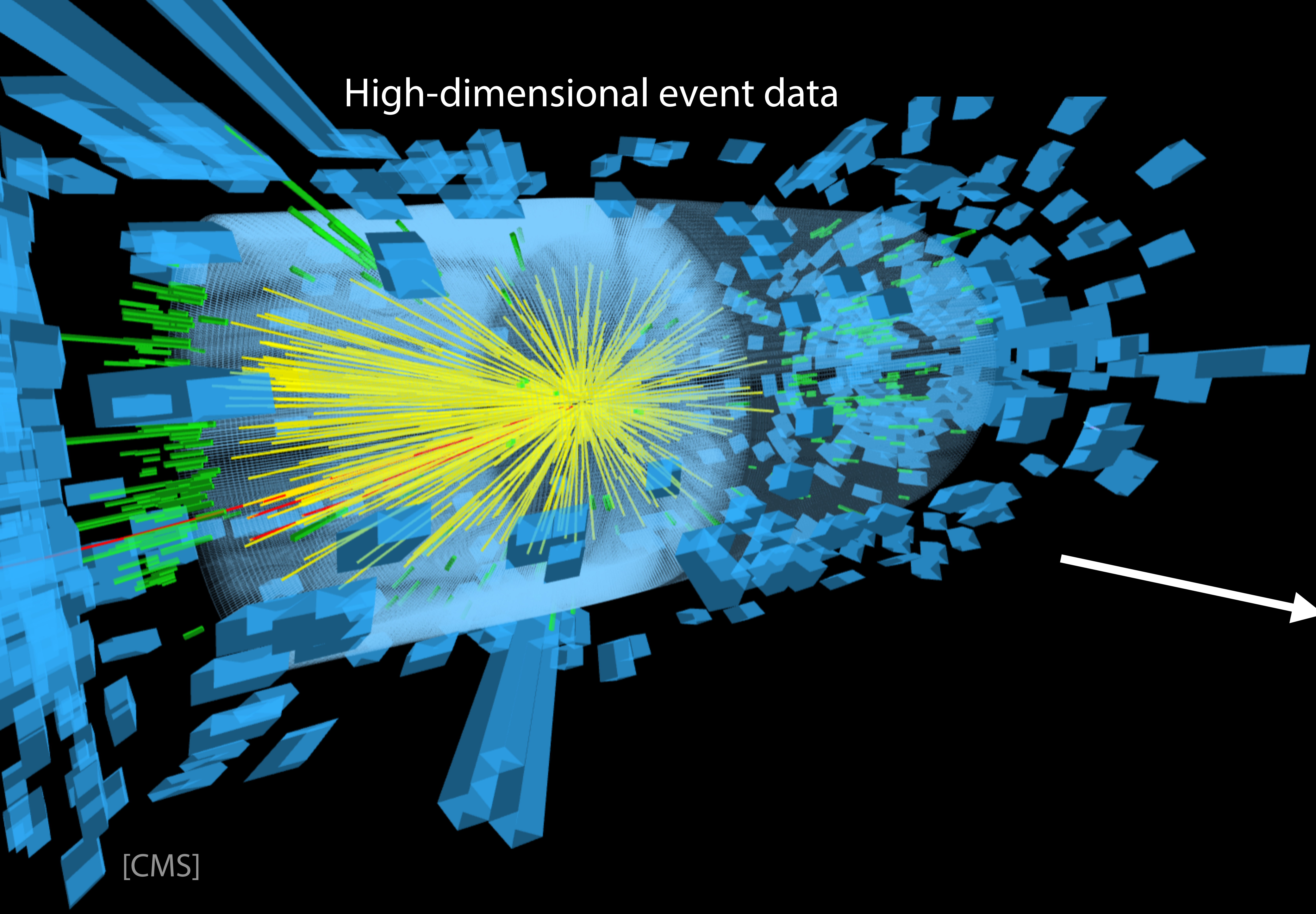
# How machine learning can help us get the most out of high-precision particle physics models

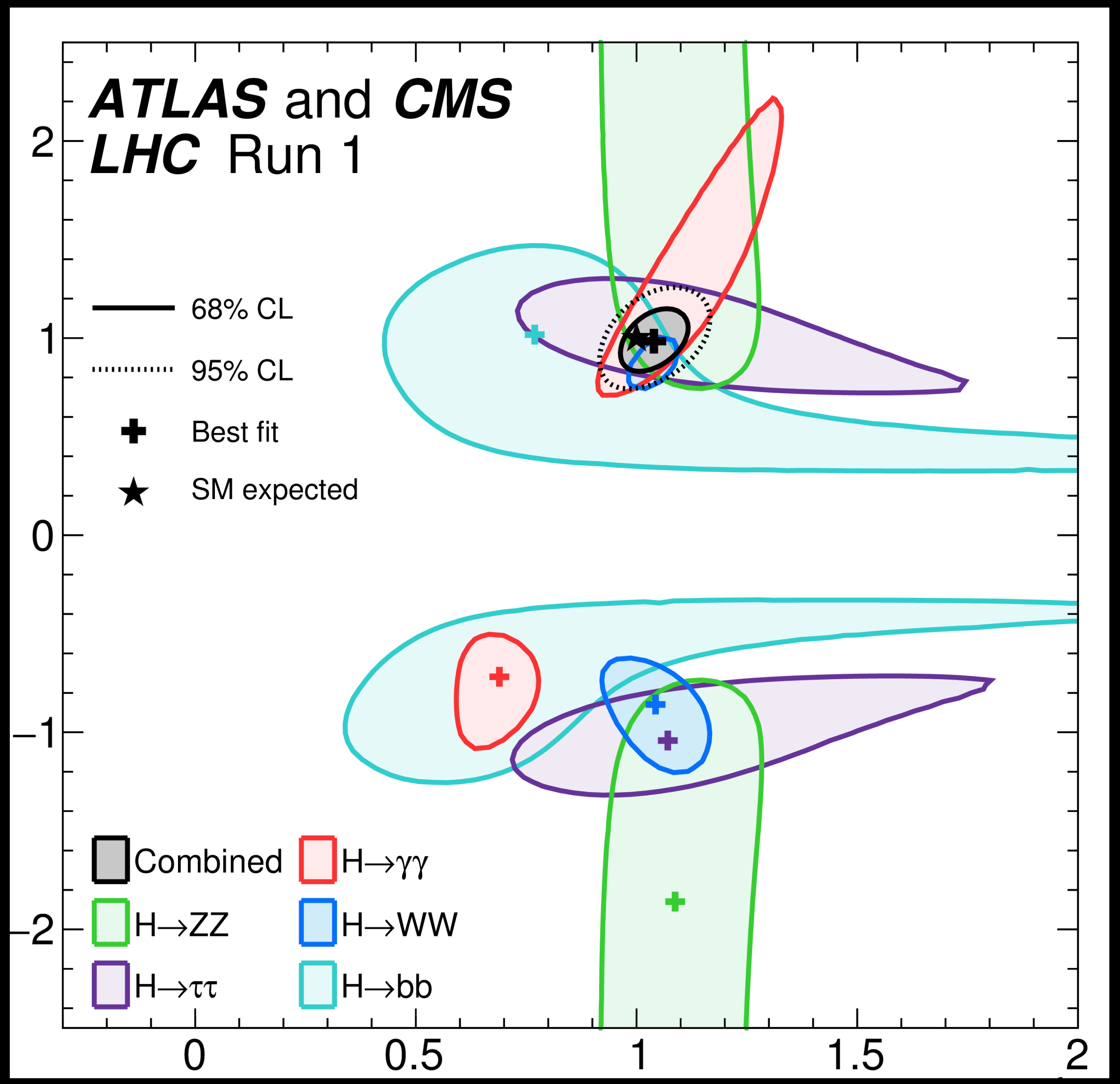
Johann Brehmer
New York University

JLab theory seminar
November 23, 2020

High-dimensional event data



[CMS]




[ATLAS, CMS 1606.02266]

