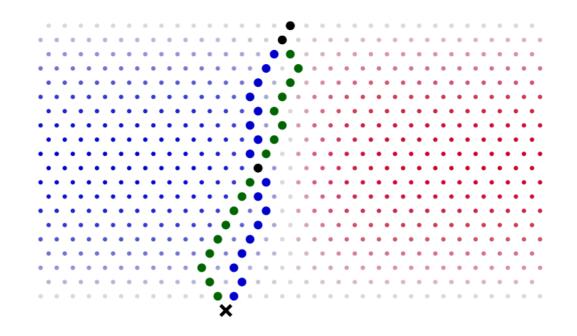
# **Neural Likelihood-free Inference**

1st Pan-European Advanced School of Statistics in HEP October 29, DESY, Hamburg

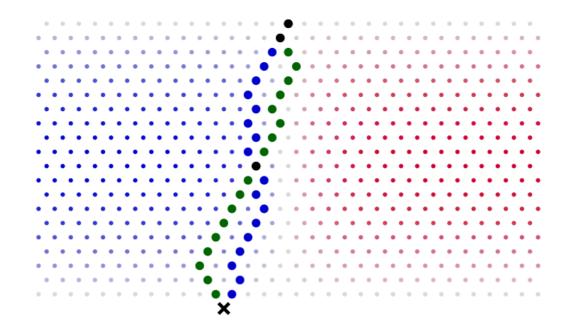
> Gilles Louppe g.louppe@uliege.be







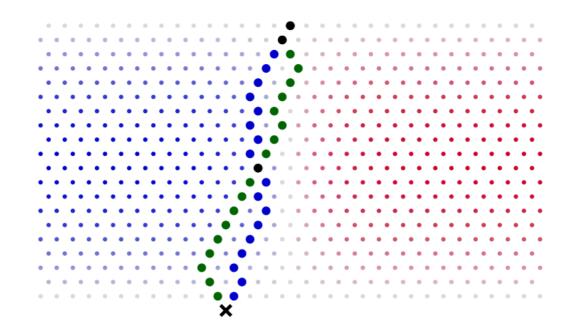
How can we estimate the probability  $\theta$  of going left when hitting a pin?



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

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

Therefore  $\hat{ heta} = rg \max \prod_{x_i} p(x_i | heta) \pi( heta).$ 

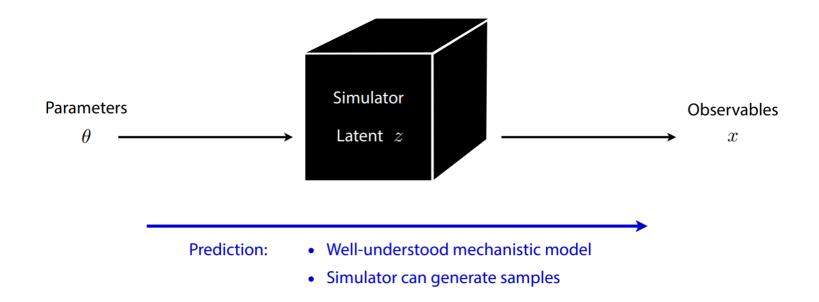


But what if we shift or remove some of the pins?

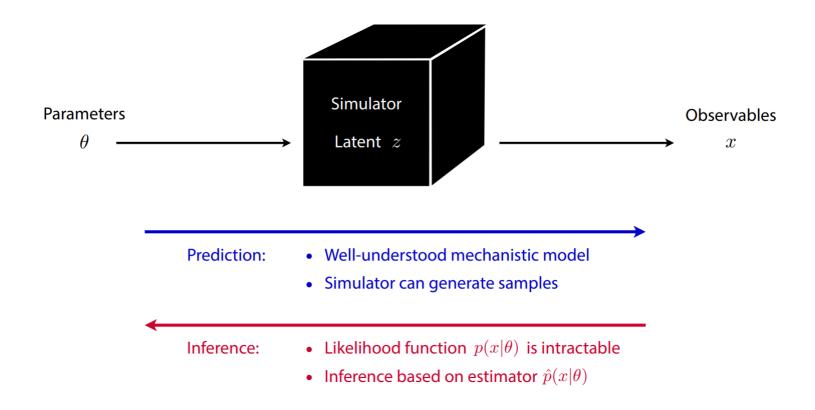
#### The Galton board is a metaphore of simulation-based science:

Galton board device	$\rightarrow$	Computer simulation
Parameters $ heta$	$\rightarrow$	Model parameters $ heta$
Buckets $x$	$\rightarrow$	Observables $x$
Random paths <i>z</i>	$\rightarrow$	Latent variables <i>z</i> (stochastic execution traces through simulator)

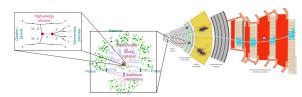
Inference in this context requires likelihood-free algorithms.



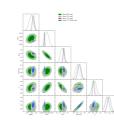
Credits: Johann Brehmer.

