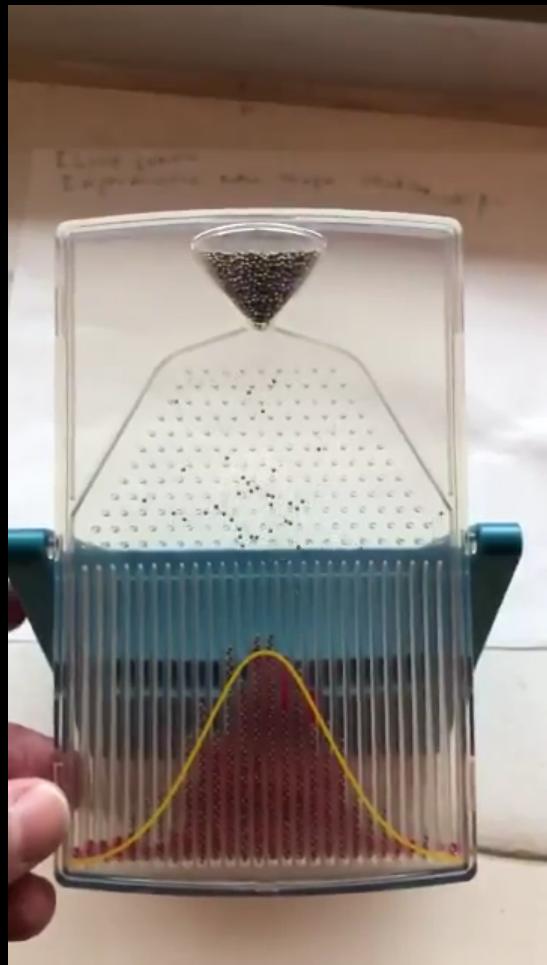


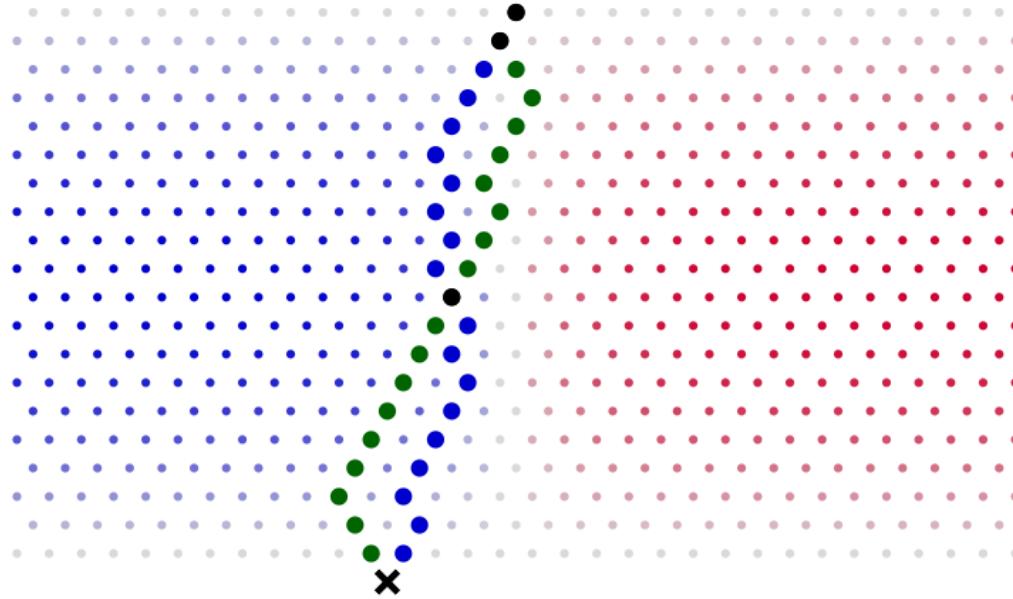
# Neural Likelihood-free Inference

PhD AI seminars  
October 21, BeCentral, Brussels

Gilles Louppe  
[g.louppe@uliege.be](mailto:g.louppe@uliege.be)

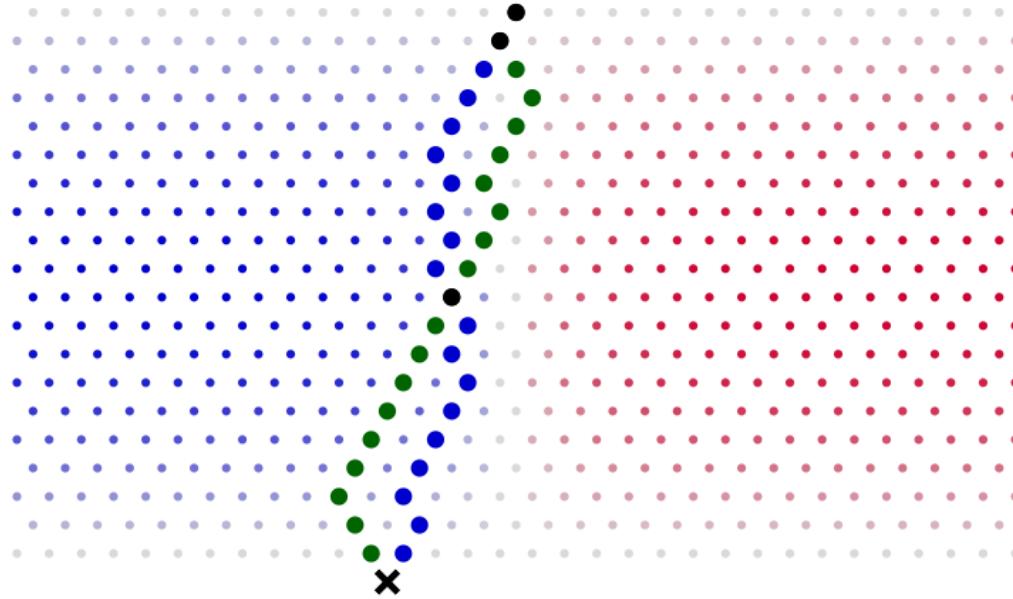






The probability of ending in bin  $x$  corresponds to the total probability of all the paths  $z$  from start to  $x$ ,

$$p(x|\theta) = \int p(x, z|\theta) dz = \binom{n}{x} \theta^x (1-\theta)^{n-x}.$$



The probability of ending in bin  $x$  corresponds to the total probability of all the paths  $z$  from start to  $x$ ,

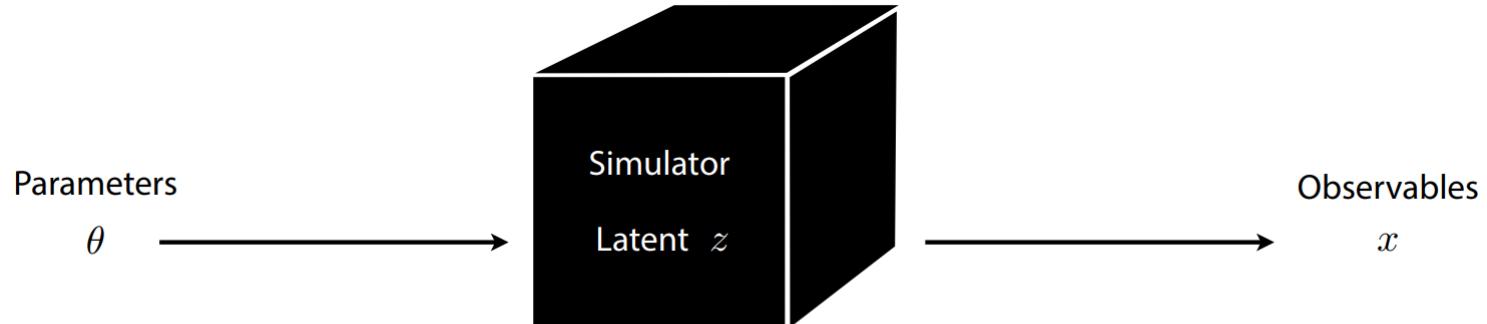
$$p(x|\theta) = \int p(x, z|\theta) dz = \binom{n}{x} \theta^x (1-\theta)^{n-x}.$$

But what if we shift or remove some of the pins?

The Galton board is a **metaphor** of simulation-based science:

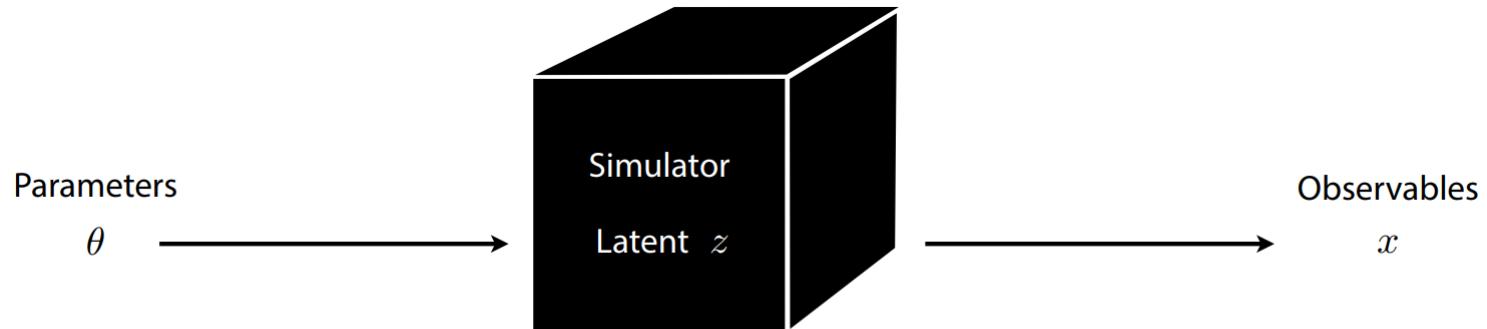
Galton board device	→	Computer simulation
Parameters $\theta$	→	Model parameters $\theta$
Buckets $x$	→	Observables $x$
Random paths $z$	→	Latent variables $z$ (stochastic execution traces through simulator)

Inference in this context requires **likelihood-free algorithms**.



Prediction:

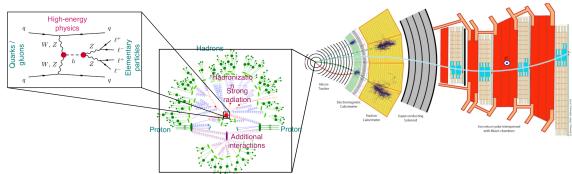
- Well-understood mechanistic model
- Simulator can generate samples



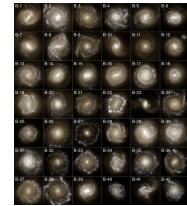
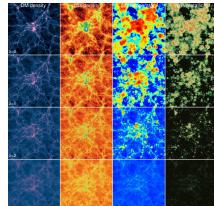
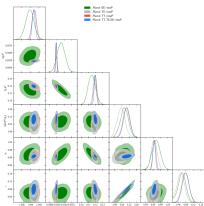
- Prediction:
- Well-understood mechanistic model
  - Simulator can generate samples

- Inference:
- Likelihood function  $p(x|\theta)$  is intractable
  - Inference based on estimator  $\hat{p}(x|\theta)$

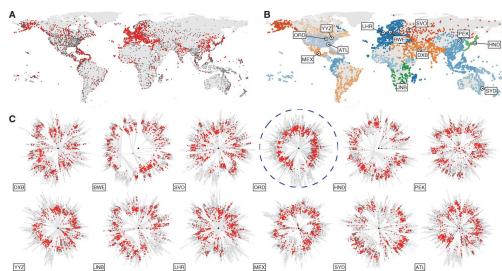
# A thriving field of research



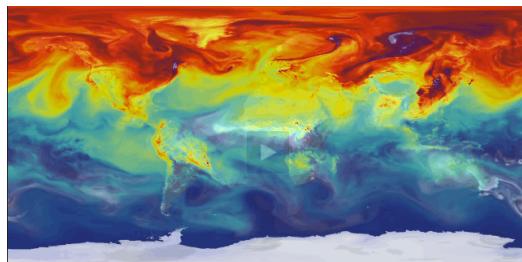
# Particle physics



## Astrophysics



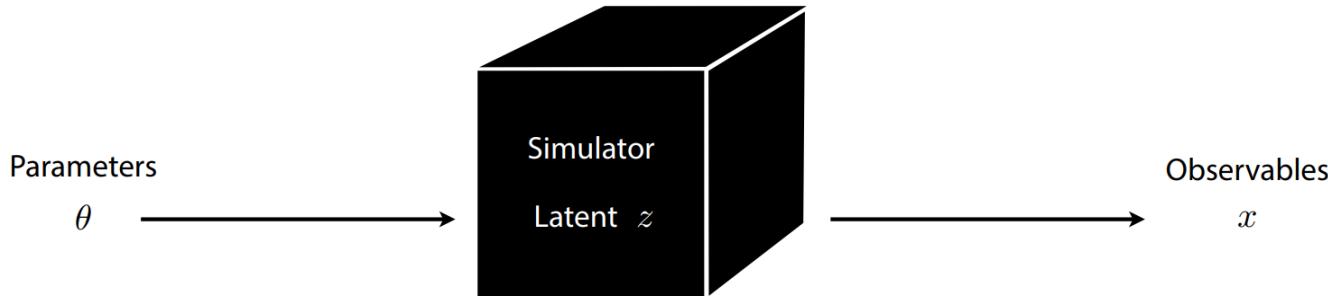
## Epidemiology



# Climatology

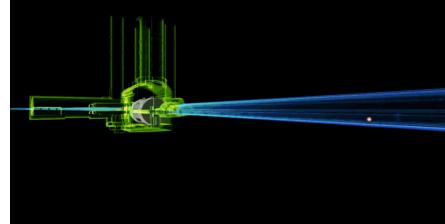
(... and many others!)

