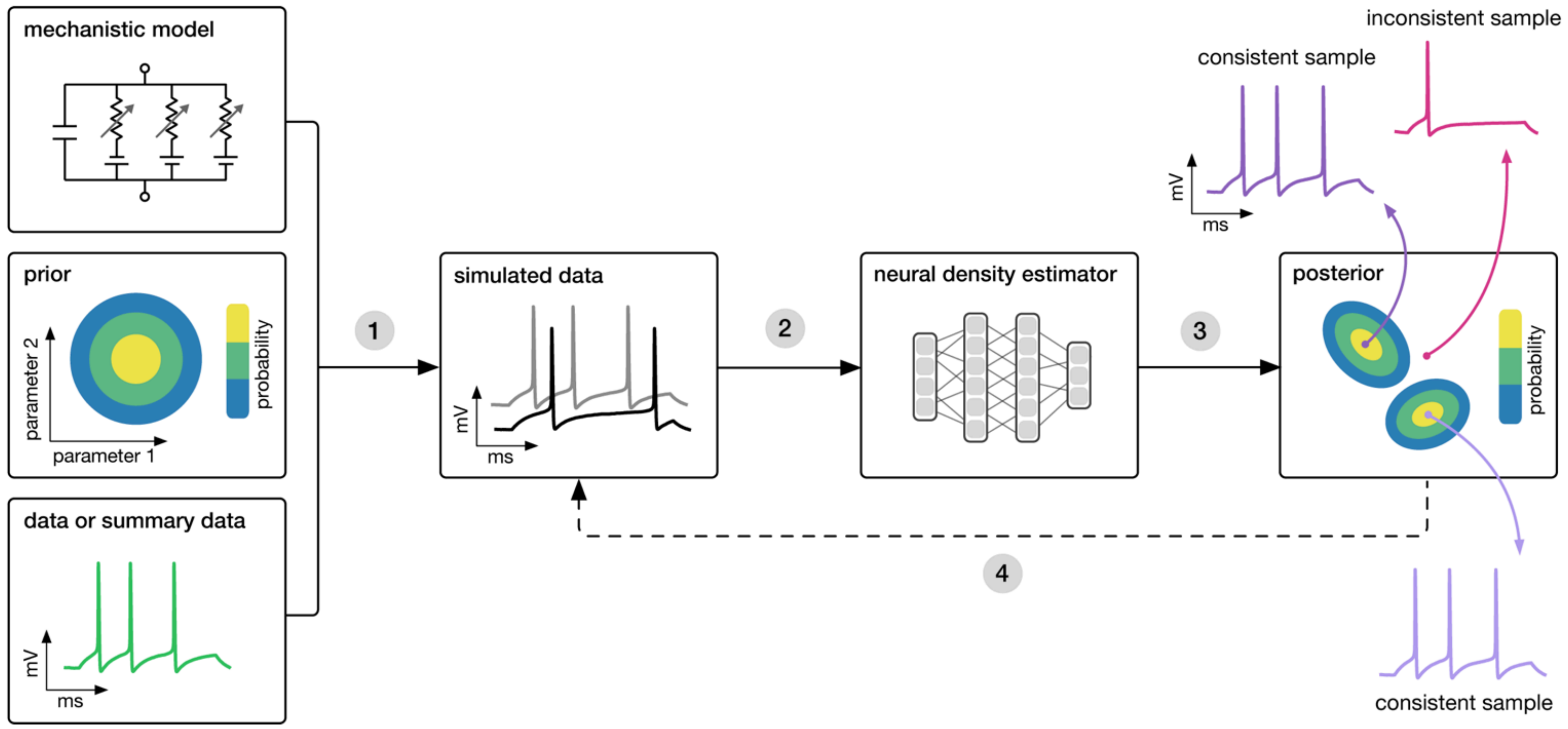
Alvaro Tejero-Cantero[e, 1], **Jan Boelts**[e, 1], **Michael Deistler**[e, 1], **Jan-Matthis Lueckmann**[e, 1], **Conor Durkan**[e, 2], **Pedro J. Gonçalves**[1, 3], **David S. Greenberg**[1, 4], and **Jakob H. Macke**[1, 5, 6]

The Journal of Open Source Software

`sbi` implements three powerful machine-learning methods that address this problem:

- Sequential Neural Posterior Estimation (SNPE),
- Sequential Neural Likelihood Estimation (SNLE), and
- Sequential Neural Ratio Estimation (SNRE).

Depending on the characteristics of the problem, e.g. the dimensionalities of the parameter space and the observation space, one of the methods will be more suitable.

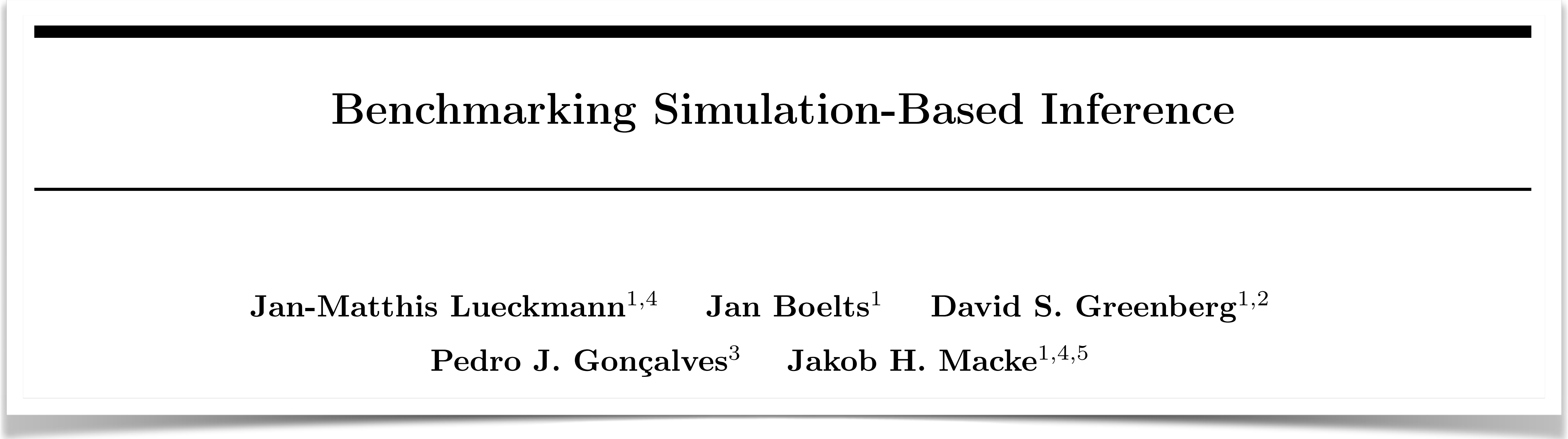


Goal: Algorithmically identify mechanistic models which are consistent with data.

Table of contents

https://www.mackelab.org/sbi/

Benchmarking

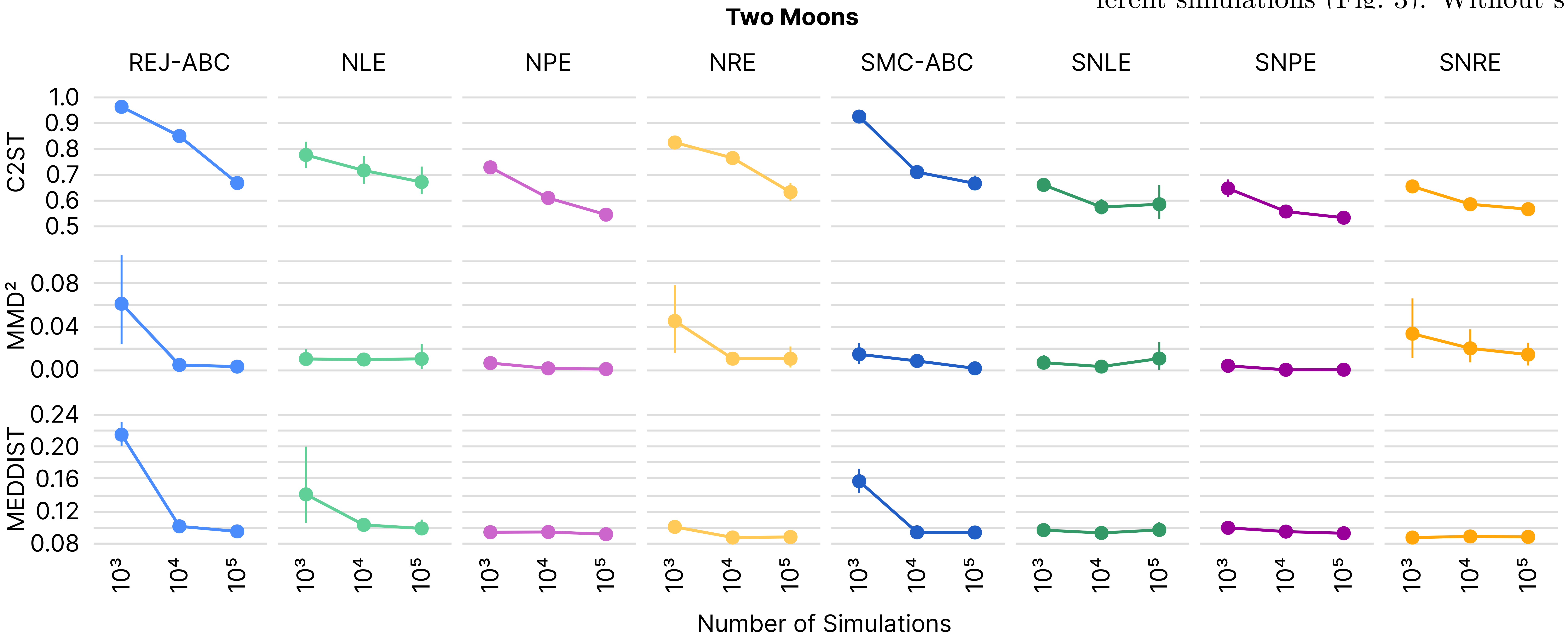


Benchmarking Simulation-Based Inference

Jan-Matthis Lueckmann[1,4] Jan Boelts[1] David S. Greenberg[1,2]
Pedro J. Gonçalves[3] Jakob H. Macke[1,4,5]

#3: Sequential estimation improves sample efficiency. Our results show that sequential algorithms outperform non-sequential ones (Fig. 3). The difference was small on simple tasks (i.e. linear Gaussian cases), yet pronounced on most others. However, we also found these methods to exhibit diminishing returns as the simulation budget grows, which points to an opportunity for future improvements.

#4: Density or ratio estimation-based algorithms generally outperform classical techniques. REJ-ABC and SMC-ABC were generally outperformed by more recent techniques which use neural networks for density- or ratio-estimation, and which can therefore efficiently interpolate between different simulations (Fig. 3). Without such model-based

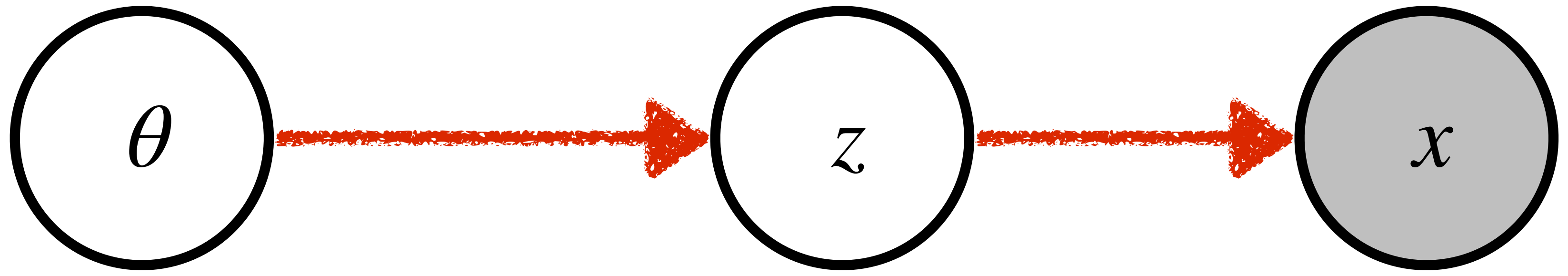


Single observation

When dealing with a single observation, there is a clear advantage to sequential techniques

- Use simulation budget in relevant regions of parameter space

#3: Sequential estimation improves sample efficiency. Our results show that sequential algorithms outperform non-sequential ones (Fig. 3). The difference was small on simple tasks (i.e. linear Gaussian cases), yet pronounced on most others. However, we also found these methods to exhibit diminishing returns as the simulation budget grows, which points to an opportunity for future improvements.



$$p(x, z \mid \theta) = p(x \mid z) p(z \mid \theta)$$

$$p(\theta \mid x) \propto \int \underbrace{p(\theta)}_{\text{prior}} \underbrace{p(x, z \mid \theta)}_{\text{likelihood}} \, dz$$

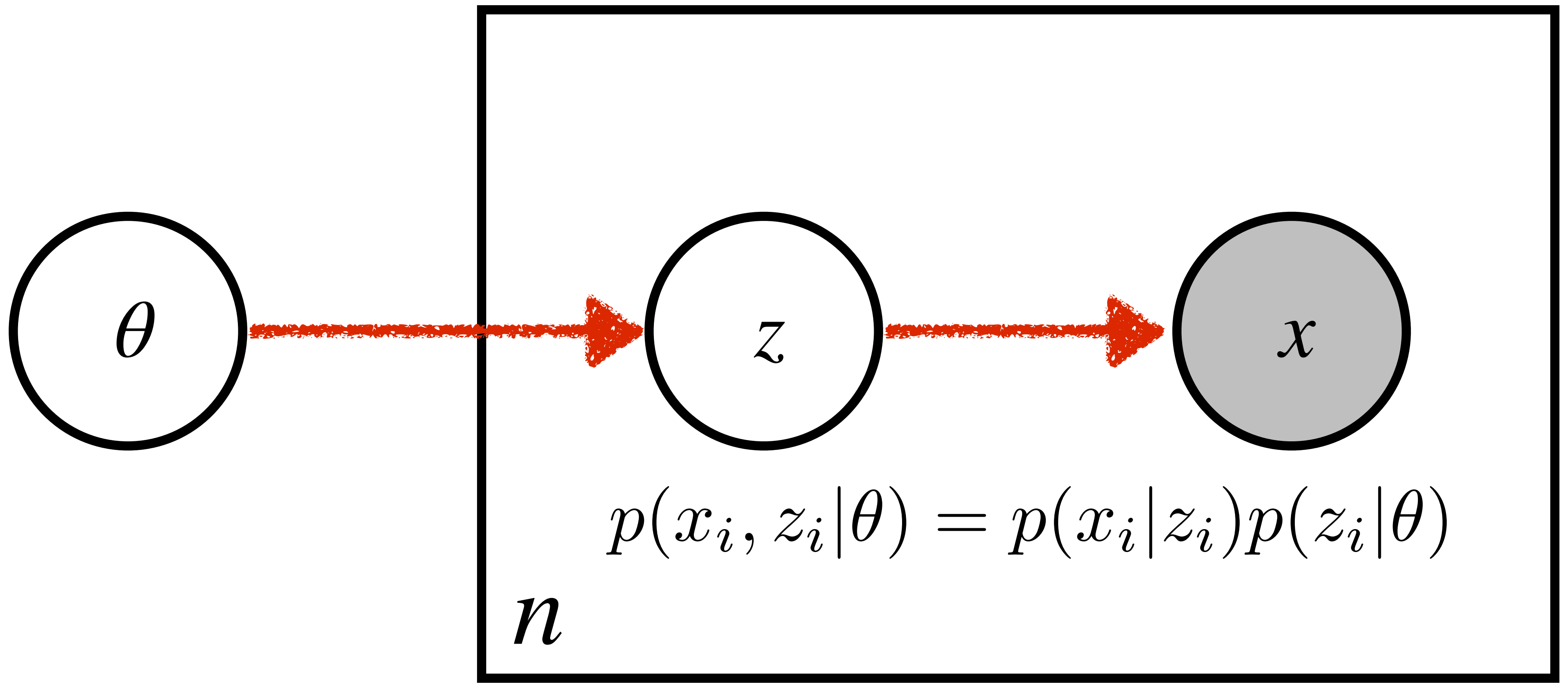
$$p(x \mid \theta) = \int p(x, z \mid \theta) dz$$

$$p(\theta \mid x) \propto \underbrace{p(\theta)}_{\text{prior}} \underbrace{p(x \mid \theta)}_{\text{likelihood}}$$

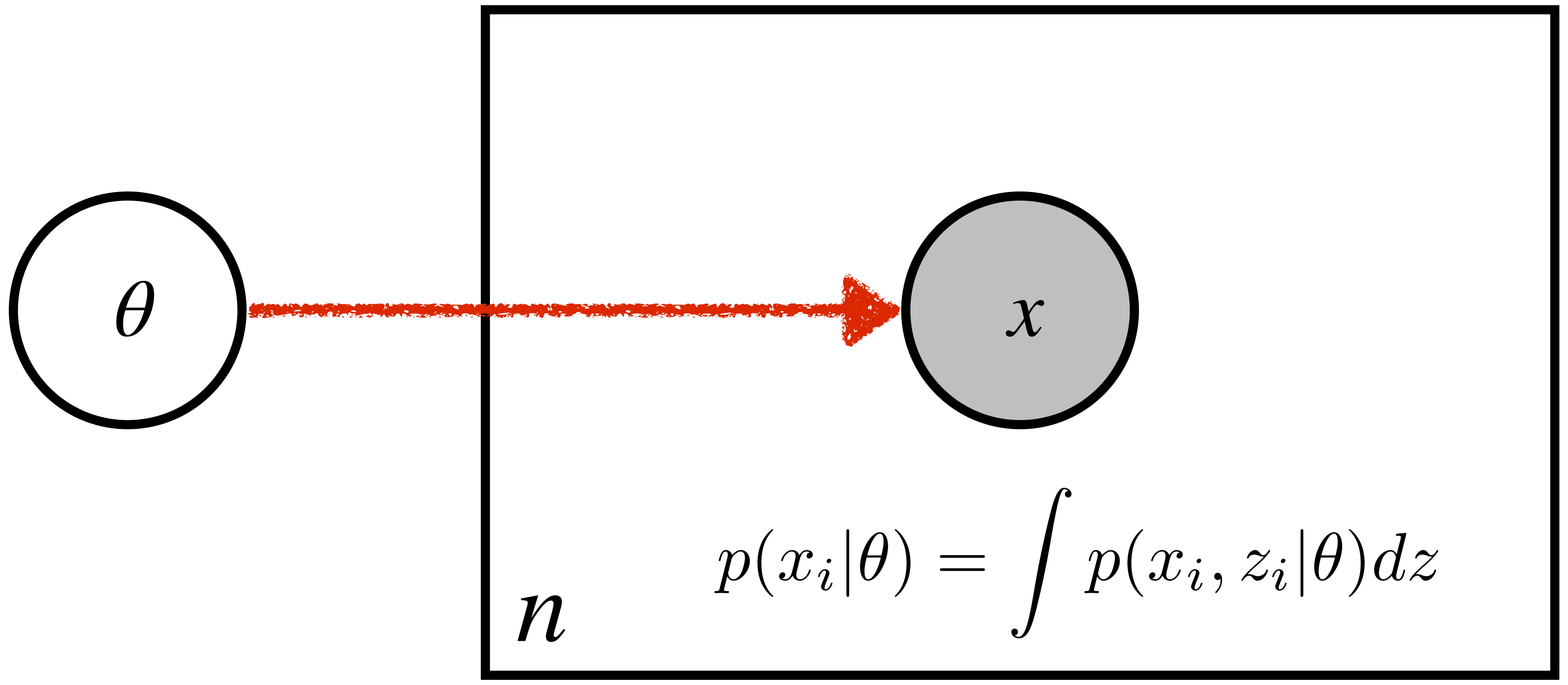
iid data and amortized likelihood

However, when dealing with iid data, there is a more advantage to learning an amortized likelihood ratio that is accurate everywhere and can be reused.

- More work needed to study tradeoff of sequential approaches with iid data



$$p(\theta \mid \{x_i\}) \propto \underbrace{p(\theta)}_{\text{prior}} \prod_{i=1}^{n} \left[\int \underbrace{p(x_i, z_i \mid \theta)}_{\text{joint likelihood}} \, dz_i \right]$$

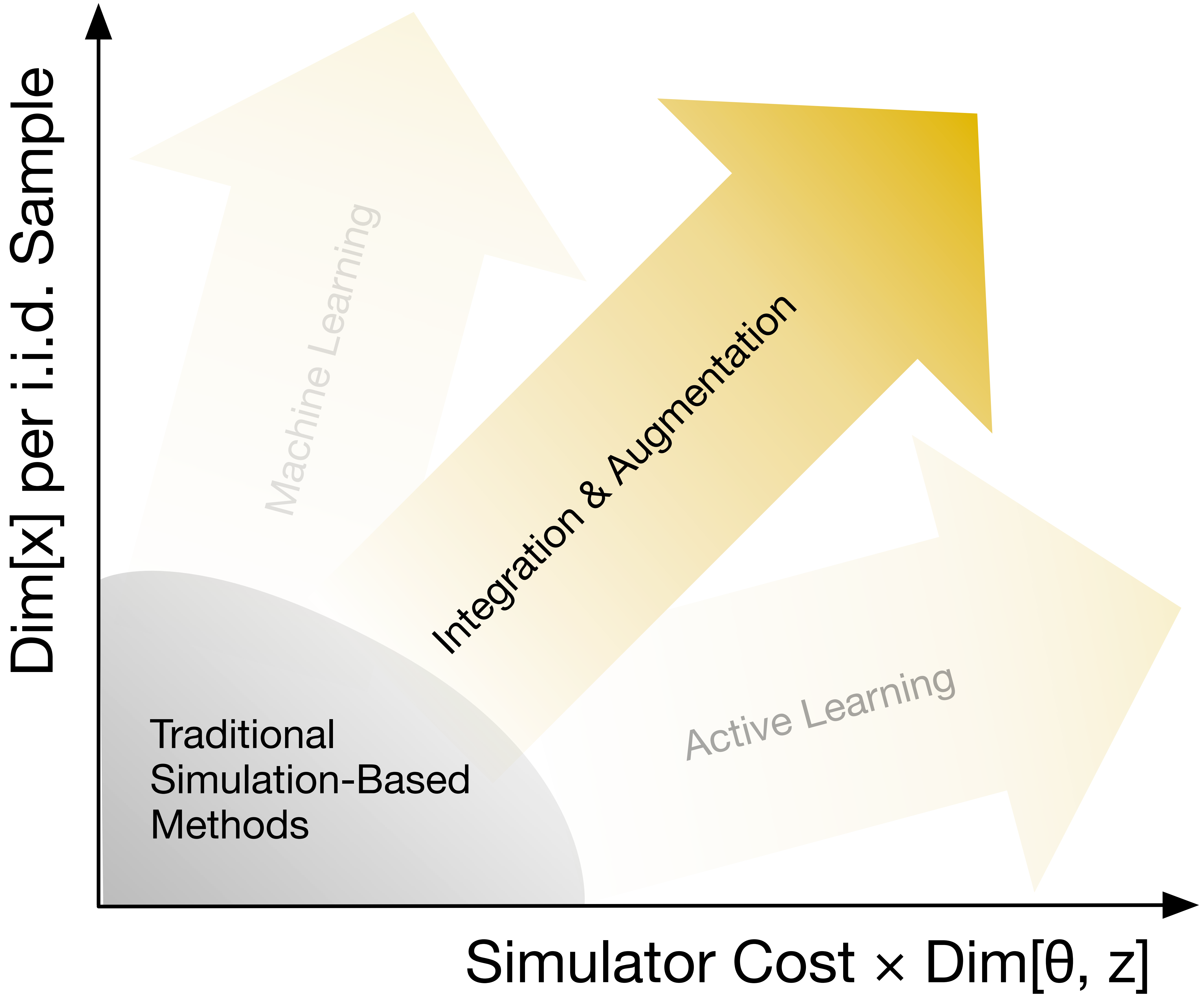


$$p(\theta \mid \{x_i\}) \propto \underbrace{p(\theta)}_{\text{prior}} \prod_{i=1}^{n} \left[\underbrace{p(x_i \mid \theta)}_{\text{amortized likelihood}} \right]$$

Opening the black box

Can we learn more efficiently for a fixed simulation budget?

- What if we open the black box?



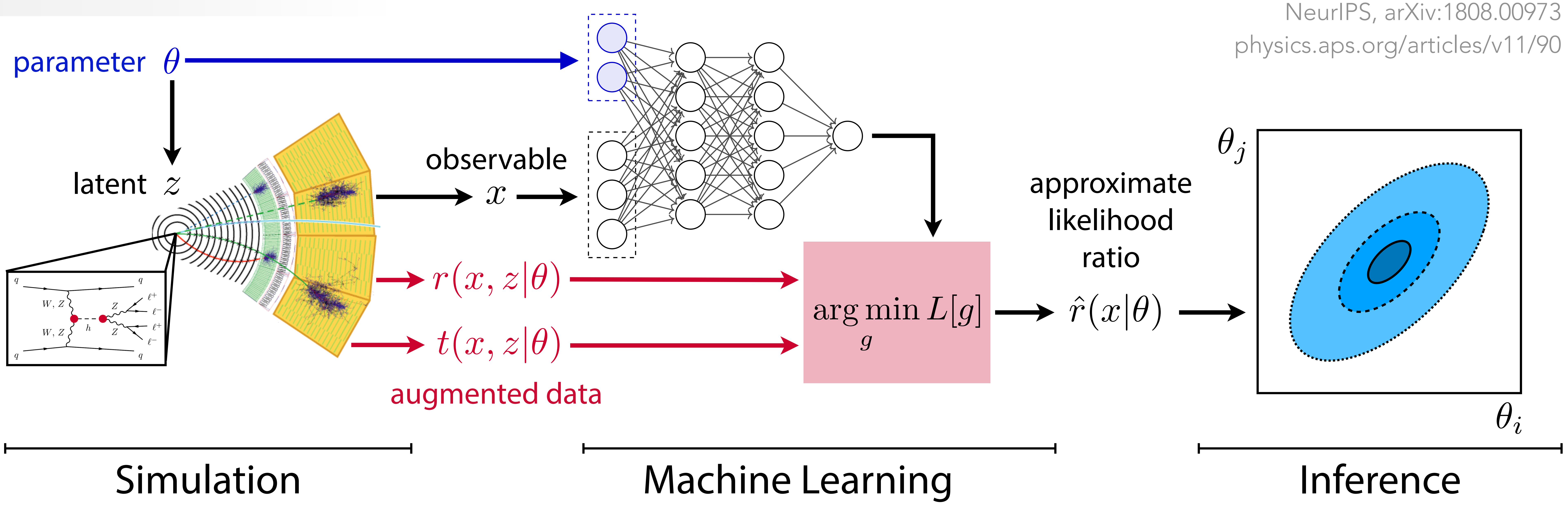
From the review

[Cranmer, J. Brehmer, G. Louppe, PNAS (2020), arXiv:1911.01429]

Fig. 3. Overview of different approaches to simulation-based inference.