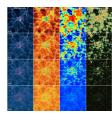


# A thriving field of research



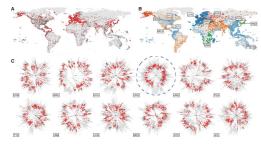
Particle physics



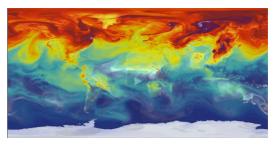




### Astrophysics



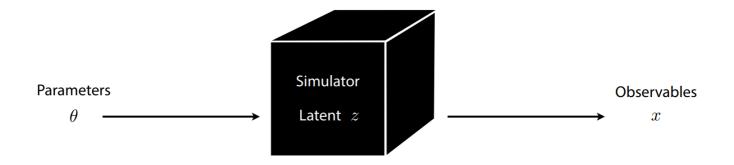
### Epidemiology



Climatology

(... and many others!)

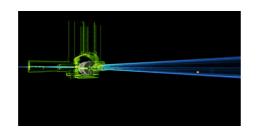
### **Particle physics**



# SM with parameters $\theta$

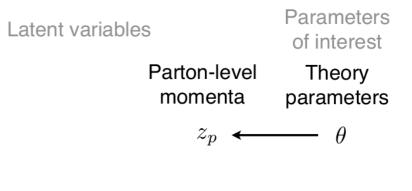
$$\begin{split} & \int_{\mathbb{R}^{n}} \int_{\mathbb{R}^{n}$$

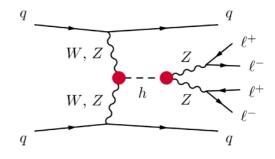
#### Simulated observables $oldsymbol{x}$



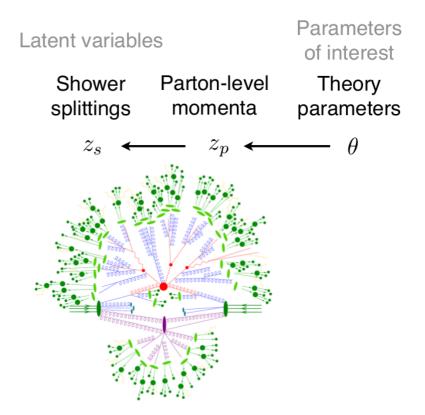
#### Real observations $x_{ m obs}$

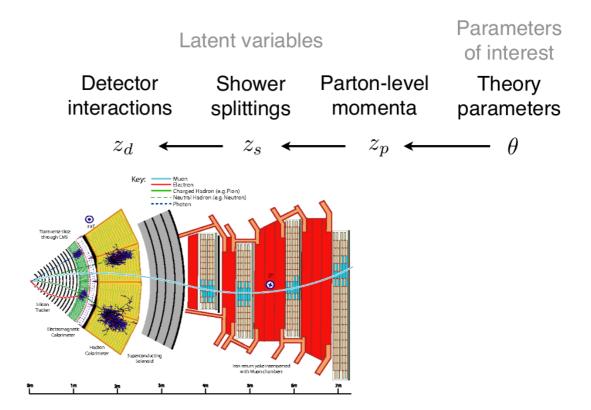


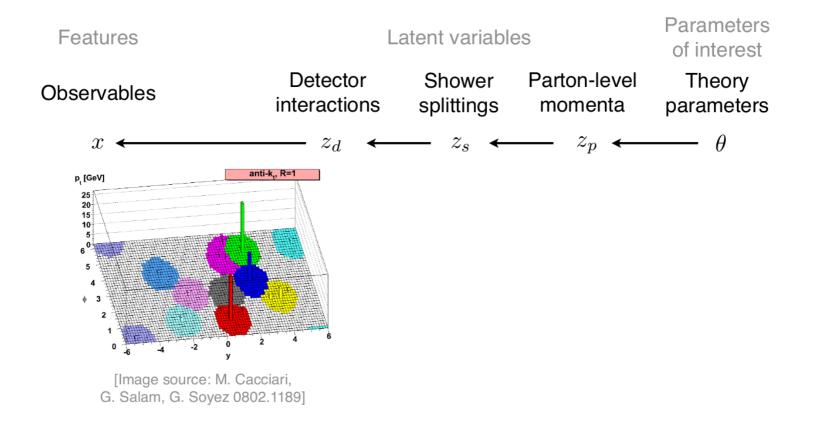




Credits: Johann Brehmer.







$$p(x| heta) = igstarrow ectsizet p(z_p| heta) p(z_s|z_p) p(z_d|z_s) p(x|z_d) dz_p dz_s dz_d$$
 $ext{intractable}$ 

## **Likelihood ratio**

The likelihood ratio

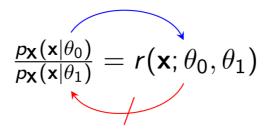
$$r(x| heta_0, heta_1)=rac{p(x| heta_0)}{p(x| heta_1)}$$

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

### **Examples**

- Frequentist hypothesis testing
- Bayesian model comparison
- Bayesian posterior sampling with MCMC
- Bayesian posterior inference through Variational Inference
- Supervised learning
- 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



Direct likelihood ratio estimation is simpler than density estimation.

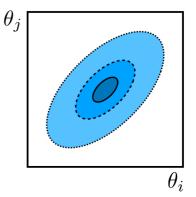
(This is fortunate, we are in the likelihood-free scenario!)