# Particle physics

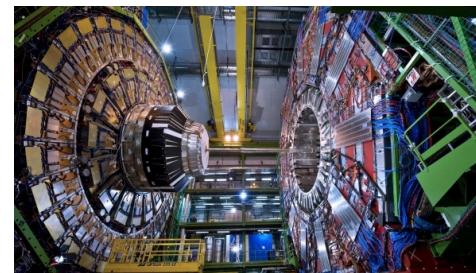


## SM with parameters $\theta$

## Simulated observables $x$



Real observations  $x_{\text{obs}}$



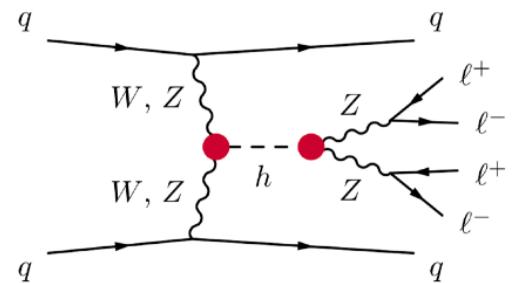
Latent variables

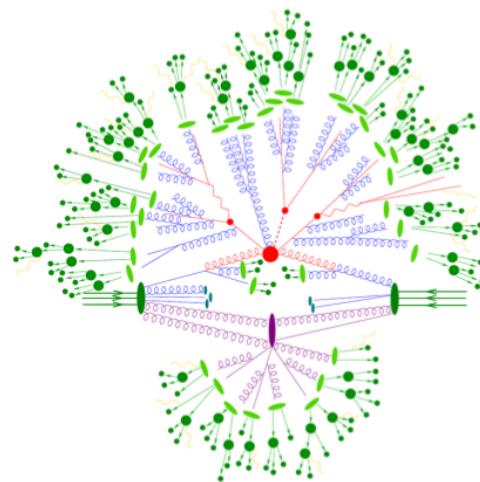
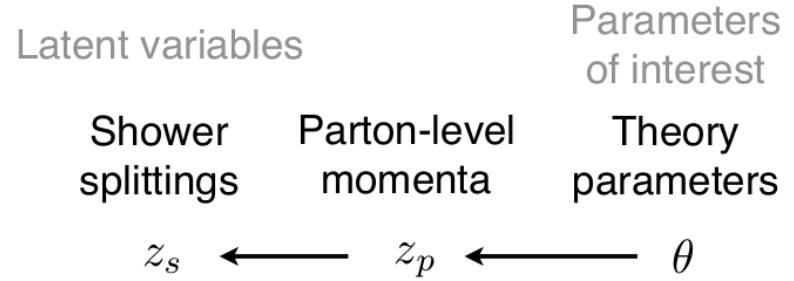
Parameters  
of interest

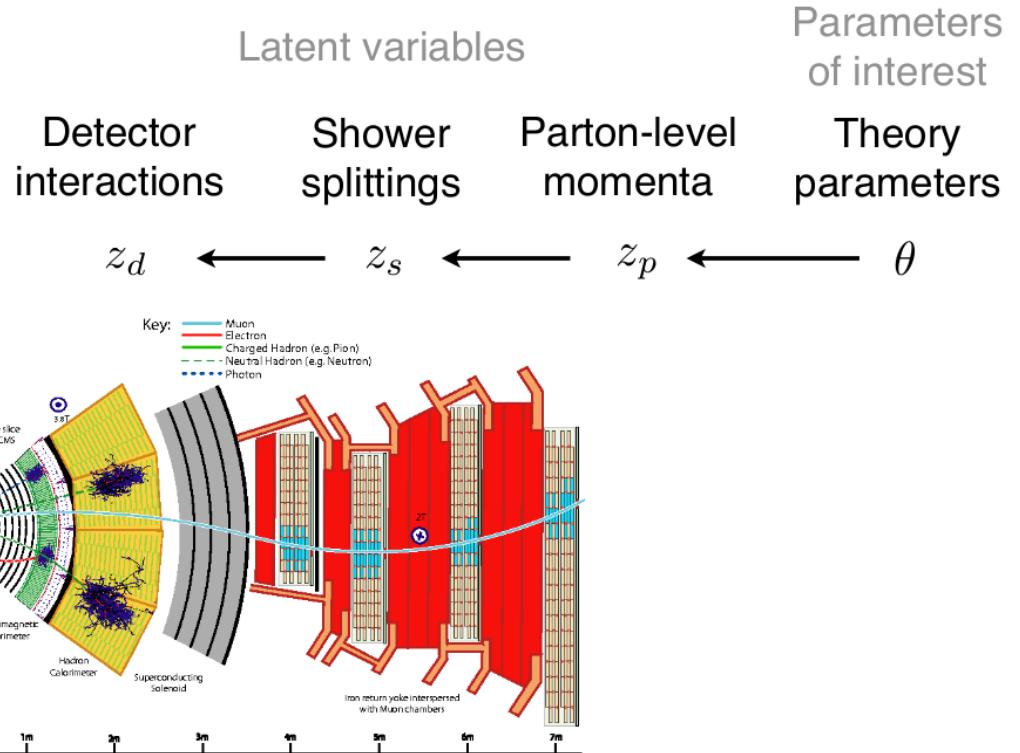
Parton-level  
momenta

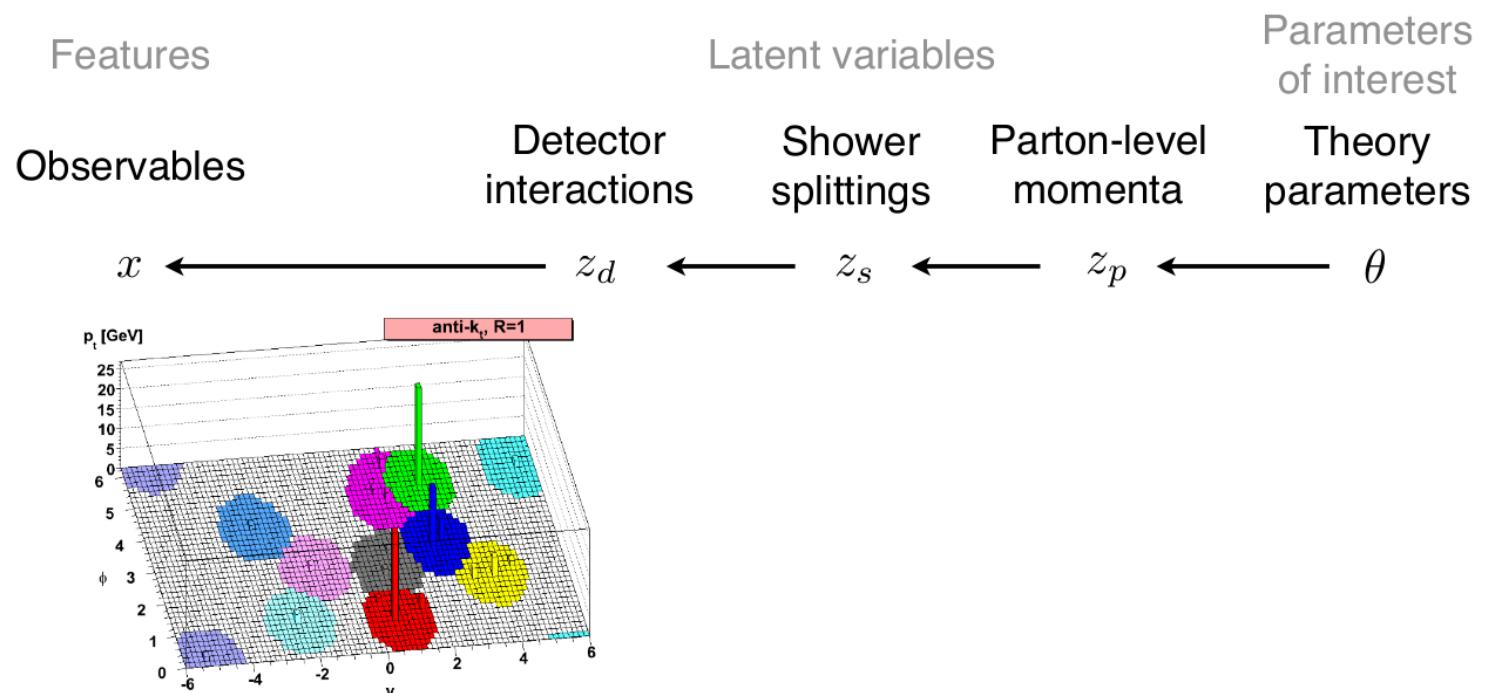
Theory  
parameters

$$z_p \leftarrow \theta$$









[Image source: M. Cacciari,  
G. Salam, G. Soyez 0802.1189]

$$p(x|\theta) = \underbrace{\iiint}_{\text{intractable}} p(z_p|\theta)p(z_s|z_p)p(z_d|z_s)p(x|z_d)dz_p dz_s dz_d$$

# Likelihood ratio

The likelihood ratio

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

is the quantity that is **central** to many **statistical inference** procedures.

## Examples

- Frequentist hypothesis testing
- Supervised learning
- Bayesian posterior sampling with MCMC
- Bayesian posterior inference through Variational Inference
- Generative adversarial networks
- Empirical Bayes with Adversarial Variational Optimization
- Optimal compression

*When solving a problem of interest, do not solve a more general problem as an intermediate step. – Vladimir Vapnik*



$$\frac{p_{\mathbf{x}}(\mathbf{x}|\theta_0)}{p_{\mathbf{x}}(\mathbf{x}|\theta_1)} = r(\mathbf{x}; \theta_0, \theta_1)$$
A diagram consisting of two curved arrows. A blue arrow points from the term  $p_{\mathbf{x}}(\mathbf{x}|\theta_0)$  to the term  $r(\mathbf{x}; \theta_0, \theta_1)$ . A red arrow points from the term  $r(\mathbf{x}; \theta_0, \theta_1)$  back up to the term  $p_{\mathbf{x}}(\mathbf{x}|\theta_0)$ .

Direct likelihood ratio estimation is simpler than density estimation.

(This is fortunate, we are in the likelihood-free scenario!)

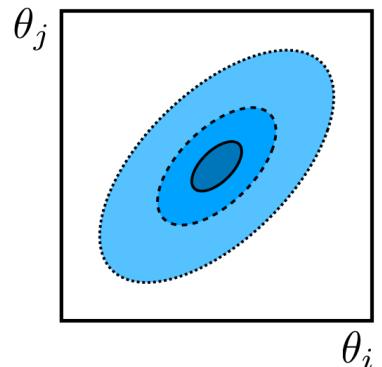
# Frequentist inference

# The frequentist (physicist's) way

The Neyman-Pearson lemma states that the likelihood ratio

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

is the **most powerful test statistic** to discriminate between a null hypothesis  $\theta_0$  and an alternative  $\theta_1$ .



IX. *On the Problem of the most Efficient Tests of Statistical Hypotheses.*

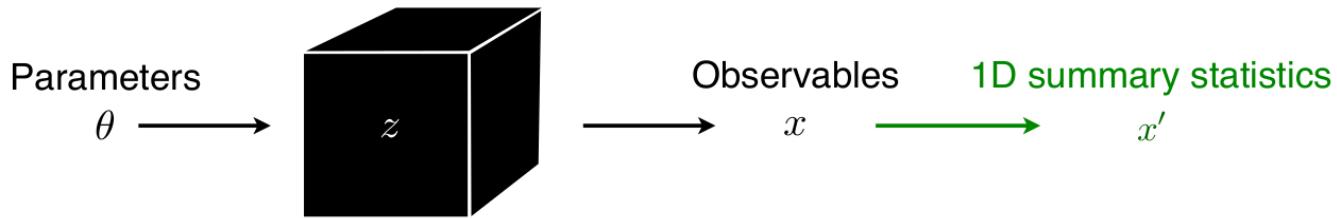
*By J. NEYMAN, Nencki Institute, Soc. Sci. Lit. Varsoviensis, and Lecturer at the Central College of Agriculture, Warsaw, and E. S. PEARSON, Department of Applied Statistics, University College, London.*

(Communicated by K. PEARSON, F.R.S.)

(Received August 31, 1932.—Read November 10, 1932.)

CONTENTS.

	PAGE.
I. Introductory . . . . .	289
II. Outline of General Theory . . . . .	293
III. Simple Hypotheses . . . . .	



Define a projection function  $s : \mathcal{X} \rightarrow \mathbb{R}$  mapping observables  $\textcolor{teal}{x}$  to a summary statistic  $\textcolor{teal}{x}' = s(x)$ .

Then, **approximate** the likelihood  $p(x|\theta)$  with the surrogate  $\hat{p}(x|\theta) = p(x'|\theta)$ .

From this it comes

$$\frac{p(x|\theta_0)}{p(x|\theta_1)} \approx \frac{\hat{p}(x|\theta_0)}{\hat{p}(x|\theta_1)} = \hat{r}(x|\theta_0, \theta_1).$$

## Wilks theorem

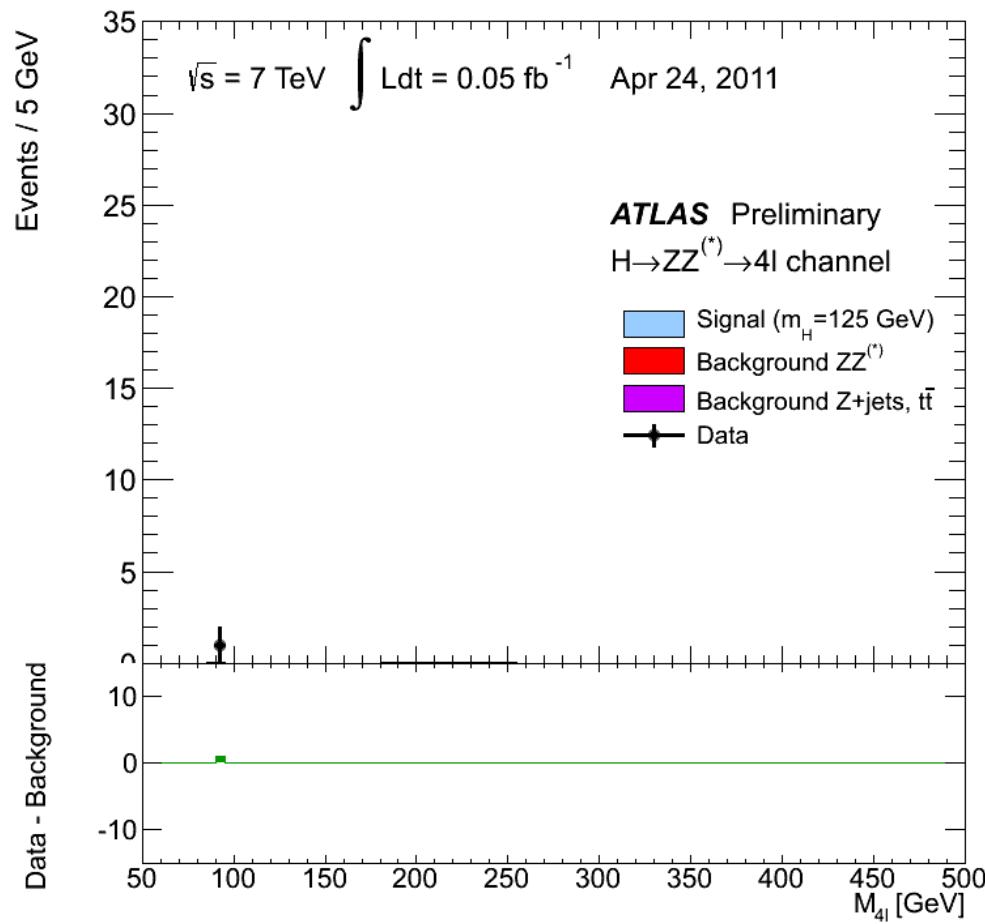
Consider the test statistic

$$q(\theta) = -2 \sum_x \log \frac{p(x|\theta)}{p(x|\hat{\theta})} = -2 \sum_x \log r(x|\theta, \hat{\theta})$$

for a fixed number  $N$  of observations  $\{x\}$  and where  $\hat{\theta}$  is the maximum likelihood estimator.