Precision constraints on new physics

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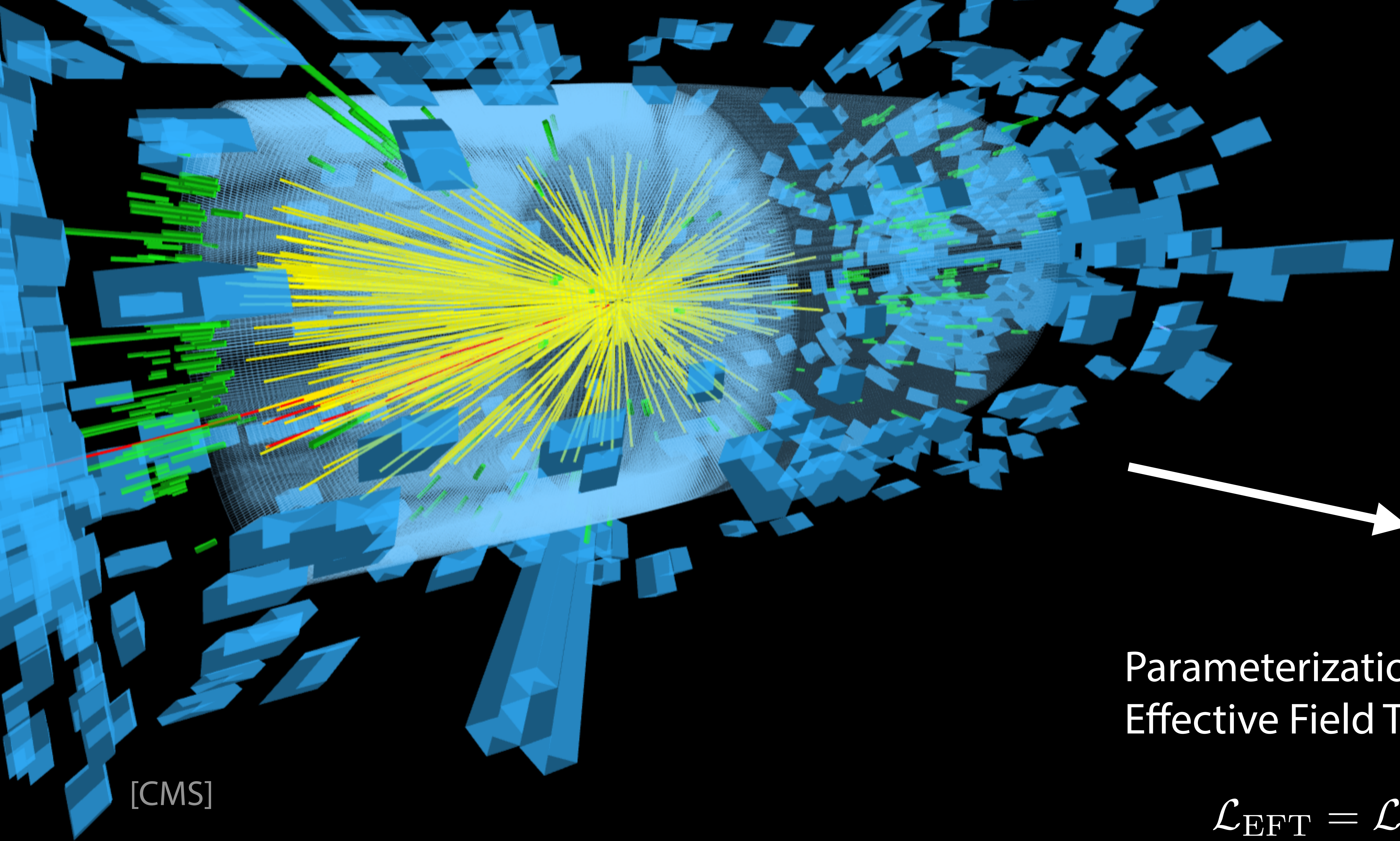
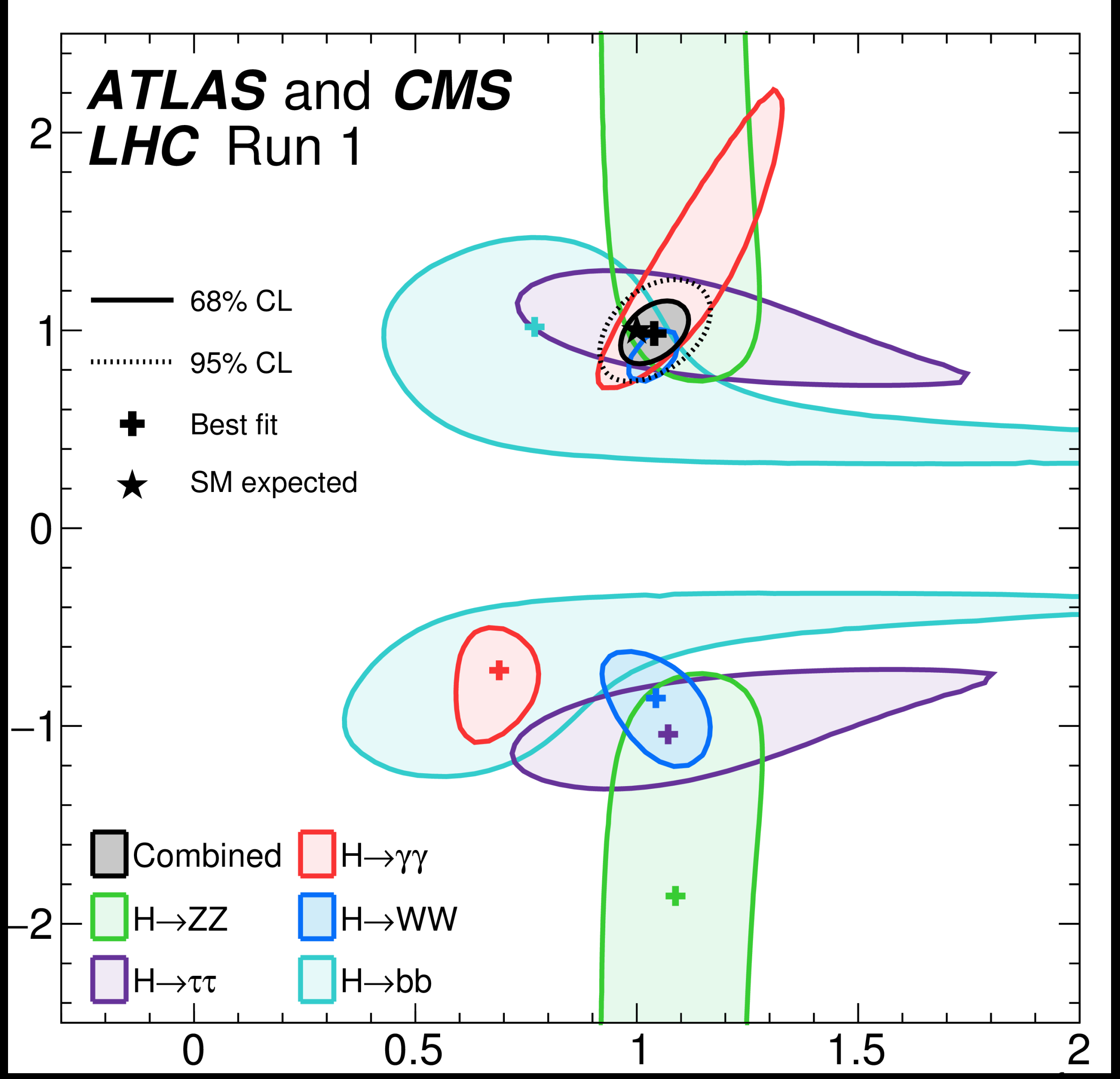


[CMS]




[ATLAS, CMS 1606.02266]