# **Frequentist inference**

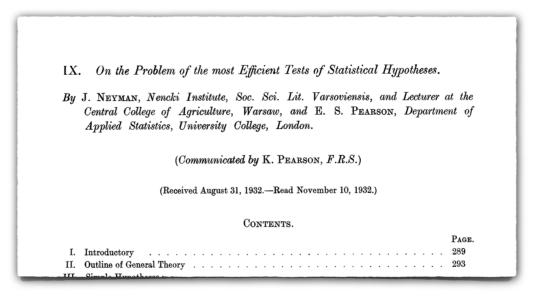
# The frequentist (physicist's) way

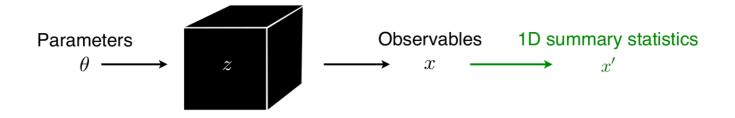
The Neyman-Pearson lemma states that the likelihood ratio

$$r(x| heta_0, heta_1) = rac{p(x| heta_0)}{p(x| heta_1)}$$



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





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

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

From this it comes

$$rac{p(x| heta_0)}{p(x| heta_1)}pproxrac{\hat{p}\left(x| heta_0
ight)}{\hat{p}\left(x| heta_1
ight)}=\hat{r}(x| heta_0, heta_1).$$

#### Wilks theorem

Consider the test statistic

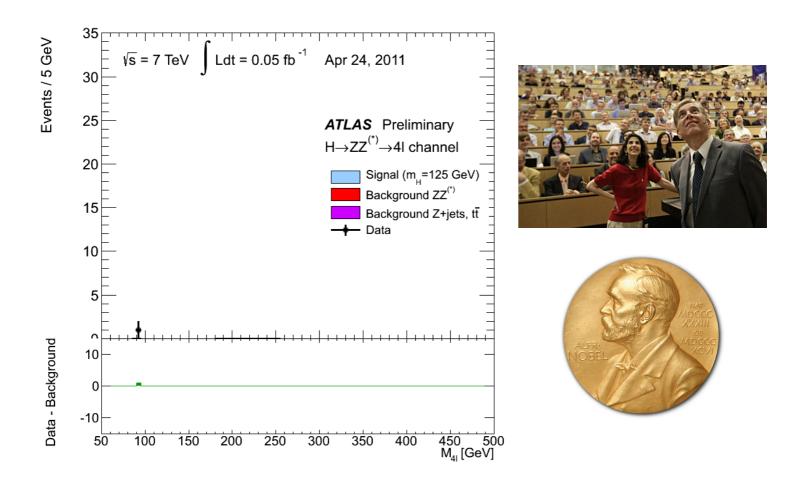
$$q( heta) = -2\sum_x \log rac{p(x| heta)}{p(x|\hat{ heta\,})} = -2\sum_x \log r(x| heta,\hat{ heta\,})$$

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

When  $N o \infty, q( heta) \sim \chi_2.$ 

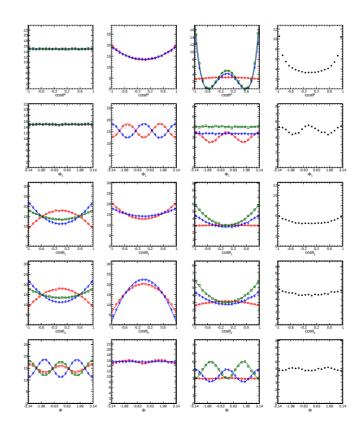
Therefore (and provided the assumptions apply!), an observed value  $q_{obs}(\theta)$  translates directly to a p-value that measures the confidence with which  $\theta$  can be excluded:

$$p_{ heta} \equiv \int_{q_{
m obs}( heta)}^{\infty} \mathrm{d}q\, p(q| heta) = 1 - F_{\chi_2}(q_{
m obs}( heta)),$$



Discovery of the Higgs boson at 5- $\sigma$ 

- 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 highdimensional histograms is not tractable.

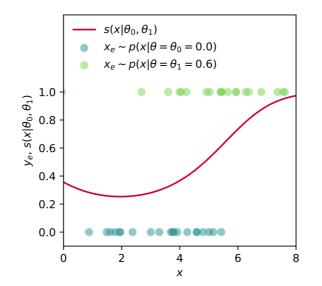




Supervised learning provides a way to automatically construct s:

- Let us consider a neural network classifier  $\hat{s}$  tasked to distinguish  $x\sim p(x| heta_0)$  from  $x\sim p(x| heta_1).$
- Train  $\hat{s}$  by minimizing the cross-entropy loss

$$egin{aligned} L_{XE}[\,\hat{s}\,] &= -\mathbb{E}_{p(x| heta)\pi( heta)}[1( heta= heta_0)\log\,\hat{s}(x) + \ &1( heta= heta_1)\log(1-\hat{s}(x))] \end{aligned}$$



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

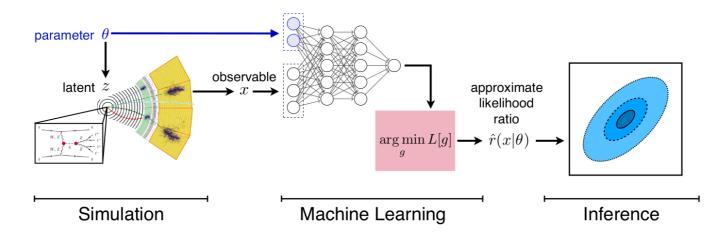
$$\hat{s}(x)pprox s^*(x)=rac{p(x| heta_1)}{p(x| heta_0)+p(x| heta_1)}.$$

Therefore,

$$r(x| heta_0, heta_1)pprox \hat{r}(x| heta_0, heta_1)=rac{1-\hat{s}(x)}{\hat{s}(x)}$$

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

Cranmer, Pavez and Louppe, 2015 [arXiv: 1506.02169].