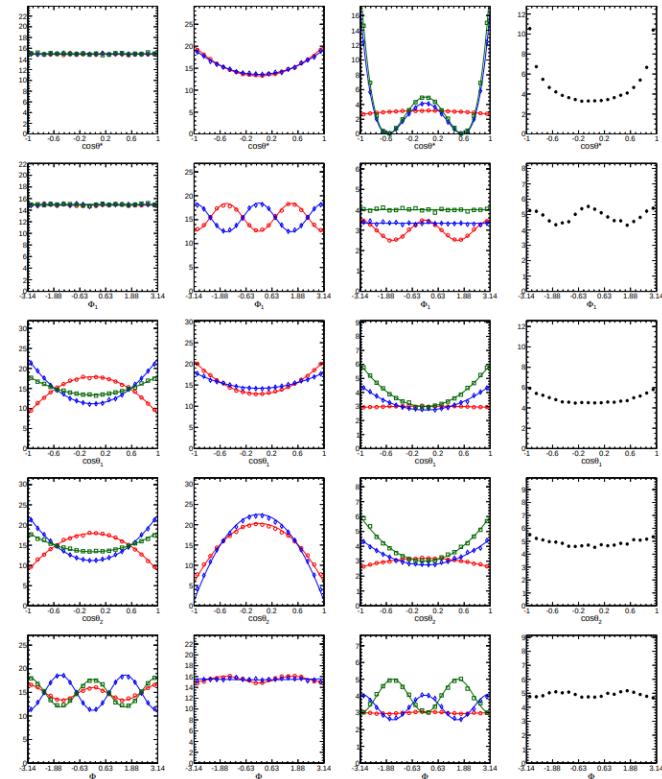
When  $N \rightarrow \infty$ ,  $q(\theta) \sim \chi_2$ . Therefore, an observed value  $q_{\text{obs}}(\theta)$  translates directly to a p-value that measures the confidence with which  $\theta$  can be excluded:

$$p_\theta \equiv \int_{q_{\text{obs}}(\theta)}^{\infty} dq p(q|\theta) = 1 - F_{\chi_2}(q_{\text{obs}}(\theta)).$$



Discovery of the Higgs boson at  $5-\sigma$  (p-value cutoff at  $3 \times 10^{-7}$ )

- Choosing the projection  $s$  is difficult and problem-dependent.
- Often there is no single good variable: compressing to any  $x'$  loses information.
- Ideally, analyze **high-dimensional**  $x'$ , including all correlations.
- Unfortunately, filling high-dimensional histograms is **not tractable**.

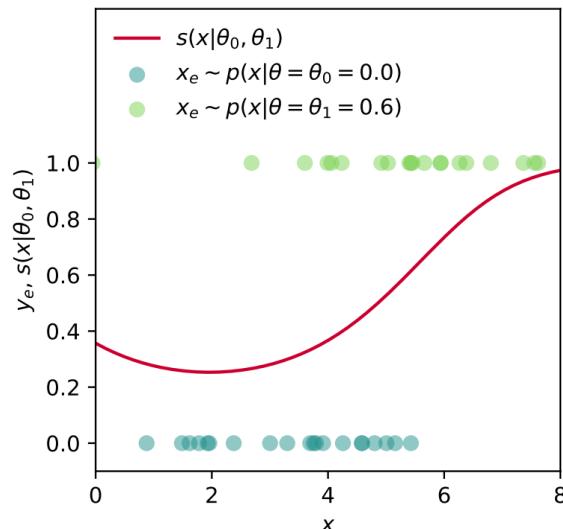


# CARL

Supervised learning provides a way to **automatically** construct  $s$ :

- Let us consider a neural network classifier  $\hat{s}$  trained to distinguish  $x \sim p(x|\theta_0)$  from  $x \sim p(x|\theta_1)$ .
- $\hat{s}$  is trained by minimizing the cross-entropy loss

$$L_{XE}[\hat{s}] = -\mathbb{E}_{p(x|\theta)\pi(\theta)}[1(\theta = \theta_0) \log \hat{s}(x) + 1(\theta = \theta_1) \log(1 - \hat{s}(x))]$$



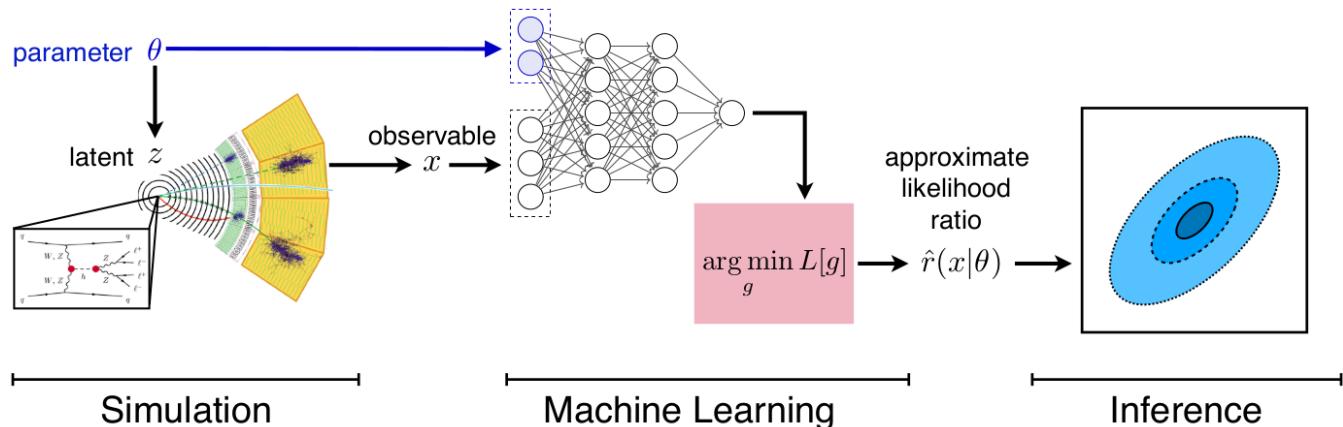
The solution  $\hat{s}$  found after training approximates the optimal classifier

$$\hat{s}(x) \approx s^*(x) = \frac{p(x|\theta_1)}{p(x|\theta_0) + p(x|\theta_1)}.$$

Therefore,

$$r(x|\theta_0, \theta_1) \approx \hat{r}(x|\theta_0, \theta_1) = \frac{1 - \hat{s}(x)}{\hat{s}(x)}$$

That is, **supervised classification** is equivalent to **likelihood ratio estimation**.



To avoid retraining a classifier  $\hat{s}$  for every  $(\theta_0, \theta_1)$  pair, fix  $\theta_1$  to  $\theta_{\text{ref}}$  and train a single **parameterized** classifier  $\hat{s}(x|\theta_0, \theta_{\text{ref}})$  where  $\theta_0$  is also given as input.

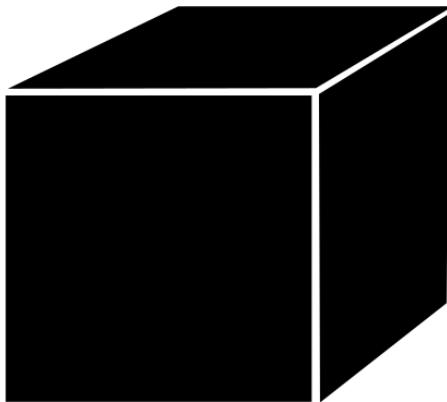
Therefore, we have

$$\hat{r}(x|\theta_0, \theta_{\text{ref}}) = \frac{1 - \hat{s}(x|\theta, \theta_{\text{ref}})}{\hat{s}(x|\theta_0, \theta_{\text{ref}})}$$

such that for any  $(\theta_0, \theta_1)$ ,

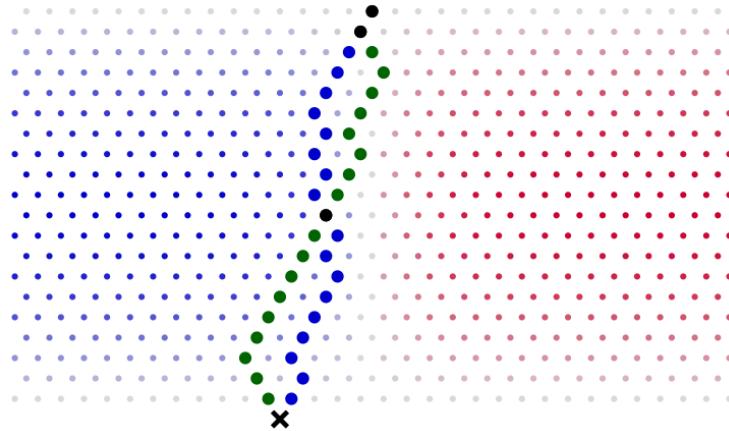
$$r(x|\theta_0, \theta_1) \approx \frac{\hat{r}(x|\theta_0, \theta_{\text{ref}})}{\hat{r}(x|\theta_1, \theta_{\text{ref}})}.$$

# Opening the black box



Traditional likelihood-free inference treats the simulator as a generative **black box**: parameters in, samples out.

But in most real-life problems, we have access to the simulator code and some understanding of the microscopic processes.



$p(x|\theta)$  is usually intractable. What about  $p(x, z|\theta)$ ?

As the trajectory  $z_1, \dots, z_T$  and the observable  $x$  are emitted, it is often possible:

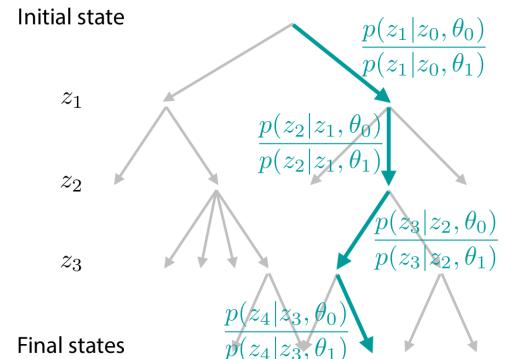
- to calculate the **joint likelihood**  $p(x, z|\theta)$ ;
- to calculate the **joint likelihood ratio**  $r(x, z|\theta_0, \theta_1)$ ;
- to calculate the **joint score**  $t(x, z|\theta_0) = \nabla_{\theta} \log p(x, z|\theta)|_{\theta_0}$ .

We call this process **mining gold** from your simulator!

## Extracting the joint likelihood ratio

- Computer simulations typically evolve along a tree-like structure of successive random branchings.
- The probabilities of each branching  $p(z_i|z_{i-1}, \theta)$  are often clearly defined in the code:

```
if random() > 0.1+2.5+model_parameter:  
    do_one_thing()  
else:  
    do_another_thing()
```



- For each run, we can calculate the probability of the chosen path for different values of the parameters and the joint likelihood-ratio:

$$r(x, z|\theta_0, \theta_1) = \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)} = \prod_i \frac{p(z_i|z_{i-1}, \theta_0)}{p(z_i|z_{i-1}, \theta_1)}$$

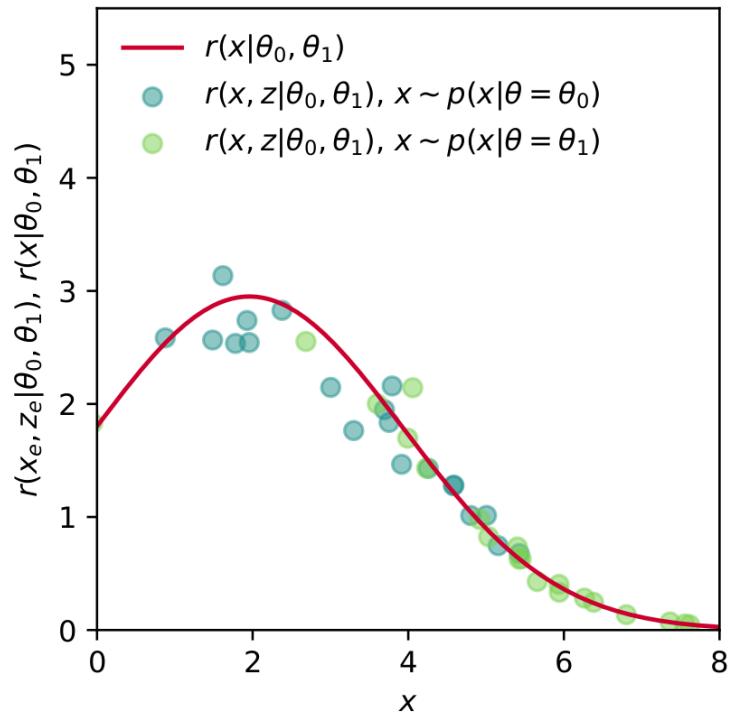
## Regressing the likelihood ratio

Observe that the joint likelihood ratios

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

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

Can we use them to approximate  $r(x | \theta_0, \theta_1)$ ?