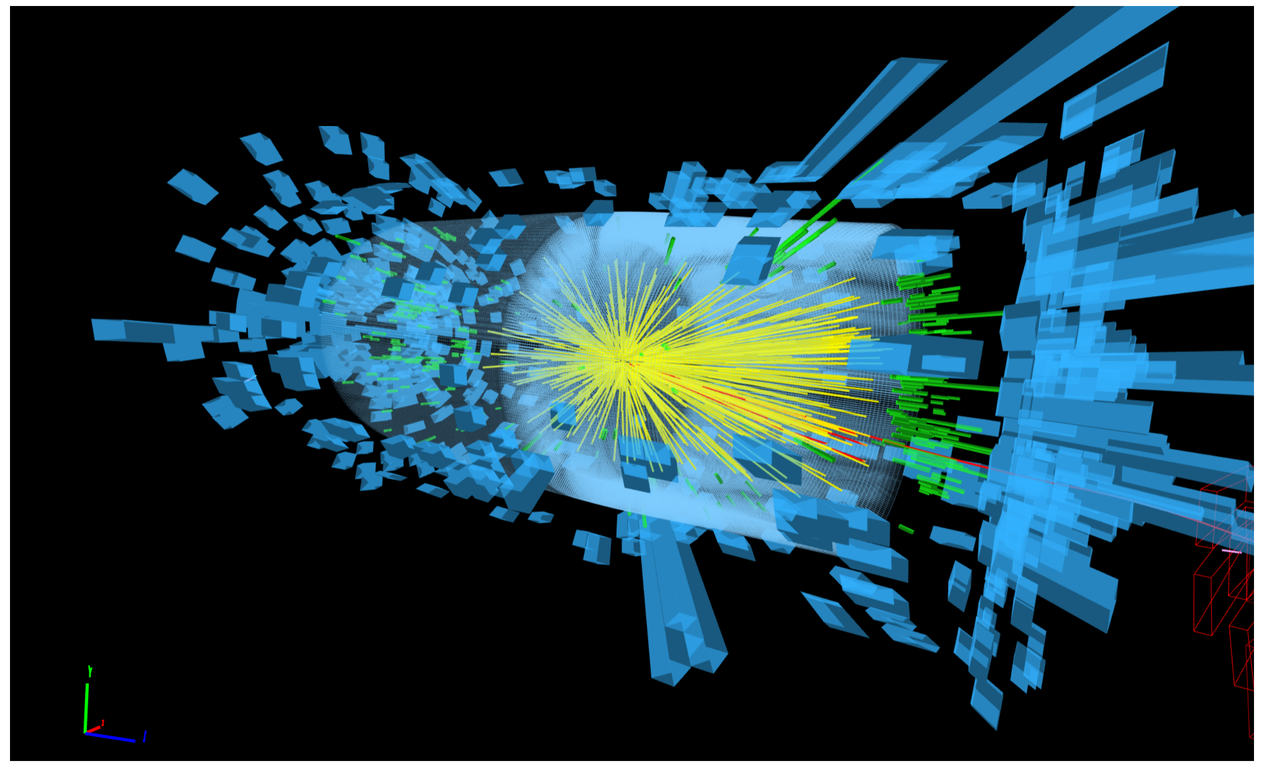
Precision constraints on new physics

Parameterization e.g. in Effective Field Theory:

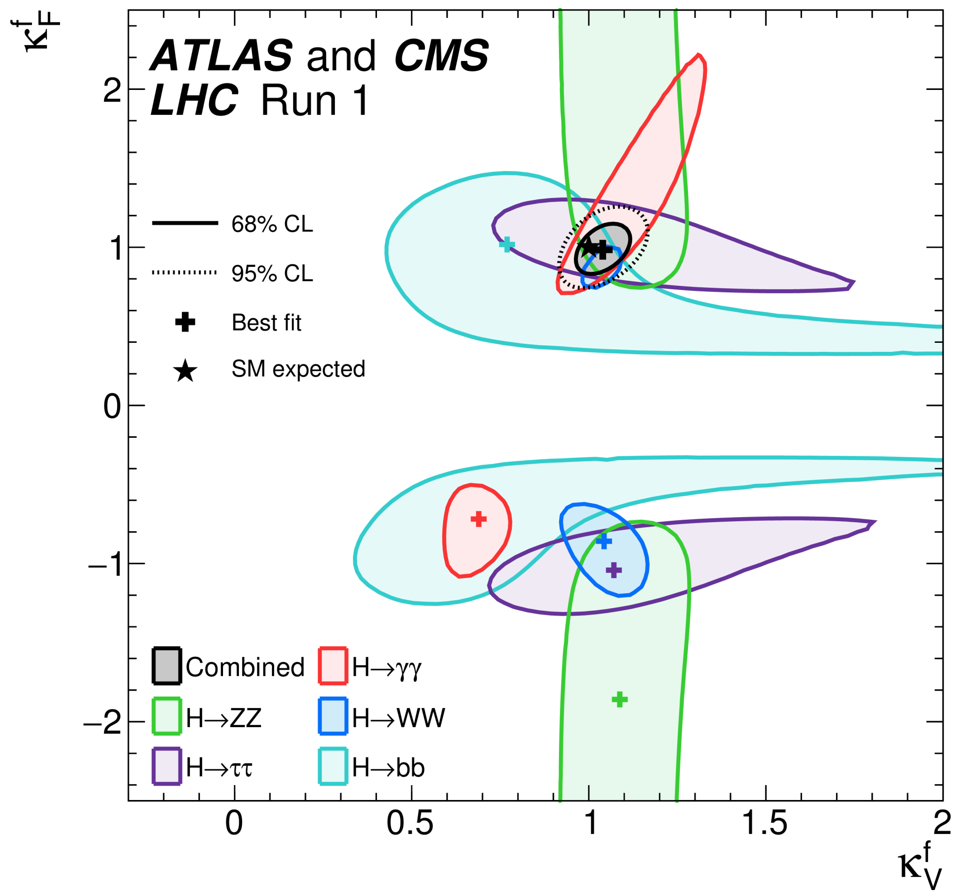
systematic expansion of new physics around Standard Model

$$\mathcal{L}_{\mathrm{EFT}} = \mathcal{L}_{\mathrm{SM}} + \sum_i \frac{f_i}{\Lambda^2}\, \mathcal{O}_i + \dots$$

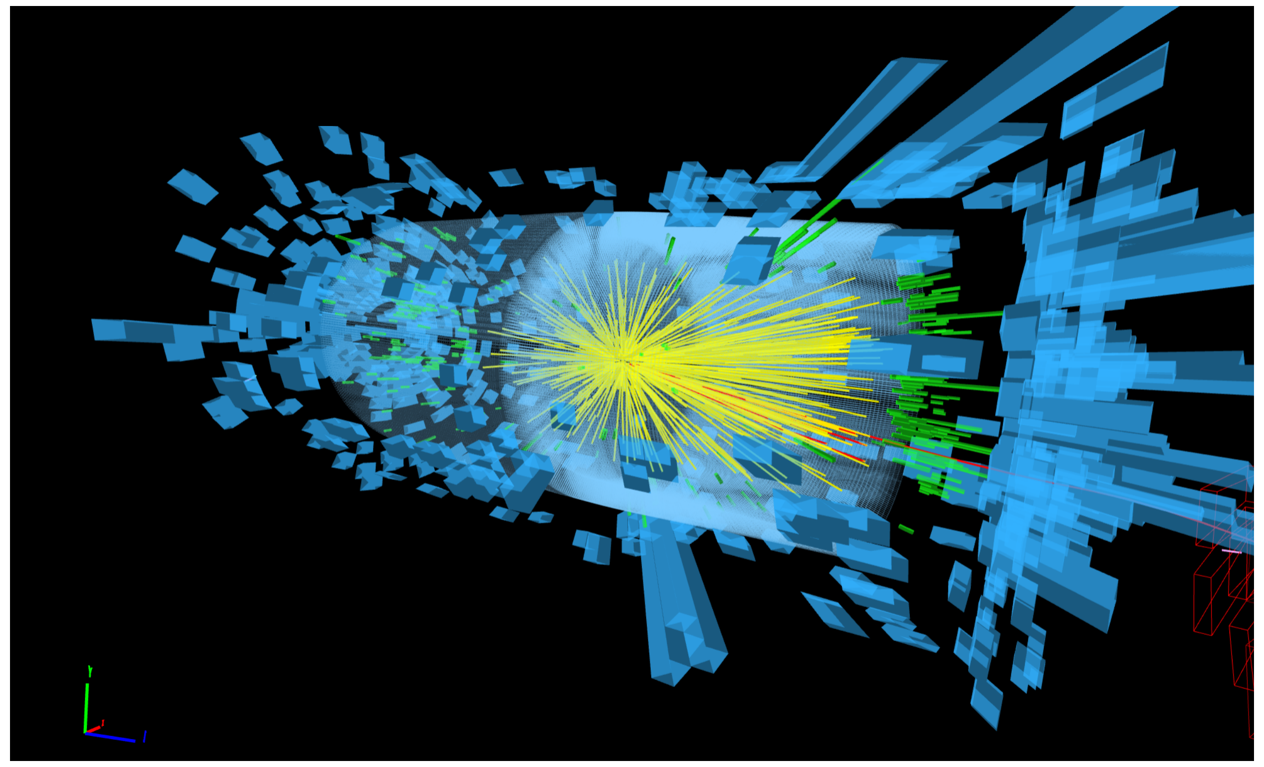
10s to 100s “universal” parameters to measure