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

Therefore, we have

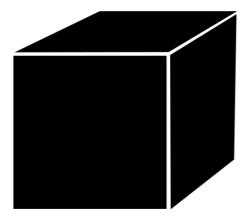
$$\hat{r}\left(x| heta_{0}, heta_{ ext{ref}}
ight)=rac{1-\hat{s}\left(x| heta_{0}, heta_{ ext{ref}}
ight)}{\hat{s}\left(x| heta_{0}, heta_{ ext{ref}}
ight)}$$

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

$$r(x| heta_0, heta_1)pprox rac{\hat{r}\left(x| heta_0, heta_{ ext{ref}}
ight)}{\hat{r}\left(x| heta_1, heta_{ ext{ref}}
ight)}.$$

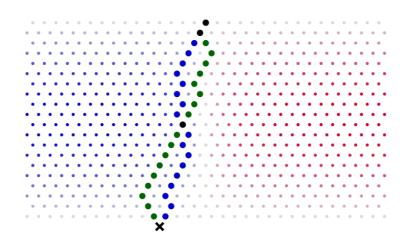
Cranmer, Pavez and Louppe, 2015 [arXiv:1506.02169].

# **Opening the black box**

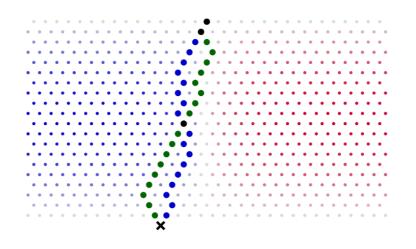




Traditional likelihood-free inference treats the simulator as a generative black box: parameters in, samples out. But in most real-life problems, we have access to the simulator code and some understanding of the microscopic processes.



p(x| heta) is usually intractable. What about p(x, z| heta)?



p(x| heta) is usually intractable. What about p(x, z| heta)?

As the trajectory  $z_1, ..., z_T$  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  $r(x,z| heta_0, heta_1);$
- to calculate the joint score  $t(x,z| heta_0) = 
  abla_ heta\log p(x,z| heta) ig|_{ heta_0}.$

We call this process mining gold from your simulator!

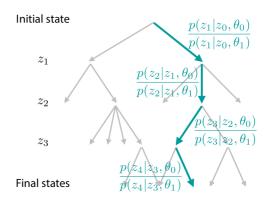
### Extracting the joint likelihood ratio

- 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:

$$r(x,z| heta_0, heta_1) = rac{p(x,z| heta_0)}{p(x,z| heta_1)} = \prod_i rac{p(z_i|z_{i-1}, heta_0)}{p(z_i|z_{i-1}, heta_1)}$$



### ALICE

When the joint likelihood ratio  $r(x, z | \theta_0, \theta_1)$  is available from the simulator, the corresponding  $s(x, z | \theta_0, \theta_1)$  are also tractable.

Therefore, the original CARL cross-entropy can be adapted to make use of the exact  $s(x,z| heta_0, heta_1)$  instead of using labels  $y\in\{0,1\}$ :

$$egin{aligned} L_{ALICE}[\hat{s}] &= -\mathbb{E}_{p(x,z)}[s(x,z| heta_0, heta_1)\log(\hat{s}(x))+ \ & (1-s(x,z| heta_0, heta_1))\log(1-\hat{s}(x))], \end{aligned}$$

where  $p(x,z) = (p(x,z| heta_0) + p(x,z| heta_1))/2.$ 



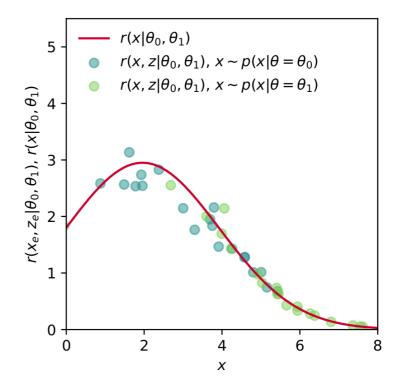
### **Regressing the likelihood ratio**

Observe that the joint likelihood ratios

$$r(x,z| heta_0, heta_1)=rac{p(x,z| heta_0)}{p(x,z| heta_1)}$$

are scattered around  $r(x| heta_0, heta_1).$ 

Can we use them to approximate  $r(x| heta_0, heta_1)$ ?