Consider the squared error of a function  $\hat{g}(x)$  that only depends on  $x$ , but is trying to approximate a function  $g(x, z)$  that also depends on the latent  $z$ :

$$L_{MSE} = \mathbb{E}_{p(x,z|\theta)} [(g(x, z) - \hat{g}(x))^2].$$

Via calculus of variations, we find that the function  $g^*(x)$  that extremizes  $L_{MSE}[g]$  is given by

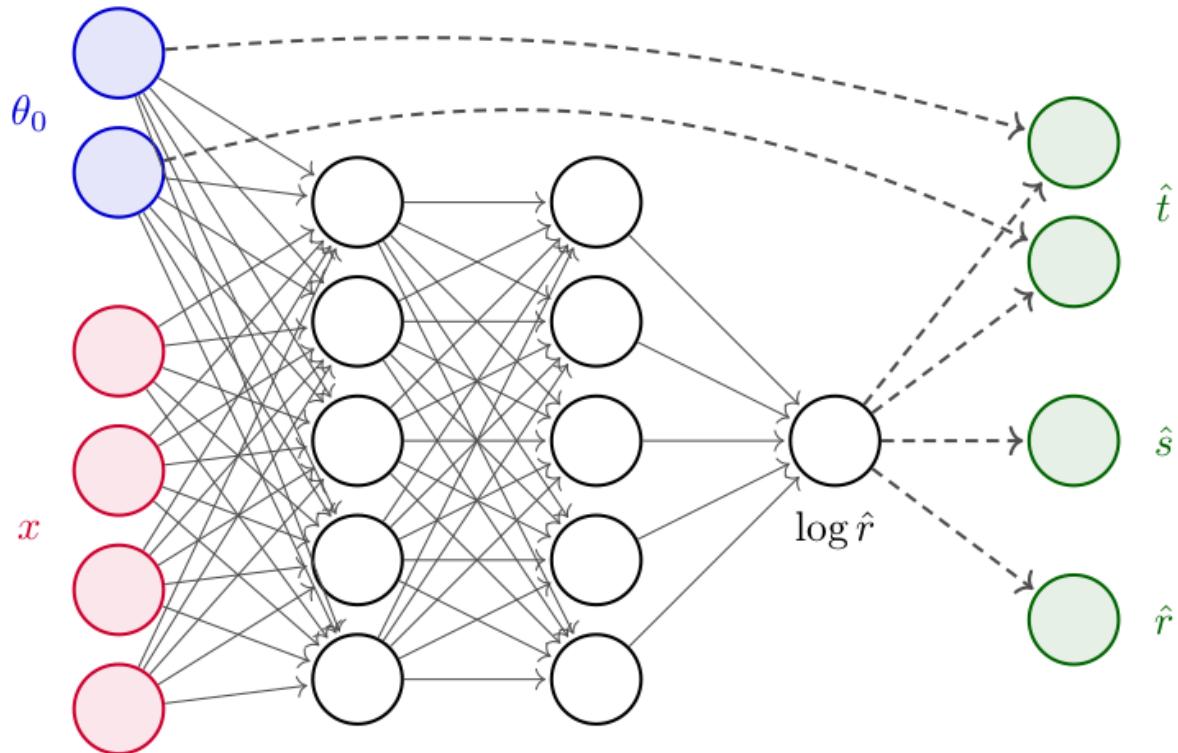
$$\begin{aligned} g^*(x) &= \frac{1}{p(x|\theta)} \int p(x, z|\theta) g(x, z) dz \\ &= \mathbb{E}_{p(z|x,\theta)} [g(x, z)] \end{aligned}$$

Therefore, by identifying the  $g(x, z)$  with the joint likelihood ratio  $r(x, z|\theta_0, \theta_1)$  and  $\theta$  with  $\theta_1$ , we define

$$L_r = \mathbb{E}_{p(x, z|\theta_1)} [(r(x, z|\theta_0, \theta_1) - \hat{r}(x))^2],$$

which is minimized by

$$\begin{aligned} r^*(x) &= \frac{1}{p(x|\theta_1)} \int p(x, z|\theta_1) \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)} dz \\ &= \frac{p(x|\theta_0)}{p(x|\theta_1)} \\ &= r(x|\theta_0, \theta_1). \end{aligned}$$



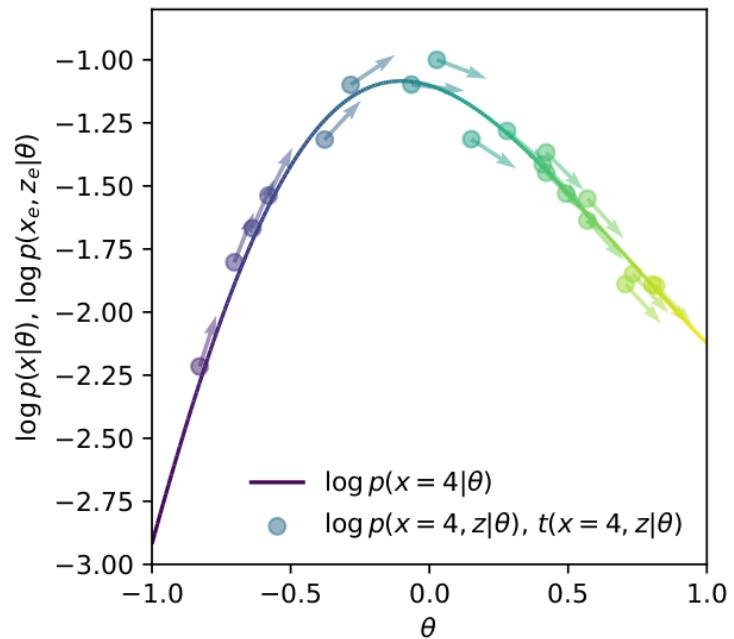
$$r^*(x|\theta_0, \theta_1) = \arg \min_{\hat{r}} L_r[\hat{r}]$$

## Regressing the score

Similarly, we can mine the simulator to extract the joint score

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

which indicates how much more or less likely  $x, z$  would be if one changed  $\theta_0$ .



Using the same trick, by identifying  $g(x, z)$  with the joint score  $t(x, z|\theta_0)$  and  $\theta$  with  $\theta_0$ , we define

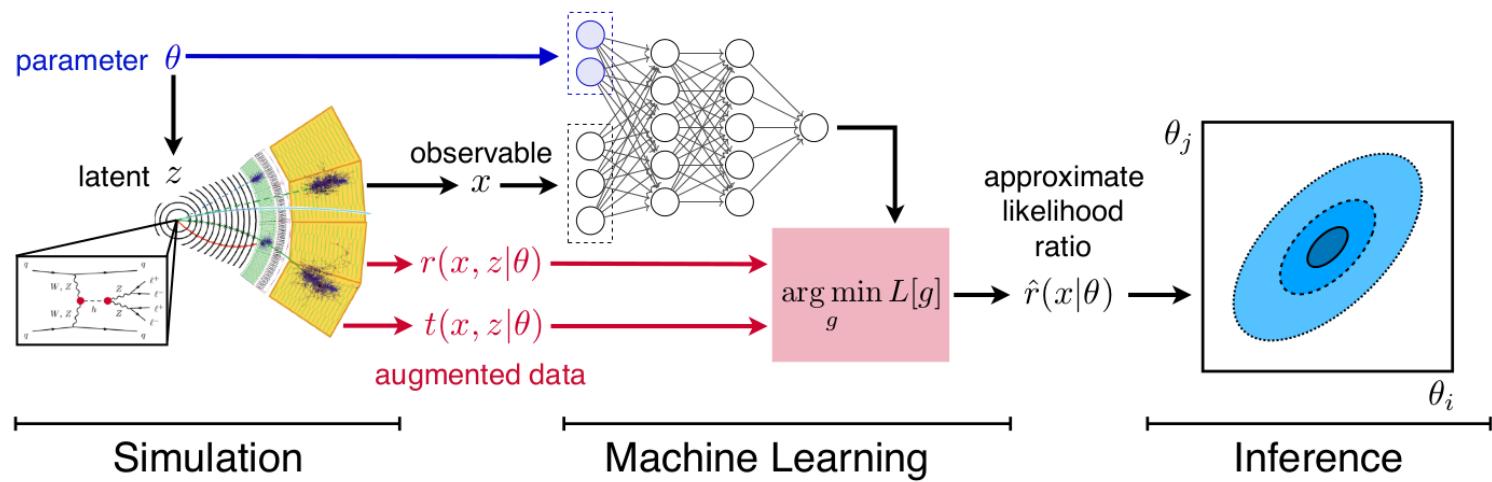
$$L_t = \mathbb{E}_{p(x,z|\theta_0)} [(t(x, z|\theta_0) - \hat{t}(x))^2],$$

which is minimized by

$$\begin{aligned} t^*(x) &= \frac{1}{p(x|\theta_0)} \int p(x, z|\theta_0) (\nabla_\theta \log p(x, z|\theta)|_{\theta_0}) dz \\ &= \frac{1}{p(x|\theta_0)} \int p(x, z|\theta_0) \frac{\nabla_\theta p(x, z|\theta)|_{\theta_0}}{p(x, z|\theta_0)} dz \\ &= \frac{\nabla_\theta p(x|\theta)|_{\theta_0}}{p(x|\theta_0)} \\ &= \nabla_\theta \log p(x|\theta)|_{\theta_0} \\ &= t(x|\theta_0). \end{aligned}$$

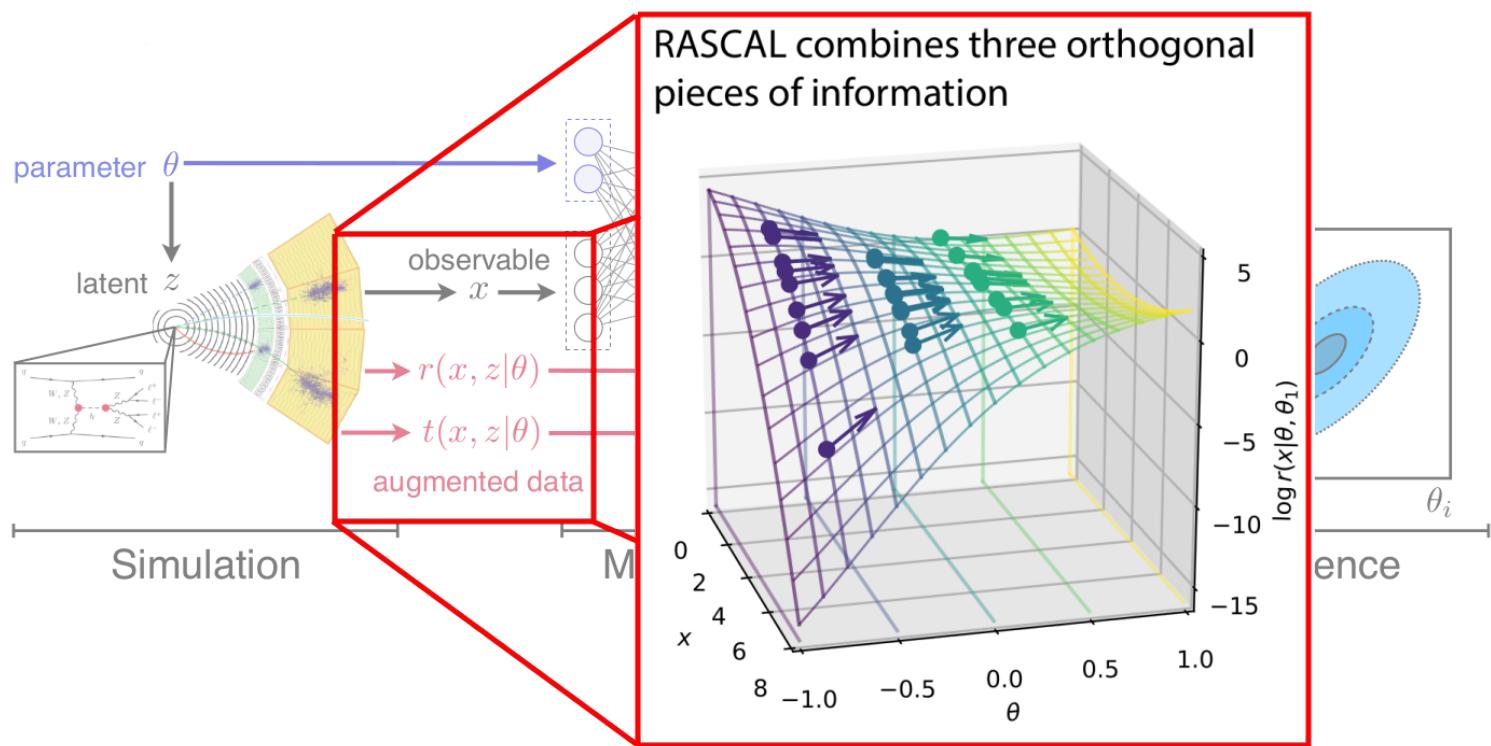
# RASCAL

$$L_{RASCAL} = L_r + L_t$$



# RASCAL

$$L_{RASCAL} = L_r + L_t$$

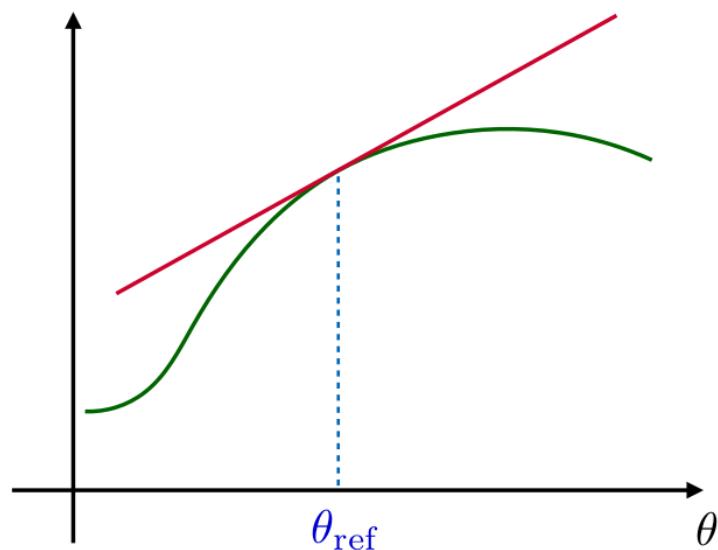


# SALLY (= optimal compression)

## The local model

In the neighborhood of  $\theta_{\text{ref}}$ , the Taylor expansion of  $\log p(x|\theta)$  is

$$\log p(x|\theta) = \log p(x|\theta_{\text{ref}}) + \underbrace{\nabla_{\theta} \log p(x|\theta) \Big|_{\theta_{\text{ref}}} \cdot (\theta - \theta_{\text{ref}})}_{t(x|\theta_{\text{ref}})} + O((\theta - \theta_{\text{ref}})^2)$$