Learning the likelihood ratio

PNAS, arXiv:1805.12244
PRL, arXiv:1805.00013
PRD, arXiv:1805.00020
NeurIPS, arXiv:1808.00973
physics.aps.org/articles/v11/90



Recently, we realized we can **extract more from the simulator**.
We can use **augmented data** to improve training

Johann Brehmer Gilles Louppe

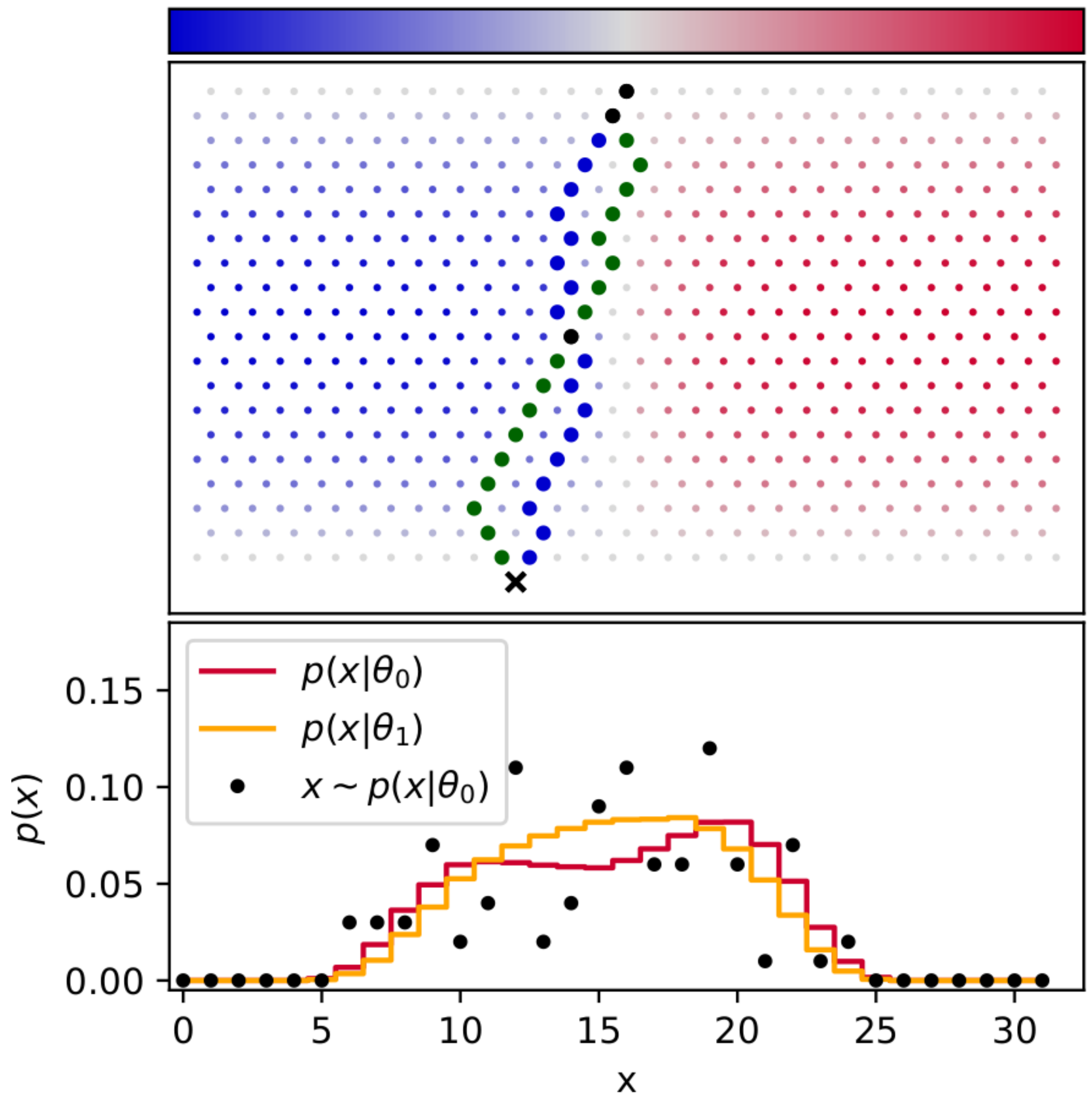
Mining Gold

Brehmer, Louppe, Pavez, KC, PNAS (2019), arXiv:1805.12244
See also Wenliang, Moskovitz, Kanagawa, Sahani, ICML2020

While implicit density is intractable

$$p(x|\theta) = \int dz p(x, z|\theta)$$

We can **augment the simulator** to calculate some quantities conditioned on latent z, which are tractable:



Joint likelihood ratio:

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

and joint score:

$$t(x, z|\theta_0) = \frac{\nabla_\theta p(x, z|\theta)|_{\theta_0}}{p(x, z|\theta_0)} = \nabla_\theta \log p(x, z|\theta)|_{\theta_0}$$

connection to REINFORCE policy gradients

The value of gold

We can calculate the joint likelihood ratio

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$

("How much more likely is this simulated event, including all intermediate states, for θ_0 compared to θ_1?")

We want the likelihood ratio function

$$r(x|\theta_0, \theta_1) \equiv \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

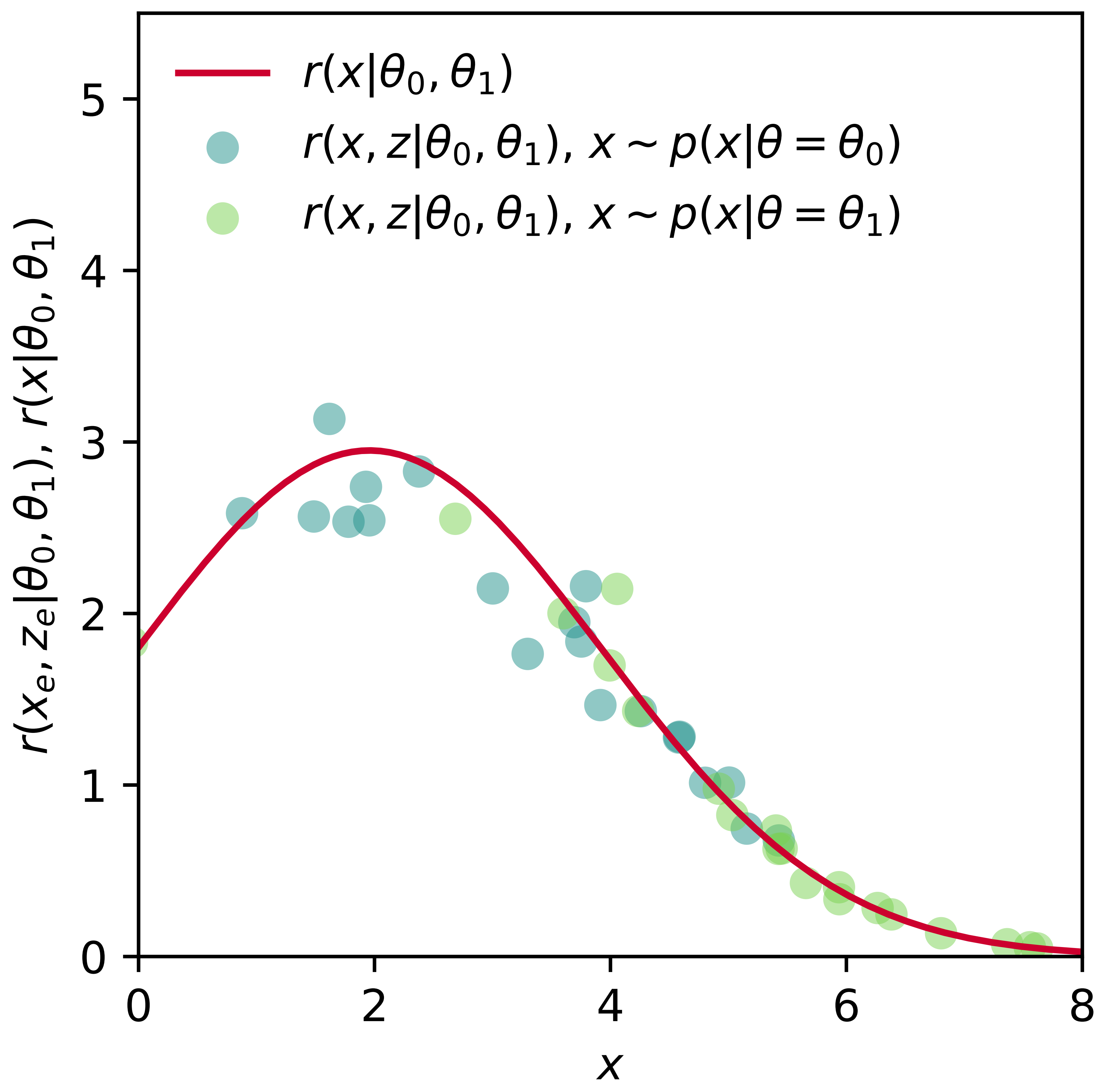
("How much more likely is the observation x for θ_0 compared to θ_1?")

The value of gold

We can calculate the joint likelihood ratio

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$

$r(x, z|\theta_0, \theta_1)$ are scattered around $r(x|\theta_0, \theta_1)$



We want the likelihood ratio function

$$r(x|\theta_0, \theta_1) \equiv \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

The value of gold

We can calculate the joint likelihood ratio

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$

We want the likelihood ratio function

$$r(x|\theta_0, \theta_1) \equiv \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

With $r(x, z|\theta_0, \theta_1)$, we define a functional like

$$L_r[\hat{r}(x|\theta_0, \theta_1)] = \int \mathrm{d}x \int \mathrm{d}z \; p(x, z|\theta_1) \left[\left(\hat{r}(x|\theta_0, \theta_1) - r(x, z|\theta_0, \theta_1) \right)^2 \right].$$

It is minimized by

$$r(x|\theta_0, \theta_1) = \arg\min_{\hat{r}(x|\theta_0, \theta_1)} L_r[\hat{r}(x|\theta_0, \theta_1)]!$$

(And we can sample from $p(x, z|\theta)$ by running the simulator.)

The value of gold

We can calculate the joint likelihood ratio

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$

We want the likelihood ratio function

$$r(x|\theta_0, \theta_1) \equiv \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

With $r(x, z|\theta_0, \theta_1)$, we define a functional like

$$L_r[\hat{r}(x|\theta_0, \theta_1)] = \int \mathrm{d}x \int \mathrm{d}z \; p(x, z|\theta_1) \left[\left(\hat{r}(x|\theta_0, \theta_1) - r(x, z|\theta_0, \theta_1) \right)^2 \right].$$

It is minimized by

$$r(x|\theta_0, \theta_1) = \arg\min_{\hat{r}(x|\theta_0, \theta_1)} L_r[\hat{r}(x|\theta_0, \theta_1)]!$$

(And we can sample from $p(x, z|\theta)$ by running the simulator.)

…. and then magic …

$$\mathbb{E}_{z \sim p(z|x, \theta_1)} [r(x, z|\theta_0, \theta_1)] = \int \mathrm{d}z \; p(z|x, \theta_1) \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)}$$

$$= \int \mathrm{d}z \; \frac{p(x, z|\theta_1)}{p(x|\theta_1)} \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)}$$

$$= r(x|\theta_0, \theta_1) \textbf{ !}$$

Learning the score

Similar to the joint likelihood ratio, from the simulator we can extract the joint score

$$t(x, z|\theta_0) \equiv \nabla_\theta \log p(x, z_d, z_s, z_p|\theta)\Big|_{\theta_0}$$

↓

We want the score

$$t(x|\theta_0) \equiv \nabla_\theta \log p(x|\theta)\Big|_{\theta_0}$$

Learning the score

Similar to the joint likelihood ratio, from the simulator we can extract the joint score

$$t(x, z|\theta_0) \equiv \nabla_\theta \log p(x, z_d, z_s, z_p|\theta)\Big|_{\theta_0}$$

We want the score

$$t(x|\theta_0) \equiv \nabla_\theta \log p(x|\theta)\Big|_{\theta_0}$$

Given $t(x, z|\theta_0)$, we define the functional

$$L_t[\hat{t}(x|\theta_0)] = \int \mathrm{d}x \int \mathrm{d}z \;\; p(x, z|\theta_0) \; \left[\left(\hat{t}(x|\theta_0) - t(x, z|\theta_0)\right)^2\right].$$

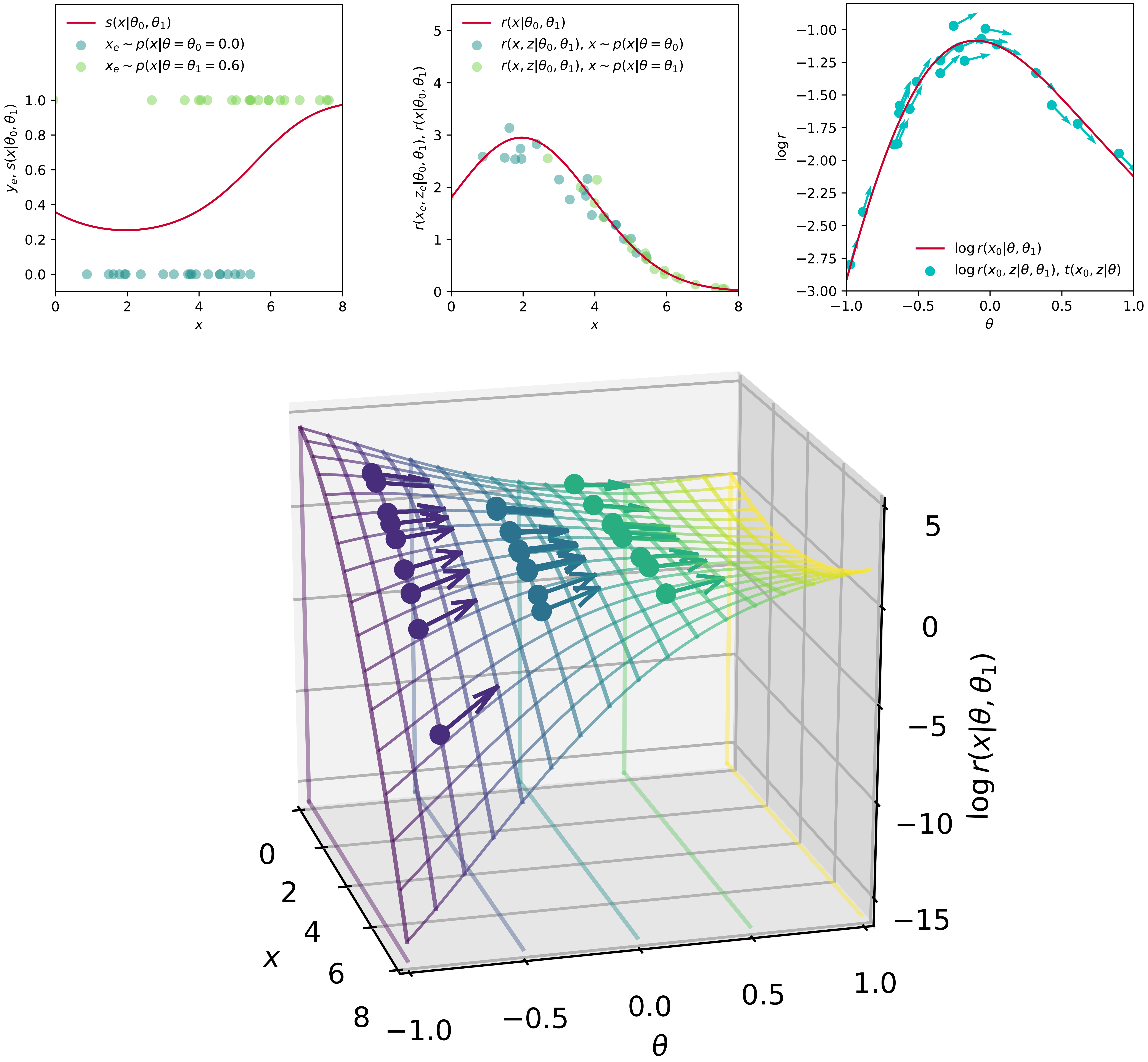
One can show it is minimized by

$$t(x|\theta_0) = \underset{\hat{t}(x|\theta_0)}{\arg\min} \, L_t[\hat{t}(x|\theta_0)].$$

Again, we implement this minimization through machine learning.

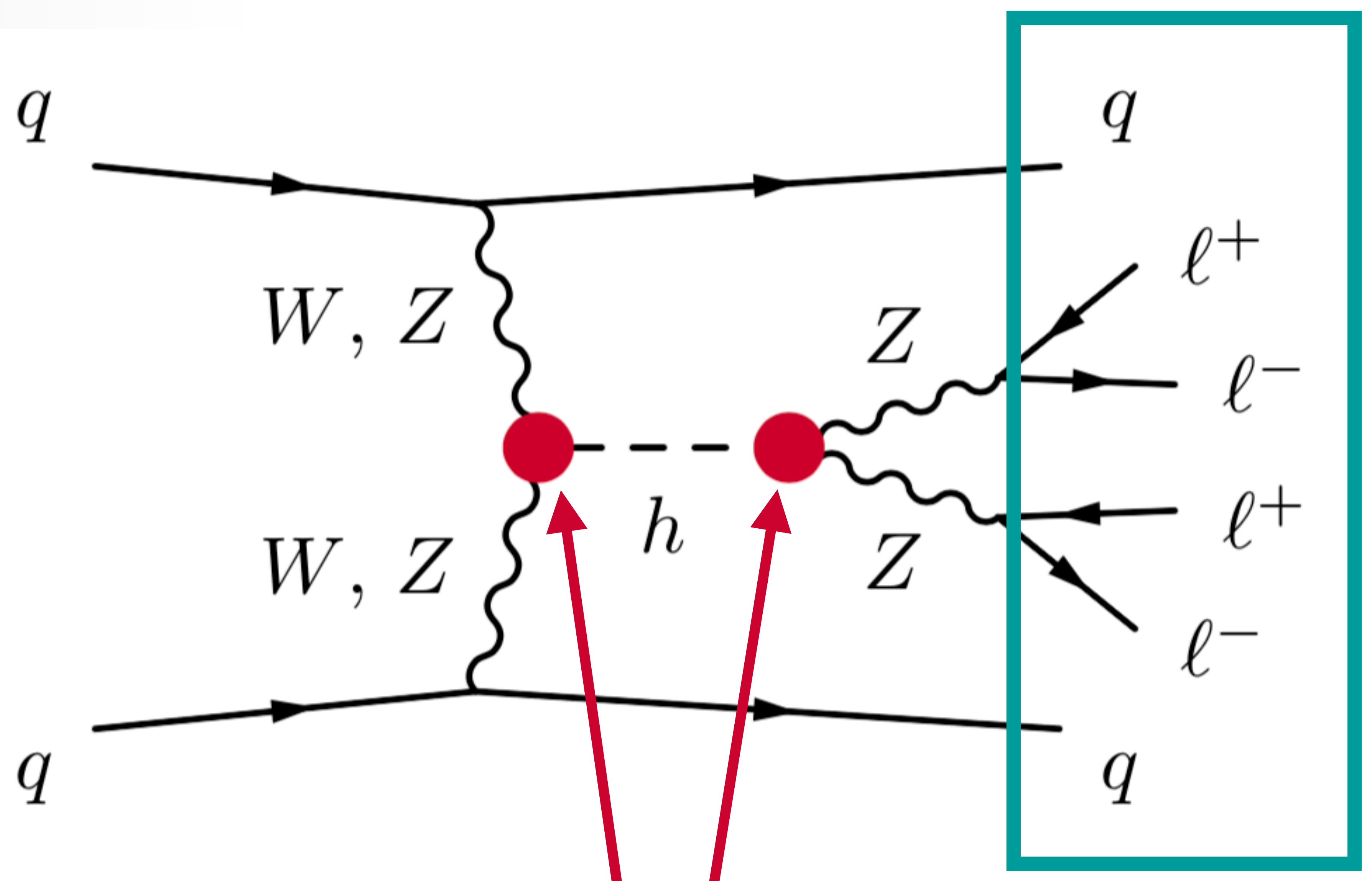
Augmented Training Data

Brehmer, Louppe, Pavez, KC, PNAS (2019), arXiv:1805.12244



Examples

Impact on Studies of The Higgs Boson



42-Dim observable **x**

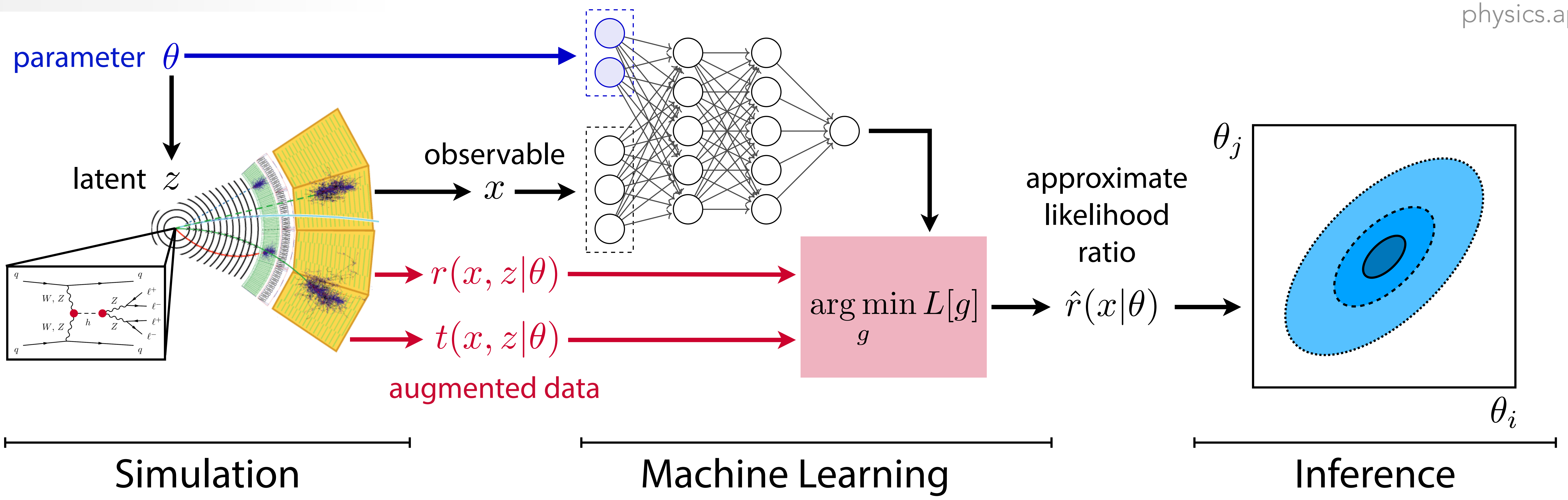
Exciting new physics might hide here!
We parameterize it with two coefficients:

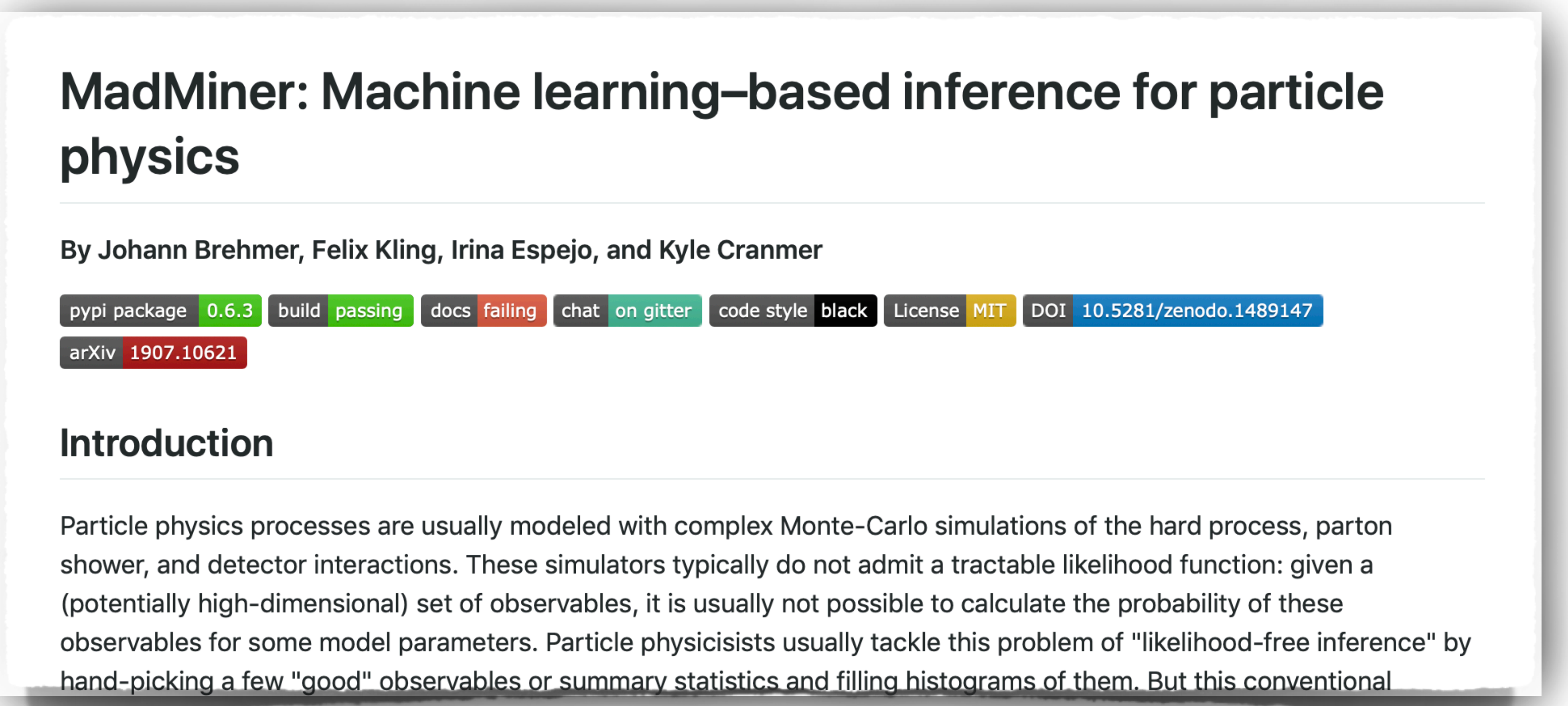
$$\mathcal{L} = \mathcal{L}_{SM} + \boxed{\frac{f_W}{\Lambda^2}} \underbrace{\frac{ig}{2} (D^\mu\phi)^\dagger \sigma^a D^\nu \phi \, W^a_{\mu\nu}}_{\mathcal{O}_W} - \boxed{\frac{f_{WW}}{\Lambda^2}} \underbrace{\frac{g^2}{4} (\phi^\dagger\phi) \, W^a_{\mu\nu} W^{\mu\nu\, a}}_{\mathcal{O}_{WW}}$$

J Brehmer, J Pavez, G Louppe, K.C. PRL & PRD 2018 [arXiv:1805.00013 & arXiv:1805.00020], CARL [arxiv:1506.02169]