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:

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

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

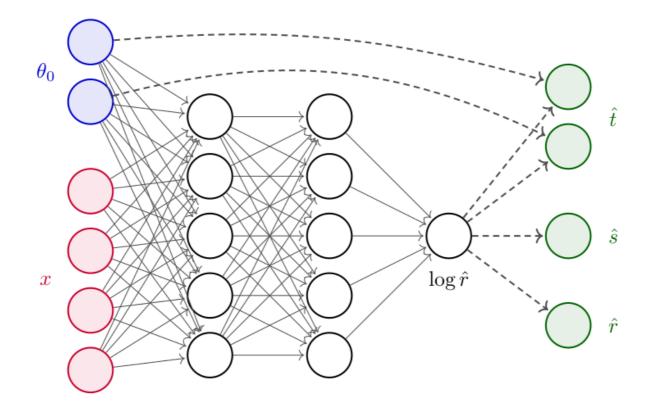
$$egin{aligned} g^*(x) &= rac{1}{p(x| heta)}\int p(x,z| heta)g(x,z)dz \ &= \mathbb{E}_{p(z|x, heta)}\left[g(x,z)
ight] \end{aligned}$$

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

$$L_r = \mathbb{E}_{p(x,z| heta_1)}\left[(r(x,z| heta_0, heta_1) - \hat{r}(x))^2
ight],$$

which is minimized by

$$egin{aligned} r^*(x) &= rac{1}{p(x| heta_1)} \int p(x,z| heta_1) rac{p(x,z| heta_0)}{p(x,z| heta_1)} dz \ &= rac{p(x| heta_0)}{p(x| heta_1)} \ &= r(x| heta_0, heta_1). \end{aligned}$$



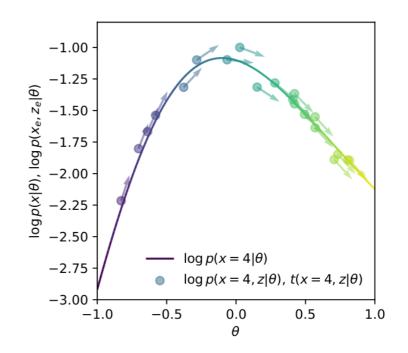
 $r^*(x| heta_0, heta_1) = rg\min_{\hat{r}} L_r[\hat{r}]$ 

#### **Regressing the score**

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

$$t(x,z| heta_0) = 
abla_ heta \log p(x,z| heta)igert_{ heta_0},$$

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  $t(x,z| heta_0)$  and heta with  $heta_0$ , we define

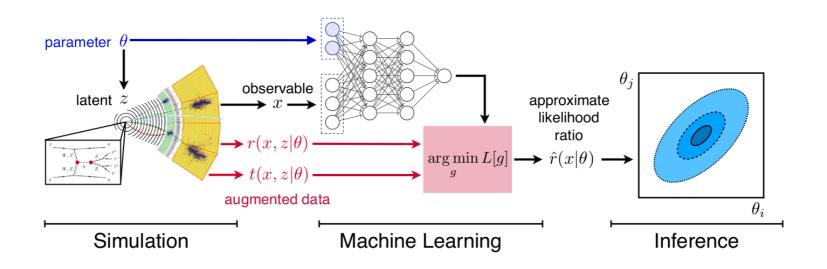
$$L_t = \mathbb{E}_{p(x,z| heta_0)}\left[(t(x,z| heta_0) - \,\hat{t}\,(x))^2
ight],$$

which is minimized by

$$egin{aligned} t^*(x) &= rac{1}{p(x| heta_0)} \int p(x,z| heta_0) (
abla_ heta \log p(x,z| heta)ig|_{ heta_0}) dz \ &= rac{1}{p(x| heta_0)} \int p(x,z| heta_0) rac{
abla_ heta p(x,z| heta)ig|_{ heta_0}}{p(x,z| heta_0)} dz \ &= rac{
abla_ heta p(x| heta)ig|_{ heta_0}}{p(x| heta_0)} \ &= 
abla_ heta \log p(x| heta)ig|_{ heta_0} \ &= t(x| heta_0). \end{aligned}$$

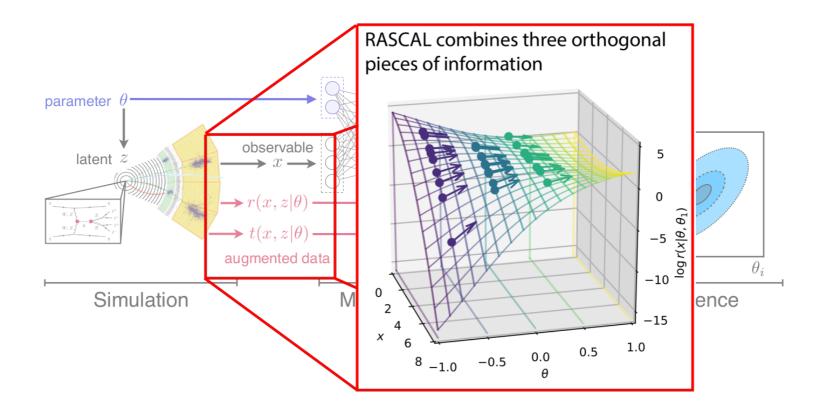


### $L_{\text{RASCAL}} = L_r + L_t$





### $L_{\text{RASCAL}} = L_r + L_t$

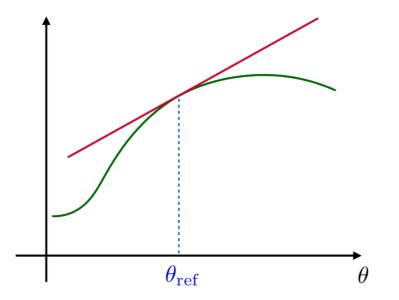


## **SALLY (= optimal compression)**

### The local model

In the neighborhood of  $heta_{
m ref}$ , the Taylor expansion of  $\log p(x| heta)$  is

$$\log p(x| heta) = \log p(x| heta_{ ext{ref}}) + \underbrace{
abla_ heta \log p(x| heta)}_{t(x| heta_{ ext{ref}})} \cdot ( heta - heta_{ ext{ref}}) + O(( heta - heta_{ ext{ref}})^2)$$