This results in the exponential model

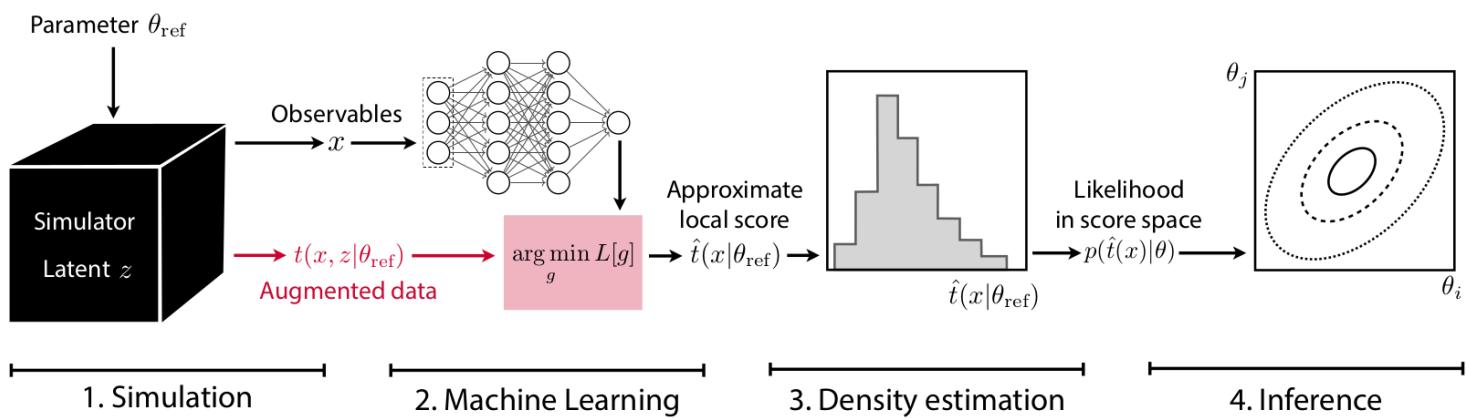
$$p_{\text{local}}(x|\theta) = \frac{1}{Z(\theta)} p(t(x|\theta_{\text{ref}})|\theta_{\text{ref}}) \exp(t(x|\theta_{\text{ref}}) \cdot (\theta - \theta_{\text{ref}}))$$

where the score  $t(x|\theta_{\text{ref}})$  are its sufficient statistics.

That is,

- knowing  $t(x|\theta_{\text{ref}})$  is just as powerful as knowing the full function  $\log p(x|\theta)$ .
- $x$  can be compressed into a single scalar  $t(x|\theta_{\text{ref}})$  without loss of power.

# SALLY



# There is more...

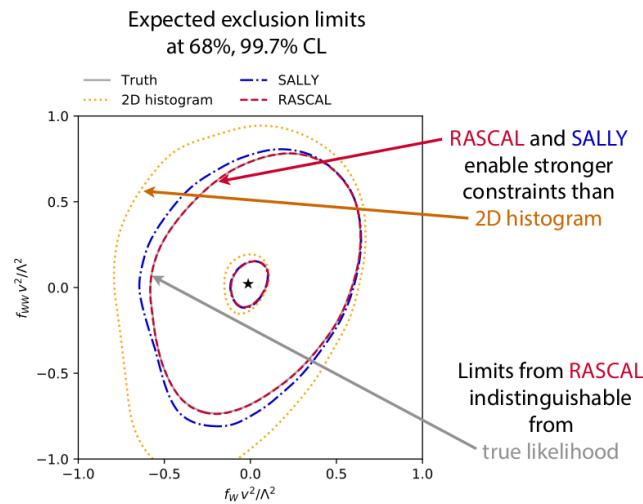
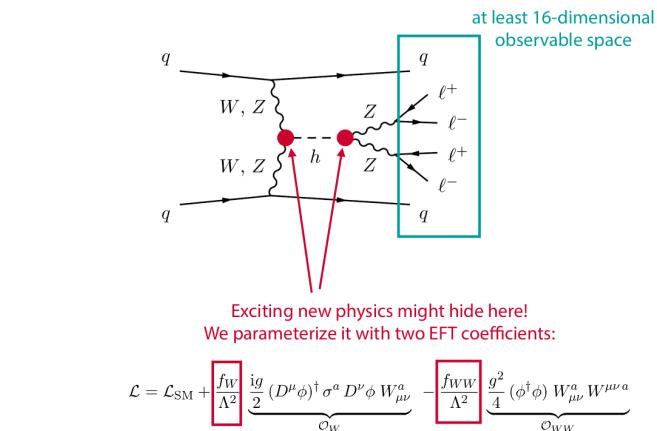
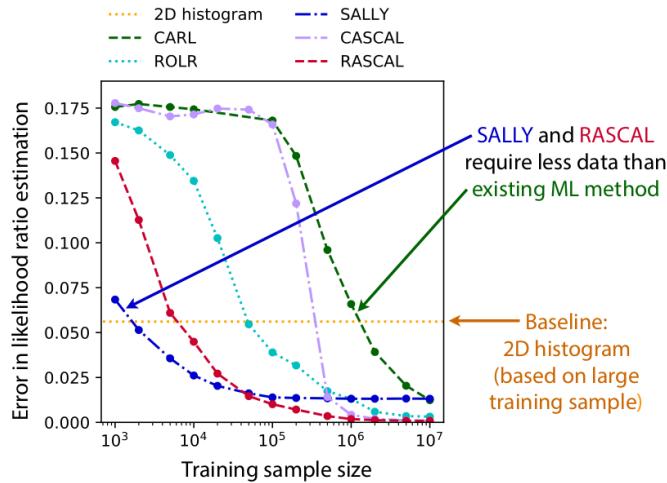
Method	Simulate	Extract		NN estimates	Asympt. exact	Generative
		$r(x, z)$	$t(x, z)$			
ROLR	$\theta_0 \sim \pi(\theta), \theta_1$	✓		$\hat{r}(x \theta_0, \theta_1)$	✓	
CASCAL	$\theta_0 \sim \pi(\theta), \theta_1$		✓	$\hat{r}(x \theta_0, \theta_1)$	✓	
ALICE	$\theta_0 \sim \pi(\theta), \theta_1$		✓	$\hat{r}(x \theta_0, \theta_1)$	✓	
RASCAL	$\theta_0 \sim \pi(\theta), \theta_1$	✓	✓	$\hat{r}(x \theta_0, \theta_1)$	✓	
ALICES	$\theta_0 \sim \pi(\theta), \theta_1$	✓	✓	$\hat{r}(x \theta_0, \theta_1)$	✓	
SCANDAL	$\theta \sim \pi(\theta)$		✓	$\hat{p}(x \theta)$	✓	✓
SALLY	$\theta_{\text{ref}}$		✓	$\hat{t}(x \theta_{\text{ref}})$	in local approx.	
SALLINO	$\theta_{\text{ref}}$		✓	$\hat{t}(x \theta_{\text{ref}})$	in local approx.	

# Examples

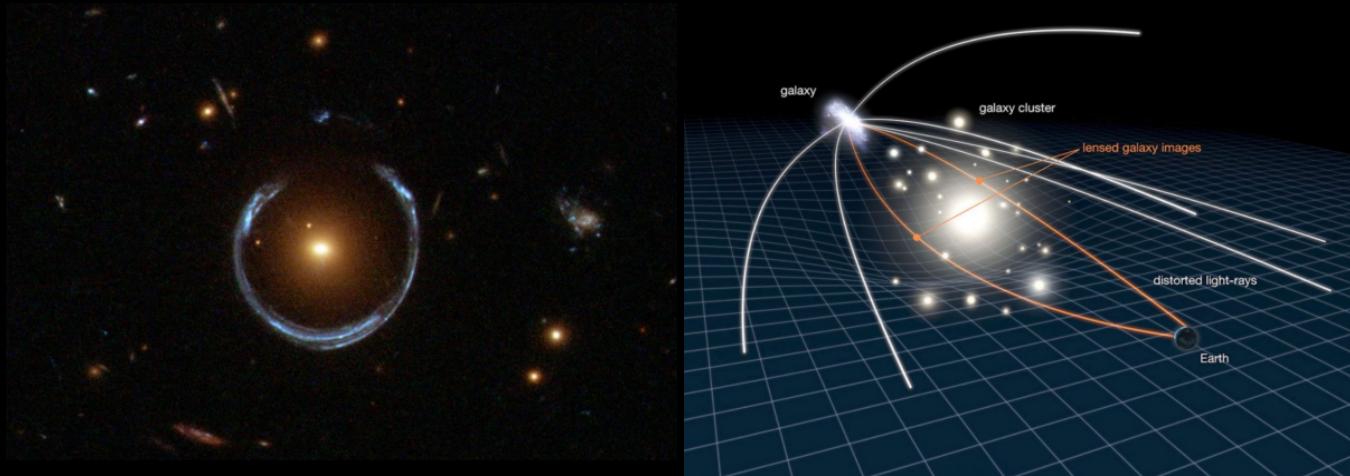
## ① Hunting new physics at particle colliders

Goal: constrain two EFT parameters

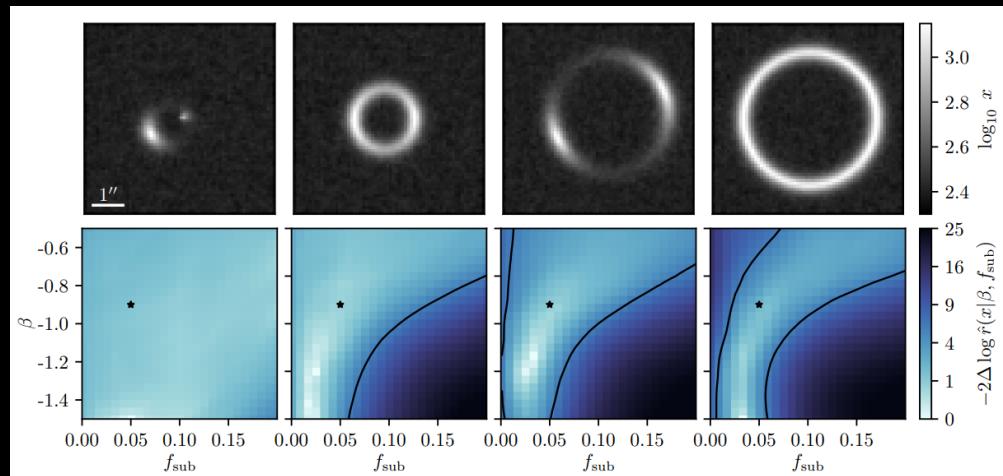
- new inference methods
- baseline: 2d histogram analysis of jet momenta and angular correlations



## ② Dark matter substructure from gravitational lensing



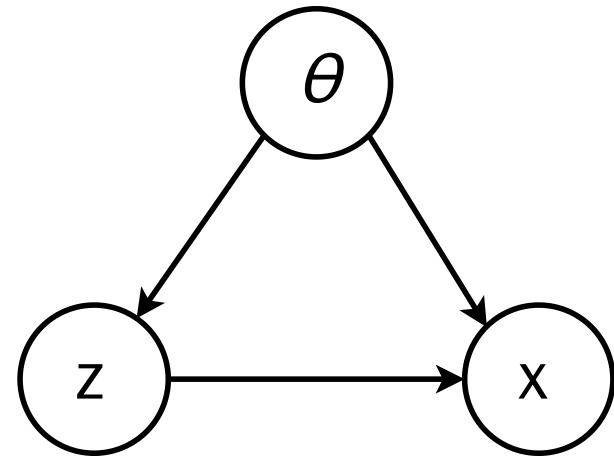
Number of dark matter subhalos and their mass and location lead to complex latent space of each image. The goal is the **inference of population parameters.**



# Bayesian inference

Bayesian inference = computing the posterior

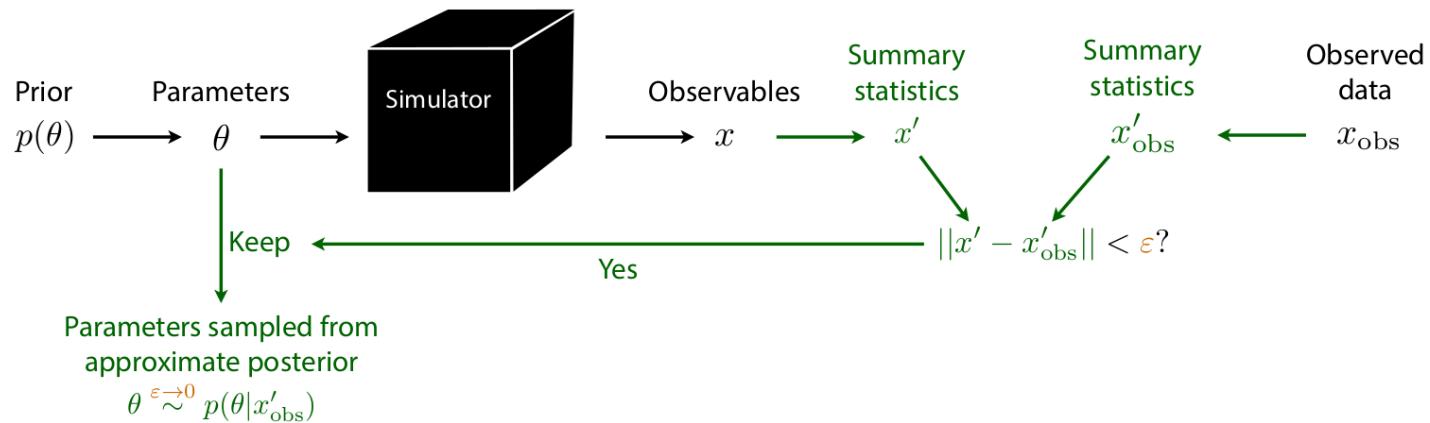
$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)}.$$



Doubly **intractable** in the likelihood-free scenario:

- Cannot evaluate the likelihood  $p(x|\theta) = \int p(x, z|\theta)dz$ .
- Cannot evaluate the evidence  $p(x) = \int p(x|\theta)p(\theta)d\theta$ .