Learning the likelihood ratio

arXiv:1805.12244
PRL, arXiv:1805.00013
PRD, arXiv:1805.00020
physics.aps.org/articles/v11/90





MadMiner: Machine learning–based inference for particle physics

By Johann Brehmer, Felix Kling, Irina Espejo, and Kyle Cranmer

pypi package 0.6.3 | build passing | docs failing | chat on gitter | code style black | License MIT | DOI 10.5281/zenodo.1489147 | arXiv 1907.10621

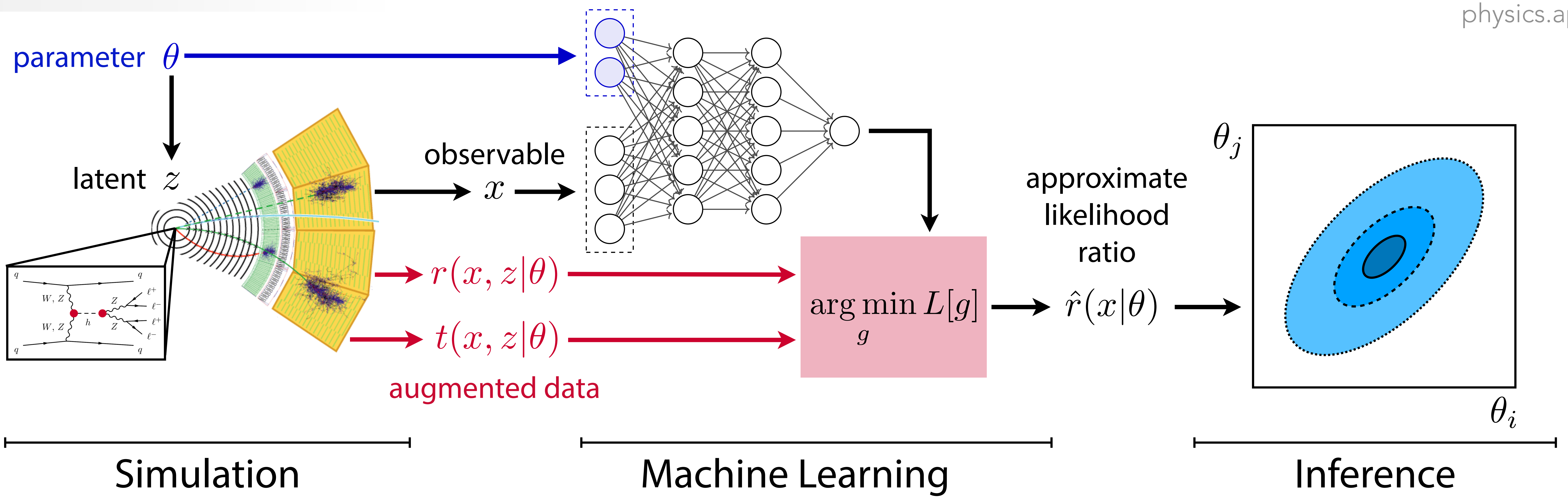
Introduction

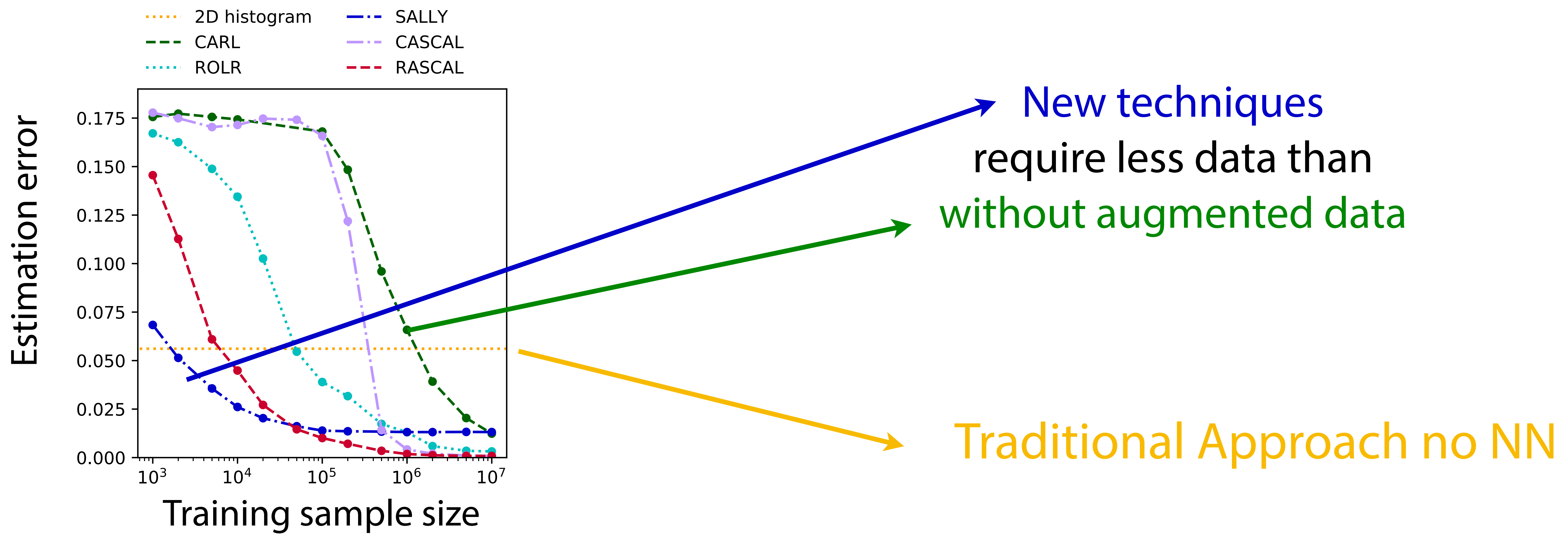
Particle physics processes are usually modeled with complex Monte-Carlo simulations of the hard process, parton shower, and detector interactions. These simulators typically do not admit a tractable likelihood function: given a (potentially high-dimensional) set of observables, it is usually not possible to calculate the probability of these observables for some model parameters. Particle physicisists usually tackle this problem of "likelihood-free inference" by hand-picking a few "good" observables or summary statistics and filling histograms of them. But this conventional

Dedicated software package interfacing with particle physics simulators:
github.com/johannbrehmer/madminer

Learning the likelihood ratio

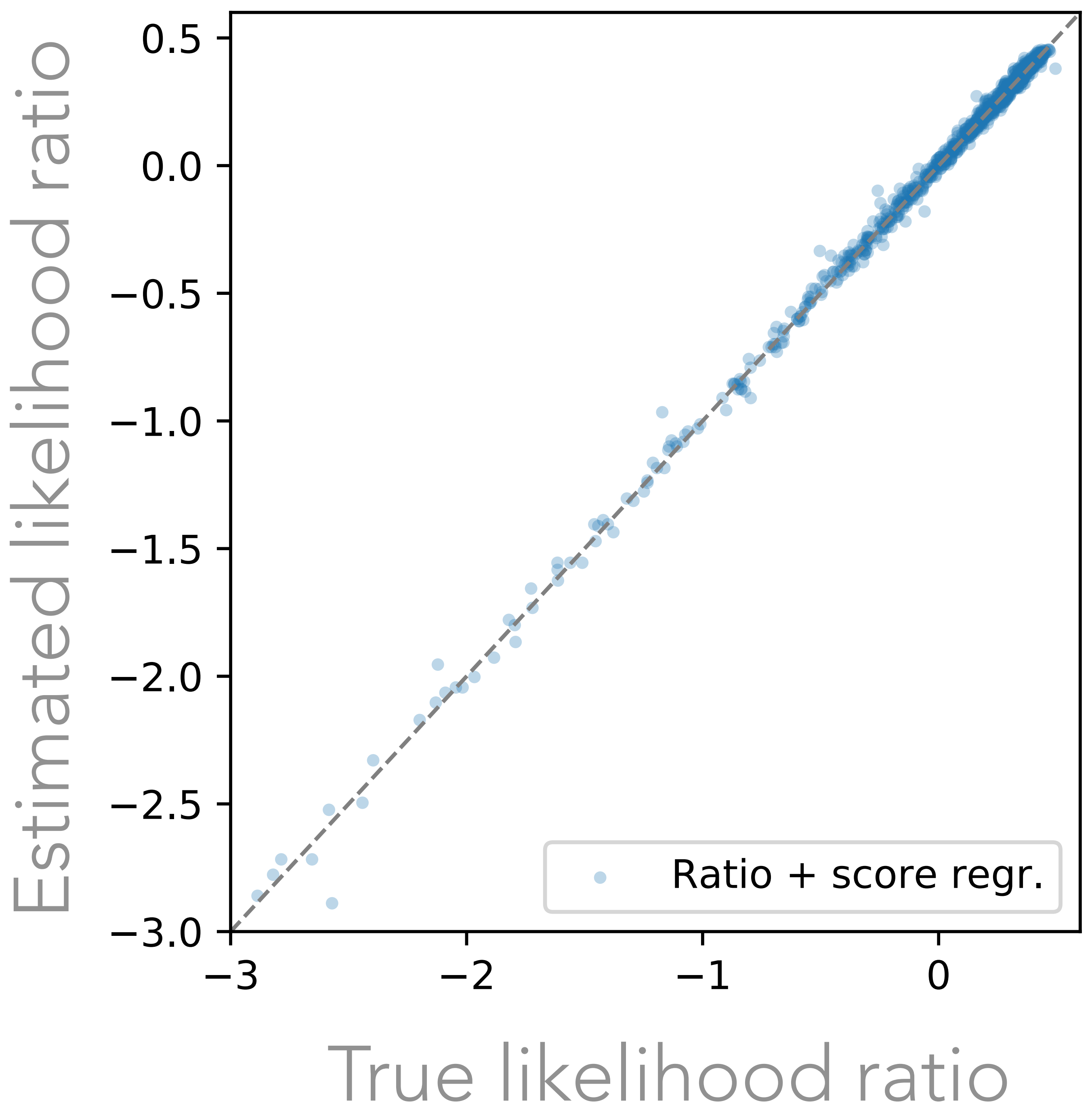
arXiv:1805.12244
PRL, arXiv:1805.00013
PRD, arXiv:1805.00020
physics.aps.org/articles/v11/90

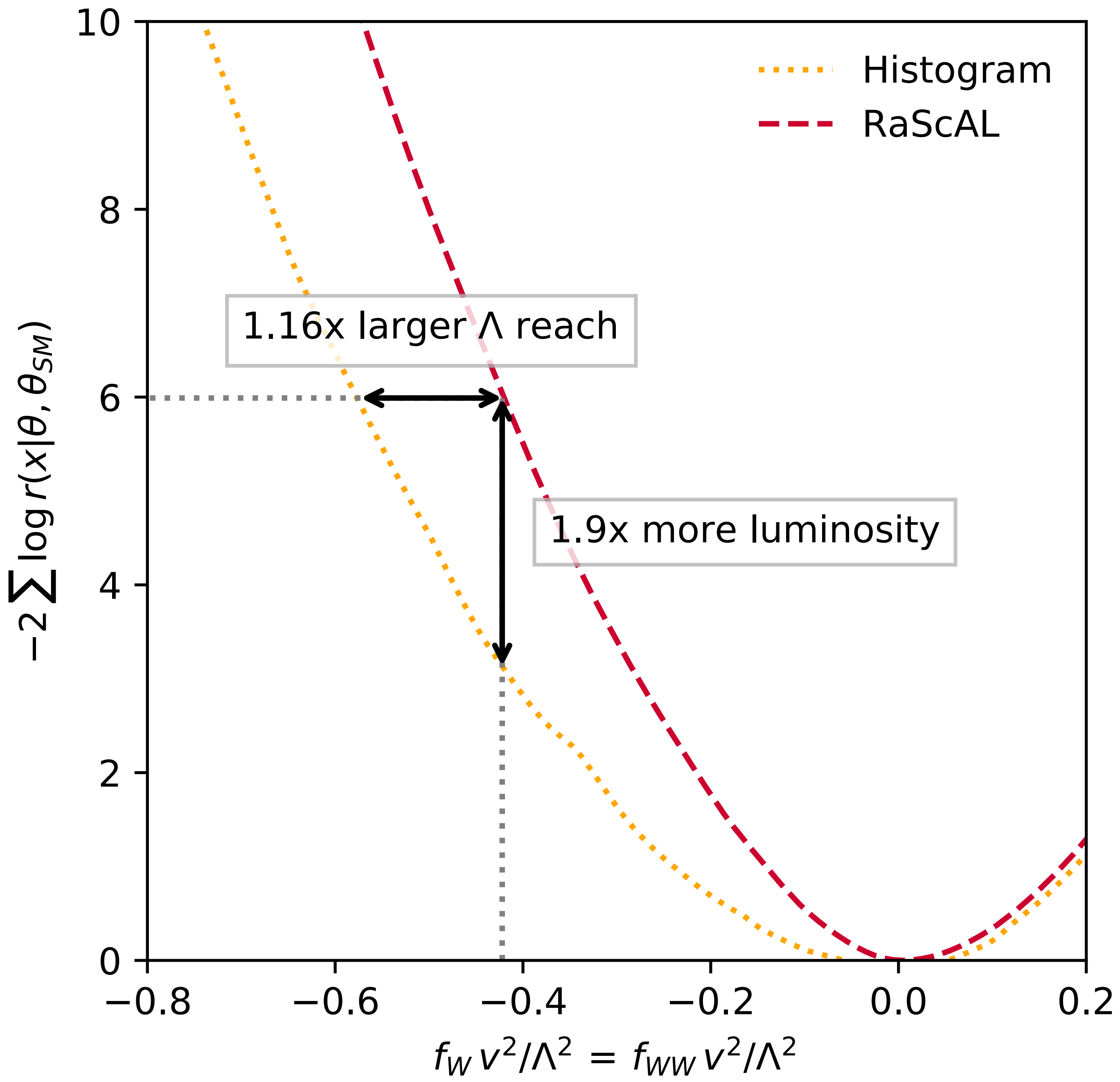




Impact on Studies of The Higgs Boson

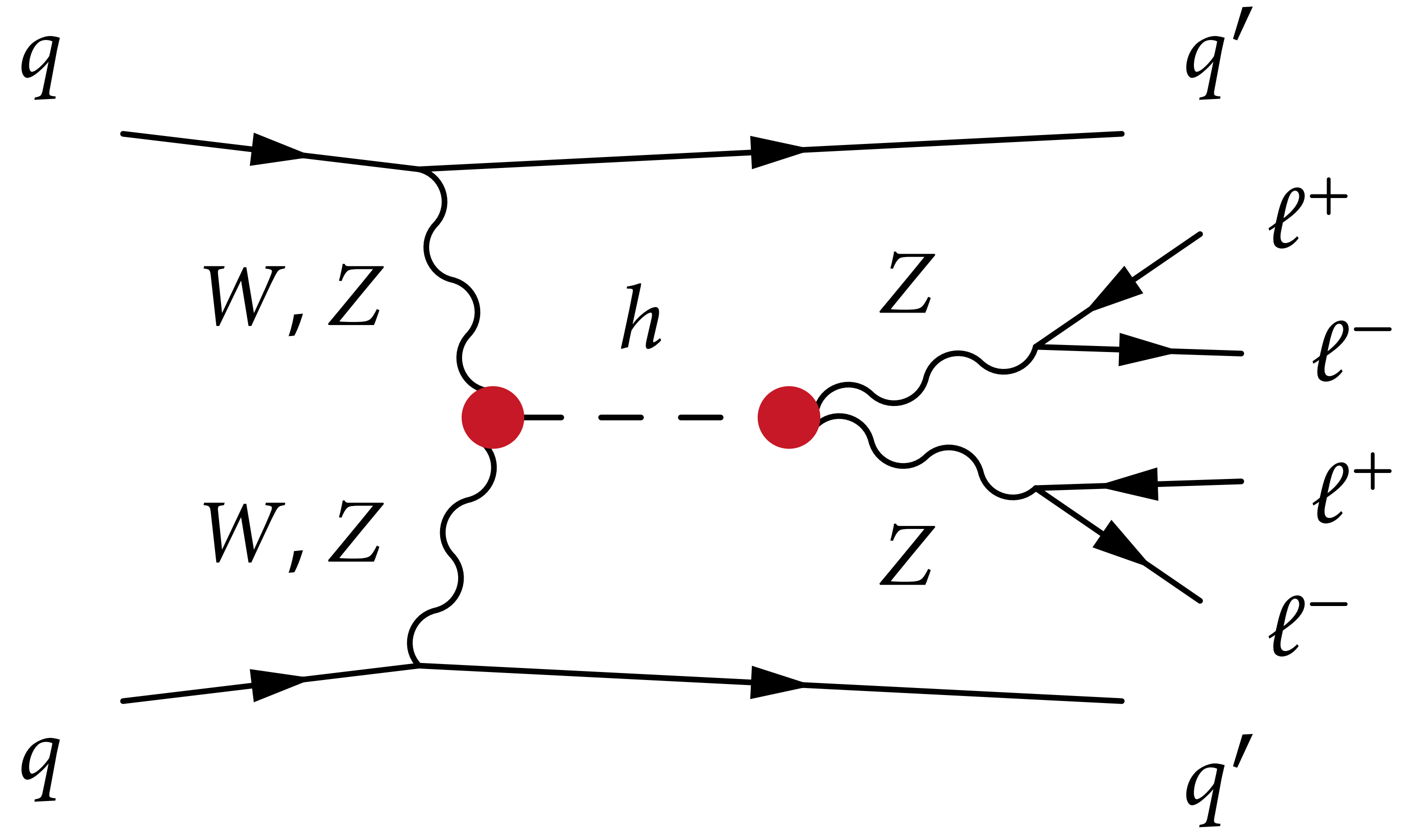
(based on a 42-Dim observation $\boldsymbol{x}$)





Accurate likelihood ratio estimates without the need for summary statistics improves sensitivity significantly

- Equivalent to 90% more LHC data!

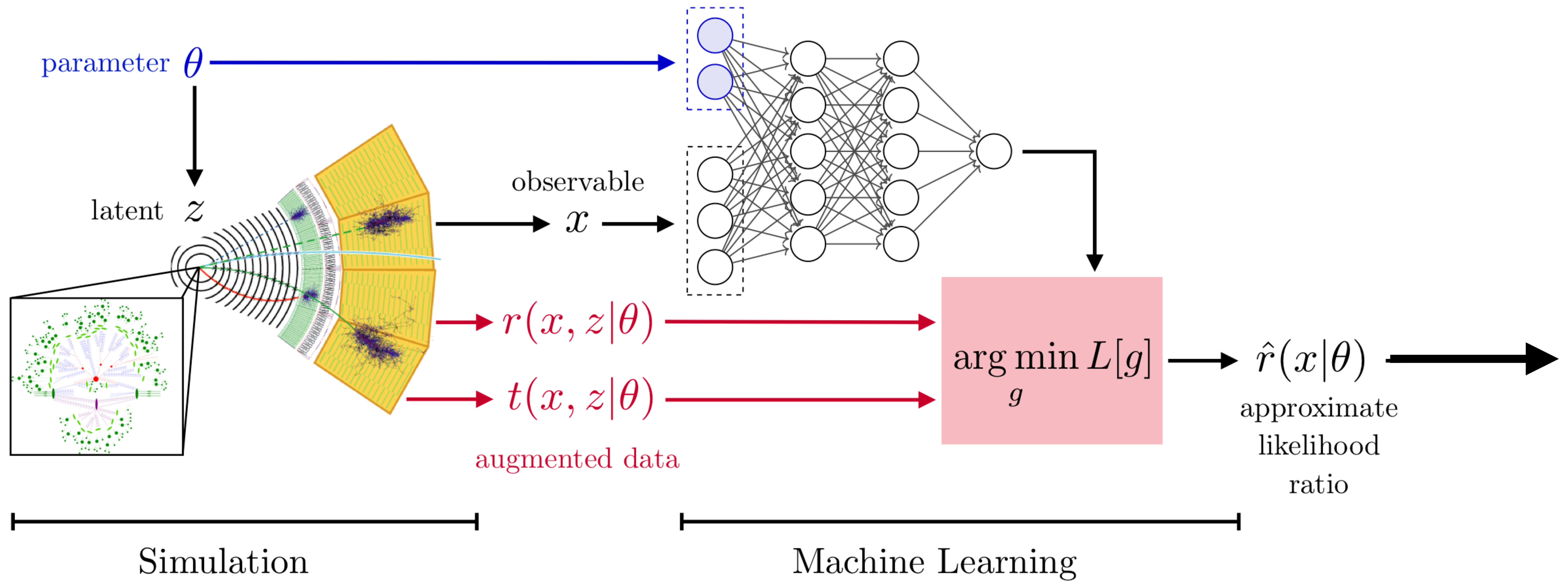


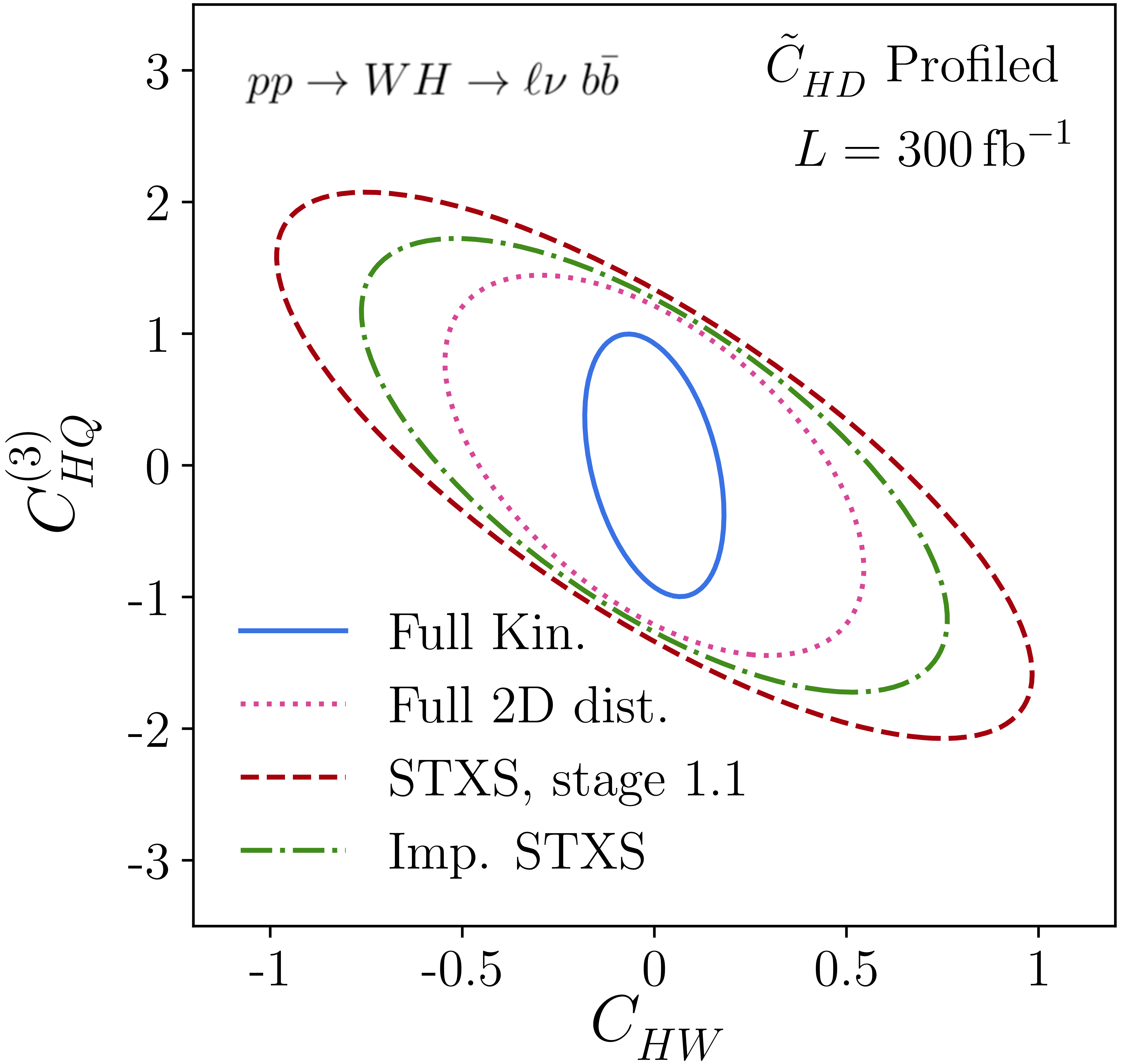
J Brehmer, J Pavez, G Louppe, K.C. PRL & PRD 2018 [arXiv:1805.00013 & arXiv:1805.00020], CARL [arxiv:1506.02169]

Impact on Studies of The Higgs Boson

Massive gains in precision of a flagship measurement at the LHC !