This results in the exponential model

$$p_{ ext{local}}(x| heta) = rac{1}{Z( heta)} p(t(x| heta_{ ext{ref}})| heta_{ ext{ref}}) \exp(t(x| heta_{ ext{ref}}) \cdot ( heta - heta_{ ext{ref}}))$$

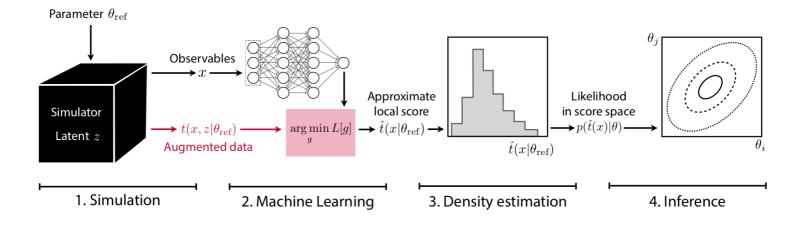
where the score  $t(x| heta_{ ext{ref}})$  are its sufficient statistics.

That is,

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

#### Brehmer, Louppe, Pavez and Cranmer, 2018 [arXiv: 1805.12244].

### SALLY



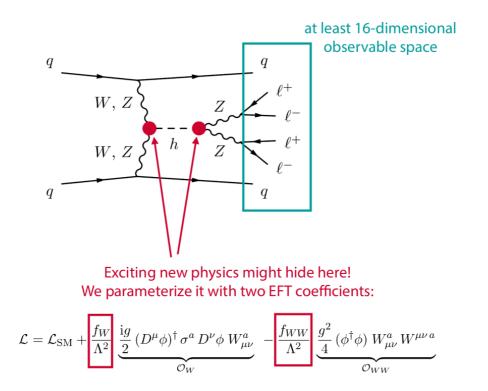
## There is more...

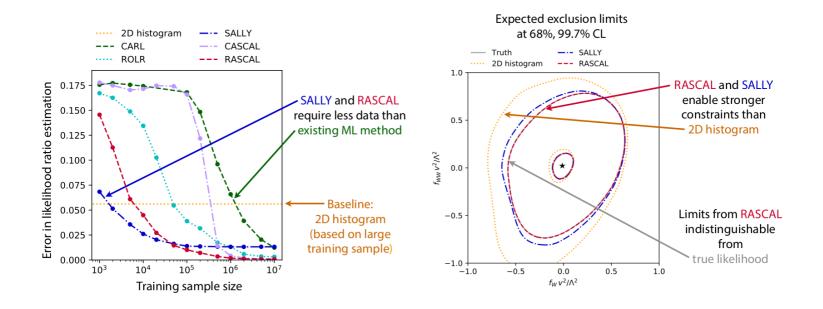
Method	Simulate	Extract $r(x,z) t(x)$		NN estimates	Asympt. exact	Generative
ROLR	$ heta_0 \sim \pi( heta)$ , $ heta_1$	$\checkmark$		$\hat{r}(x  heta_0, heta_1)$	$\checkmark$	
CASCAL	$ heta_0 \sim \pi( heta)$ , $ heta_1$		$\checkmark$	$\hat{r}(x  heta_0, heta_1)$	$\checkmark$	
ALICE	$ heta_0 \sim \pi( heta)$ , $ heta_1$		$\checkmark$	$\hat{r}(x  heta_0, heta_1)$	$\checkmark$	
RASCAL	$ heta_0 \sim \pi( heta)$ , $ heta_1$	$\checkmark$	$\checkmark$	$\hat{r}(x  heta_0, heta_1)$	$\checkmark$	
ALICES	$ heta_0 \sim \pi( heta)$ , $ heta_1$	$\checkmark$	$\checkmark$	$\hat{r}(x  heta_0, heta_1)$	$\checkmark$	
SCANDAL	$\theta \sim \pi(\theta)$		$\checkmark$	$\hat{p}(x  heta)$	$\checkmark$	$\checkmark$
SALLY	$ heta_{ref}$		$\checkmark$	$\hat{t}(x  heta_{ref})$	in local approx.	
SALLINO	$ heta_{ref}$		$\checkmark$	$\hat{t}(x  heta_{ref})$	in local approx.	