High-dimensional
event data $x$




Constraints on
parameters $\theta$

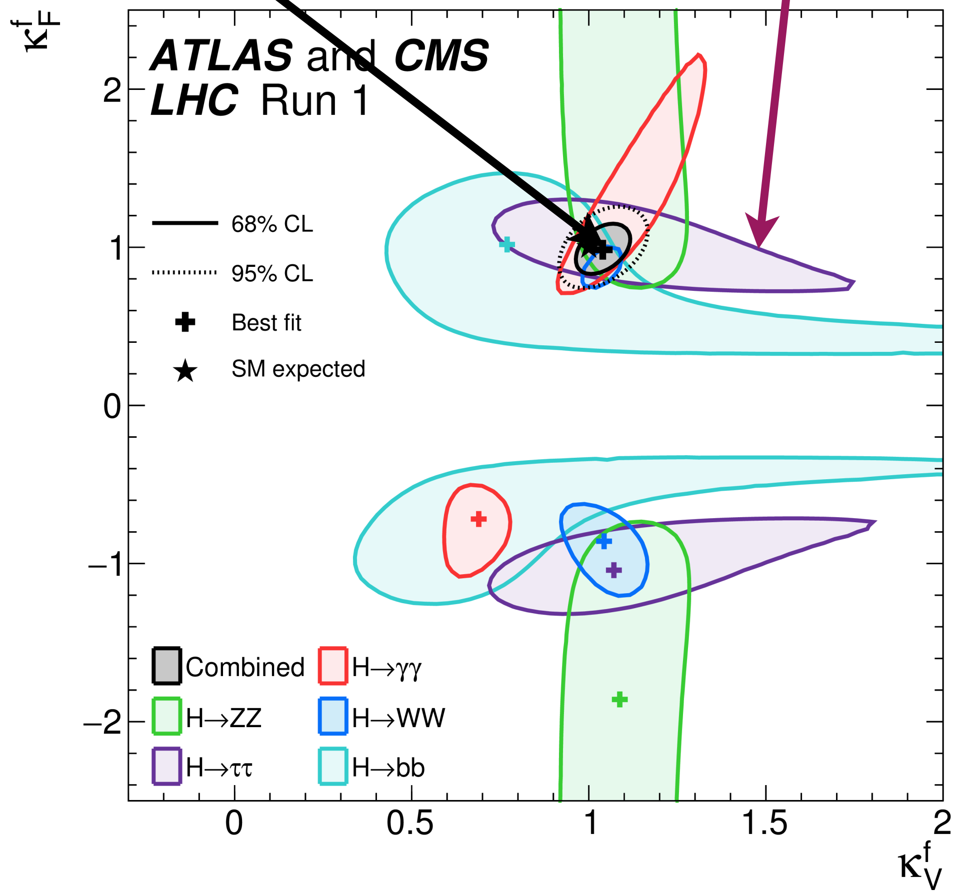


High-dimensional
event data $x$

Likelihood function
$p(x|\theta)$

Maximum-likelihood
estimator

Confidence limits based
on likelihood ratio tests

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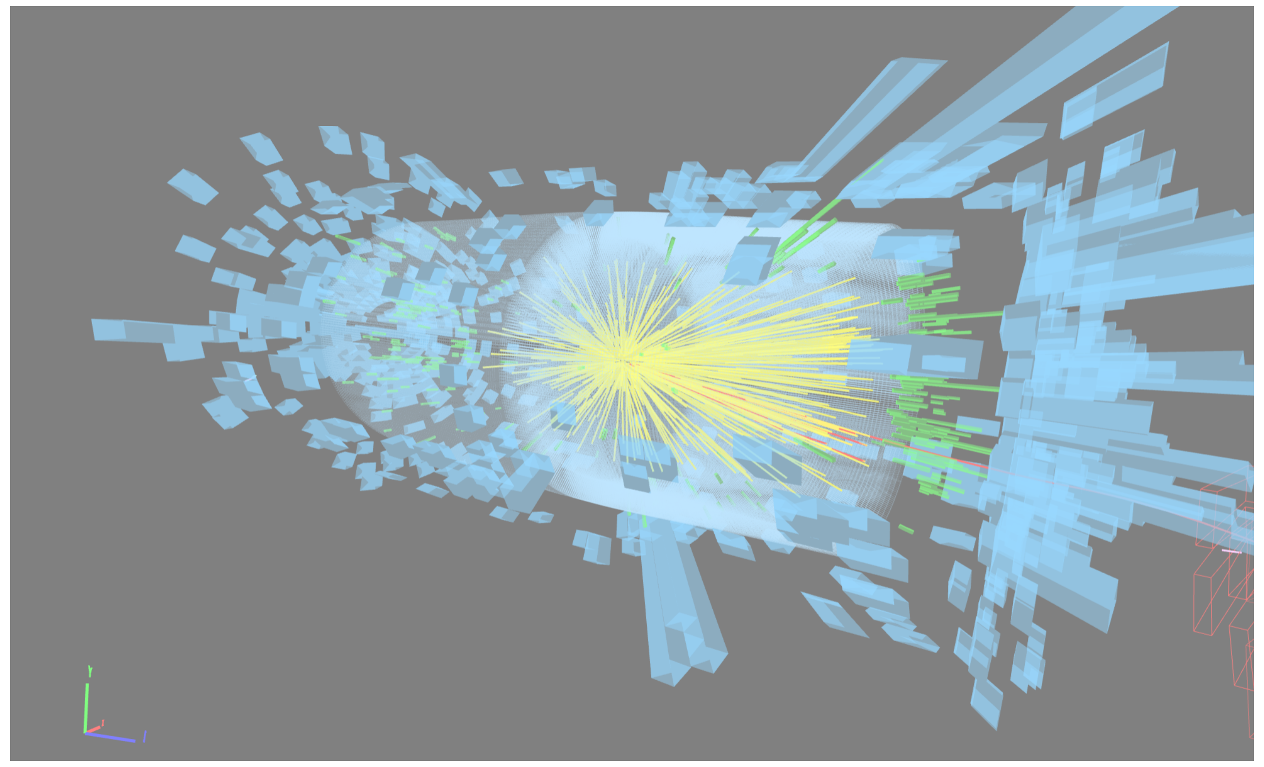
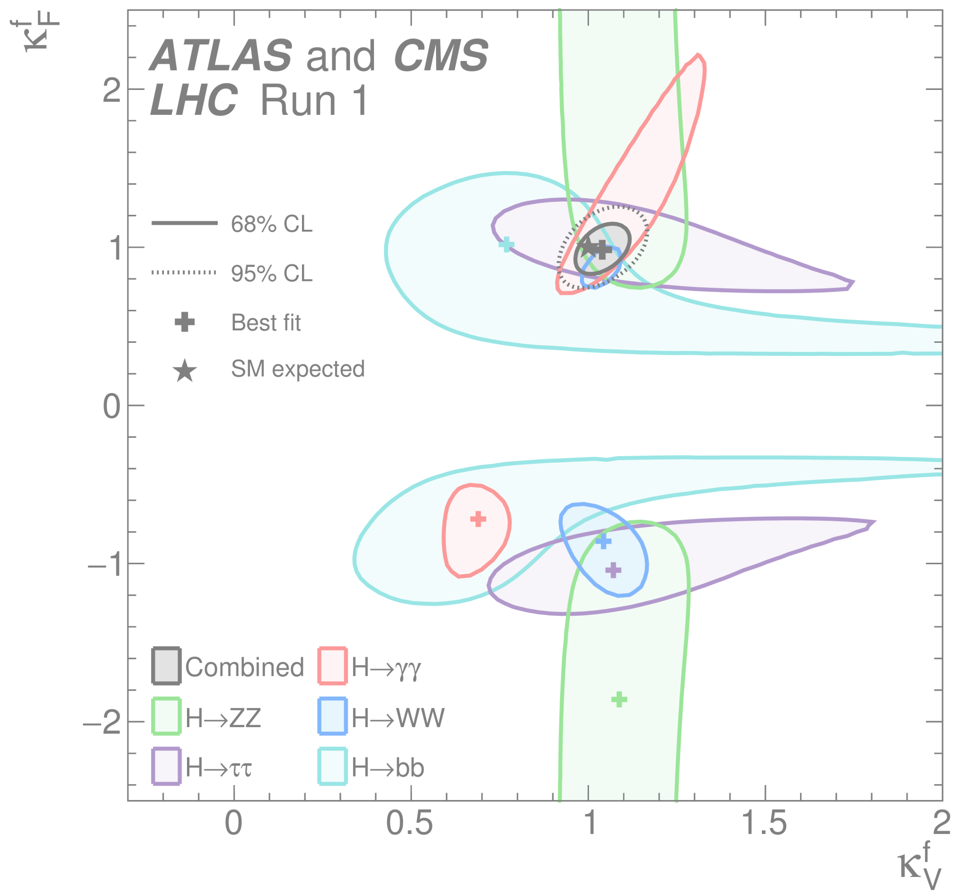