Equivalent increasing data collected by LHC by several factors





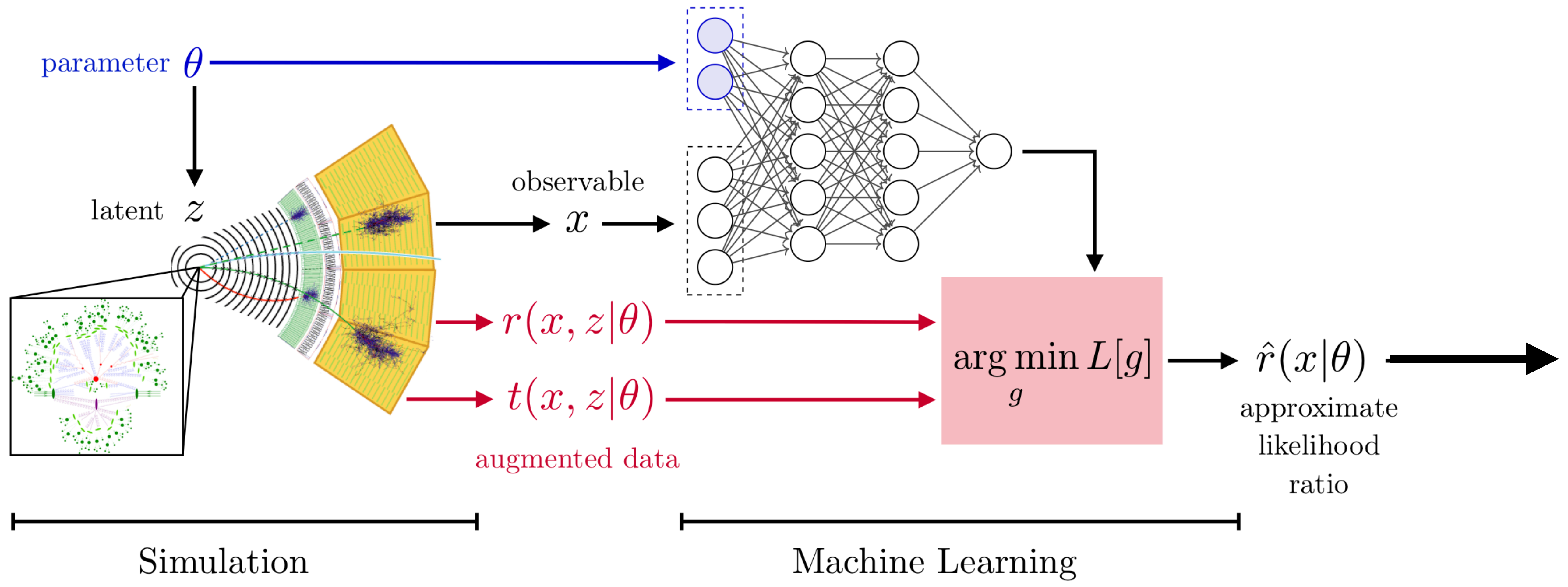
[J. Brehmer, S. Dawson, S. Homiller, F. Kling, T. Plehn 1908.06980]

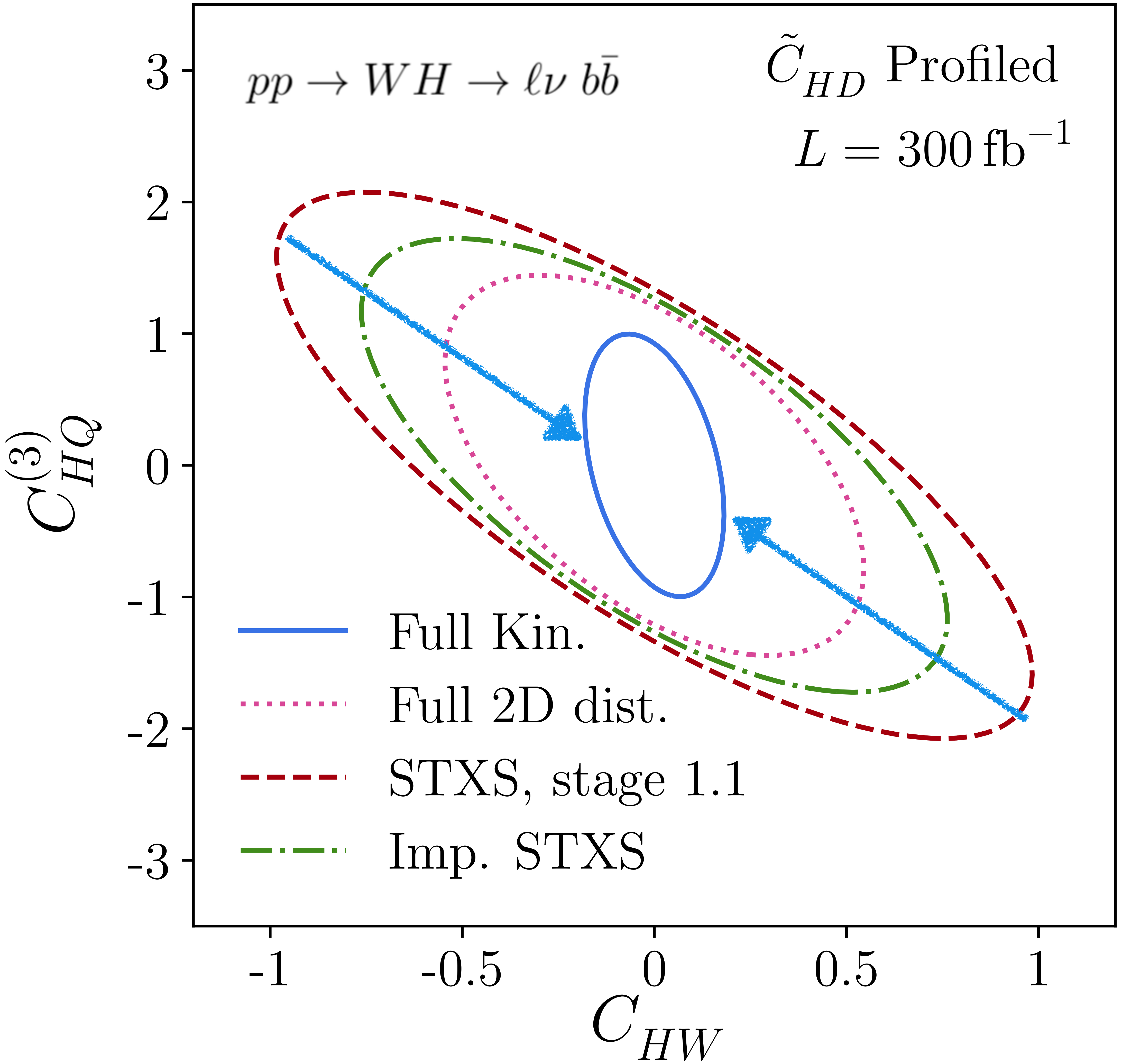
[J. Brehmer, F. Kling, I. Espejo, K. Cranmer 1907.10621]

Impact on Studies of The Higgs Boson

Massive gains in precision of a flagship measurement at the LHC !

Equivalent increasing data collected by LHC by several factors





[J. Brehmer, S. Dawson, S. Homiller, F. Kling, T. Plehn 1908.06980]

[J. Brehmer, F. Kling, I. Espejo, K. Cranmer 1907.10621]

Dark Matter Substructure

Abundance of DM subhalos vs mass:

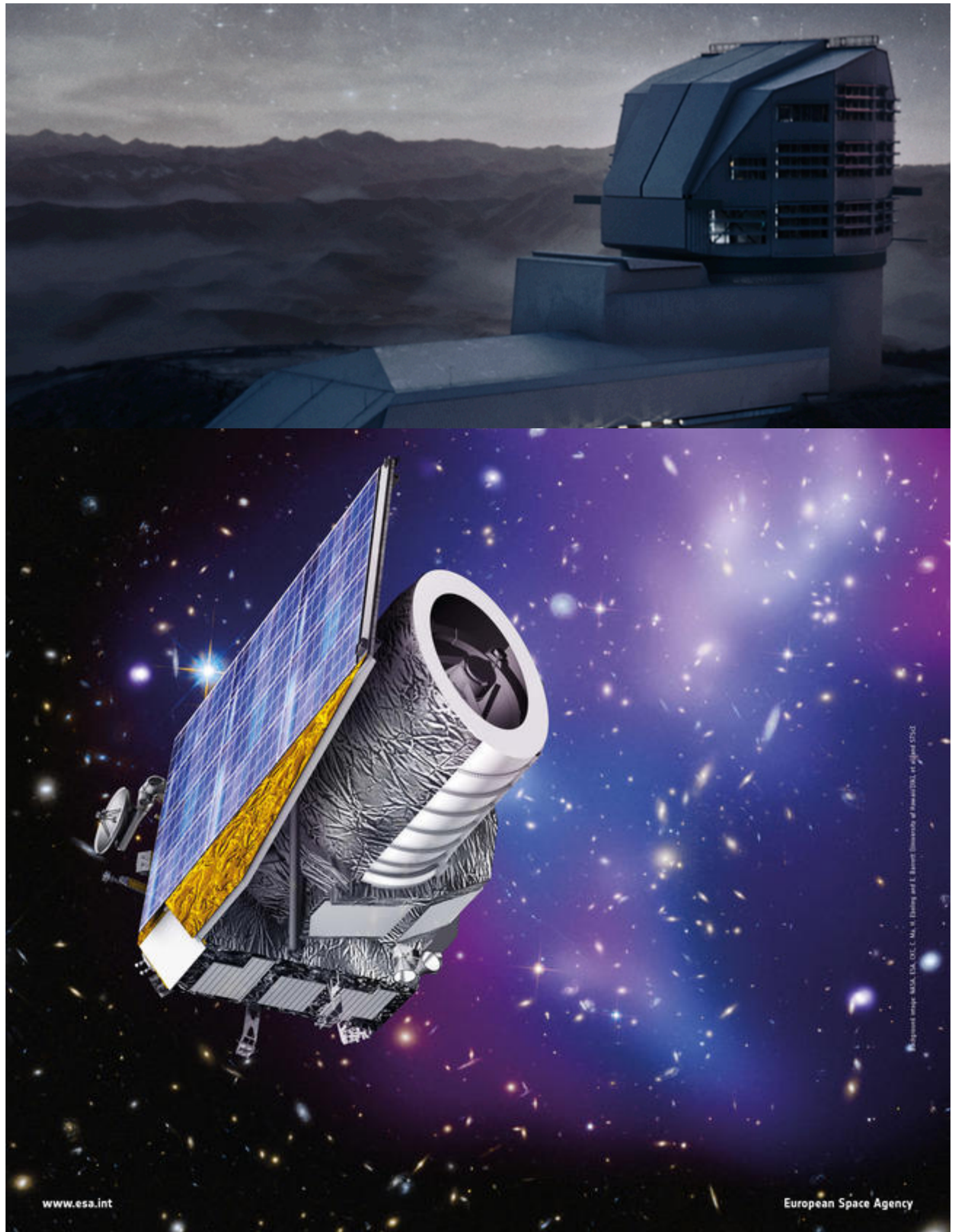
[R. *Dunstan et al* 1109.6291]

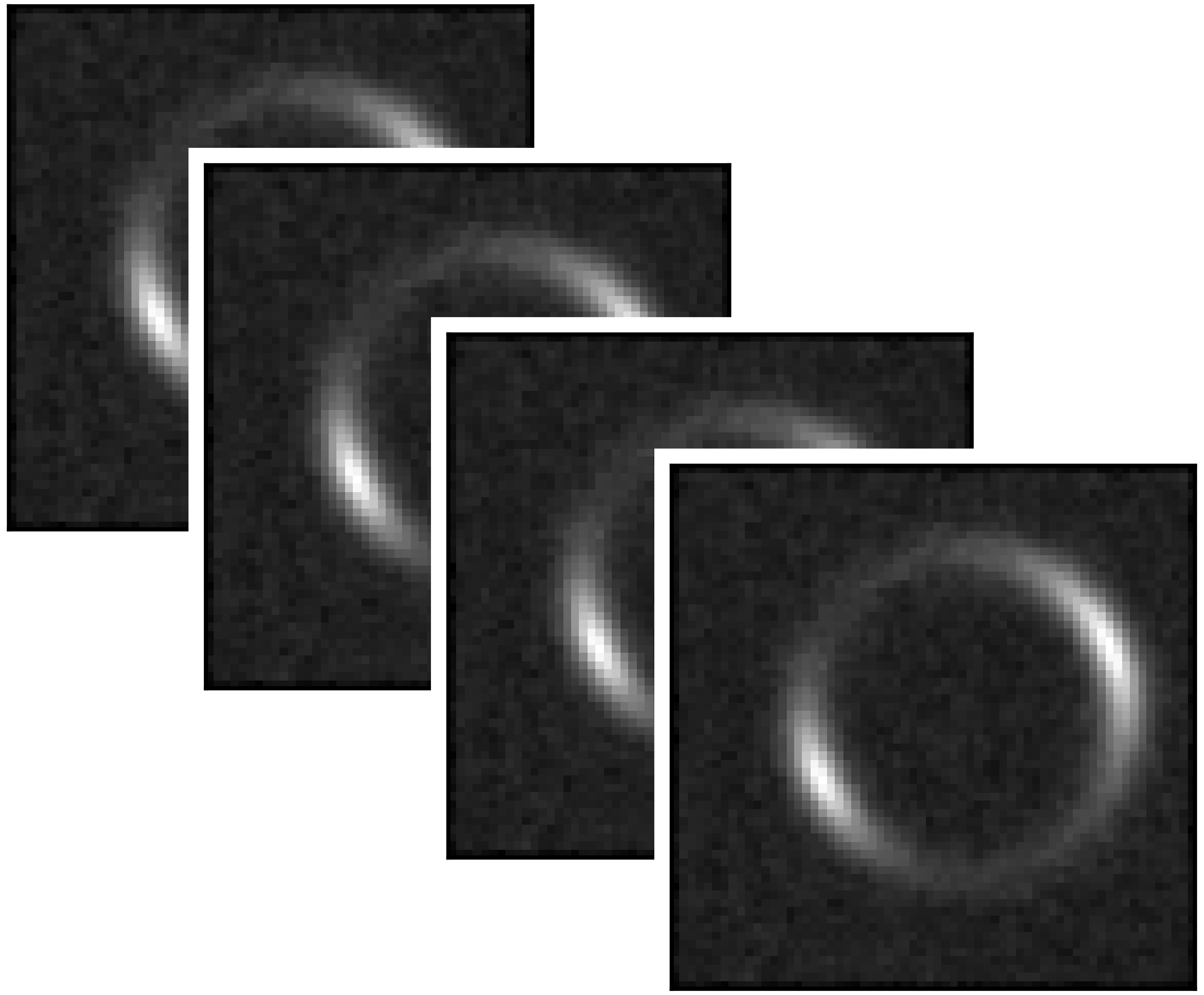
[T. Brown, J.Tumlinson]


galaxy
galaxy cluster
lensed galaxy images
distorted light-rays
Earth

Scalable inference for small subhalos

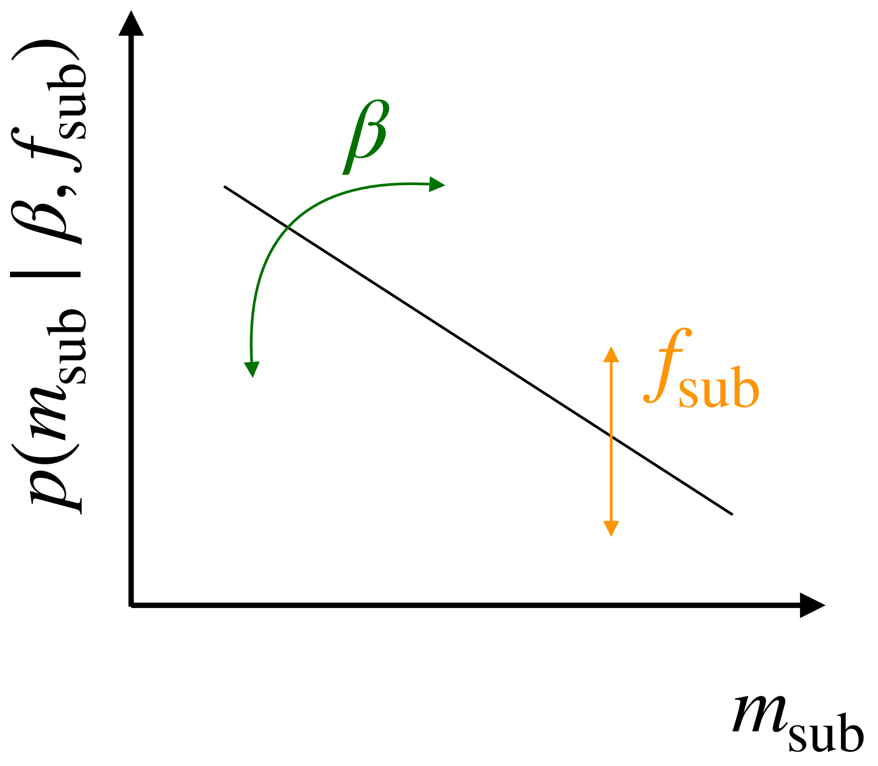
Future surveys (LSST, Euclid) are expected to deliver large samples of galaxy-galaxy strong lenses [Collett et al 1507.02657]



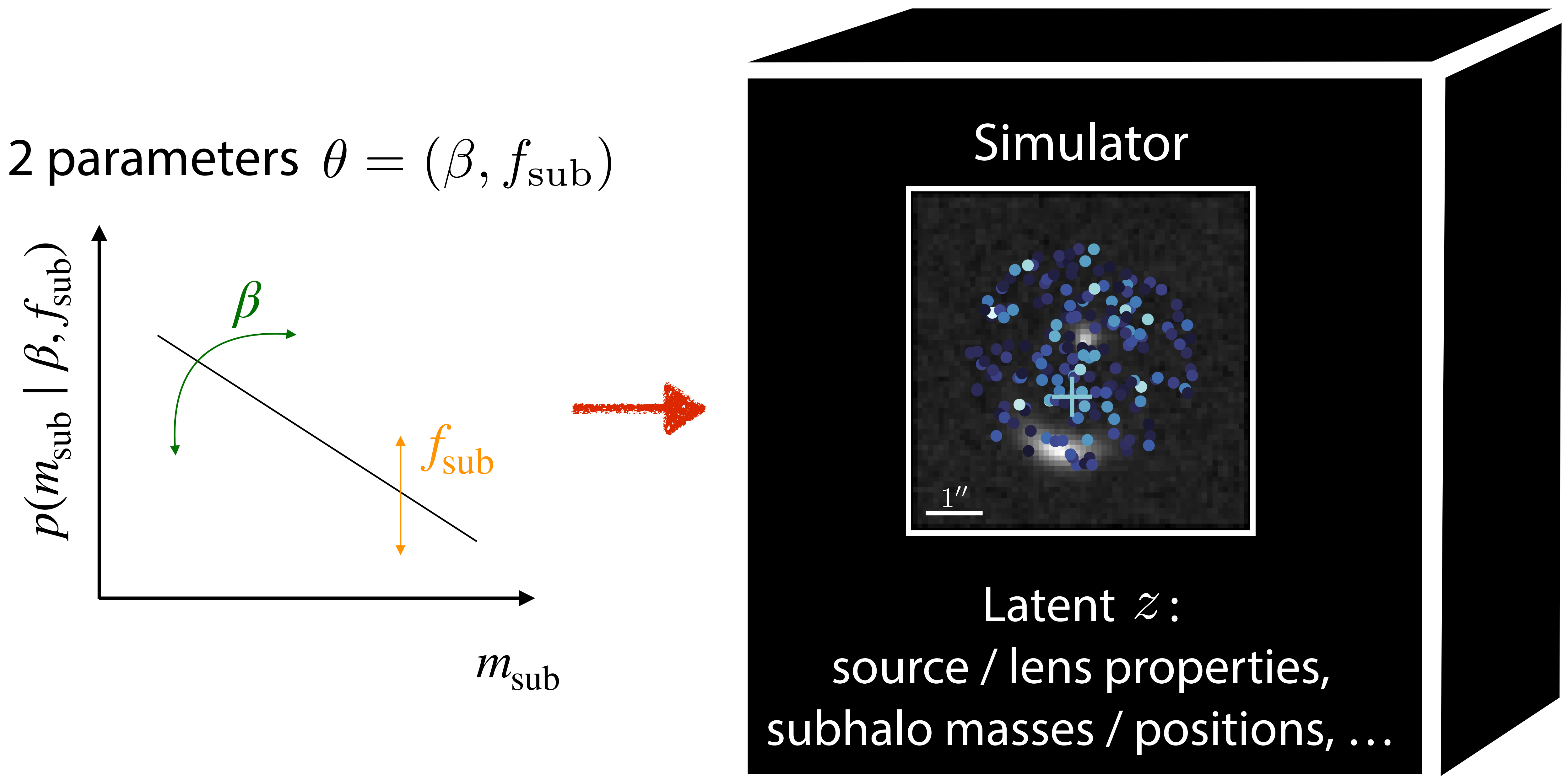


Simulation-based inference for strong lensing

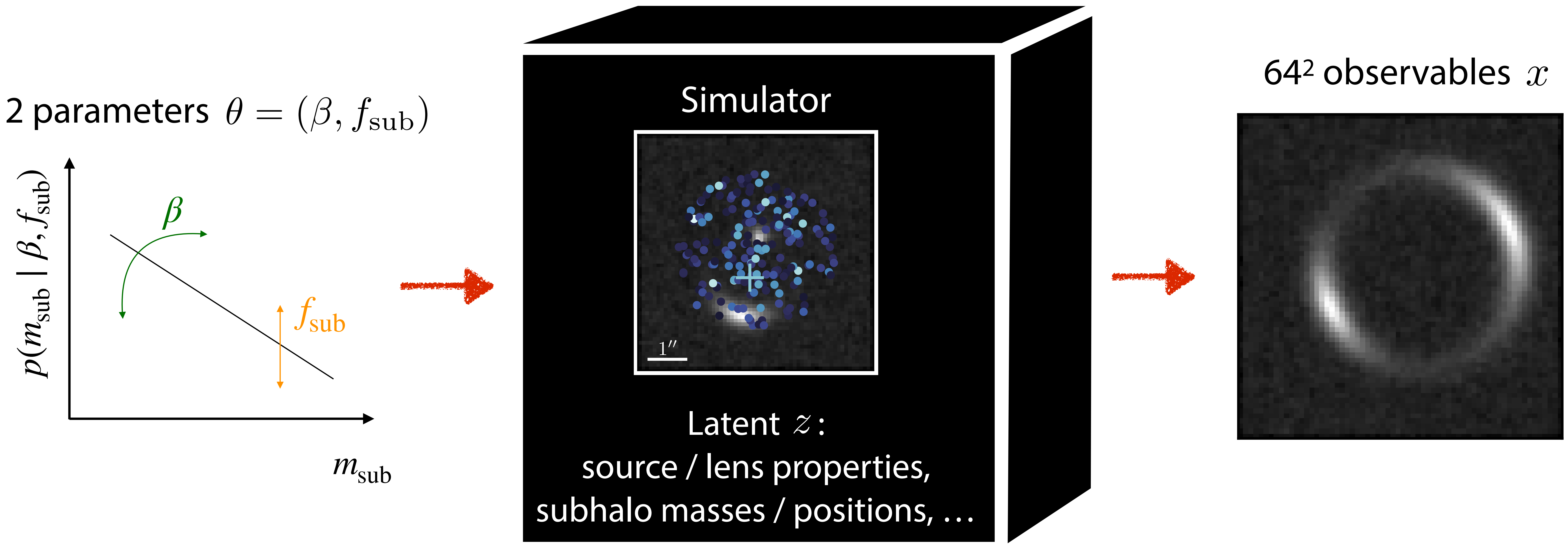
2 parameters $\theta = (\beta, f_{\rm sub})$



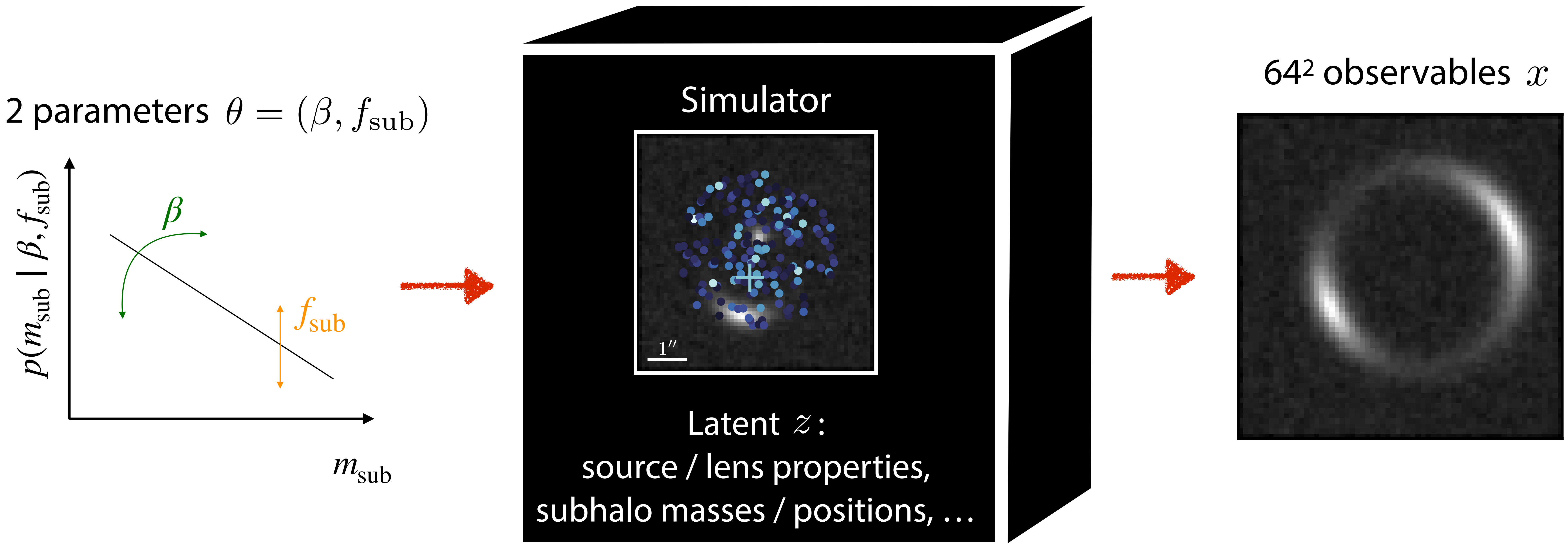
Simulation-based inference for strong lensing