### **Examples**

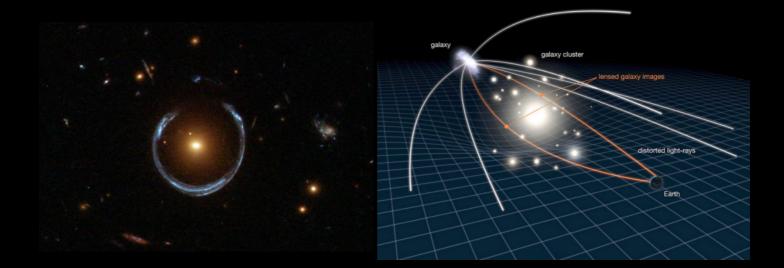
### 1 Hunting new physics at particle colliders

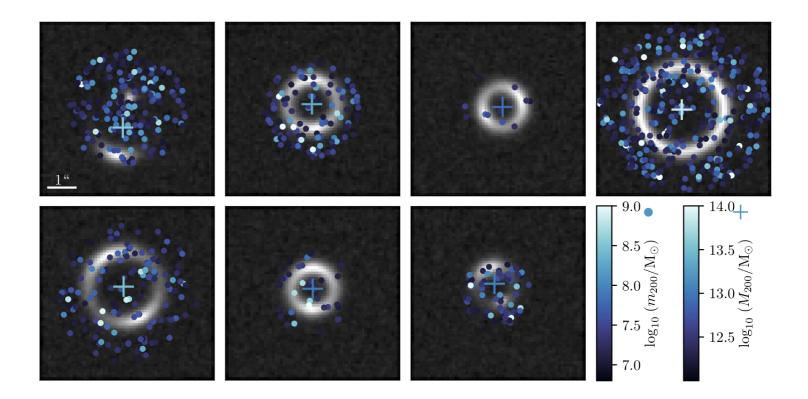
The goal is to constrain two EFT parameters and compare against traditional histogram analysis.



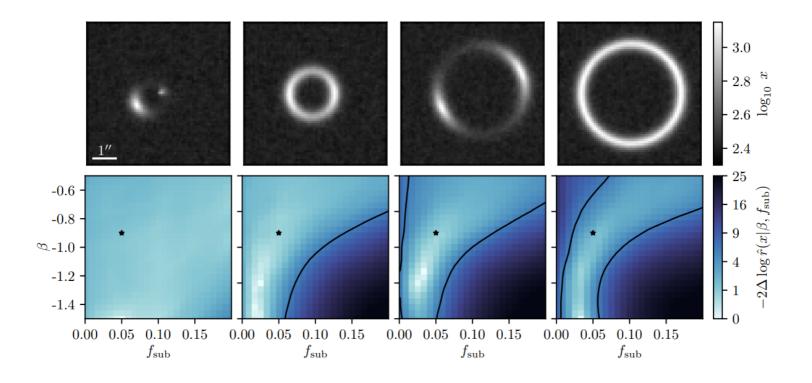


### **②** Dark matter substructure from gravitational lensing





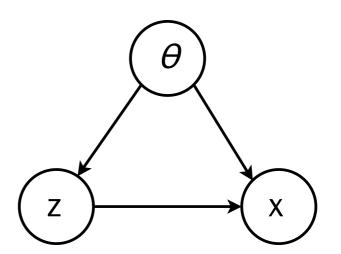
Number of dark matter subhalos and their mass and location lead to complex latent space of each image. The goal is the **inference of population parameters.** 



## **Bayesian inference**

Bayesian inference = computing the posterior

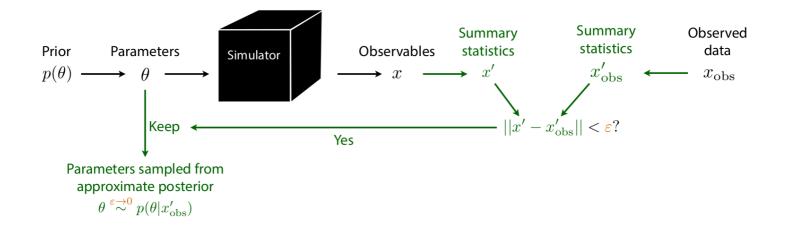
 $p( heta|x) = rac{p(x| heta)p( heta)}{p(x)}.$ 



Doubly intractable in the likelihood-free scenario:

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

$$p( heta|x) = rac{p(x| heta)p( heta)}{p(x)} = r(x| heta)p( heta) pprox \hat{r}(x| heta)p( heta),$$

where  $r(x| heta) = rac{p(x| heta)}{p(x)}$  is the likelihood-to-evidence ratio.

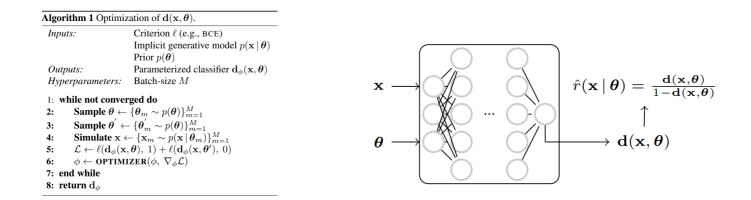
## **Amortizing Bayes**

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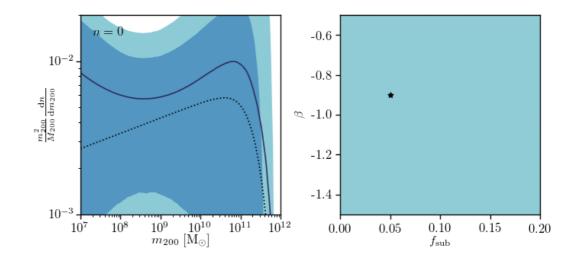
$$p( heta|x) = rac{p(x| heta)p( heta)}{p(x)} = r(x| heta)p( heta) pprox \hat{r}(x| heta)p( heta),$$

where  $r(x| heta) = rac{p(x| heta)}{p(x)}$  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.