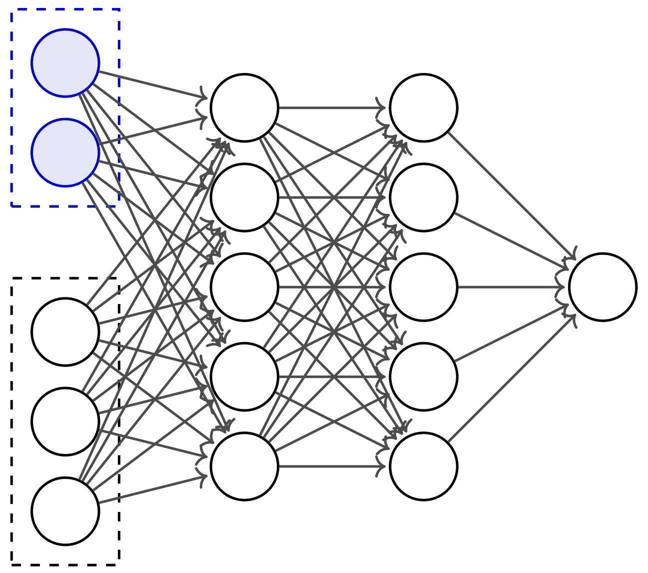
High-dimensional event data $x$

Likelihood function
$p(x|\theta)$

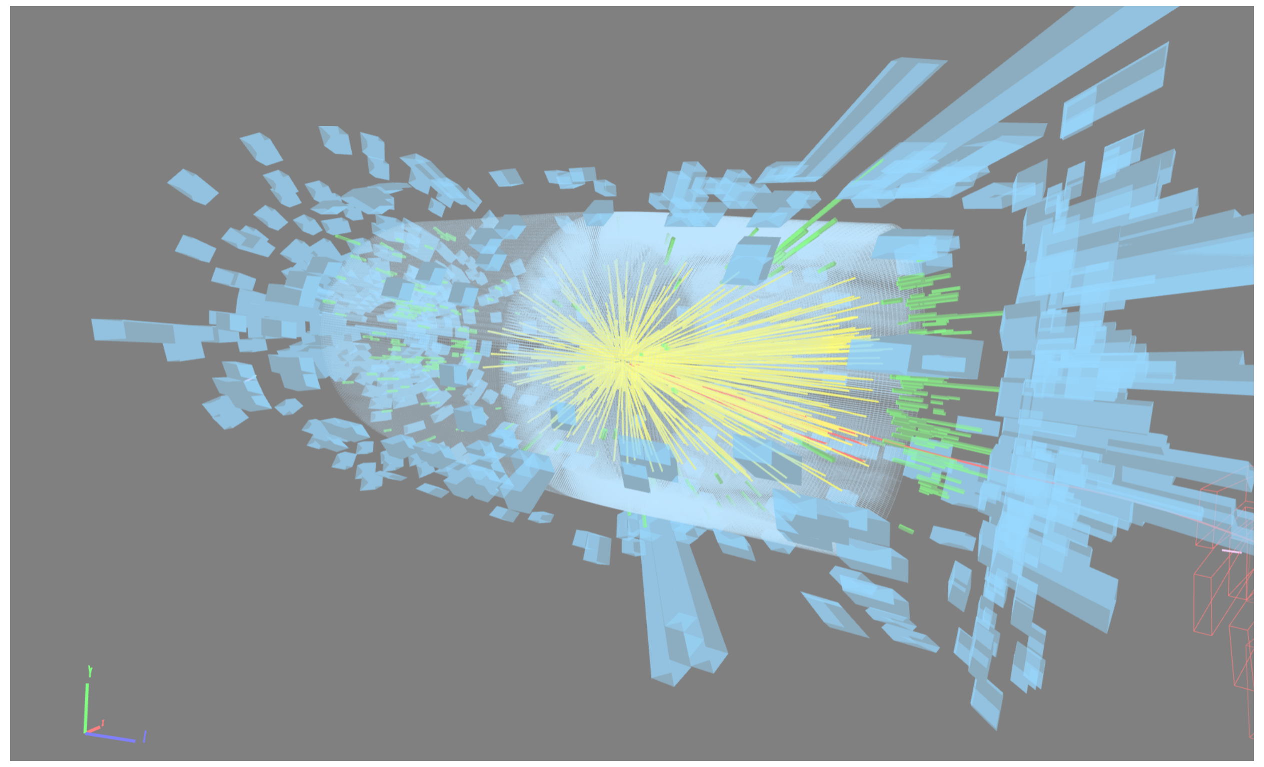



Constraints on parameters $\theta$

Surprisingly, when we want to use high-dimensional data and have to deal with the detector response, we do not have a good way to calculate the likelihood.



Machine learning



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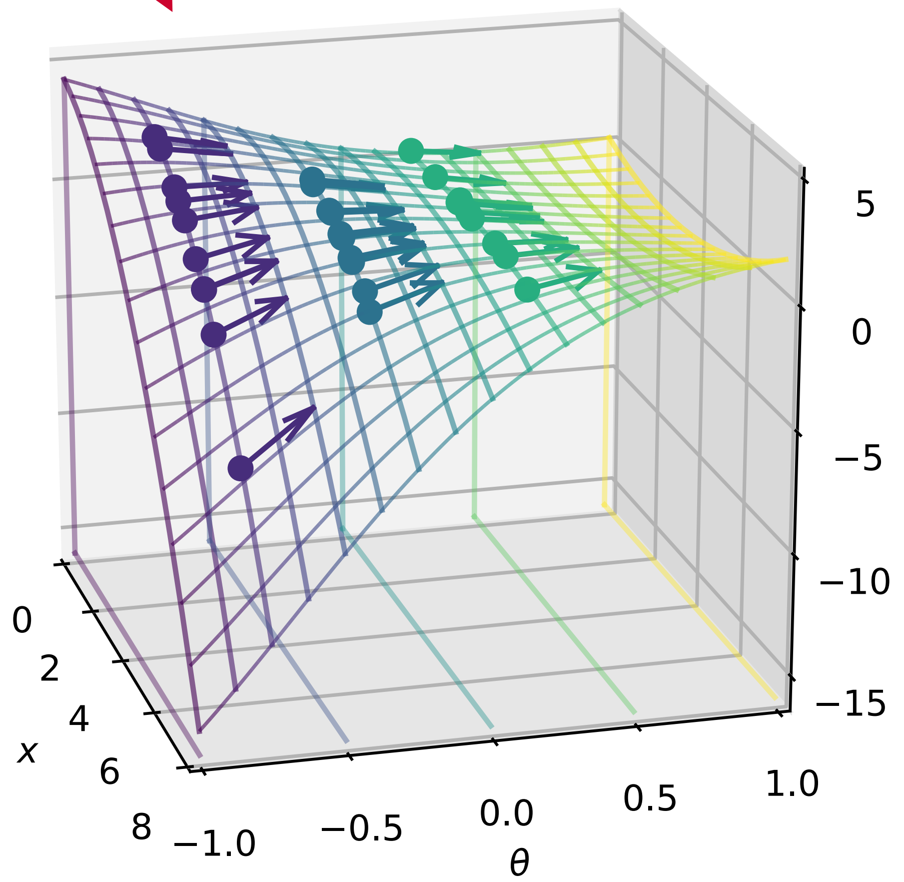
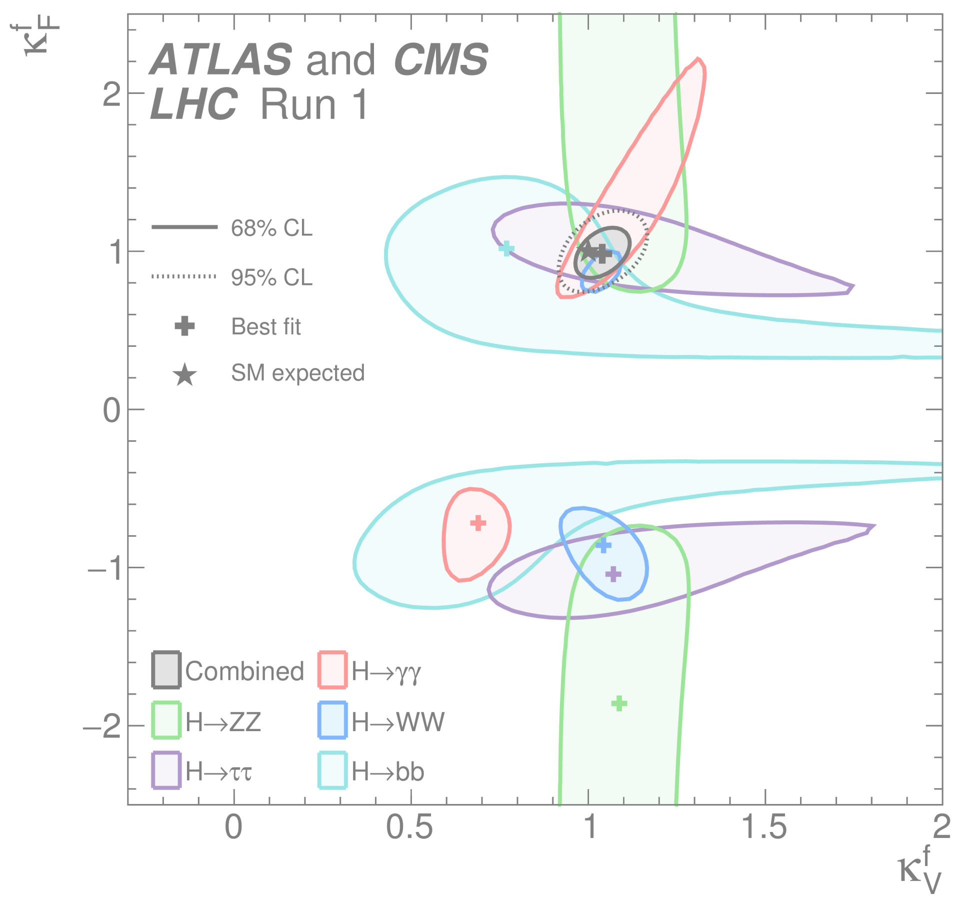