# Approximate Bayesian Computation (ABC)



## Issues

- How to choose  $x'?$   $\epsilon?$   $\|\cdot\|?$
- No tractable posterior.
- Need to run new simulations for new data or new prior.

# Amortizing Bayes

The Bayes rule can be rewritten as

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)} = r(x|\theta)p(\theta) \approx \hat{r}(x|\theta)p(\theta),$$

where  $r(x|\theta) = \frac{p(x|\theta)}{p(x)}$  is the likelihood-to-evidence ratio.

# Amortizing Bayes

The Bayes rule can be rewritten as

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)} = r(x|\theta)p(\theta) \approx \hat{r}(x|\theta)p(\theta),$$

where  $r(x|\theta) = \frac{p(x|\theta)}{p(x)}$  is the likelihood-to-evidence ratio.

As before, the likelihood-to-evidence ratio can be approximated e.g. from a neural network classifier trained to distinguish  $x \sim p(x|\theta)$  from  $x \sim p(x)$ , hence enabling direct and **amortized** posterior evaluation.

**Algorithm 1** Optimization of  $d(x, \theta)$ .

---

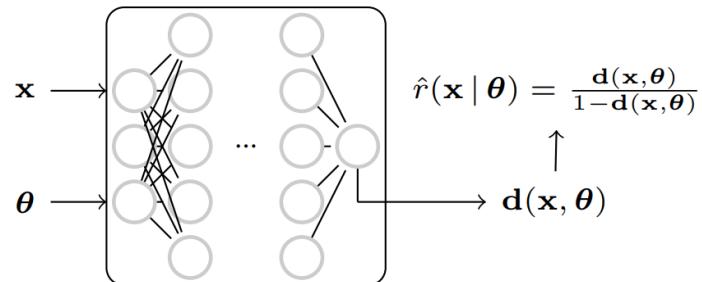
*Inputs:* Criterion  $\ell$  (e.g., BCE)  
Implicit generative model  $p(x|\theta)$   
Prior  $p(\theta)$

*Outputs:* Parameterized classifier  $d_\phi(x, \theta)$

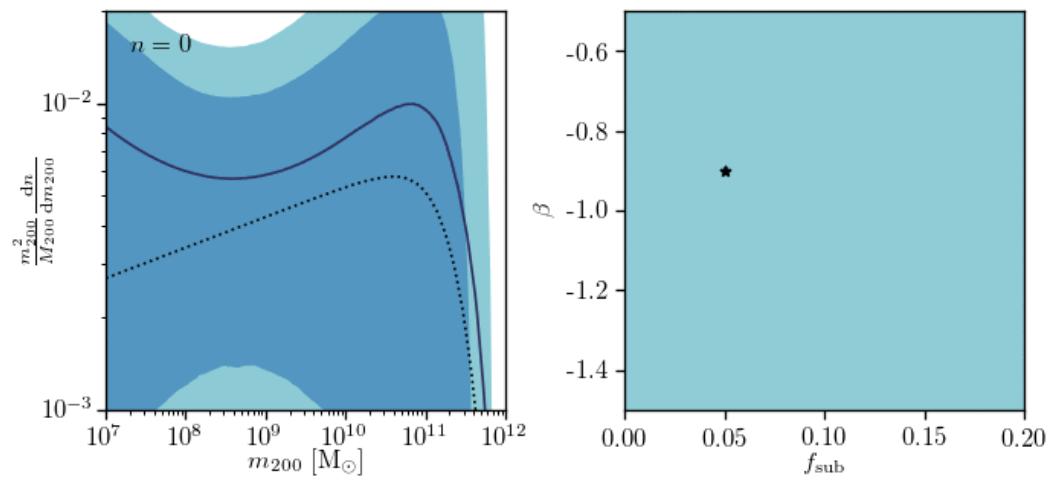
*Hyperparameters:* Batch-size  $M$

- 1: **while** not converged **do**
- 2:    Sample  $\theta \leftarrow \{\theta_m \sim p(\theta)\}_{m=1}^M$
- 3:    Sample  $\theta' \leftarrow \{\theta'_m \sim p(\theta)\}_{m=1}^M$
- 4:    Simulate  $x \leftarrow \{x_m \sim p(x|\theta_m)\}_{m=1}^M$
- 5:     $\mathcal{L} \leftarrow \ell(d_\phi(x, \theta), 1) + \ell(d_\phi(x, \theta'), 0)$
- 6:     $\phi \leftarrow \text{OPTIMIZER}(\phi, \nabla_\phi \mathcal{L})$
- 7: **end while**
- 8: **return**  $d_\phi$

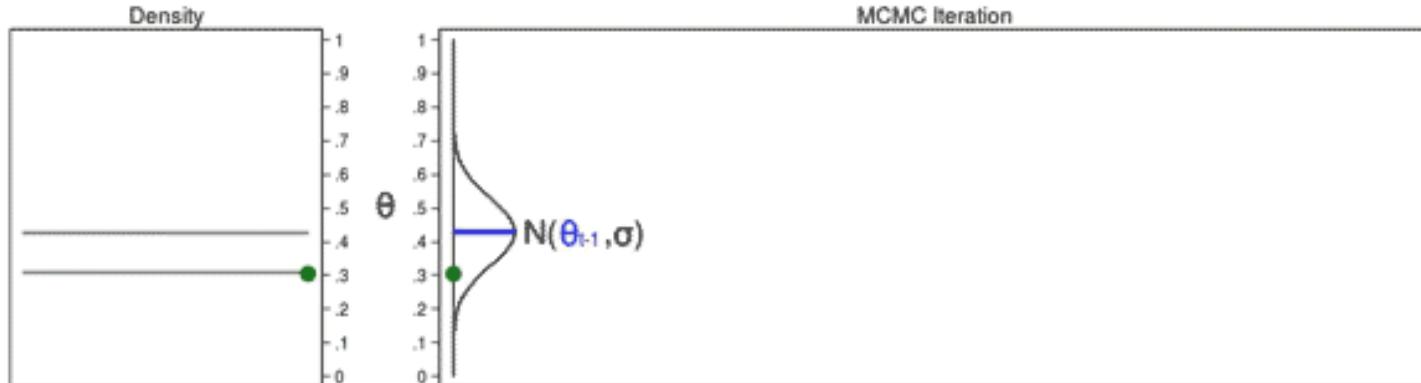
---



## Bayesian inference of dark matter subhalo population parameters



# MCMC posterior sampling



$$\text{Step 1: } r(\theta_{\text{new}}, \theta_{t-1}) = \frac{\text{Posterior}(\theta_{\text{new}})}{\text{Posterior}(\theta_{t-1})} = \frac{\text{Beta}(1,1, 0.306) \times \text{Binomial}(10,4, 0.306)}{\text{Beta}(1,1, 0.429) \times \text{Binomial}(10,4, 0.429)} = 0.834$$

$$\text{Step 2: Acceptance probability } \alpha(\theta_{\text{new}}, \theta_{t-1}) = \min[r(\theta_{\text{new}}, \theta_{t-1}), 1] = \min[0.834, 1] = 0.834$$

Step 3: Draw  $u \sim \text{Uniform}(0,1) = 0.617$

Step 4: If  $u < \alpha(\theta_{\text{new}}, \theta_{t-1}) \rightarrow$  If  $0.617 < 0.834$  Then  $\theta_t = \theta_{\text{new}} = 0.306$   
Otherwise  $\theta_t = \theta_{t-1} = 0.429$

## Likelihood-free MCMC

MCMC samplers require the evaluation of the posterior ratios:

$$\begin{aligned}\frac{p(\theta_{\text{new}}|x)}{p(\theta_{t-1}|x)} &= \frac{p(x|\theta_{\text{new}})p(\theta_{\text{new}})/p(x)}{p(x|\theta_{t-1})p(\theta_{t-1})/p(x)} \\ &= \frac{p(x|\theta_{\text{new}})p(\theta_{\text{new}})}{p(x|\theta_{t-1})p(\theta_{t-1})} \\ &= r(x|\theta_{\text{new}}, \theta_{t-1}) \frac{p(\theta_{\text{new}})}{p(\theta_{t-1})}\end{aligned}$$

Again, MCMC samplers can be made likelihood-free by plugging a learned approximation  $\hat{r}(x|\theta_{\text{new}}, \theta_{t-1})$  of the likelihood ratio.

For MCMC, best results are obtained when using ratios of likelihood-to-evidence ratios:

$$\hat{r}(x|\theta_{\text{new}}, \theta_{t-1}) = \frac{\hat{r}(x|\theta_{\text{new}})}{\hat{r}(x|\theta_{t-1})}$$

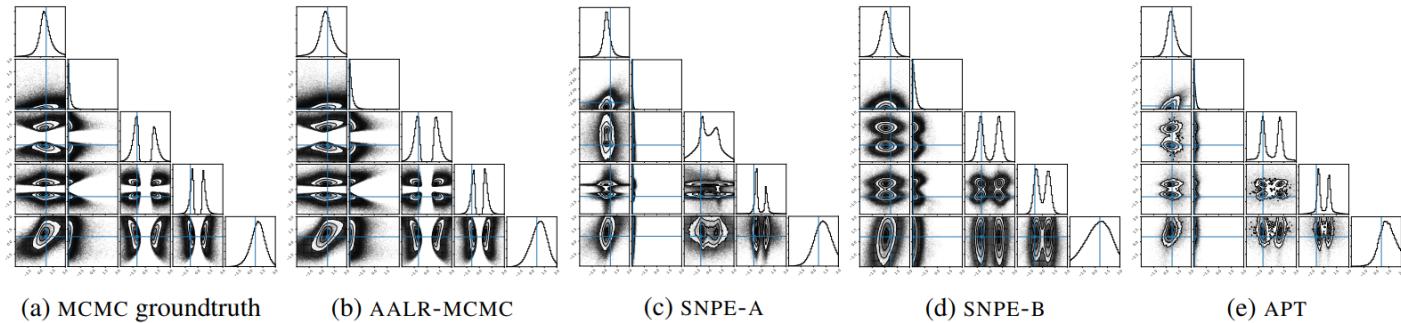
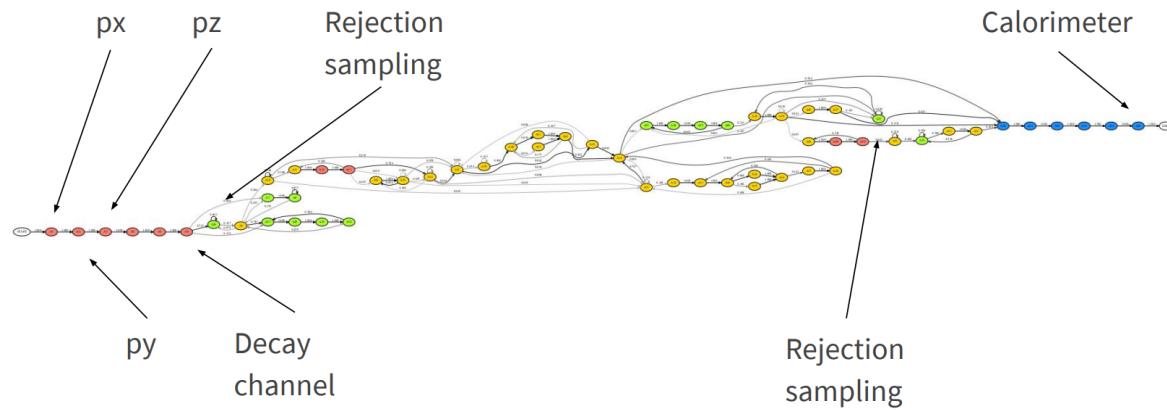


Figure 3: Posteriors from the tractable benchmark. The experiments are repeated 25 times and the approximate posteriors are subsampled from those runs. AALR-MCMC shares the same structure with the MCMC truth, demonstrating its accuracy. Some runs of the other methods were not consistent, contributing to the variance observed in Table 2.

Algorithm	MMD	ROC AUC
AALR-MCMC (ours)	<b>0.05</b> $\pm$ 0.005	<b>0.59</b> $\pm$ 0.0010
ABC ( $\epsilon = 32$ )	0.51 $\pm$ 0.001	0.99 $\pm$ 0.0001
ABC ( $\epsilon = 16$ )	0.50 $\pm$ 0.003	0.99 $\pm$ 0.0002
ABC ( $\epsilon = 8$ )	0.39 $\pm$ 0.001	0.99 $\pm$ 0.0003
ABC ( $\epsilon = 4$ )	0.29 $\pm$ 0.004	0.98 $\pm$ 0.0007
APT	0.17 $\pm$ 0.036	0.86 $\pm$ 0.0008
AALR-MCMC (LRT)	0.53 $\pm$ 0.004	0.99 $\pm$ 0.0001
SNPE-A	0.21 $\pm$ 0.070	0.97 $\pm$ 0.0098
SNPE-B	0.20 $\pm$ 0.061	0.92 $\pm$ 0.0181

Table 2: AALR-MCMC outperforms all other methods. Numerical errors introduced by MCMC might have contributed to these results. A comparison of the PDFs between the true posterior and our ratio estimator are shown in Figure 11 (Appendix D.2). The MMD scores are in agreement with [41].

# Probabilistic programming



53

A probabilistic program defines a joint distribution of **unobserved  $x$**  and **observed  $y$**  variables  $p(x, y)$ .