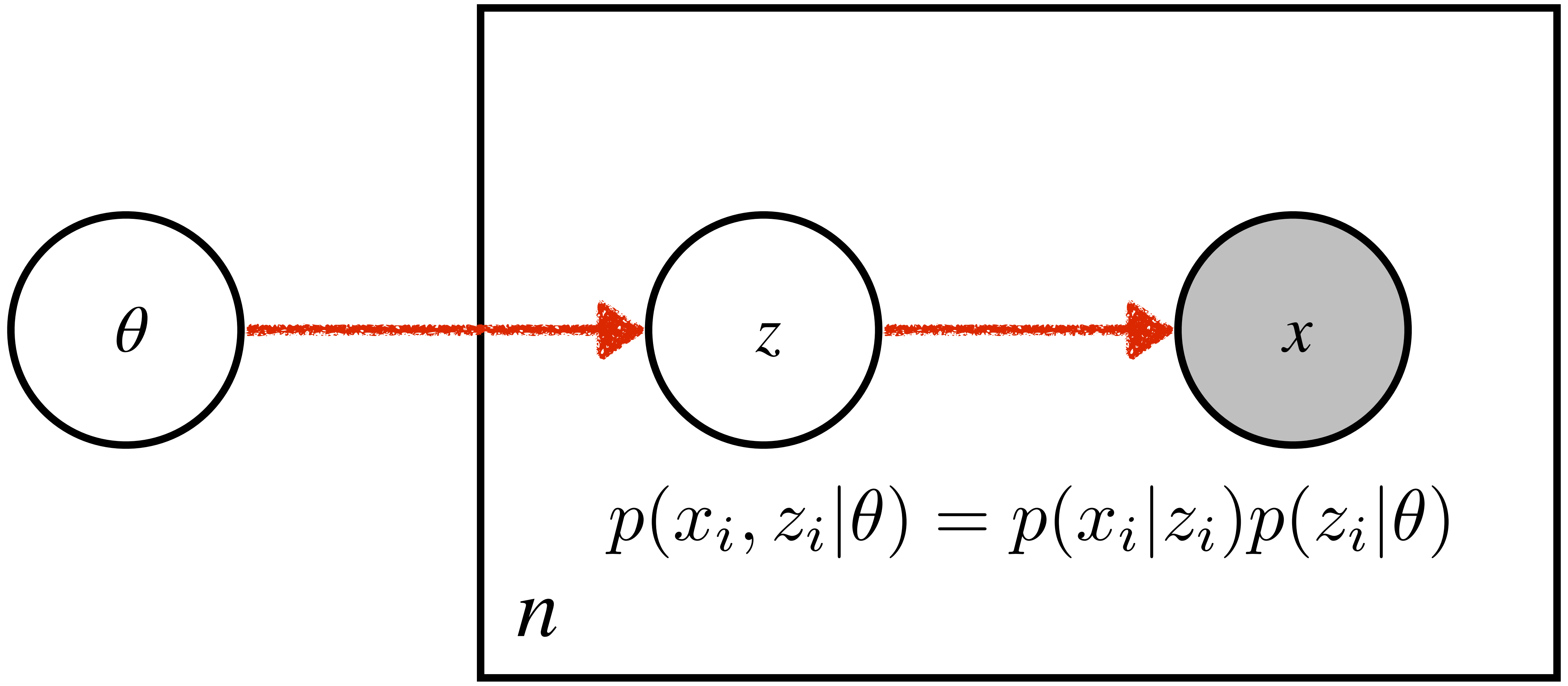


Simulation-based inference for strong lensing

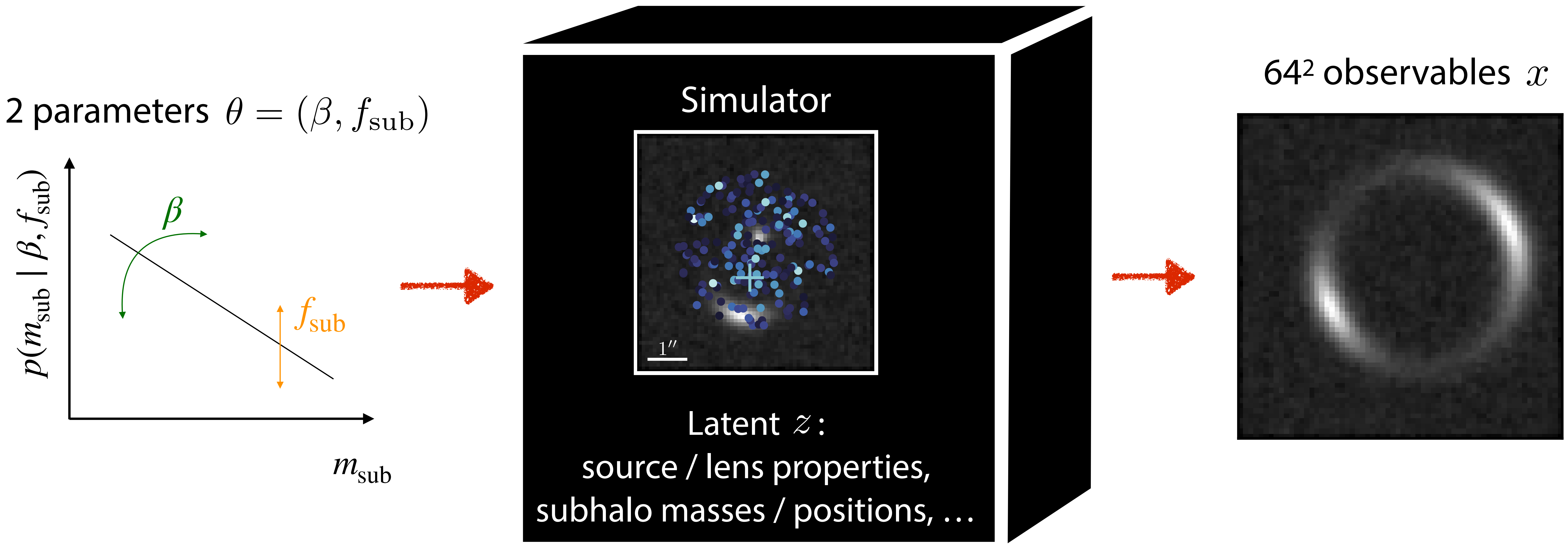


Simulation-based inference for strong lensing





Simulation-based inference for strong lensing

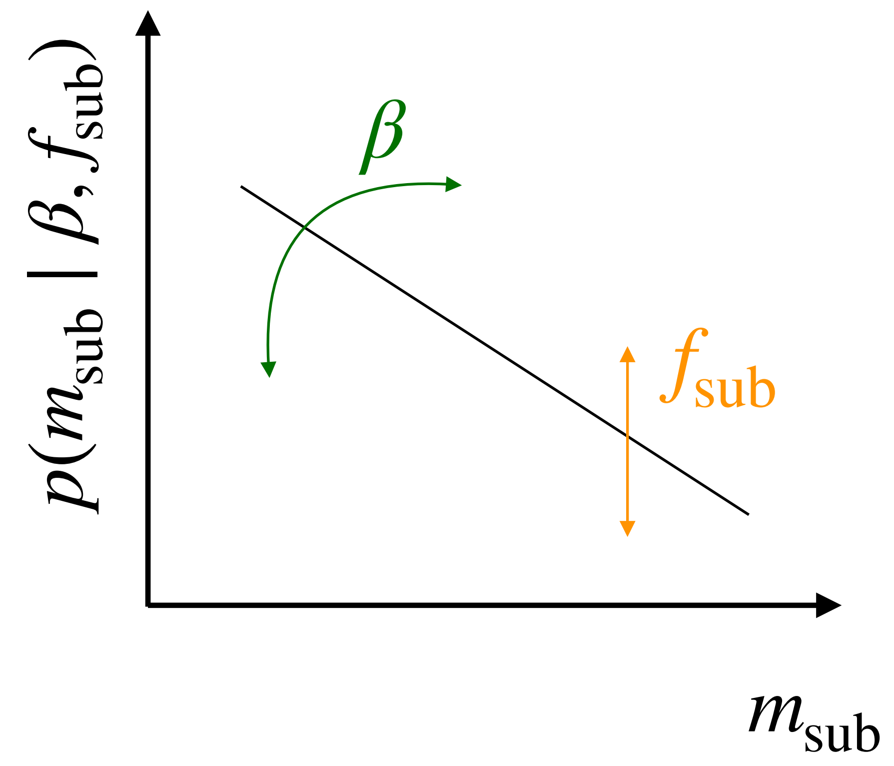


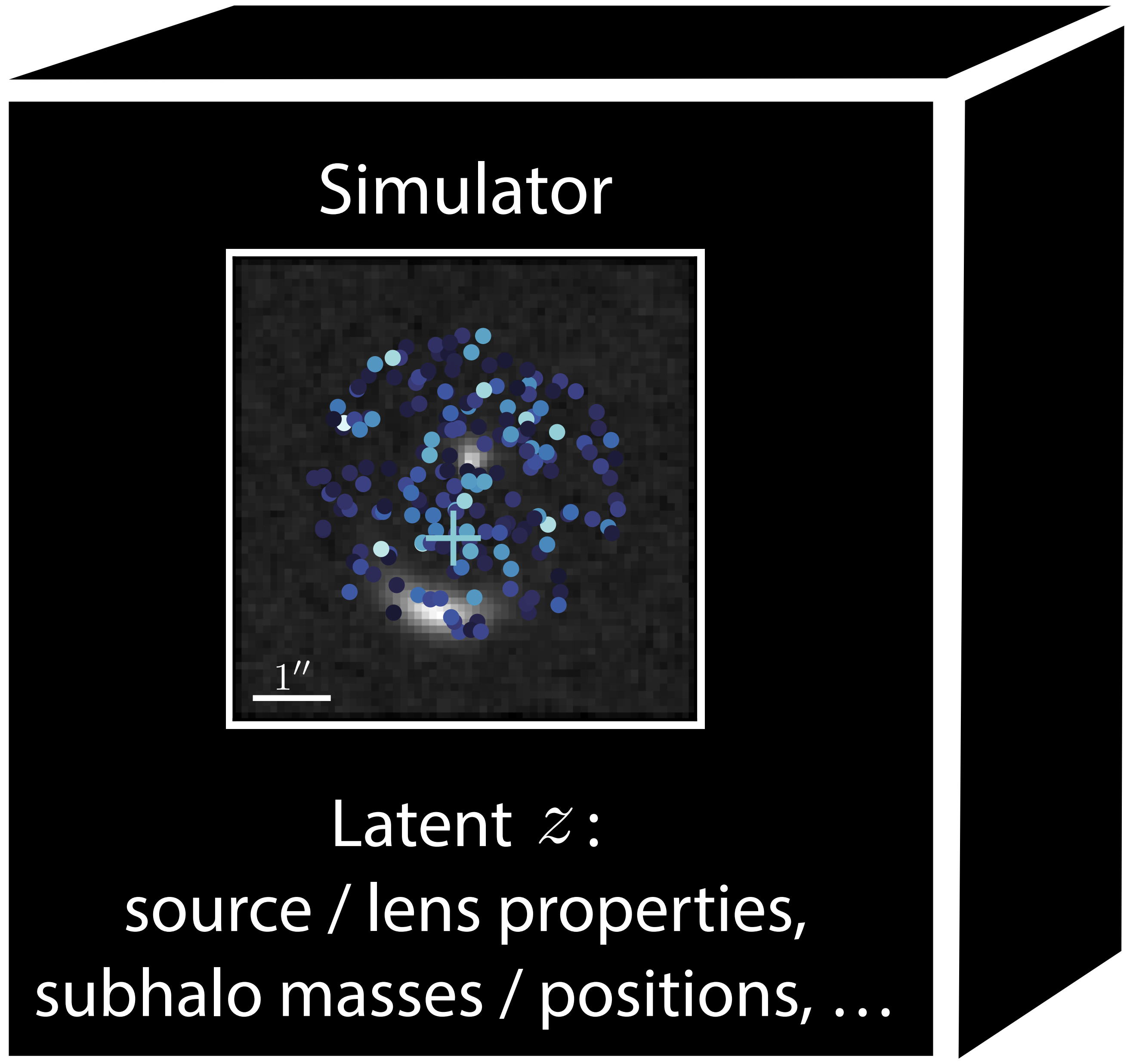
⇒ Need inference technique that

- scales to many lenses (fast evaluation)
- captures subtle effects in high-dimensional image data
- can deal with a large number of subhalos (latent variables)

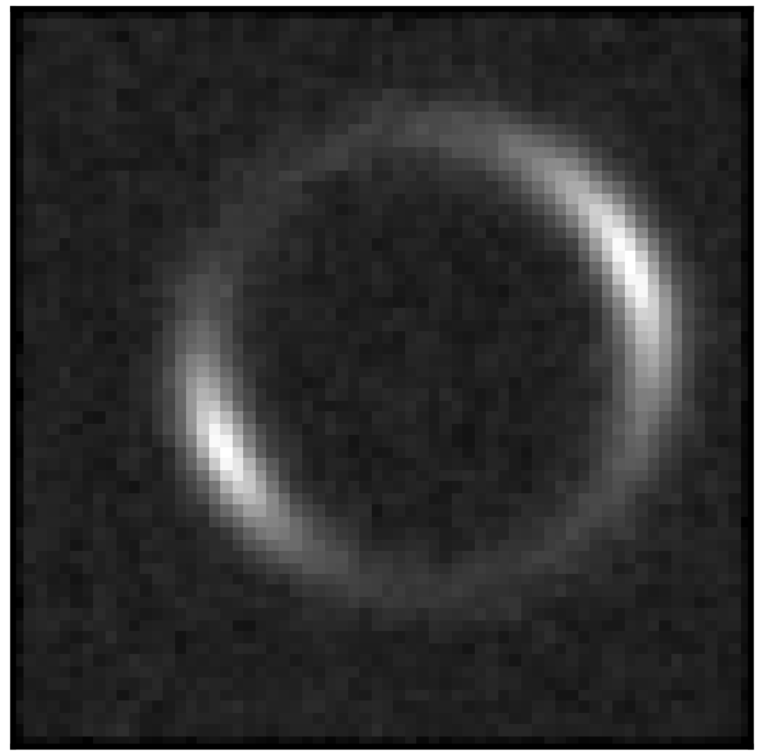
Simulation-based inference for strong lensing

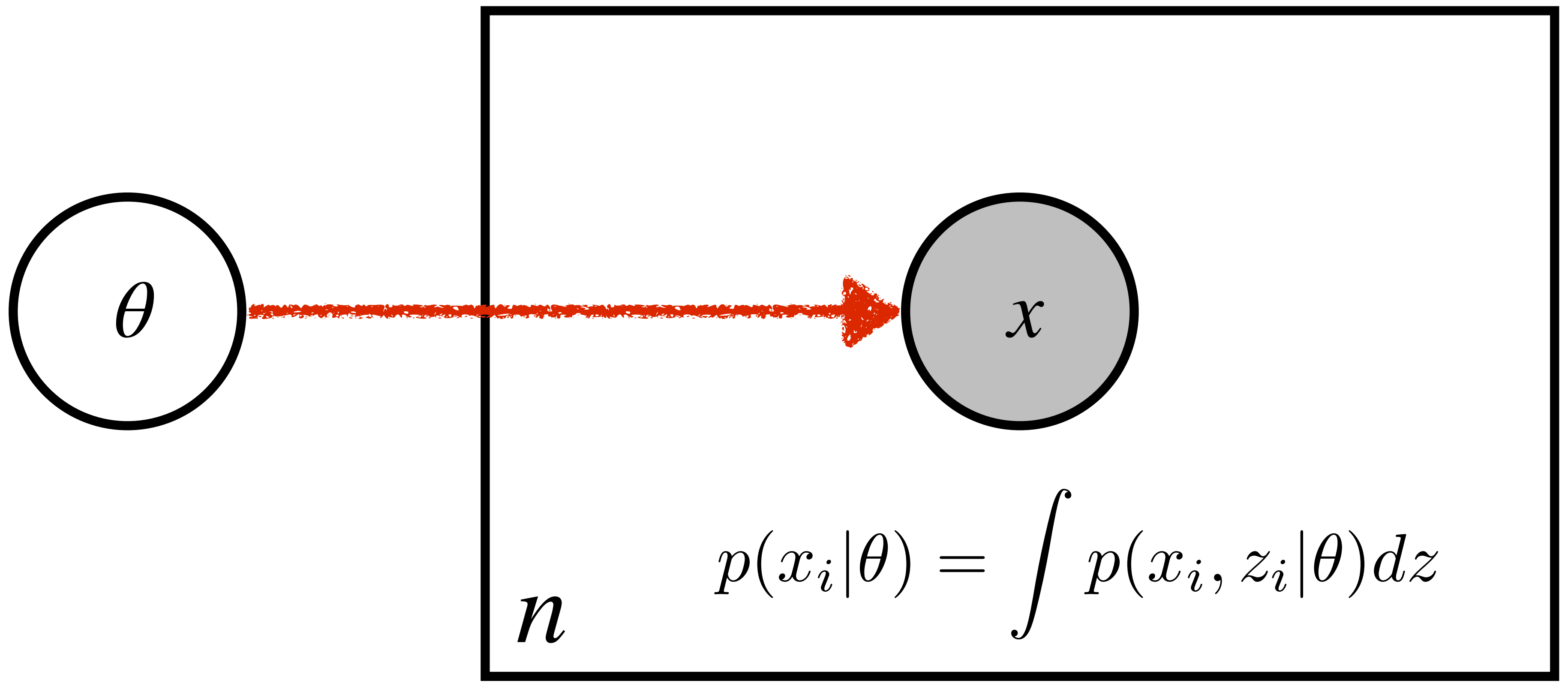
2 parameters $\theta = (\beta, f_{\rm sub})$





64^2 observables x

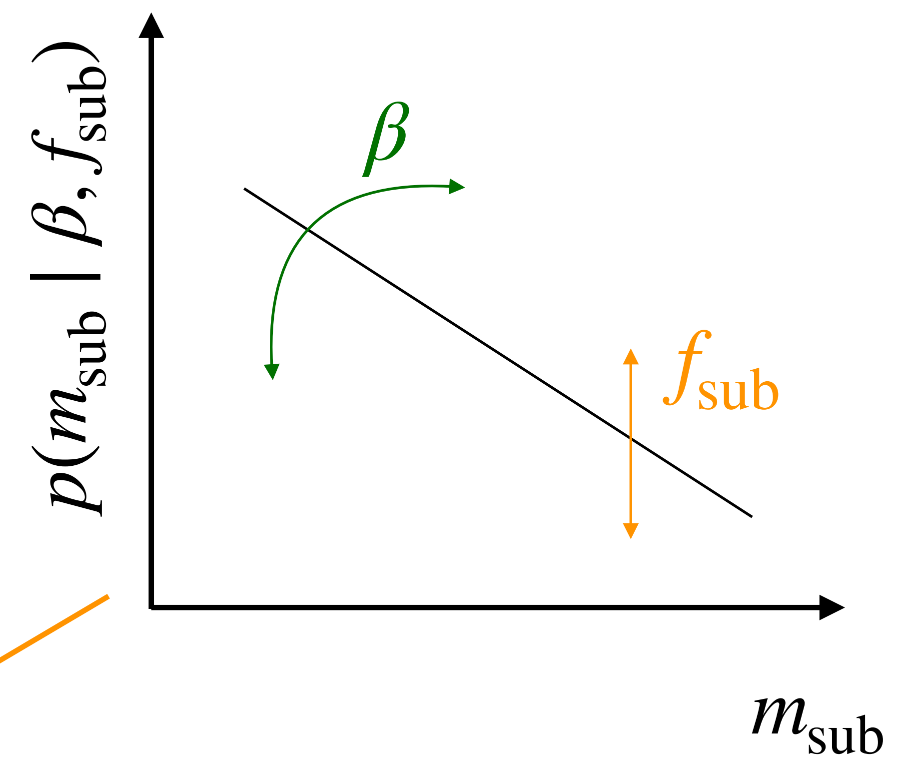




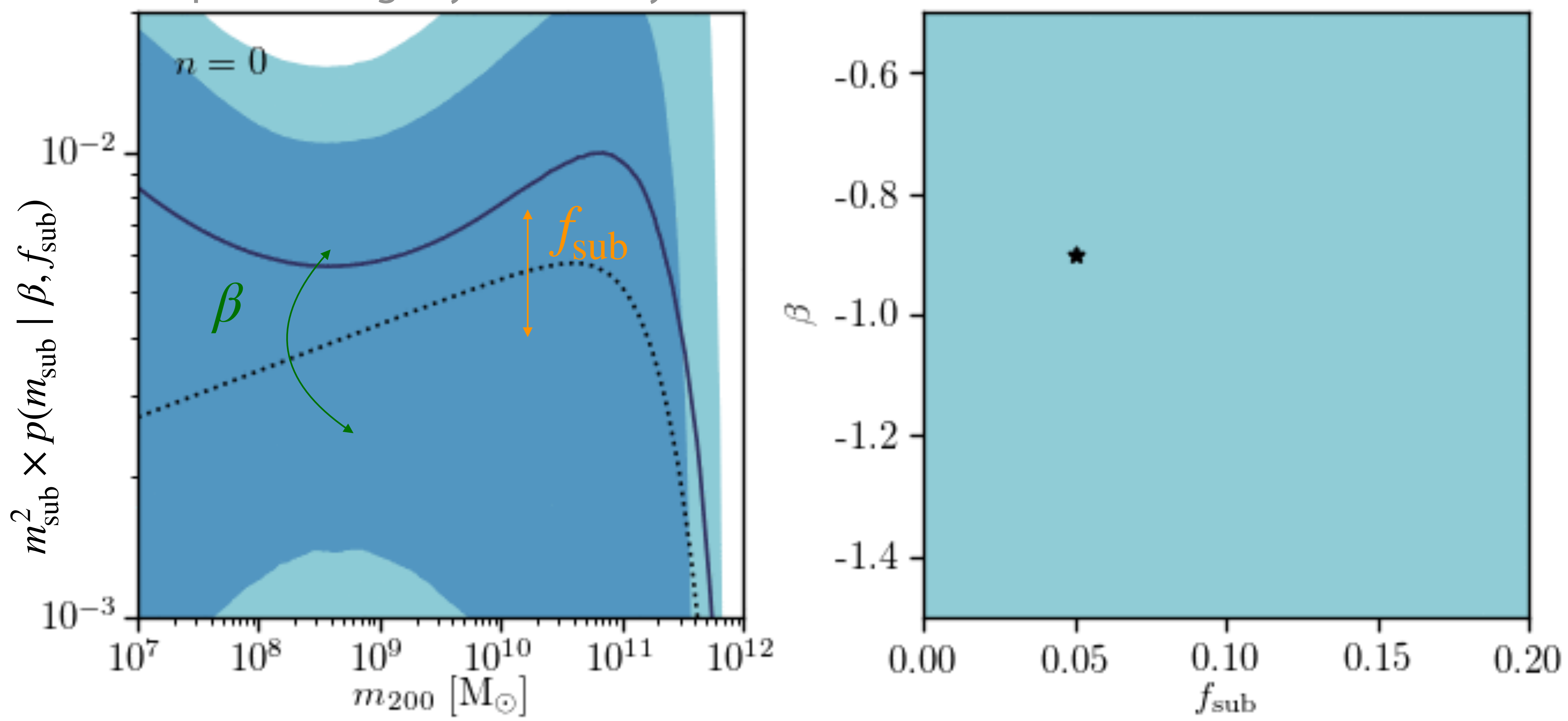
$$p(\theta \mid \{x_i\}) \propto \underbrace{p(\theta)}_{\text{prior}} \prod_{i=1}^{n} \left[\underbrace{p(x_i \mid \theta)}_{\text{amortized likelihood}} \right]$$

Posterior from amortized likelihood ratio

Watch how the posterior for two population parameters concentrate around true value used to generate mock data.



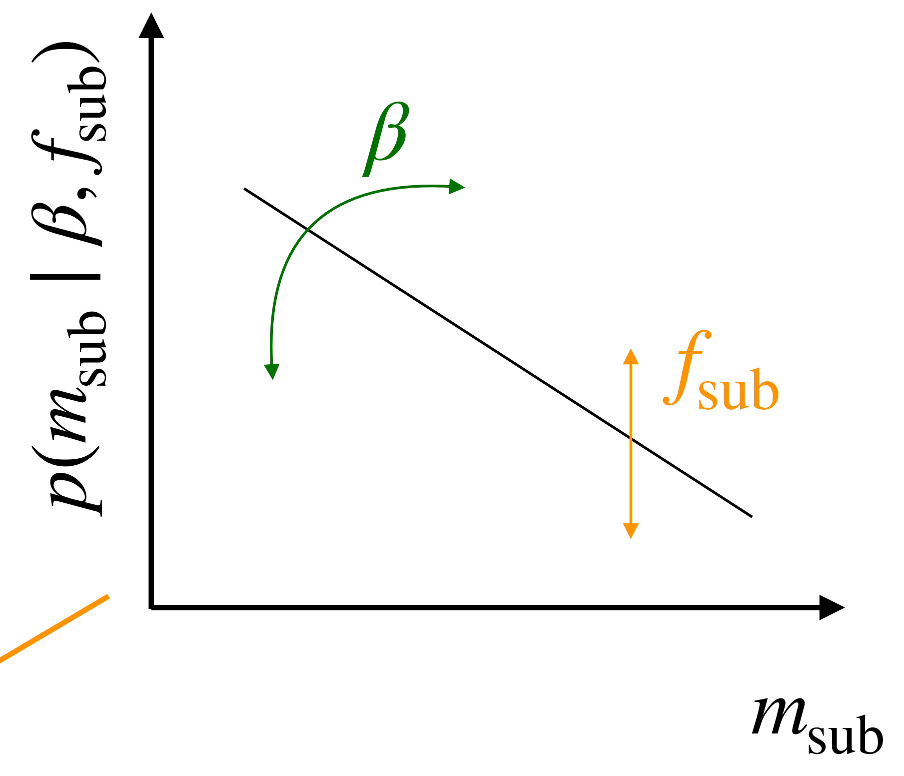
(plotted slightly differently)



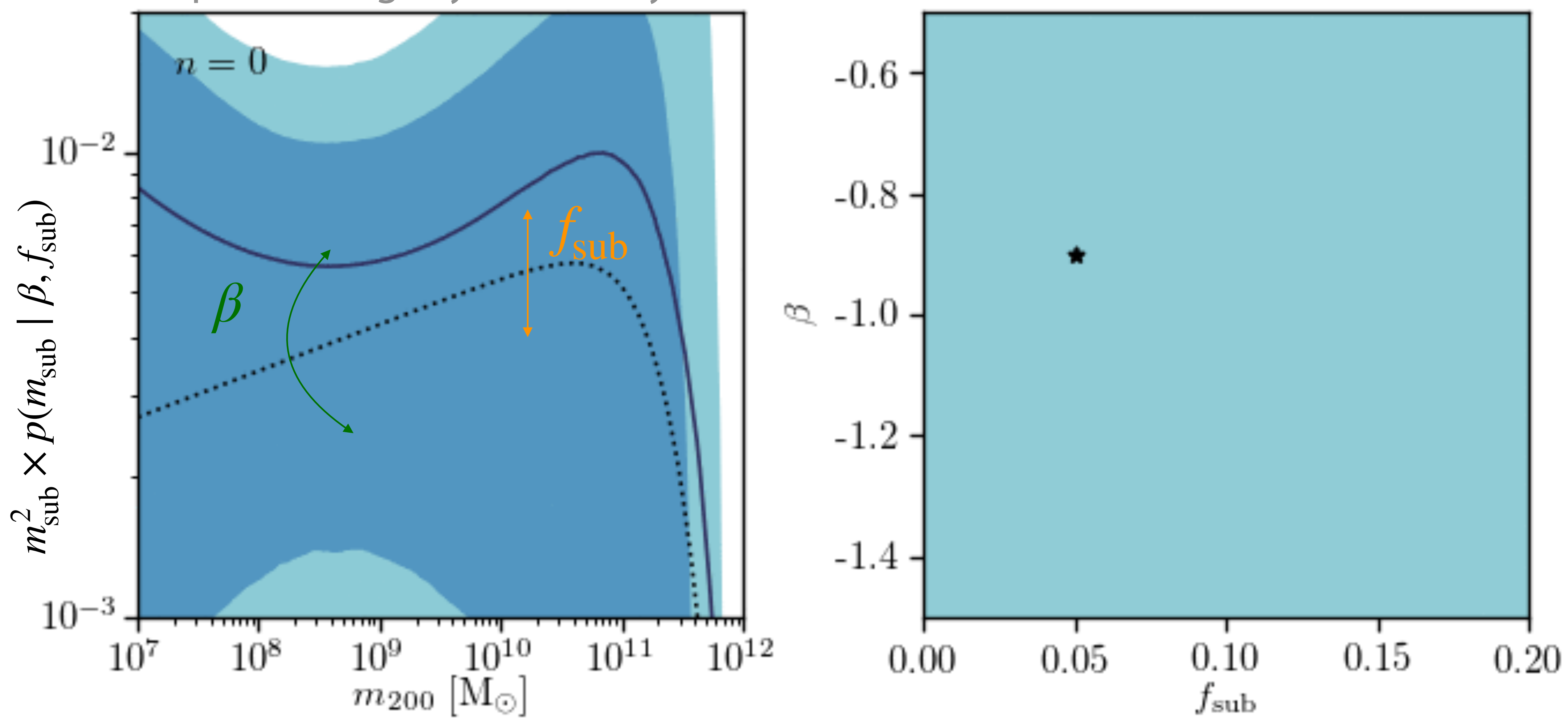
Sid Mishra-Sharma Johann Brehmer Gilles Louppe Joeri Hermans, K. Cranmer. published in ApJ, 886 (2019) arXiv:1909.02005

Posterior from amortized likelihood ratio

Watch how the posterior for two population parameters concentrate around true value used to generate mock data.