Estimator of the likelihood $p(x|\theta)$

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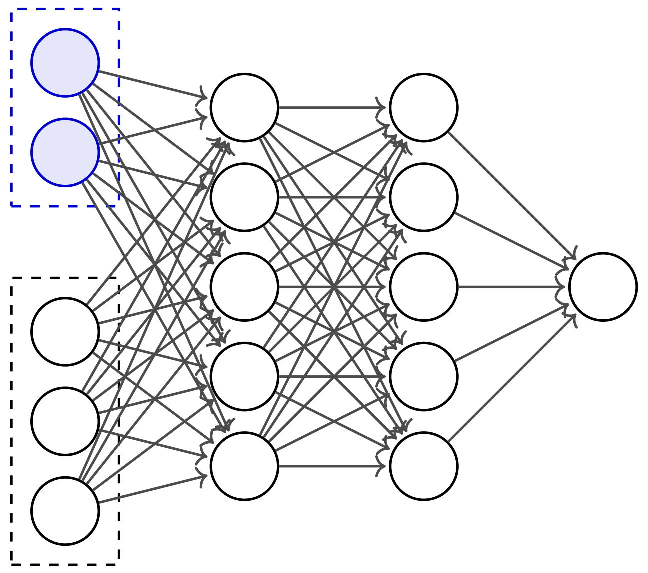

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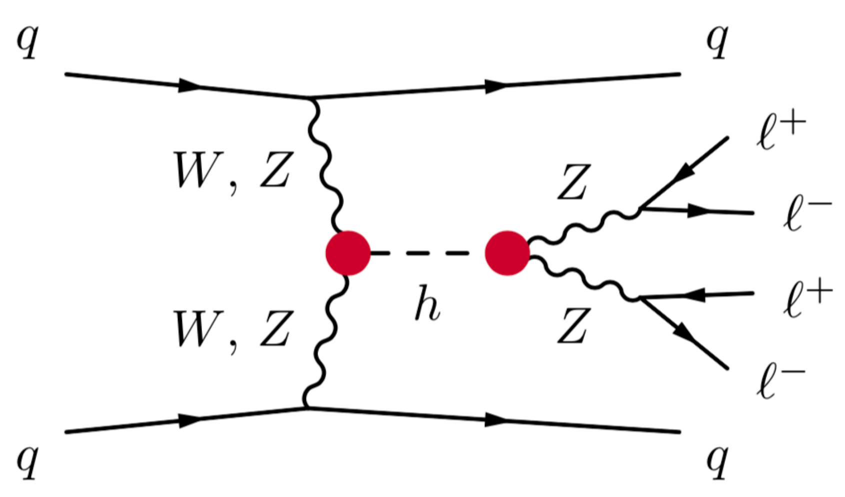
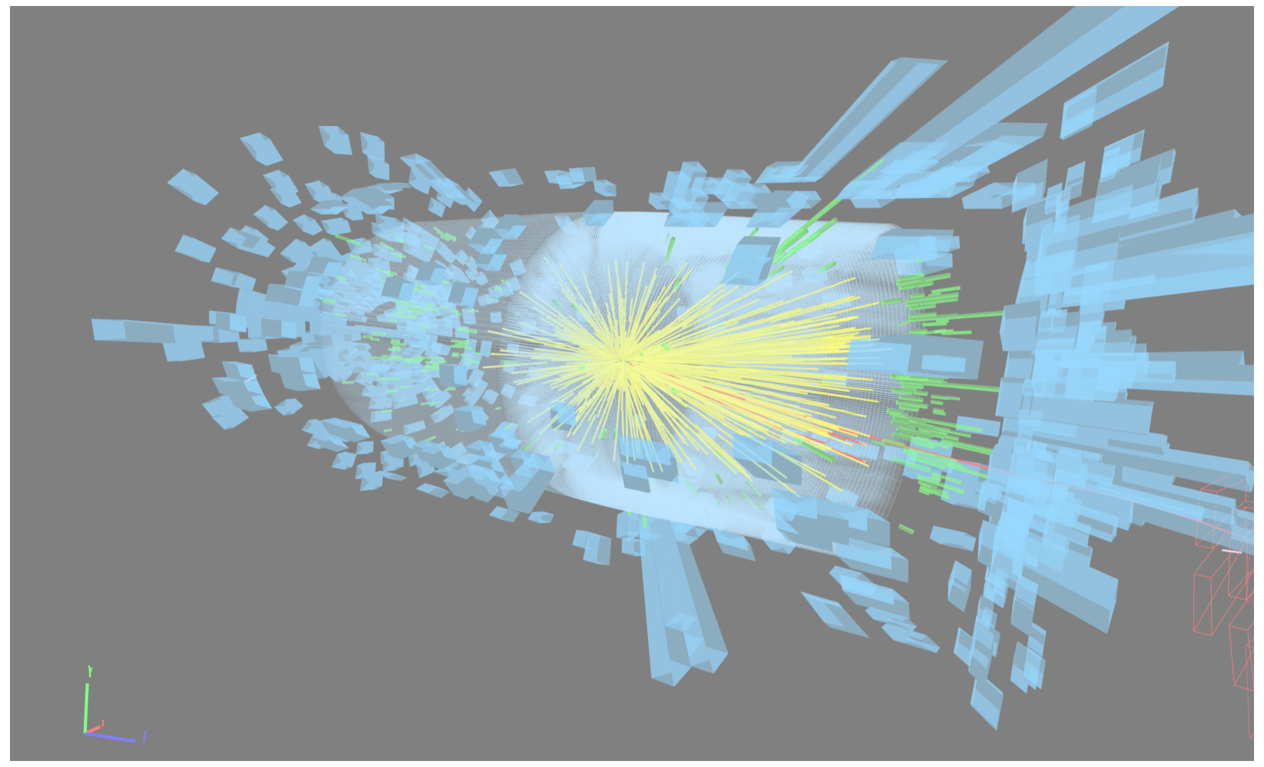



Physics insight:
matrix element information



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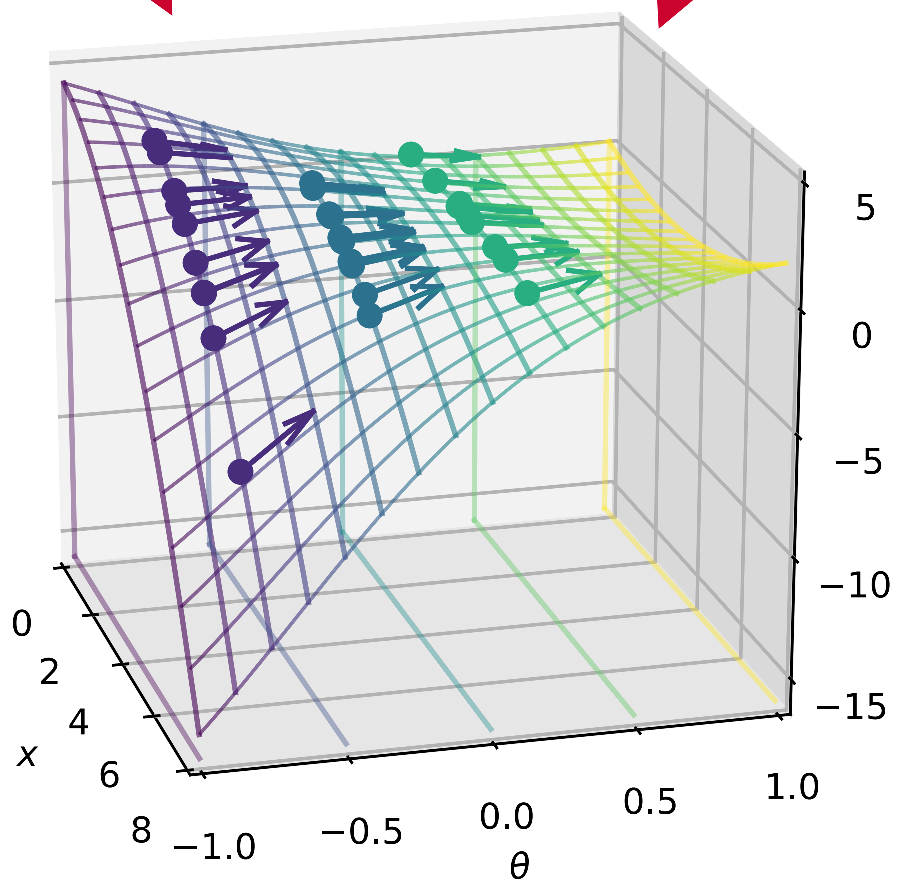