Probabilistic programming extends ordinary programming with two added constructs:

- Sampling from distributions
- Conditioning random variables by specifying observed values

**Inference engines** give us distributions over unobserved variables, given observed variables (data)

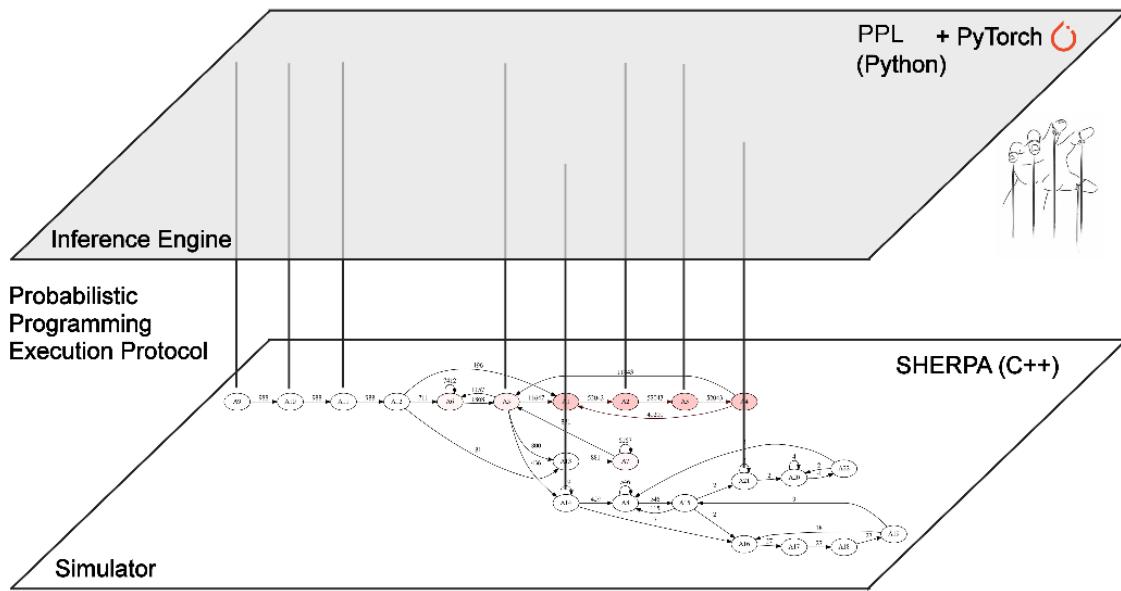
$$p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$

## Probabilistic programming languages

- Anglican (Clojure)
- Church (Scheme)
- Edward, TensorFlow Probability (Python, TensorFlow)
- Pyro (Python, PyTorch)
- Figaro (Scala)
- Infer.NET (C#)
- LibBi (C++ template library)
- PyMC3 (Python)
- Stan (C++)
- WebPPL (JavaScript)

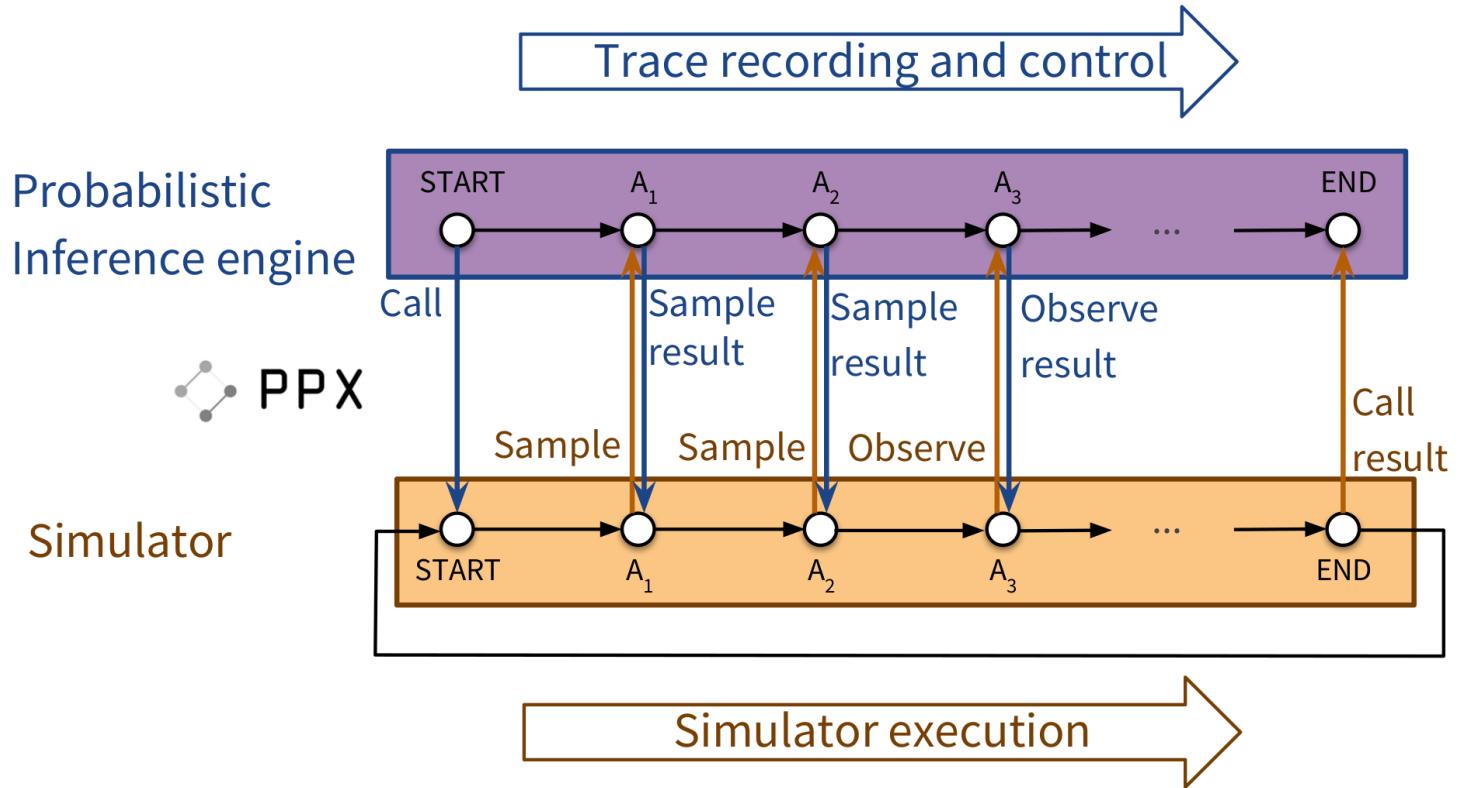
A stochastic simulator implicitly defines a probability distribution by sampling pseudo-random numbers.

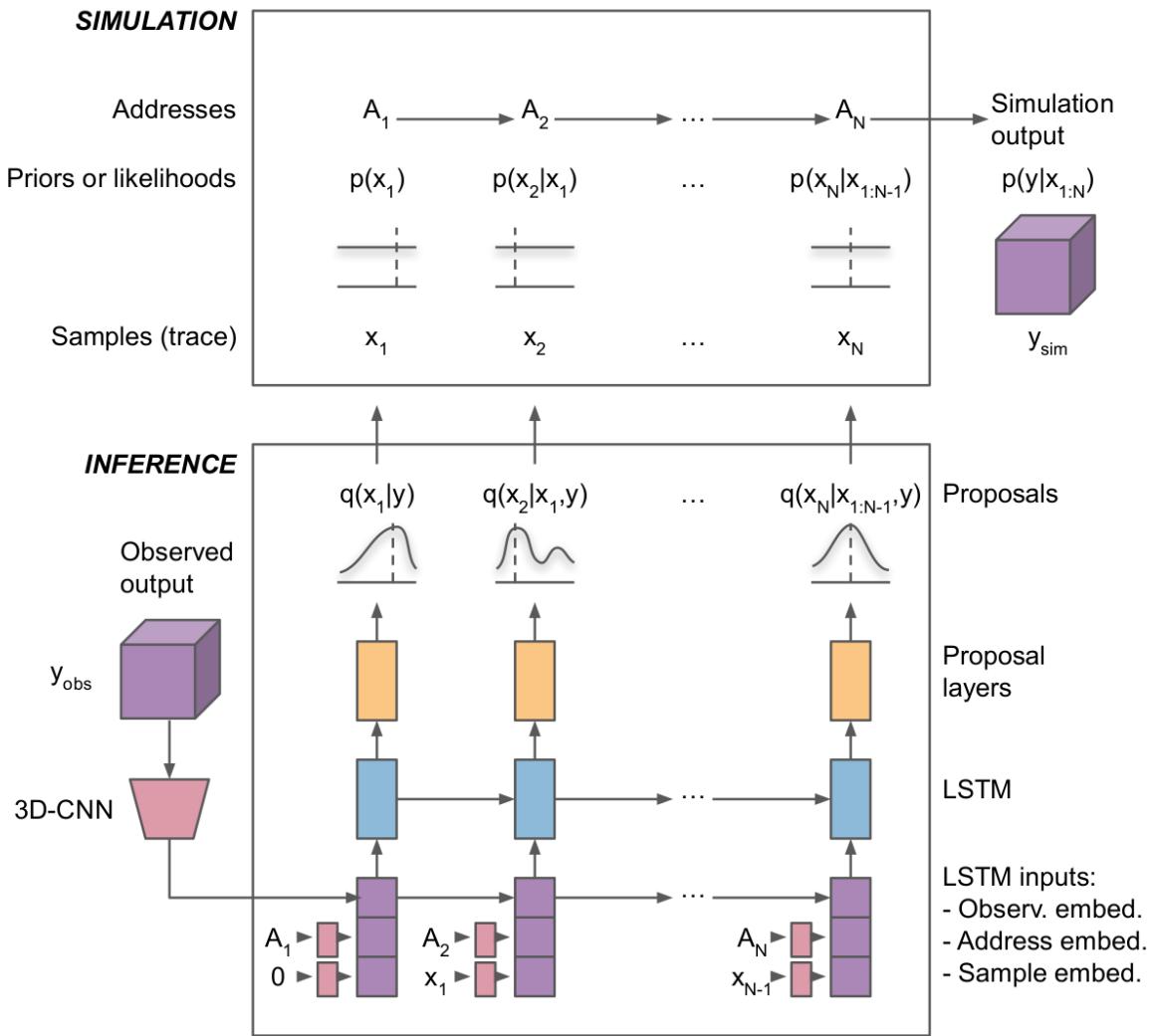
**Scientific simulators are probabilistic programs!**



## Key idea

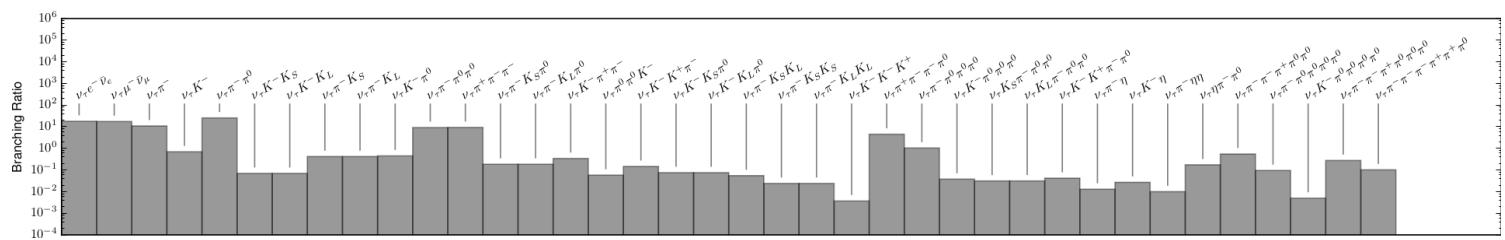
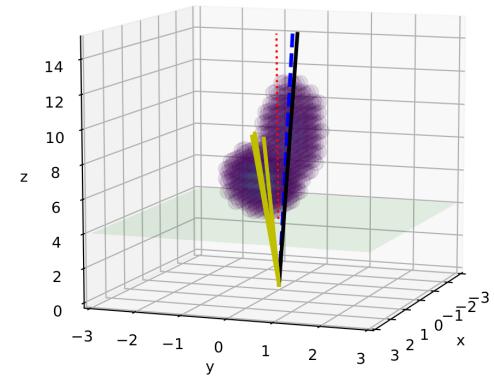
Let a neural network take full control of the internals of the simulation program by hijacking all calls to the random number generator.



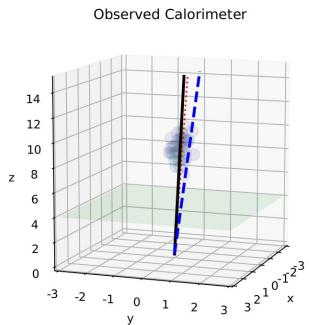


## ③ Taking control of Sherpa (particle physics simulator)

- $\tau$  decay in Sherpa, 38 decay channels, coupled with an approximate calorimeter simulation in C++.
  - Observations are 3D calorimeter depositions.
  - Latent variables (Monte Carlo truth) of interest: decay channel,  $px$ ,  $py$ ,  $pz$  momenta, final state momenta and IDs.