(plotted slightly differently)



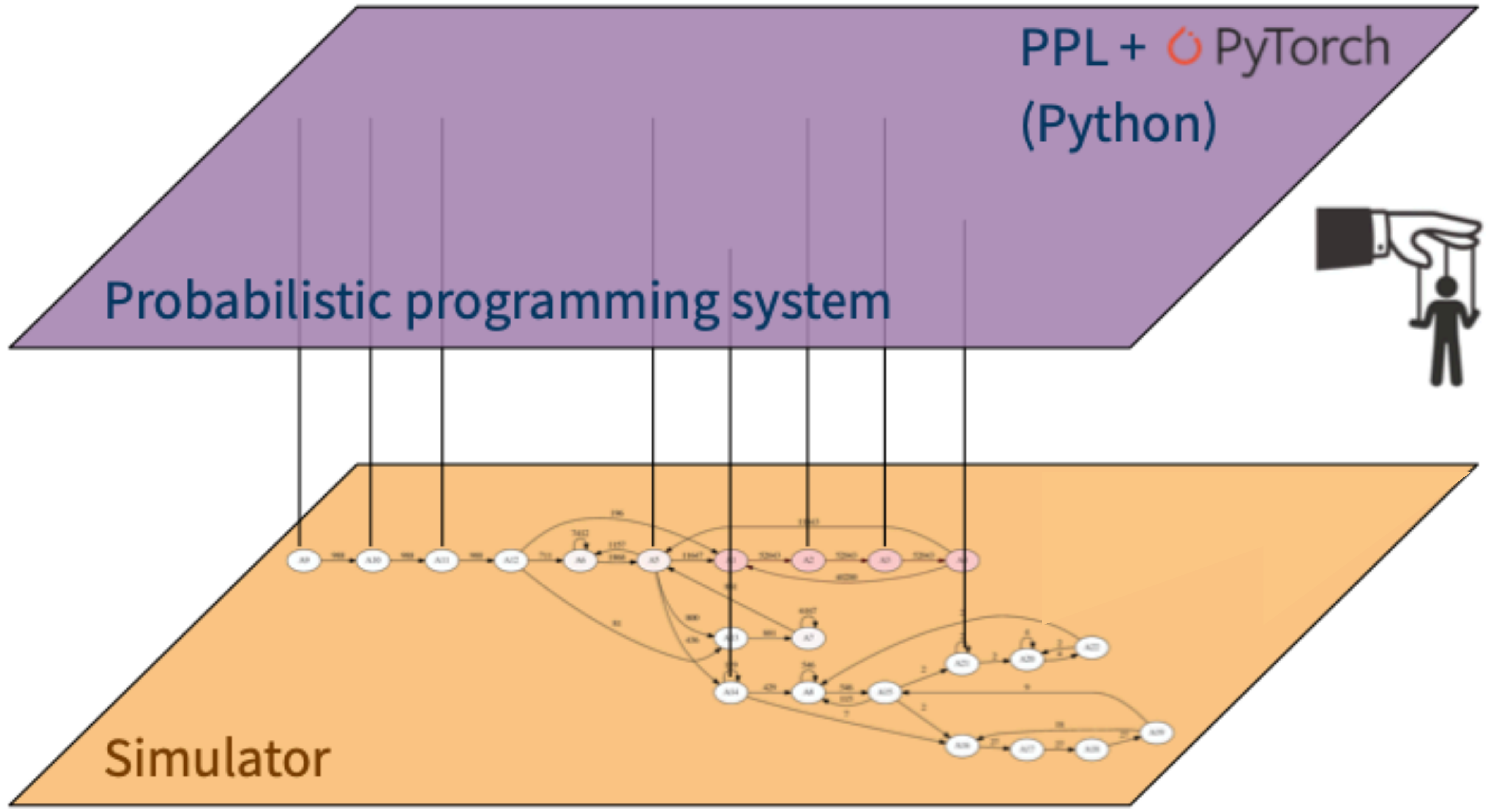
Sid Mishra-Sharma Johann Brehmer Gilles Louppe Joeri Hermans, K. Cranmer. published in ApJ, 886 (2019) arXiv:1909.02005

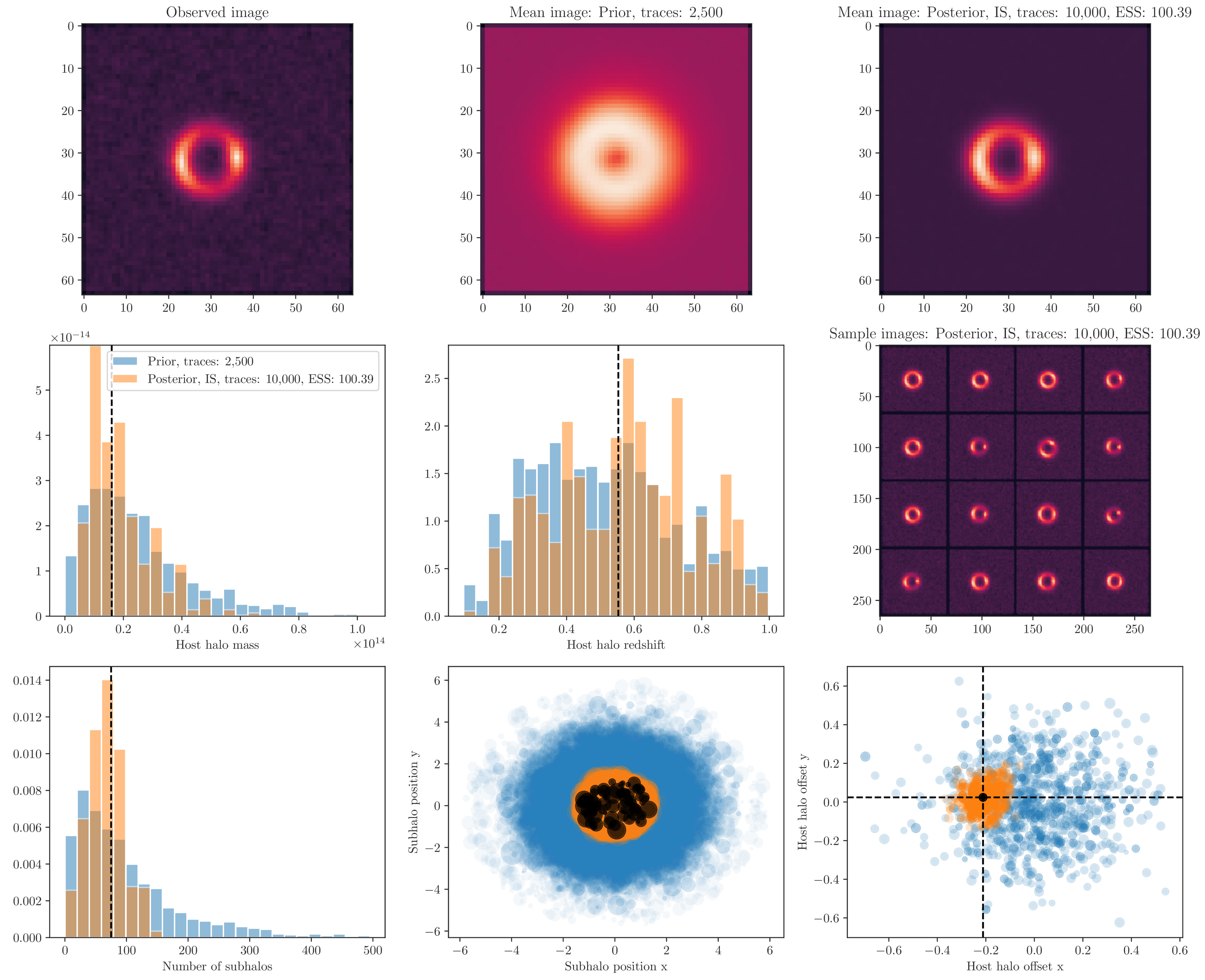
Prob Prog for Dark Matter & Gravitational Lensing

PRELIMINARY!

Here we use probabilistic programming to infer the latent variables z, the details of sub halo for a particular image

- prior $p(z)$
- posterior $p(z \mid x)$ for an observed image





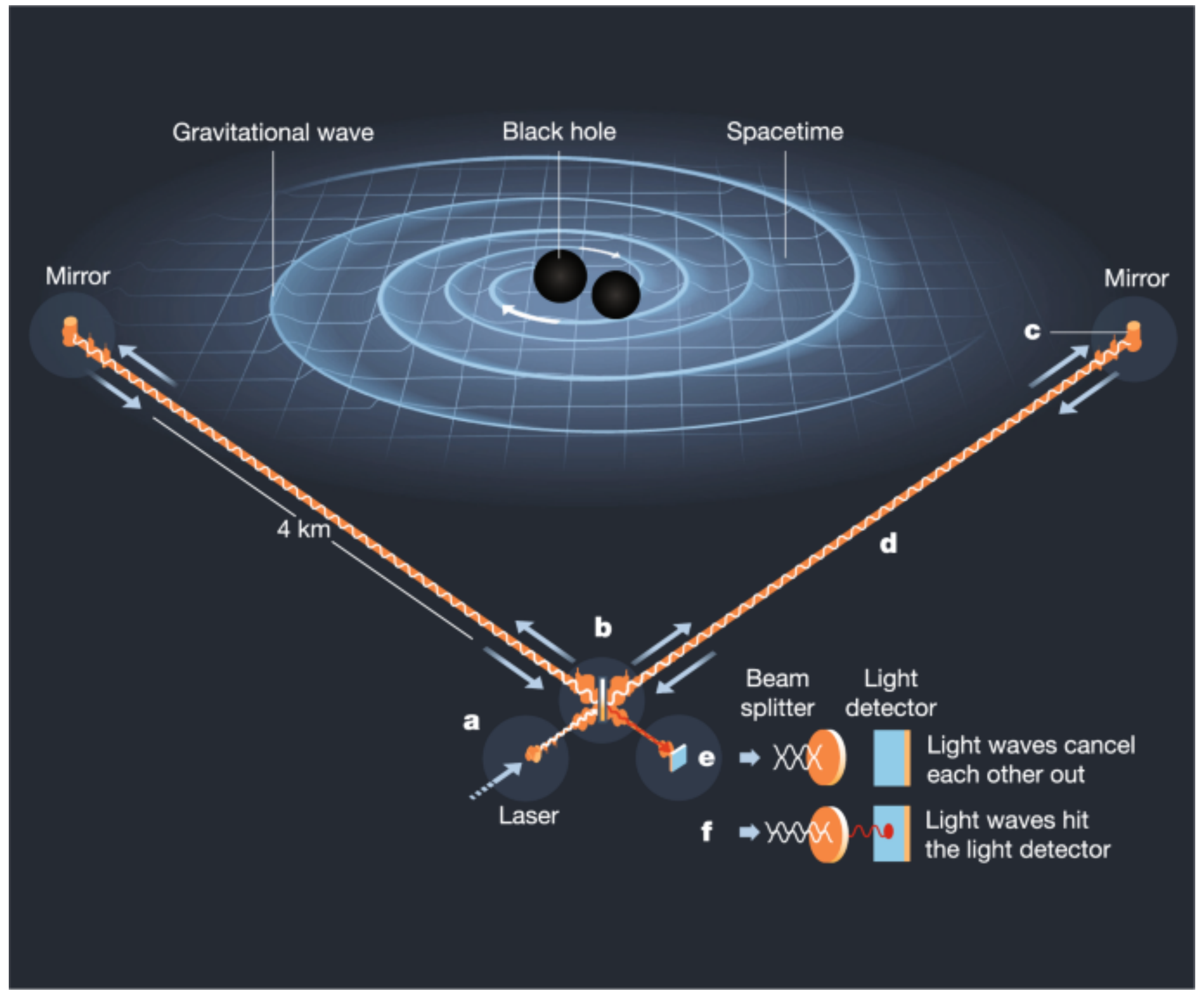

Sid Mishra-Sharma

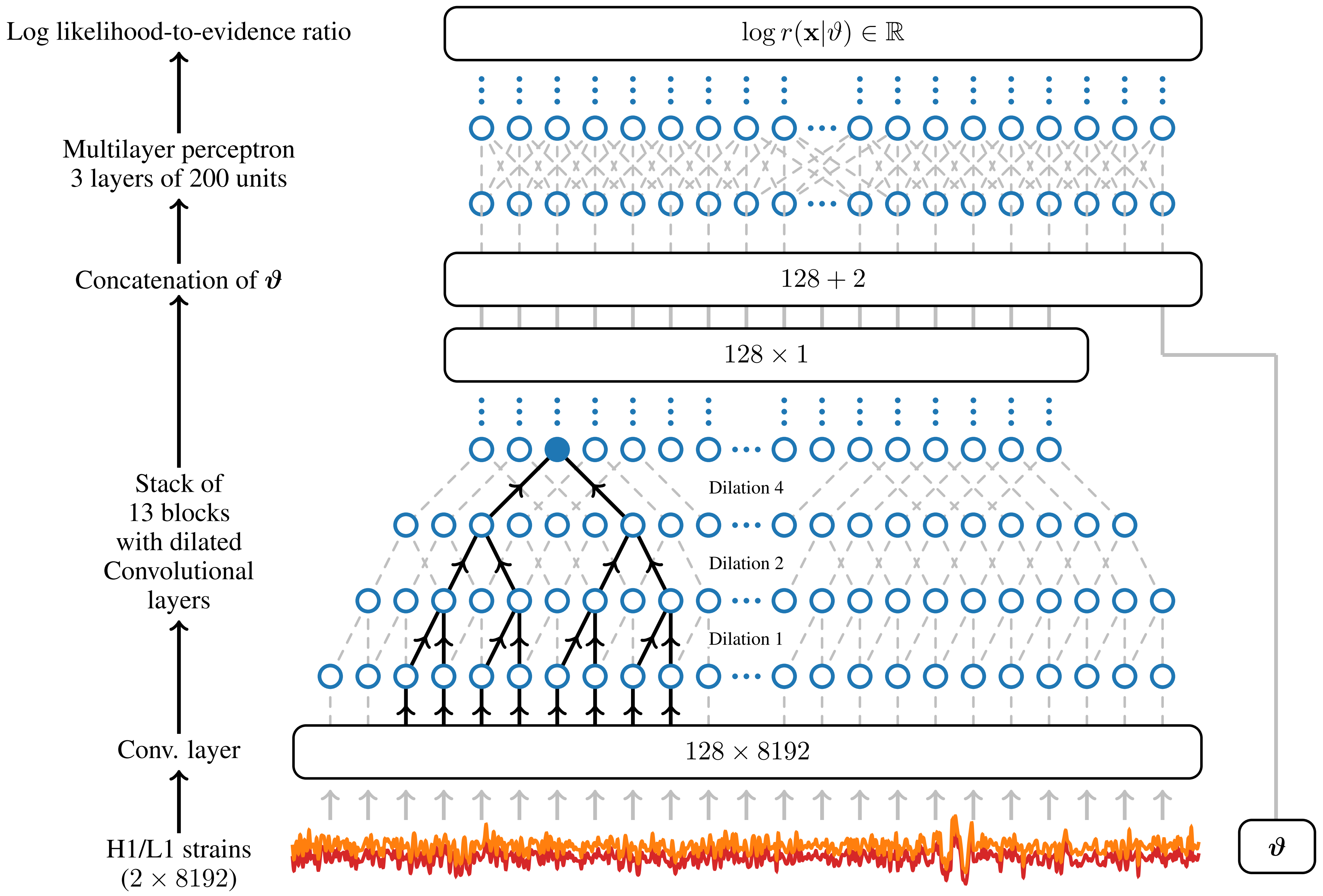

Johann Brehmer


Andreas Munk


Atılım Güneş Baydin

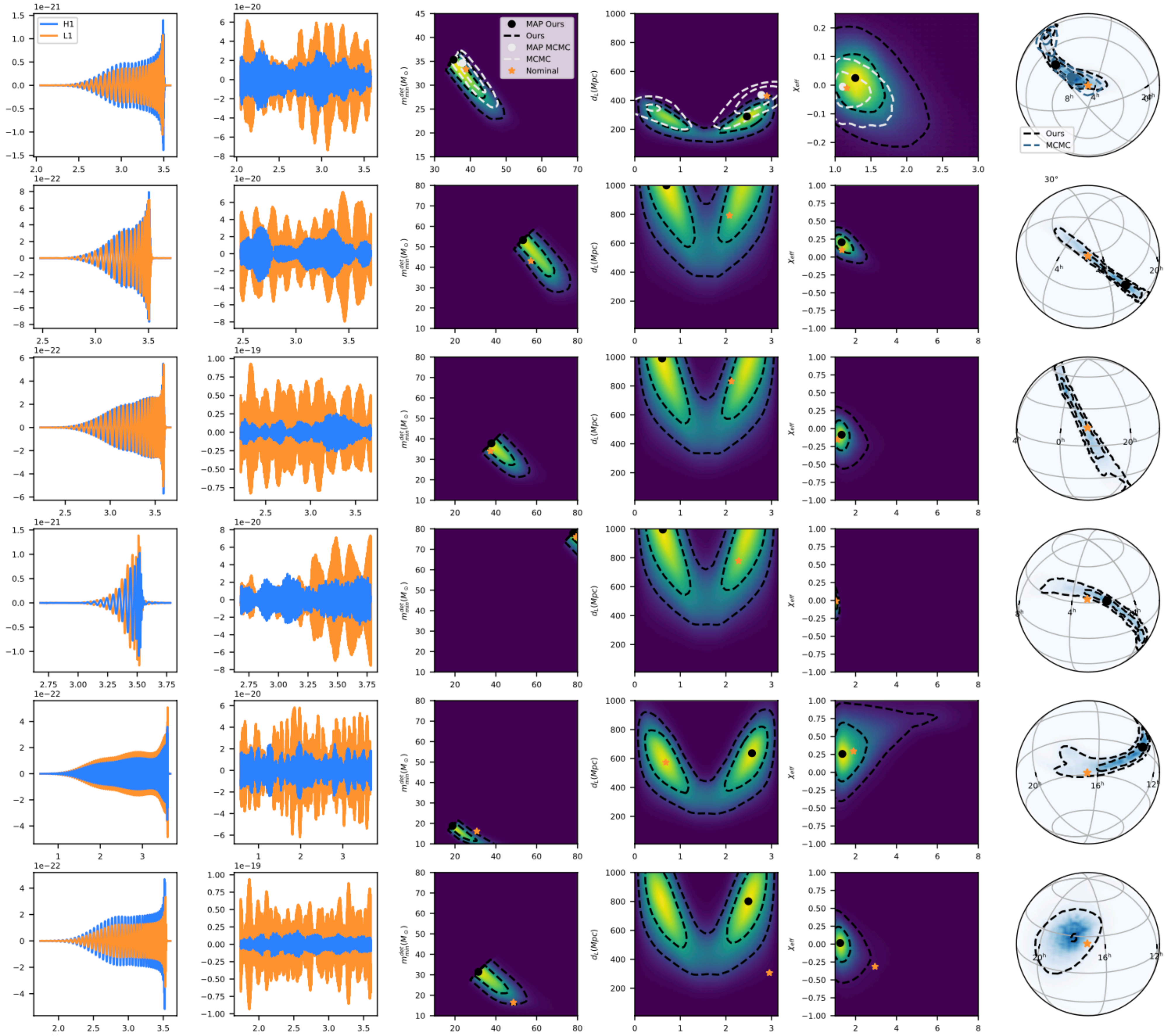
Gravitational Wave Astronomy



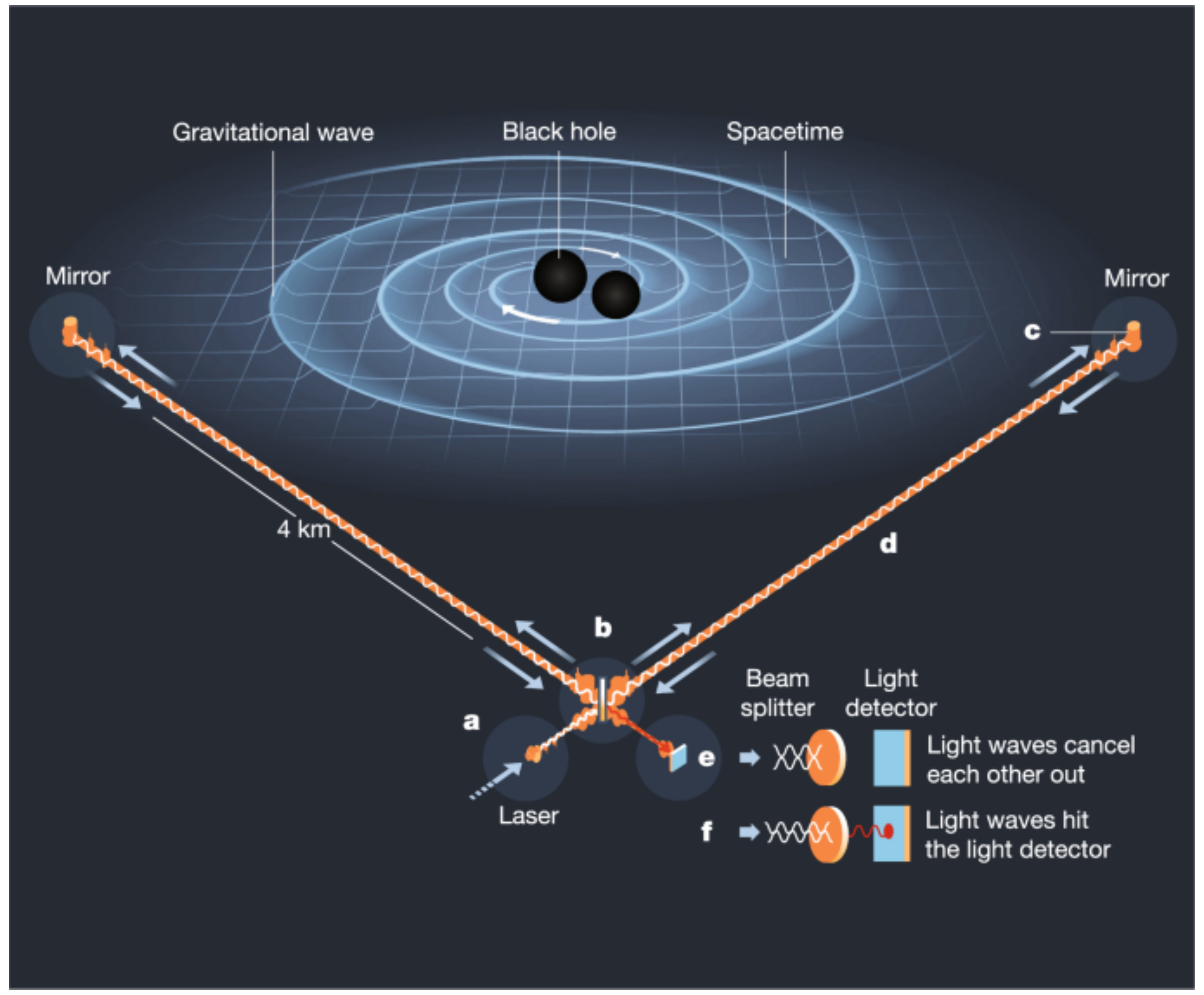


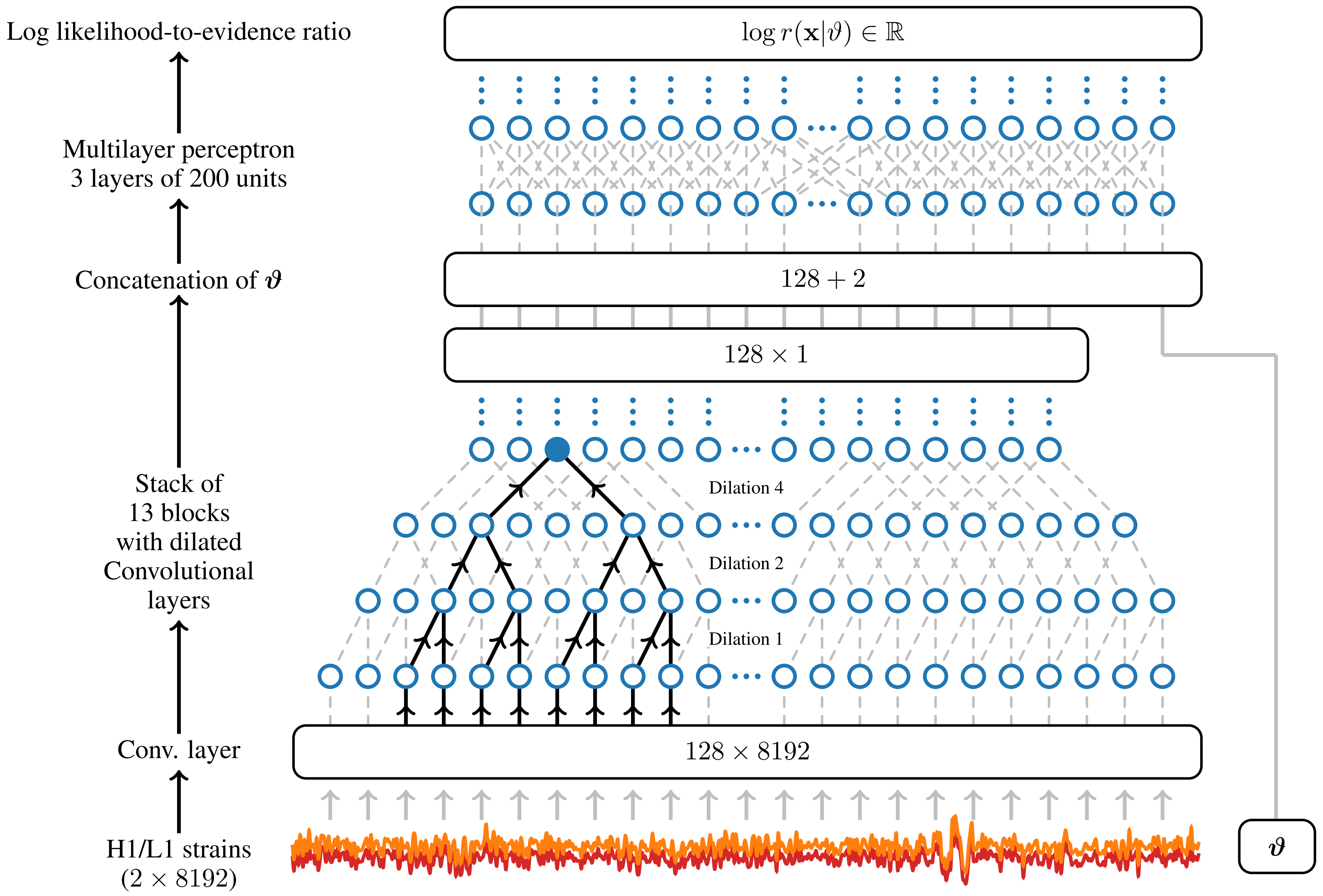
Lightning-Fast Gravitational Wave Parameter Inference through Neural Amortization

Delaunoy, Wehenkel, Hinderer, Nissanke, Weniger, Williamson, Louppe
[arXiv:2010.12931]



Gravitational Wave Astronomy





[28] H. Gabbard, C. Messenger, I. S. Heng, F. Tonolini, and R. Murray-Smith, Bayesian parameter estimation using conditional variational autoencoders for gravitational-wave astronomy (2019), arXiv:1909.06296 [astro-ph.IM].