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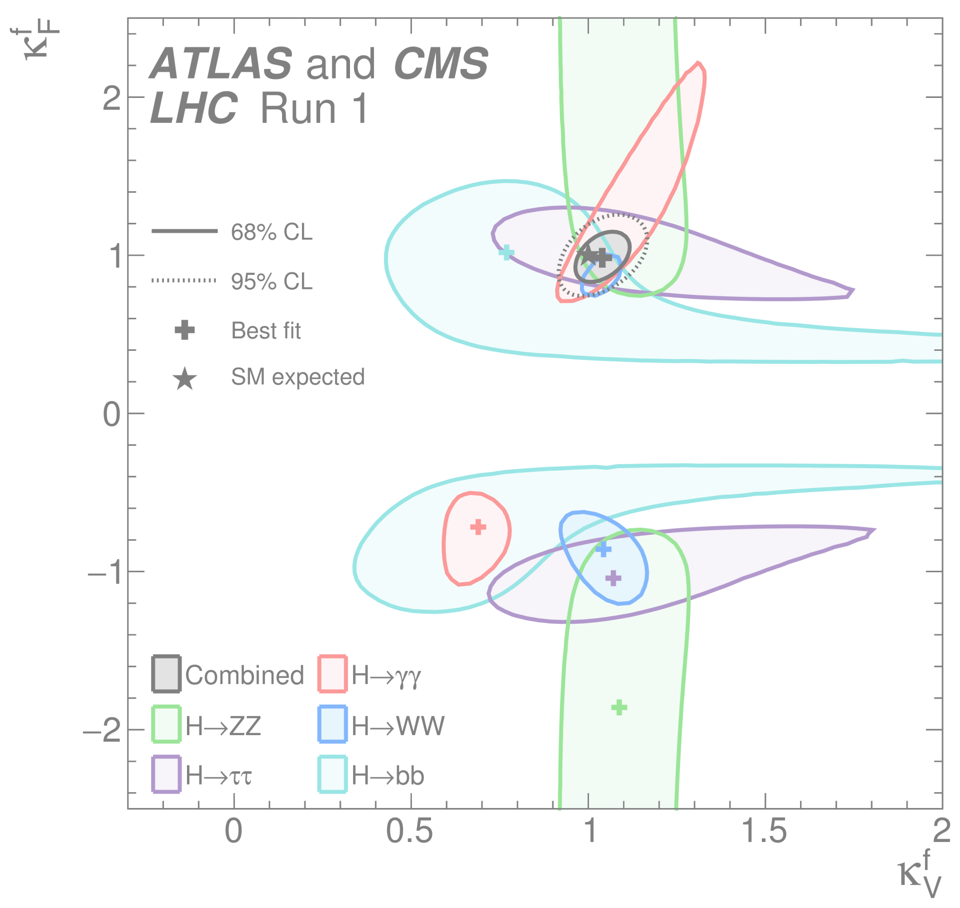


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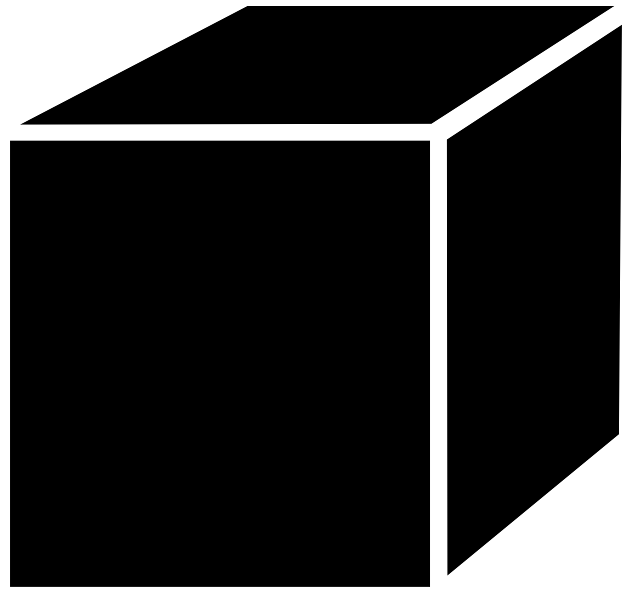
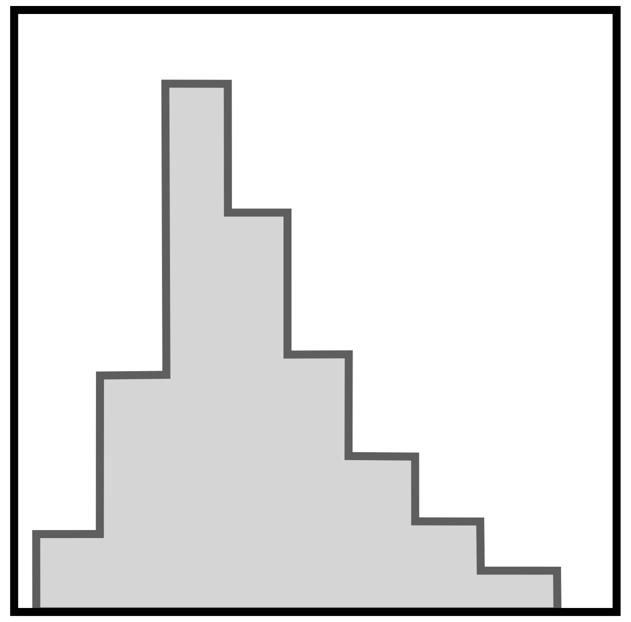
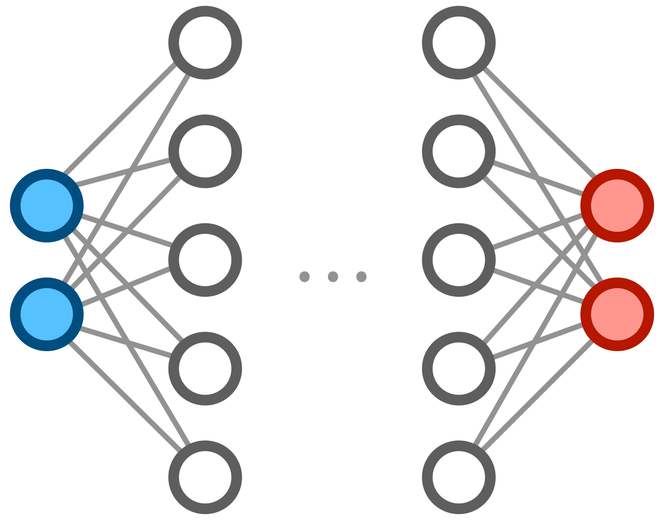


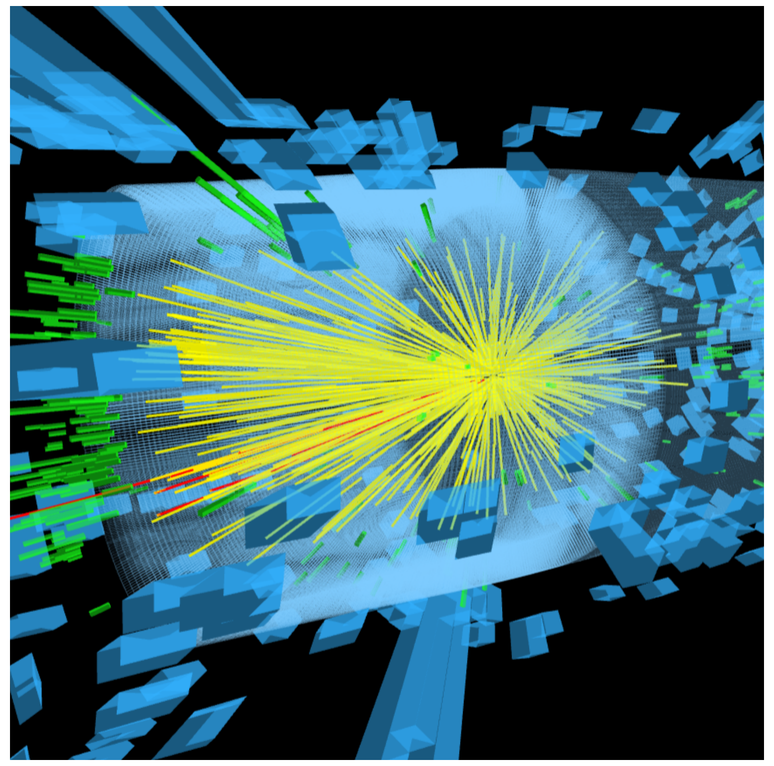
1. The simulation-based inference problem