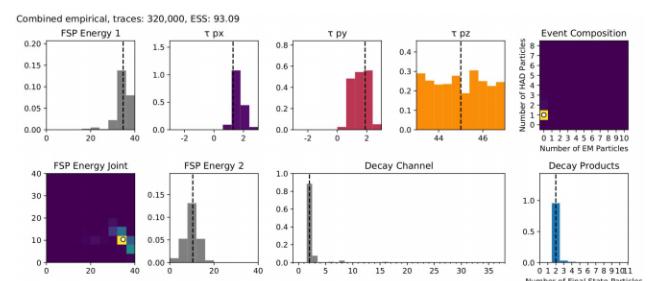
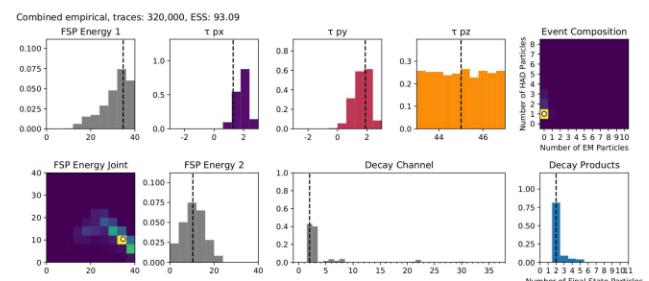
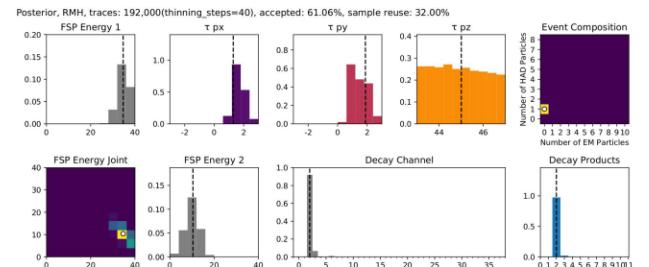
# Inference results

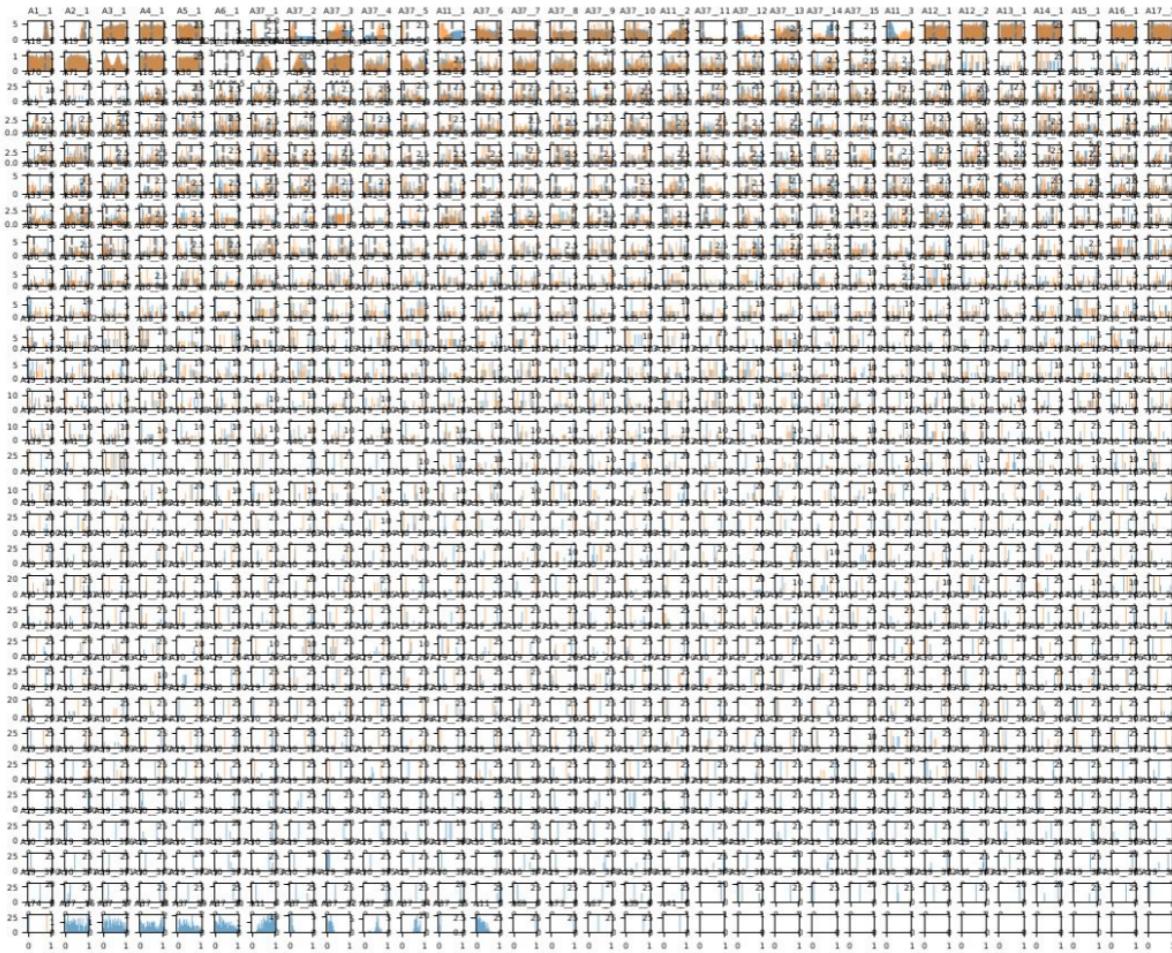


MCMC true posterior  
(7.7M single node)

IC proposal  
from trained NN

IC posterior  
after importance  
weighting

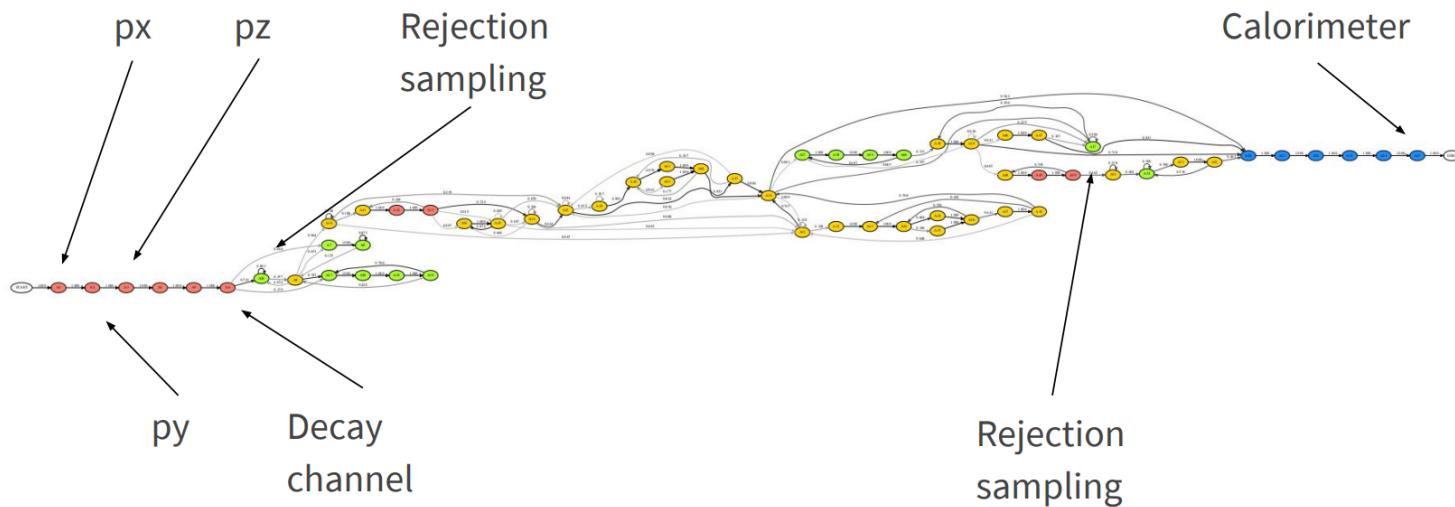


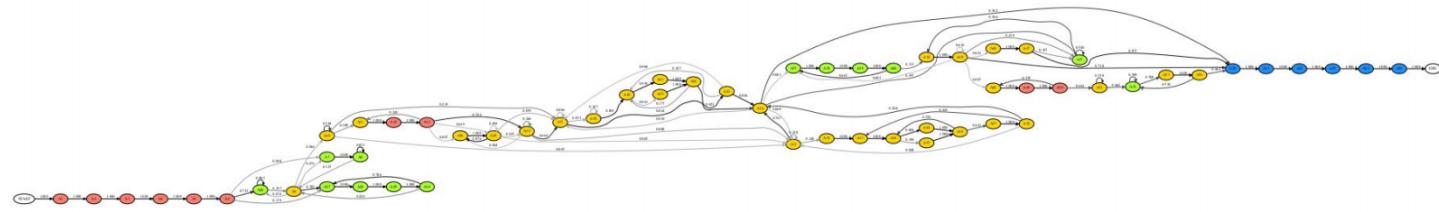


We obtain posteriors over the whole Sherpa address space, 1000s of addresses.

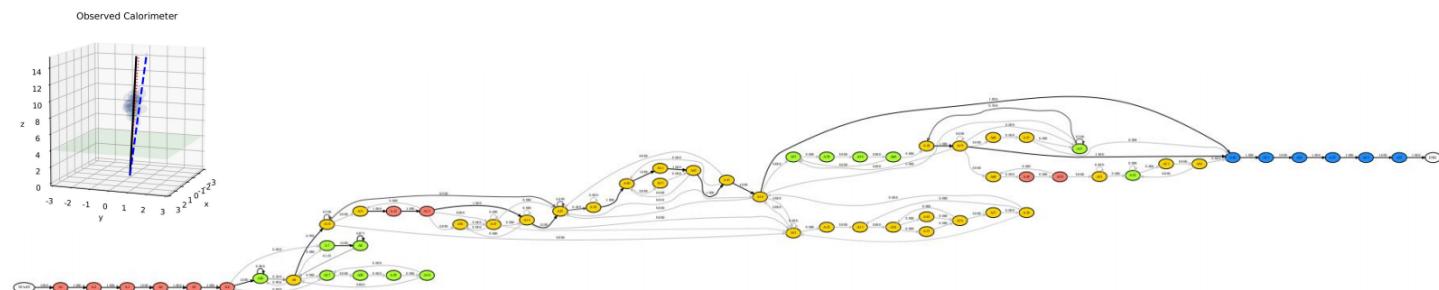
## Interpretability

Latent probabilistic structure of the 250 most frequent trace types:





(a) Prior execution  $p(\mathbf{x})$ .

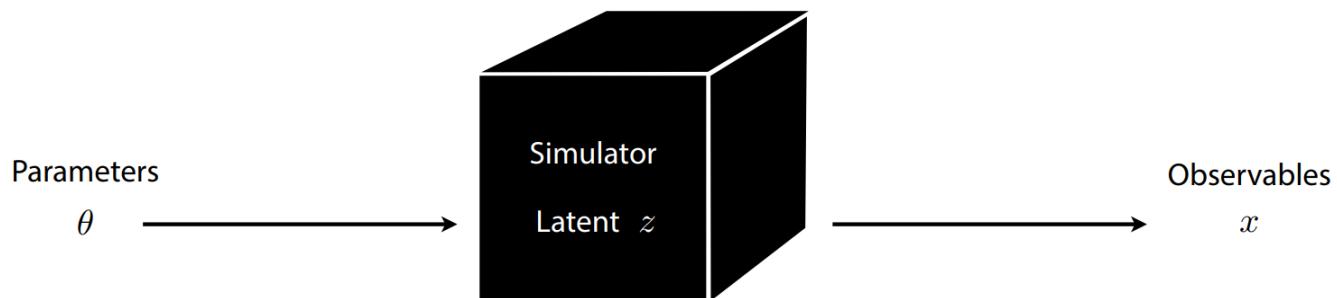


(b) Posterior execution  $p(\mathbf{x}|\mathbf{y})$  conditioned on a given calorimeter observation  $\mathbf{y}$ .

# Summary

# Summary

- Much of modern science is based on "likelihood-free" simulations.
- The likelihood-ratio is central to many statistical inference procedures, regardless of your religion.
- Supervised learning enables likelihood-ratio estimation.
- Better likelihood-ratio estimates can be achieved by mining simulators.
- Probabilistic programming enables posterior inference in scientific simulators.



# Collaborators



Kyle Cranmer



Juan Pavez



Johann  
Brehmer



Joeri  
Hermans



Antoine  
Wehenkel



Siddarth  
Mishra-  
Sharma



Lukas  
Heinrich



Atilim Güneş  
Baydin



Wahid Bhimji



Frank Wood

# References

- Brehmer, J., Mishra-Sharma, S., Hermans, J., Louppe, G., Cranmer, K. (2019). Mining for Dark Matter Substructure: Inferring subhalo population properties from strong lenses with machine learning. arXiv preprint arXiv 1909.02005.
- Hermans, J., Begy, V., & Louppe, G. (2019). Likelihood-free MCMC with Approximate Likelihood Ratios. arXiv preprint arXiv:1903.04057.
- Baydin, A. G., Shao, L., Bhimji, W., Heinrich, L., Meadows, L., Liu, J., ... & Ma, M. (2019). Etalumis: Bringing Probabilistic Programming to Scientific Simulators at Scale. arXiv preprint arXiv:1907.03382.
- Stoye, M., Brehmer, J., Louppe, G., Pavez, J., & Cranmer, K. (2018). Likelihood-free inference with an improved cross-entropy estimator. arXiv preprint arXiv:1808.00973.
- Baydin, A. G., Heinrich, L., Bhimji, W., Gram-Hansen, B., Louppe, G., Shao, L., ... & Wood, F. (2018). Efficient Probabilistic Inference in the Quest for Physics Beyond the Standard Model. arXiv preprint arXiv:1807.07706.
- Brehmer, J., Louppe, G., Pavez, J., & Cranmer, K. (2018). Mining gold from implicit models to improve likelihood-free inference. arXiv preprint arXiv:1805.12244.
- Brehmer, J., Cranmer, K., Louppe, G., & Pavez, J. (2018). Constraining Effective Field Theories with Machine Learning. arXiv preprint arXiv:1805.00013.
- Brehmer, J., Cranmer, K., Louppe, G., & Pavez, J. (2018). A Guide to Constraining Effective Field Theories with Machine Learning. arXiv preprint arXiv:1805.00020.
- Casado, M. L., Baydin, A. G., Rubio, D. M., Le, T. A., Wood, F., Heinrich, L., ... & Bhimji, W. (2017). Improvements to Inference Compilation for Probabilistic Programming in Large-Scale Scientific Simulators. arXiv preprint arXiv:1712.07901.
- Louppe, G., Hermans, J., & Cranmer, K. (2017). Adversarial Variational Optimization of Non-Differentiable Simulators. arXiv preprint arXiv:1707.07113.
- Cranmer, K., Pavez, J., & Louppe, G. (2015). Approximating likelihood ratios with calibrated discriminative classifiers. arXiv preprint arXiv:1506.02169.

The end.