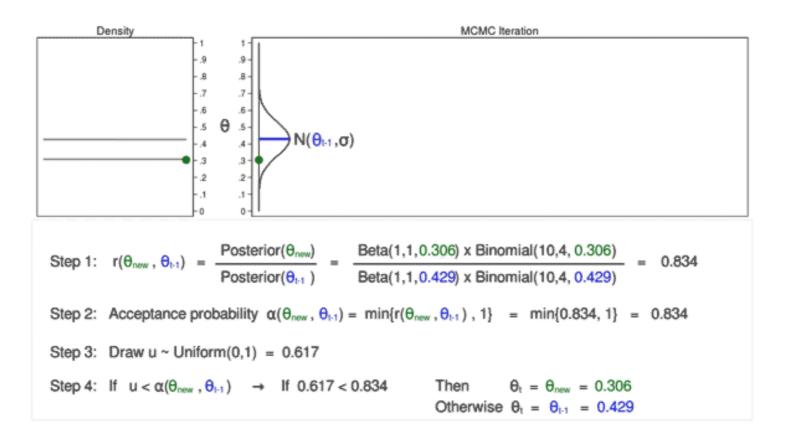


### Bayesian inference of dark matter subhalo population parameters



Brehmer, Mishra-Sharma, Hermans, Louppe, and Cranmer, 2019 [arXiv: 1909.02005].

## **MCMC posterior sampling**



### Likelihood-free MCMC

MCMC samplers require the evaluation of the posterior ratios:

$$egin{aligned} rac{p( heta_{ ext{new}}|x)}{p( heta_{t-1}|x)} &= rac{p(x| heta_{ ext{new}})p( heta_{ ext{new}})/p(x)}{p(x| heta_{t-1})p( heta_{t-1})/p(x)} \ &= rac{p(x| heta_{ ext{new}})p( heta_{ ext{new}})}{p(x| heta_{t-1})p( heta_{t-1})} \ &= r(x| heta_{ ext{new}}, heta_{t-1})rac{p( heta_{ ext{new}})/p( heta_{ ext{new}})}{p( heta_{ ext{new}}, heta_{ ext{new}})} \end{aligned}$$

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:

$$\hat{r}(x| heta_{ ext{new}}, heta_{t-1}) = rac{\hat{r}(x| heta_{ ext{new}})}{\hat{r}(x| heta_{t-1})}$$

Hermans, Begy and Louppe, 2019 [arXiv:1903.04057].

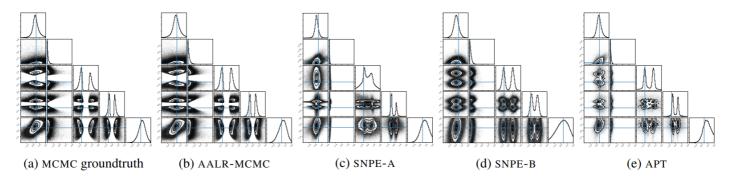
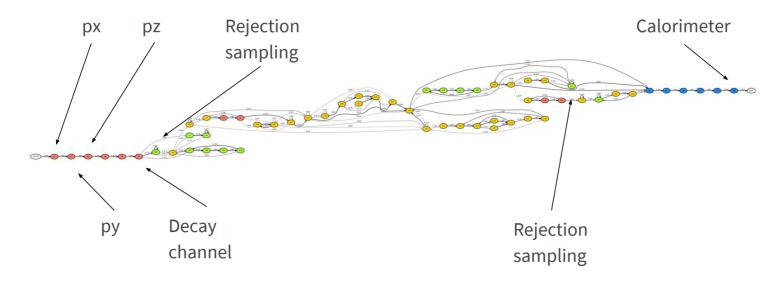


Figure 3: Posteriors from the tractable benchmark. The experiments are repeated 25 times and the approximate posteriors are subsampled from those runs. AALR-MCMC shares the same structure with the MCMC truth, demonstrating its accuracy. Some runs of the other methods were not consistent, contributing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

Algorithm	MMD	ROC AUC	
AALR-MCMC (ours)	$0.05 \pm 0.005$	$0.59 \pm 0.0010$	
ABC ( $\epsilon = 32$ )	$0.51\pm0.001$	$0.99 \pm 0.0001$	
ABC ( $\epsilon = 16$ )	$0.50\pm0.003$	$0.99 \pm 0.0002$	
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	$0.20\pm0.061$	$0.92\pm0.0181$	

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**



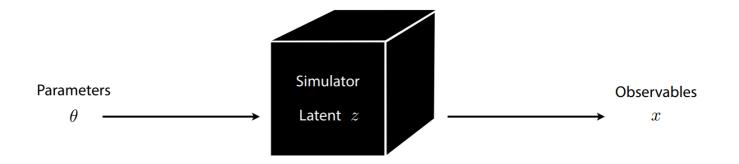
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#### See Lukas' talk after the coffee break!



## **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**





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The end.