[29] A. J. K. Chua and M. Vallisneri, Learning Bayesian posteriors with neural networks for gravitational-wave inference, Phys. Rev. Lett. **124**, 041102 (2020), arXiv:1909.05966 [gr-qc].

[30] C. Chatterjee, L. Wen, K. Vinsen, M. Kovalam, and A. Datta, Using Deep Learning to Localize Gravitational Wave Sources, Phys. Rev. D **100**, 103025 (2019), arXiv:1909.06367 [astro-ph.IM].

[31] S. R. Green, C. Simpson, and J. Gair, Gravitational-wave parameter estimation with autoregressive neural network flows, Phys. Rev. D **102**, 104057 (2020), arXiv:2002.07656 [astro-ph.IM].

[32] S. R. Green and J. Gair, Complete parameter inference for GW150914 using deep learning, Mach. Learn. Sci. Tech. **2**, 03LT01 (2021), arXiv:2008.03312 [astro-ph.IM].

[33] A. Delaunoy, A. Wehenkel, T. Hinderer, S. Nissanke, C. Weniger, A. R. Williamson, and G. Louppe, Lightning-Fast Gravitational Wave Parameter Inference through Neural Amortization, (2020), arXiv:2010.12931 [astro-ph.IM].

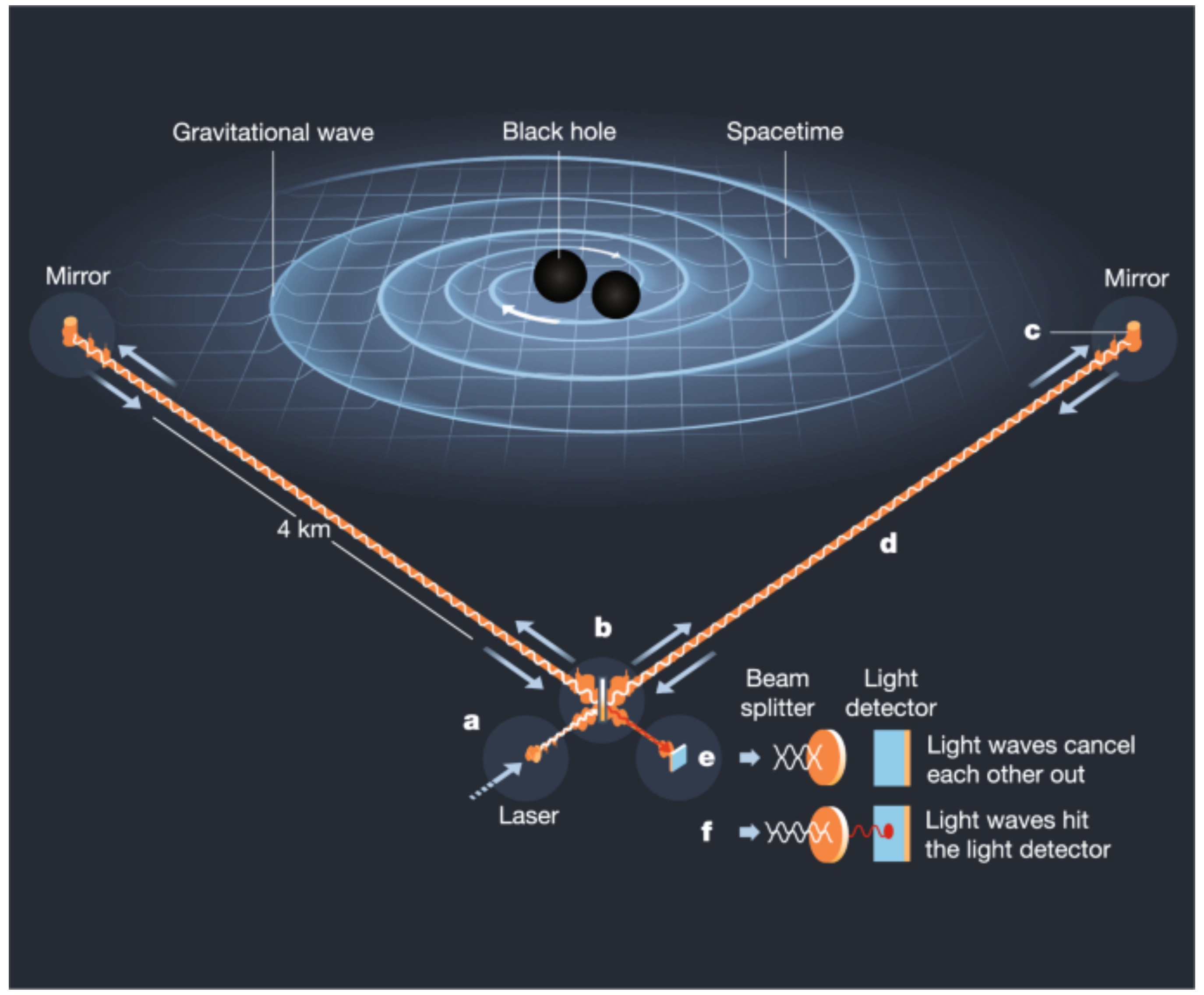
[34] P. G. Krastev, K. Gill, V. A. Villar, and E. Berger, Detection and Parameter Estimation of Gravitational Waves from Binary Neutron-Star Mergers in Real LIGO Data using Deep Learning, Phys. Lett. B **815**, 136161 (2021), arXiv:2012.13101 [astro-ph.IM].

[35] H. Shen, E. A. Huerta, E. O'Shea, P. Kumar, and Z. Zhao, Statistically-informed deep learning for gravitational wave parameter estimation, (2021), arXiv:1903.01998v3 [gr-qc].

[36] E. Cuoco, J. Powell, M. Cavaglià, K. Ackley, M. Bejger, C. Chatterjee, M. Coughlin, S. Coughlin, P. Easter, R. Essick, *et al.*, Enhancing gravitational-wave science with machine learning, Machine Learning: Science and Technology **2**, 011002 (2020), arXiv:2005.03745 [astro-ph.HE].

[36] E. Cuoco, J. Powell, M. Cavaglià, K. Ackley, M. Bejger, C. Chatterjee, M. Coughlin, S. Coughlin, P. Easter, R. Essick, *et al.*, Enhancing gravitational-wave science with machine learning, Machine Learning: Science and Technology **2**, 011002 (2020), arXiv:2005.03745 [astro-ph.HE].

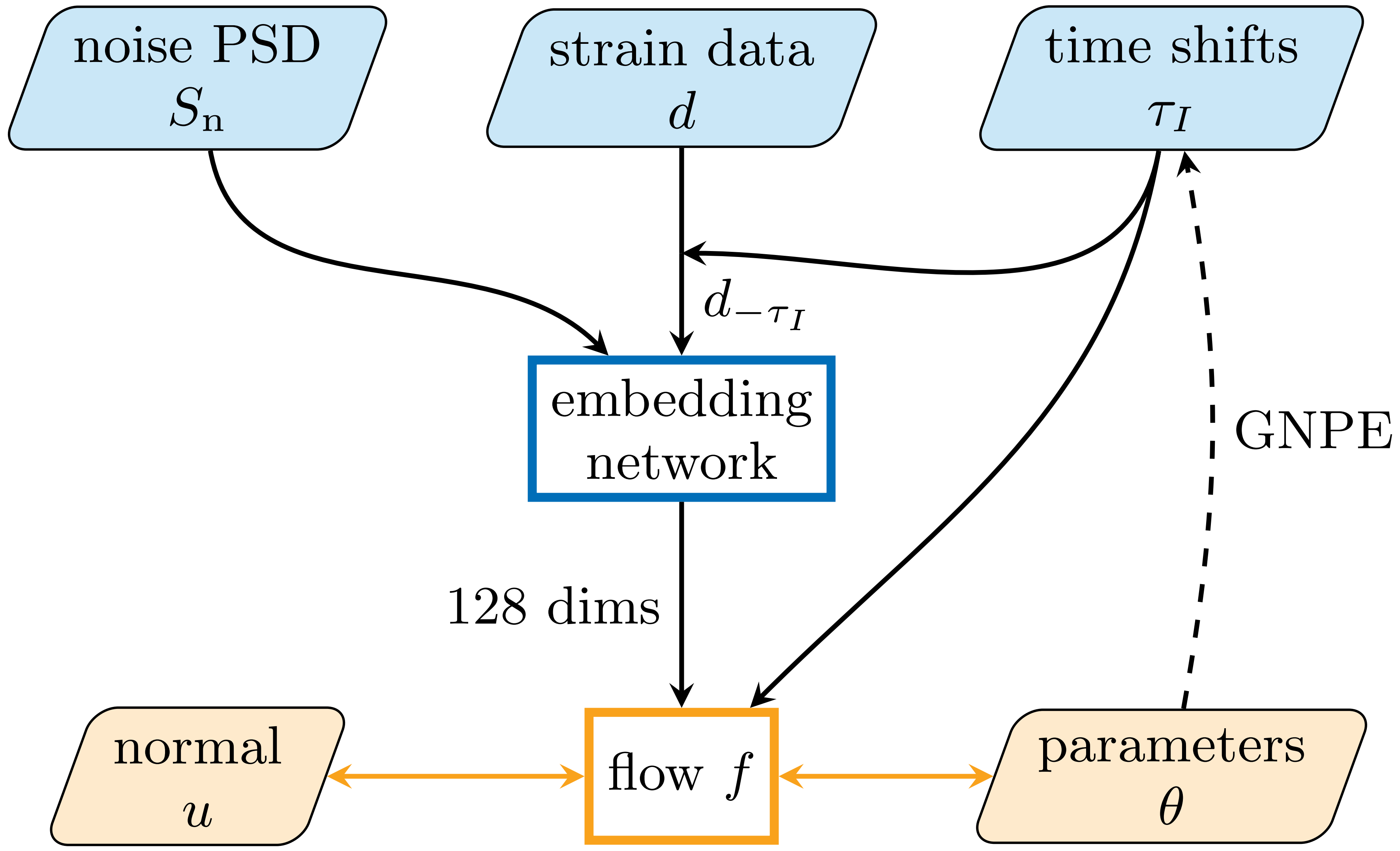
Gravitational Wave Astronomy



Real-time gravitational-wave science with neural posterior estimation

Maximilian Dax,[1,*] Stephen R. Green,[2,†] Jonathan Gair,[2,‡]
Jakob H. Macke,[1,3] Alessandra Buonanno,[2,4] and Bernhard Schölkopf[1]

[1] *Max Planck Institute for Intelligent Systems, Max-Planck-Ring 4, 72076 Tübingen, Germany*
[2] *Max Planck Institute for Gravitational Physics (Albert Einstein Institute), Am Mühlenberg 1, 14476 Potsdam, Germany*
[3] *Machine Learning in Science, University of Tübingen, 72076 Tübingen, Germany*
[4] *Department of Physics, University of Maryland, College Park, MD 20742, USA*



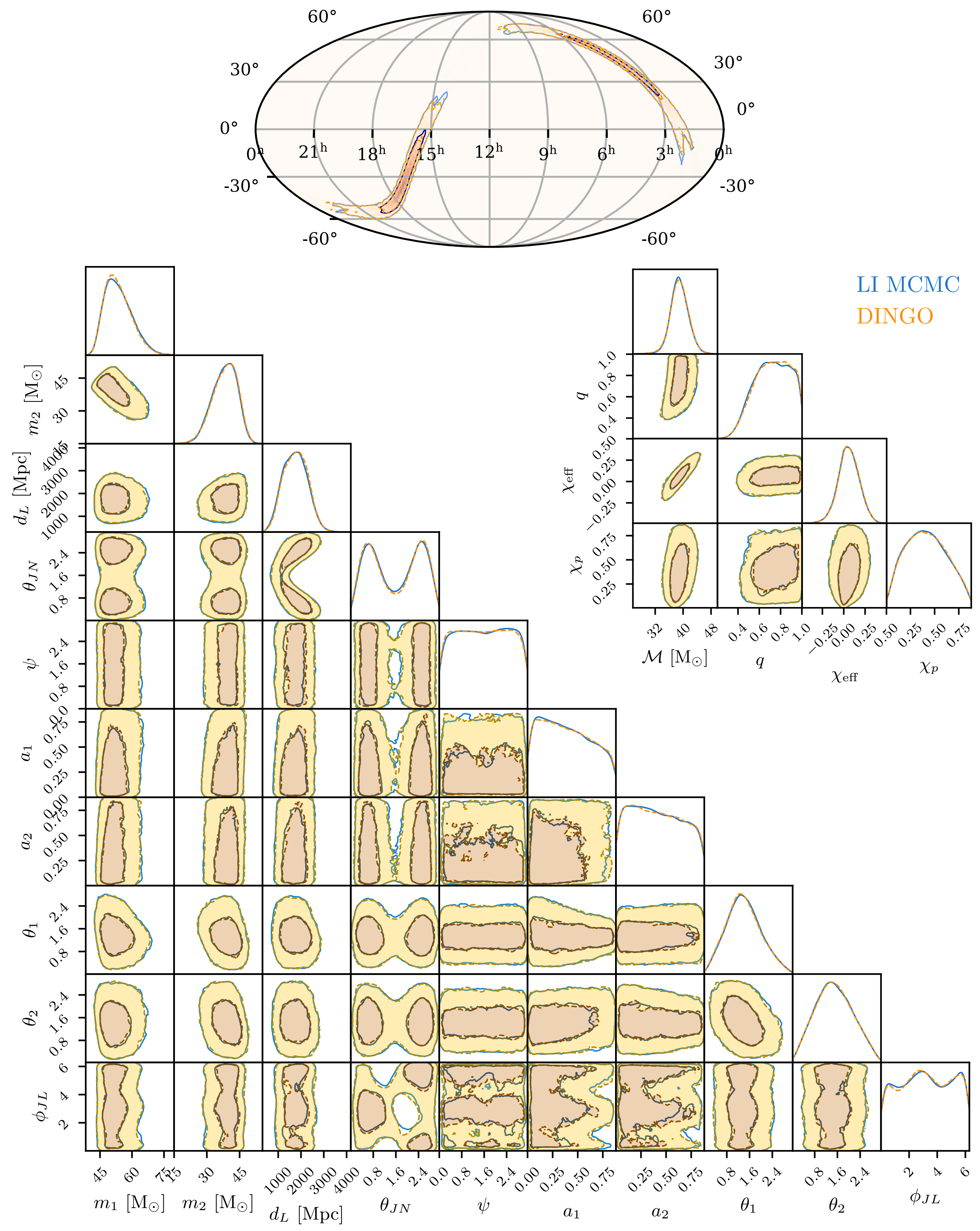
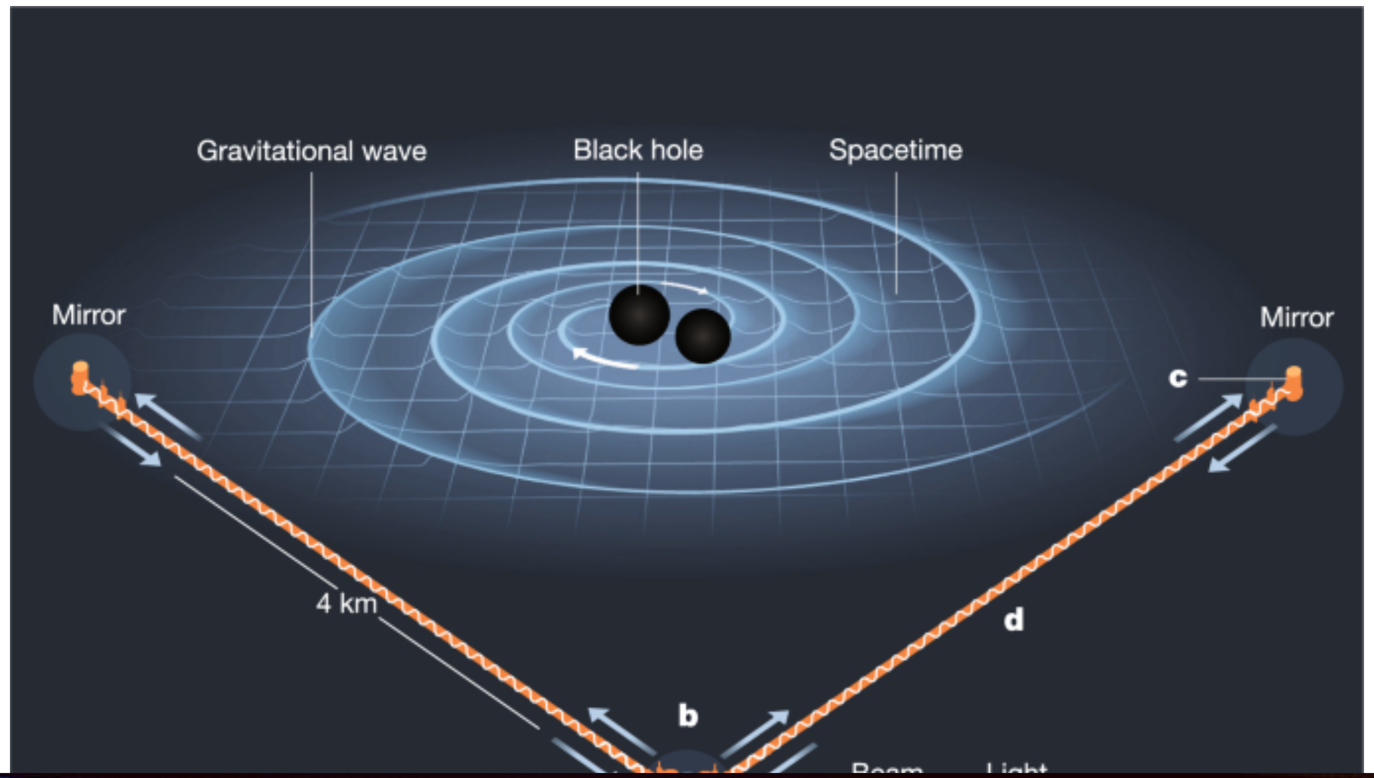


Figure 15. GW170823.

Gravitational Wave Astronomy



Real-time gravitational-wave science with neural posterior estimation

Maximilian Dax,[1,*] Stephen R. Green,[2,†] Jonathan Gair,[2,‡]
Jakob H. Macke,[1,3] Alessandra Buonanno,[2,4] and Bernhard Schölkopf[1]

[1] *Max Planck Institute for Intelligent Systems, Max-Planck-Ring 4, 72076 Tübingen, Germany*
[2] *Max Planck Institute for Gravitational Physics (Albert Einstein Institute), Am Mühlenberg 1, 14476 Potsdam, Germany*
[3] *Machine Learning in Science, University of Tübingen, 72076 Tübingen, Germany*
[4] *Department of Physics, University of Maryland, College Park, MD 20742, USA*

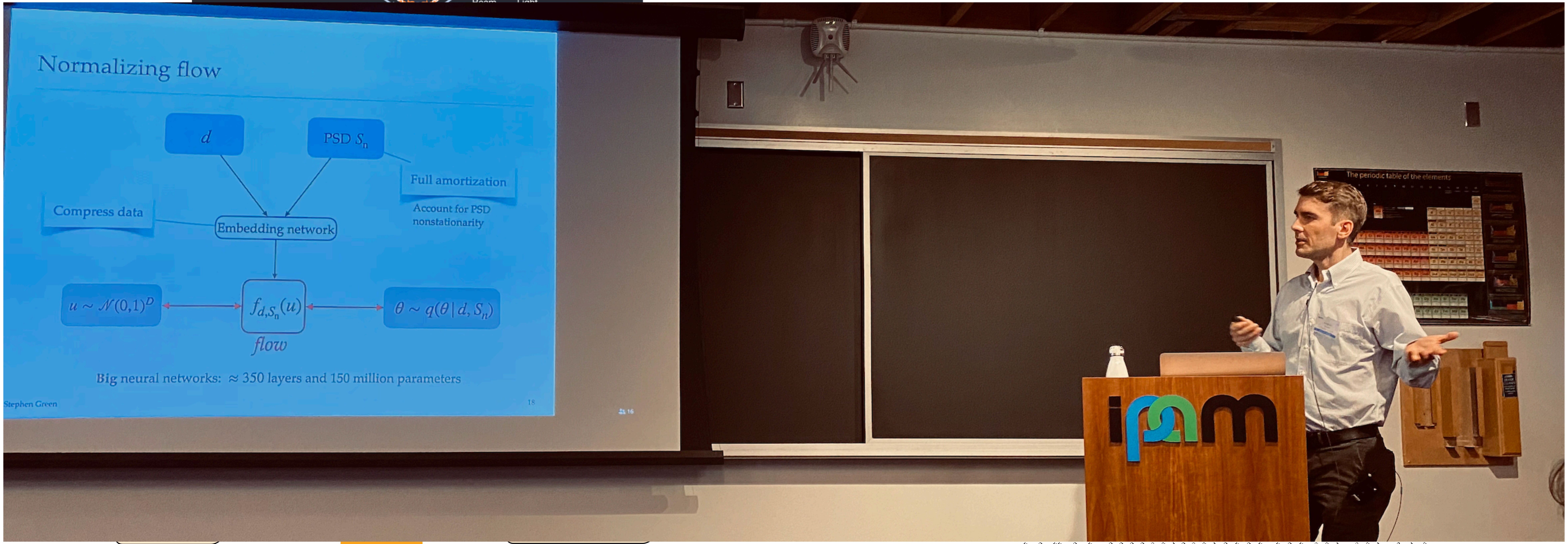
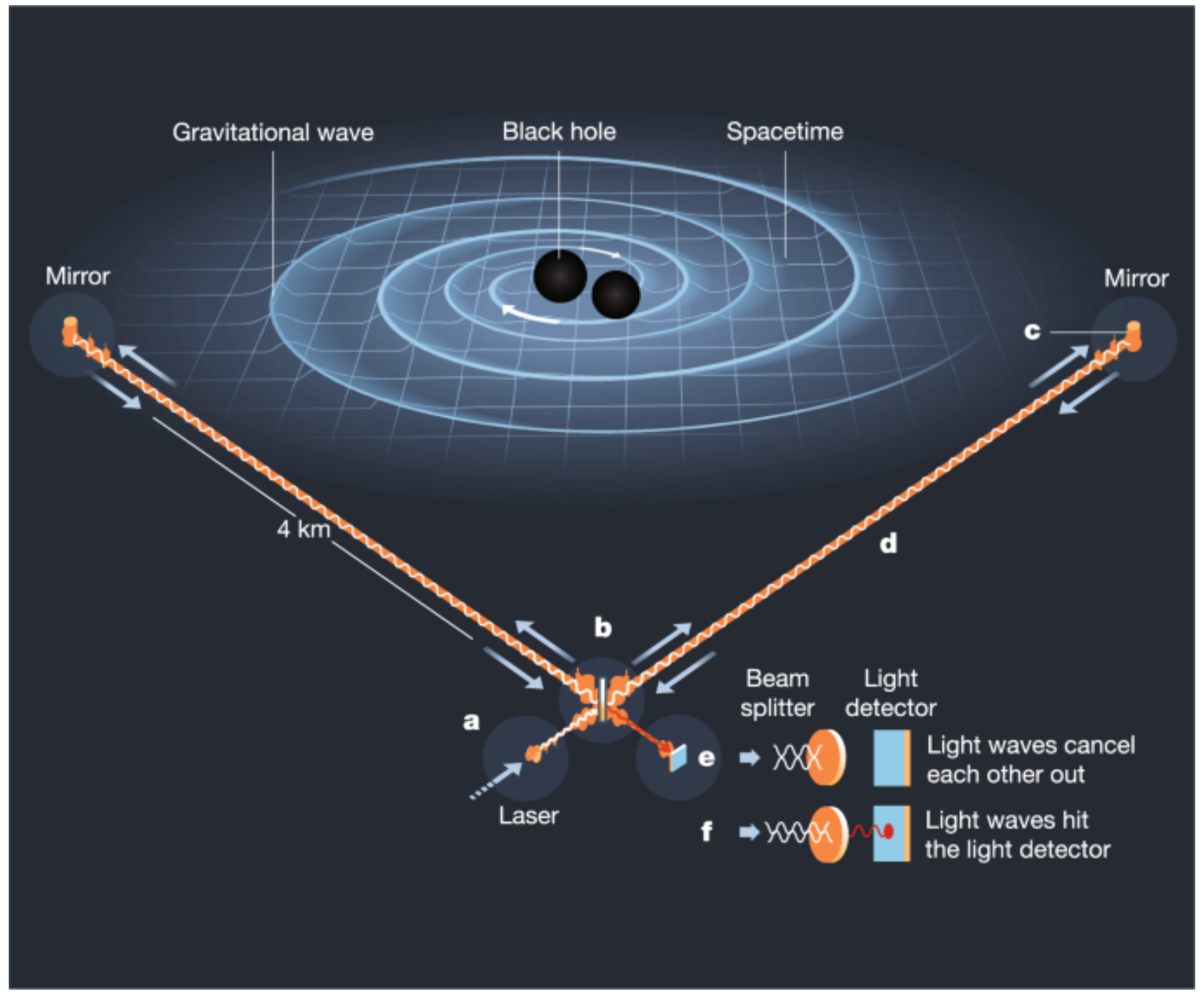
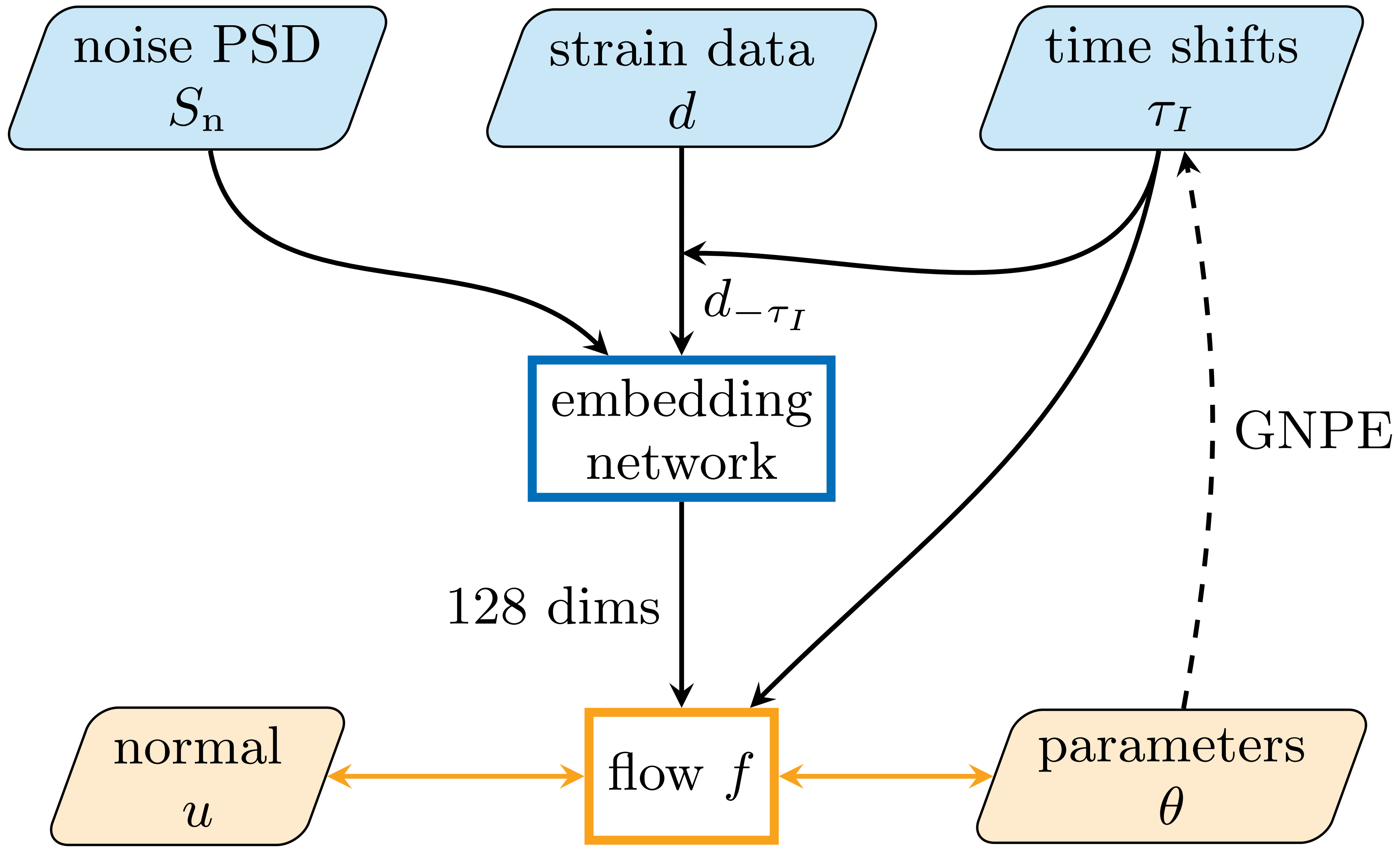


Figure 15. GW170823.





Remark / Alternative framing

- Can think of noise model as having nuisance parameters ν
- Including off-source measurement S_n can be thought of as combining likelihoods for on-source and off-source

$$p(d, S_n \mid \theta, \nu) = p(d \mid \theta, \nu) p(S_n \mid \nu)$$

- Joint posterior given by

$$p(\theta, \nu \mid d, S_n) \propto p(d, S_n \mid \theta, \nu) \pi(\theta) \pi(\nu)$$

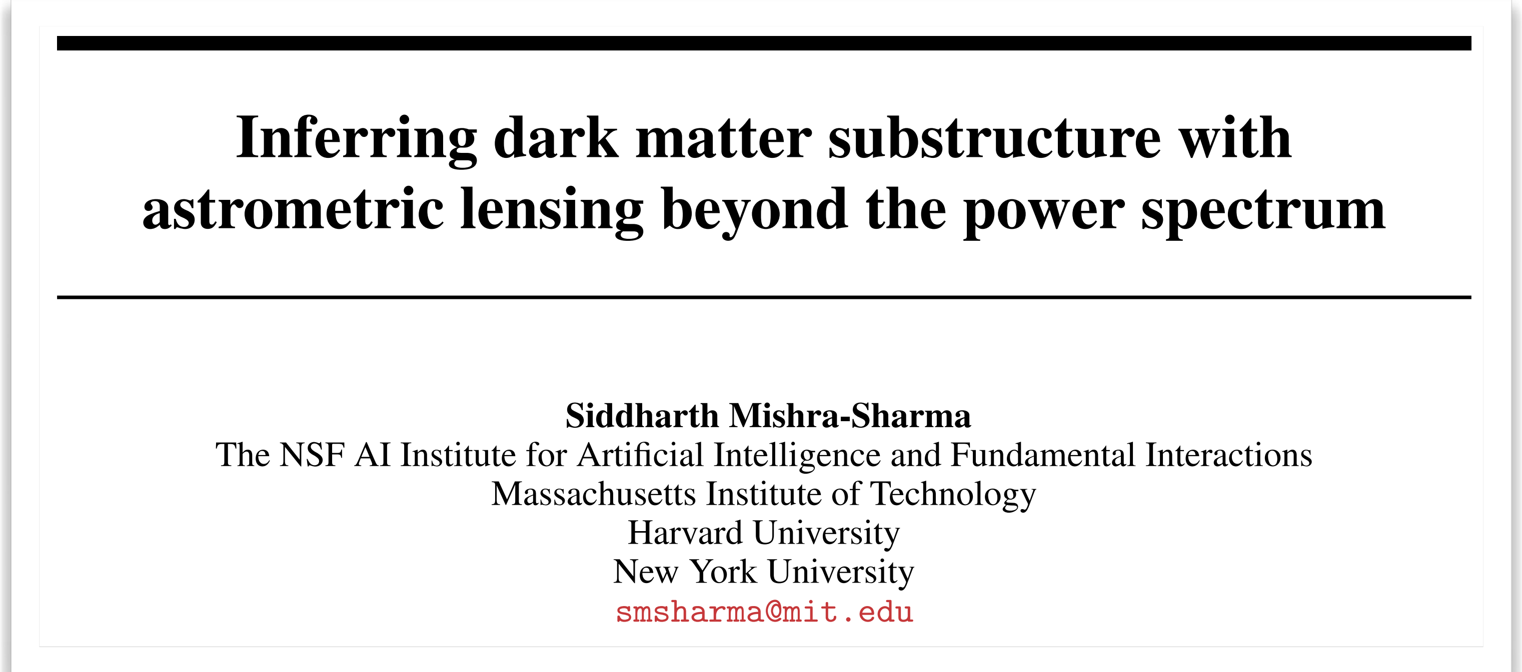
- Final posterior given by

$$p(\theta \mid d, S_n) = \int d\nu\, p(\theta, \nu \mid d, S_n)$$

Another recent examples

Sid Mishra-Sharma

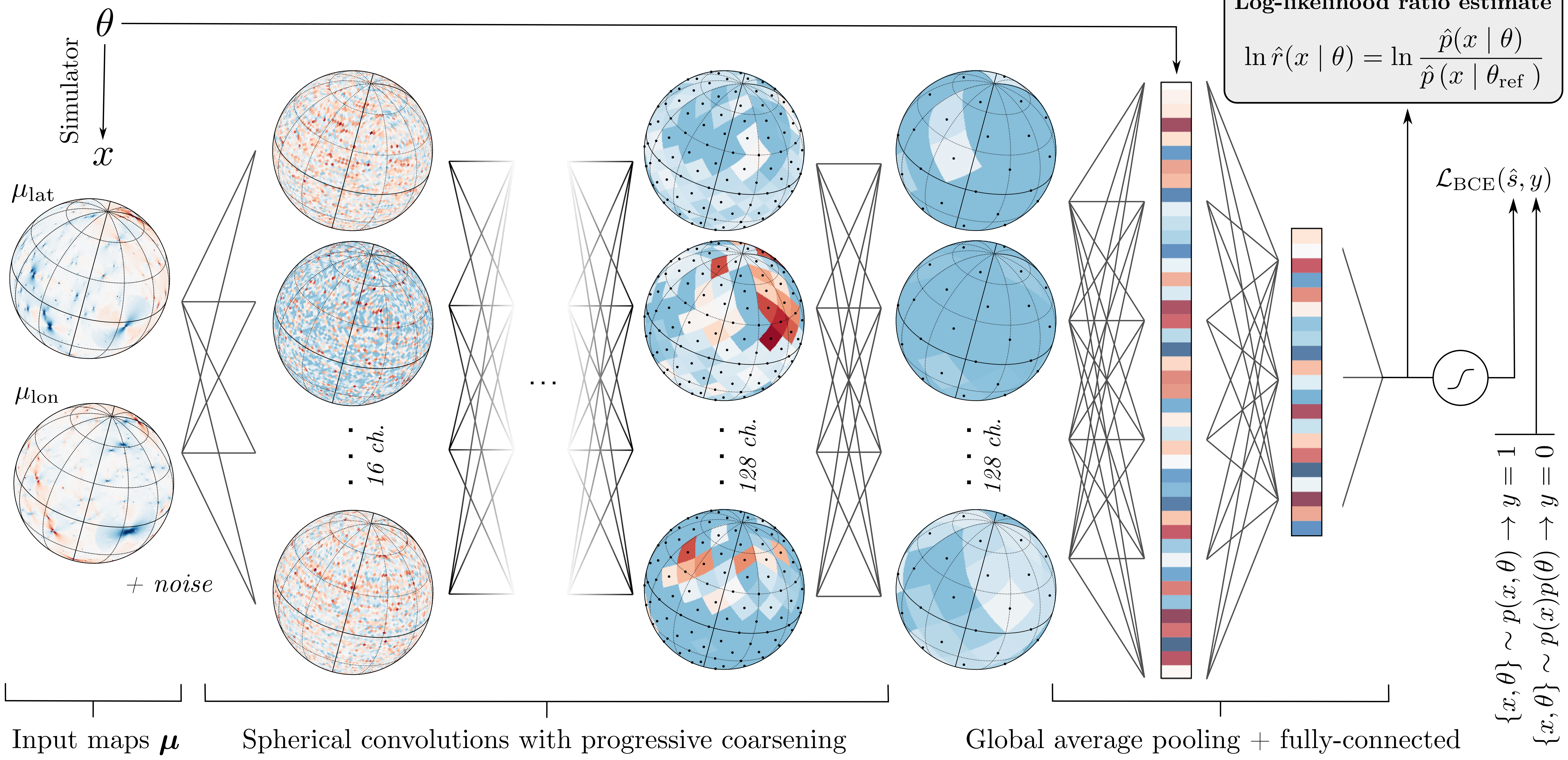
- Neural ratio estimation
- Targets population-level parameters (fraction of dark matter in sub halos)
- Feature extractor / embedding network / learned summary statistics with inductive bias (spherical CNN)
- Aimed at future Gaia data



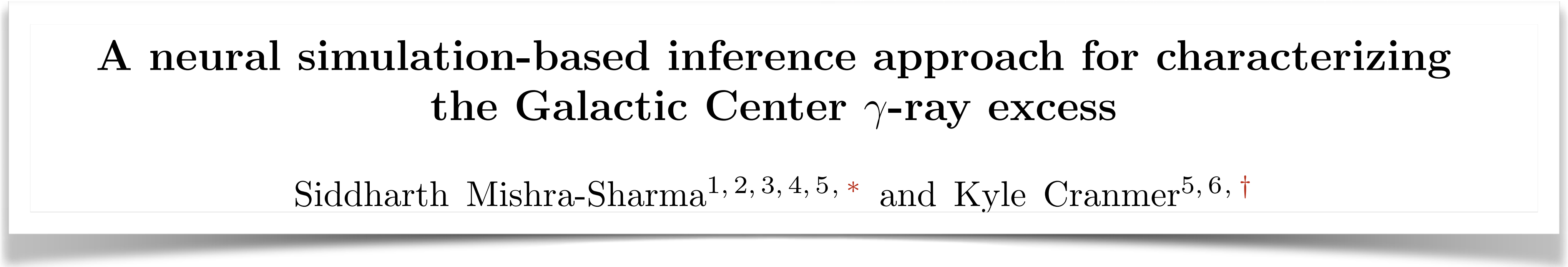
Inferring dark matter substructure with astrometric lensing beyond the power spectrum

Siddharth Mishra-Sharma
The NSF AI Institute for Artificial Intelligence and Fundamental Interactions
Massachusetts Institute of Technology
Harvard University
New York University
smsharma@mit.edu

[arXiv:2110.01620]



Another recent examples

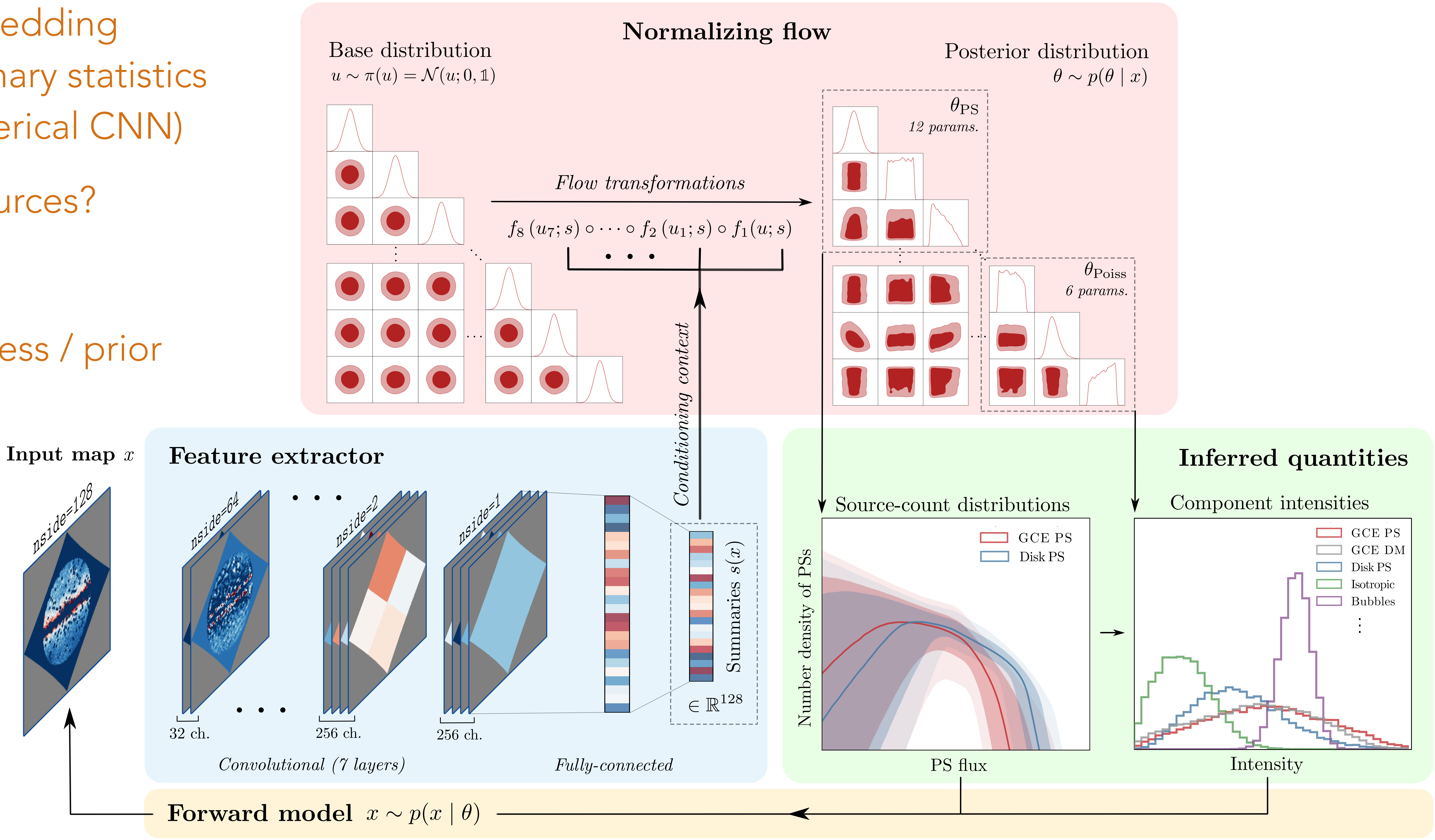

A neural simulation-based inference approach for characterizing the Galactic Center γ-ray excess

Siddharth Mishra-Sharma[1,2,3,4,5,*] and Kyle Cranmer[5,6,†]


Sid Mishra-Sharma

[arXiv:2110.06931]

- Neural posterior estimation
- Feature extractor / embedding network / learned summary statistics with inductive bias (spherical CNN)
- Dark matter or point sources?
- Real Fermi data
- Many checks of robustness / prior sensitivity etc.



MCMC-style exactness with approximate posteriors

https://arxiv.org/abs/1904.12072 https://arxiv.org/abs/2105.12603
https://arxiv.org/abs/2107.00734 https://arxiv.org/abs/2106.05934
https://arxiv.org/abs/2003.06413

One can also make a hybrid

- If $q(\theta \mid x)$ is the approximate posterior surrogate
- And $\tilde{p}(x \mid \theta) = p(x \mid \theta)\pi(\theta)$ is the un-normalized posterior (likelihood x prior)
- One can get "exact" samples in the MCMC sense by using $\theta' \sim q(\theta \mid x)$ as a proposal and accept/reject based on $\dfrac{q(\theta \mid x)\tilde{p}(\theta' \mid x)}{q(\theta \mid x)\tilde{p}(\theta' \mid x)}$
- Very efficient, dramatically reduced no auto-correlation time.

Flow-based generative models for Markov chain Monte Carlo in lattice field theory

M. S. Albergo,[1,2,3] G. Kanwar,[4] and P. E. Shanahan[4,1]
[1]Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada
[2]Cavendish Laboratories, University of Cambridge, Cambridge CB3 0HE, U.K.
[3]University of Waterloo, Waterloo, Ontario N2L 3G1, Canada
[4]Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.

A Markov chain update scheme using a machine-learned *flow-based generative model* is proposed for Monte Carlo sampling in lattice field theories. The generative model may be optimized (trained) to produce samples from a distribution approximating the desired Boltzmann distribution determined by the lattice action of the theory being studied. Training the model systematically improves autocorrelation times in the Markov chain, even in regions of parameter space where standard Markov chain Monte Carlo algorithms exhibit critical slowing down in producing decorrelated updates. Moreover, the model may be trained without existing samples from the desired distribution. The algorithm is compared with HMC and local Metropolis sampling for ϕ^4 theory in two dimensions.

Flow-based sampling for multimodal distributions in lattice field theory

Daniel C. Hackett,[1,2] Chung-Chun Hsieh,[3] Michael S. Albergo,[4] Denis Boyda,[5,1,2]
Jiunn-Wei Chen,[3,6,7] Kai-Feng Chen,[3] Kyle Cranmer,[4] Gurtej Kanwar,[1,2] and Phiala E. Shanahan[1,2]
[1]Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA
[2]The NSF AI Institute for Artificial Intelligence and Fundamental Interactions
[3]Department of Physics and Center for Theoretical Physics, National Taiwan University, Taipei, Taiwan 106
[4]Center for Cosmology and Particle Physics, New York University, New York, NY 10003, USA
[5]Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont IL 60439, USA
[6]Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan
[7]Leung Center for Cosmology and Particle Astrophysics, National Taiwan University, Taipei, Taiwan 106
(Dated: July 5, 2021)

Flow-based generative models for Markov chain Monte Carlo in lattice field theory

M. S. Albergo,[1,2,3] G. Kanwar,[4] and P. E. Shanahan[4,1]
[1]Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada
[2]Cavendish Laboratories, University of Cambridge, Cambridge CB3 0HE, U.K.
[3]University of Waterloo, Waterloo, Ontario N2L 3G1, Canada
[4]Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.

A Markov chain update scheme using a machine-learned *flow-based generative model* is proposed for Monte Carlo sampling in lattice field theories. The generative model may be optimized (trained) to produce samples from a distribution approximating the desired Boltzmann distribution determined by the lattice action of the theory being studied. Training the model systematically improves autocorrelation times in the Markov chain, even in regions of parameter space where standard Markov chain Monte Carlo algorithms exhibit critical slowing down in producing decorrelated updates. Moreover, the model may be trained without existing samples from the desired distribution. The algorithm is compared with HMC and local Metropolis sampling for ϕ^4 theory in two dimensions.

Adaptive Monte Carlo augmented with normalizing flows

Marylou Gabrié
*Flatiron Institute, New York, NY and Center for Data Science, New York University, New York, NY**

Grant M. Rotskoff
Dept. of Chemistry, Stanford University, Stanford, CA 94305†

Eric Vanden-Eijnden
Courant Institute, New York University, New York, NY 10012‡

RESEARCH

RESEARCH ARTICLE SUMMARY

MACHINE LEARNING

Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning

Frank Noé*†, Simon Olsson*, Jonas Köhler*, Hao Wu

INTRODUCTION: Statistical mechanics aims to compute the average behavior of physical systems on the basis of their microscopic constituents. For example, what is the probability that a protein will be folded at a given temperature? If we could answer such questions efficiently, then we could not only comprehend the workings of molecules and materials, but we could also design drug molecules and materials with new properties in a principled way.

To this end, we need to compute statistics of the equilibrium states of many-body systems. In the protein-folding example, this means to consider each of the astronomically many ways to place all protein atoms in space, to compute the probability of each such "configuration" in the equilibrium ensemble, and then to compare the total probability of unfolded and folded configurations.

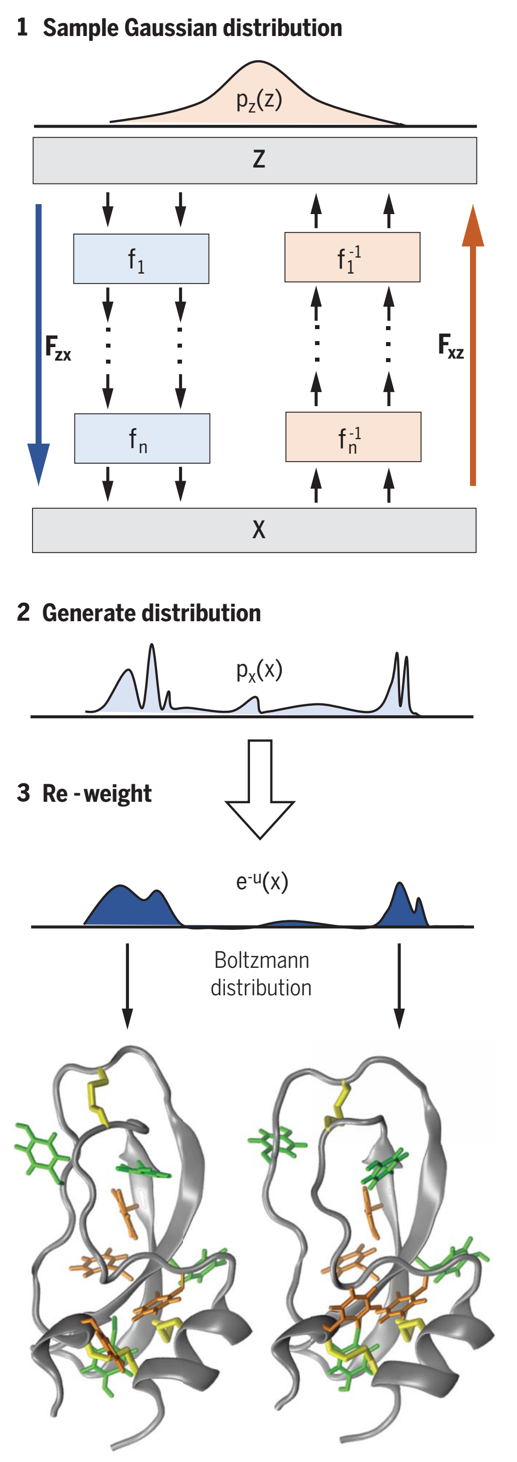
As enumeration of all configurations is infeasible, one instead must attempt to sample them from their equilibrium distribution. However, we currently have no way to generate equilibrium samples of many-body systems in "one shot." The main approach is thus to start with one configuration, e.g., the folded protein state, and make tiny changes to it over time, e.g., by using Markov-chain Monte Carlo or molecular dynamics (MD). However, these simulations get trapped in metastable (long-lived) states: For example, sampling a single folding or unfolding event with atomistic MD may take a year on a supercomputer.

RATIONALE: Here, we combine deep machine learning and statistical mechanics to develop Boltzmann generators. Boltzmann generators are trained on the energy function of a many-body system and learn to provide unbiased, one-shot samples from its equilibrium state. This is achieved by training an invertible neural network to learn a coordinate transformation from a system's configurations to a so-called latent space representation, in which the low-energy configurations of different states are close to each other and can be easily sampled. Because of the invertibility, every latent space sample can be back-transformed to a system configuration with high Boltzmann probability (Fig. 1). We then employ statistical mechanics, which offers a rich set of tools for reweighting the distribution generated by the neural network to the Boltzmann distribution.

RESULTS: Boltzmann generators can be trained to directly generate independent samples of low-energy structures of condensed-matter systems and protein molecules. When initialized with a few structures from different metastable states, Boltzmann generators can generate statistically independent samples from these states and efficiently compute the free-energy differences between them. This capability could be used to compute relative stabilities between different experimental structures of protein or other organic molecules, which is currently a very challenging problem. Boltzmann generators can also learn a notion of "reaction coordinates": Simple linear interpolations between points in latent space have a high probability of corresponding to physically realistic, low-energy transition pathways. Finally, by using established sampling methods such as Metropolis Monte Carlo in the latent space variables, Boltzmann generators can discover new states and gradually explore state space.

ON OUR WEBSITE
Read the full article at http://dx.doi.org/10.1126/science.aaw1147

CONCLUSION: Boltzmann generators can overcome rare event–sampling problems in many-body systems by learning to generate unbiased equilibrium samples from different metastable states in one shot. They differ conceptually from established enhanced sampling methods, as no reaction coordinates are needed to drive them between metastable states. However, by applying existing sampling methods in the latent spaces learned by Boltzmann generators, a plethora of new opportunities opens up to design efficient sampling methods for many-body systems. ■



Boltzmann generators overcome sampling problems between long-lived states. The Boltzmann generator works as follows: 1. We sample from a simple (e.g., Gaussian) distribution. 2. An invertible deep neural network is trained to transform this simple distribution to a distribution $p_X(x)$ that is similar to the desired Boltzmann distribution of the system of interest. 3. To compute thermodynamics quantities, the samples are reweighted to the Boltzmann distribution using statistical mechanics methods.

The list of author affiliations is available in the full article online.
*These authors contributed equally to this work.
†Corresponding author. Email: frank.noe@fu-berlin.de
Cite this article as F. Noé *et al.*, *Science* 365, eaaw1147 (2019). DOI: 10.1126/science.aaw1147

Noé *et al.*, *Science* 365, 1001 (2019) 6 September 2019 1 of 1

Inductive Bias

Compositionality

Relationships

Symmetry

Causality

Separation

Insight of data generating process informs inductive bias on architecture

Conclusions

Simulation-based inference is a great fit for gravitational wave astronomy

- Amortized inference has many advantages
- There are possibilities for hybrids where fast inference with surrogate is calibrated with more forward simulations or used to accelerate MCMC

The product of inference doesn't need to be samples from the posterior

- With NPE you can actually convey and evaluate the posterior $p(\theta \mid x)$
- If you want to do population level inference, it may be better to isolate individual terms the likelihood (avoid double counting the prior)
- You can skip explicit inference of latents associated to individual objects

Support

NSF

MSDSE
MOORE - SLOAN
DATA SCIENCE ENVIRONMENTS

BSF
United States – Israel
Binational Science Foundation

dianahep

iris hep
Institute for Research and Innovation in Software for High Energy Physics

The SCAILFIN Project
scailfin.github.io