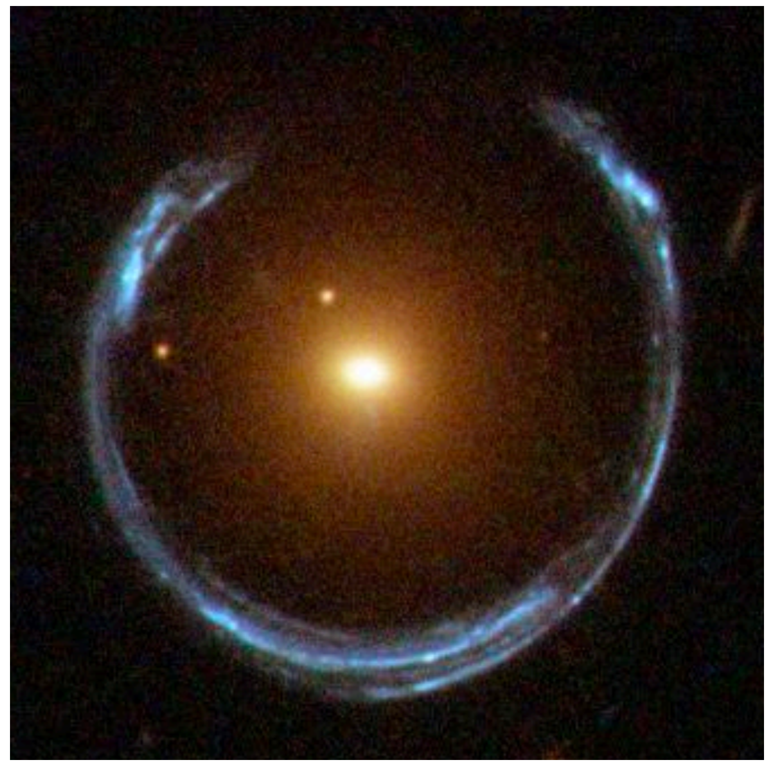
2. Why has that not stopped us before?



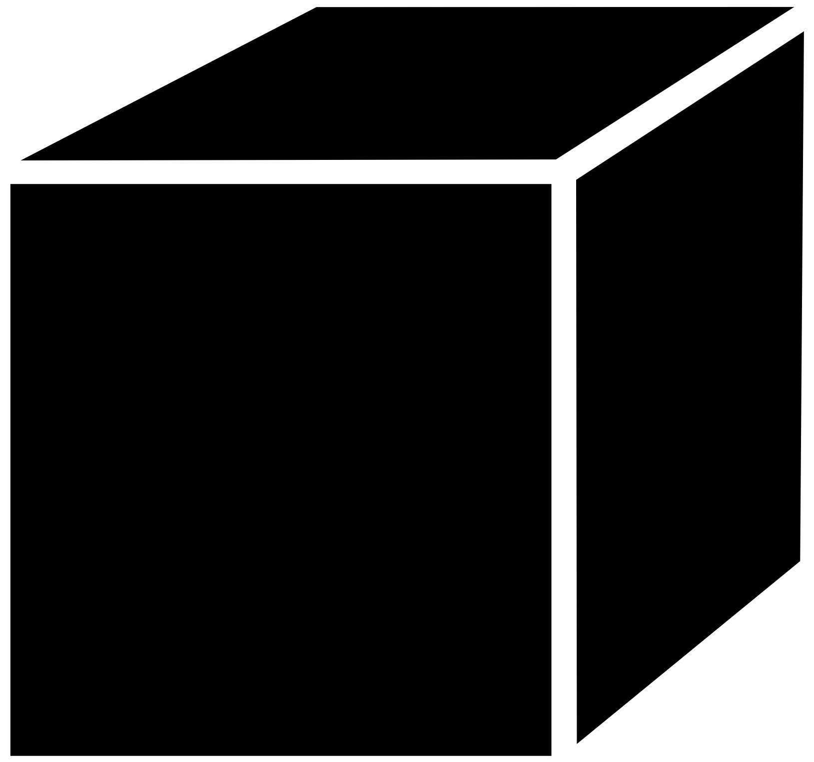
3. Machine learning methods



4. Examples



5. Beyond the LHC



1. LHC measurements as a simulation-based inference problem

# Modelling LHC processes

Theory
parameters
$\theta$

Evolution

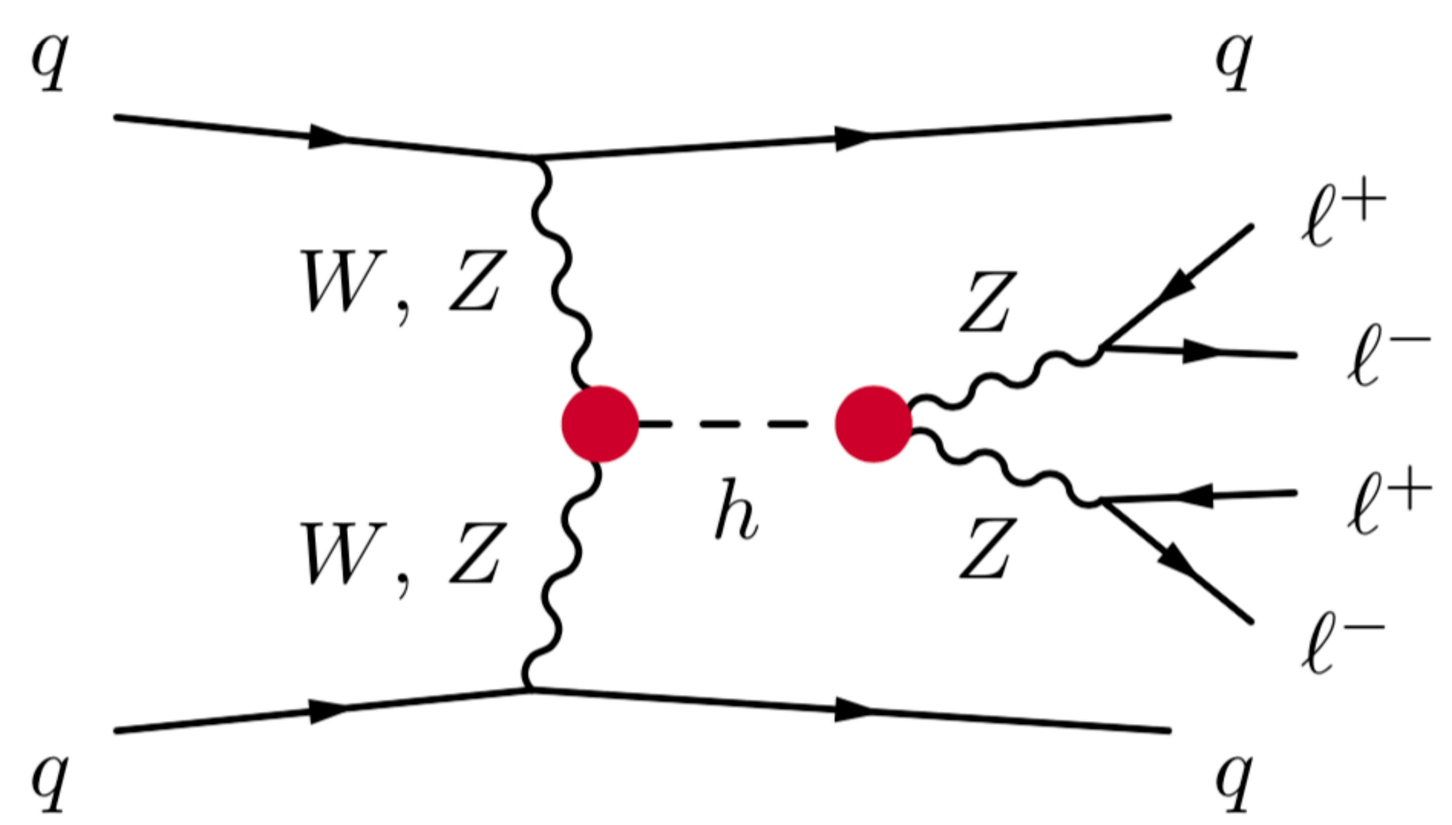
# Modelling LHC processes

Latent variables

Parton-level momenta

Theory parameters

$z_p \longleftarrow \theta$



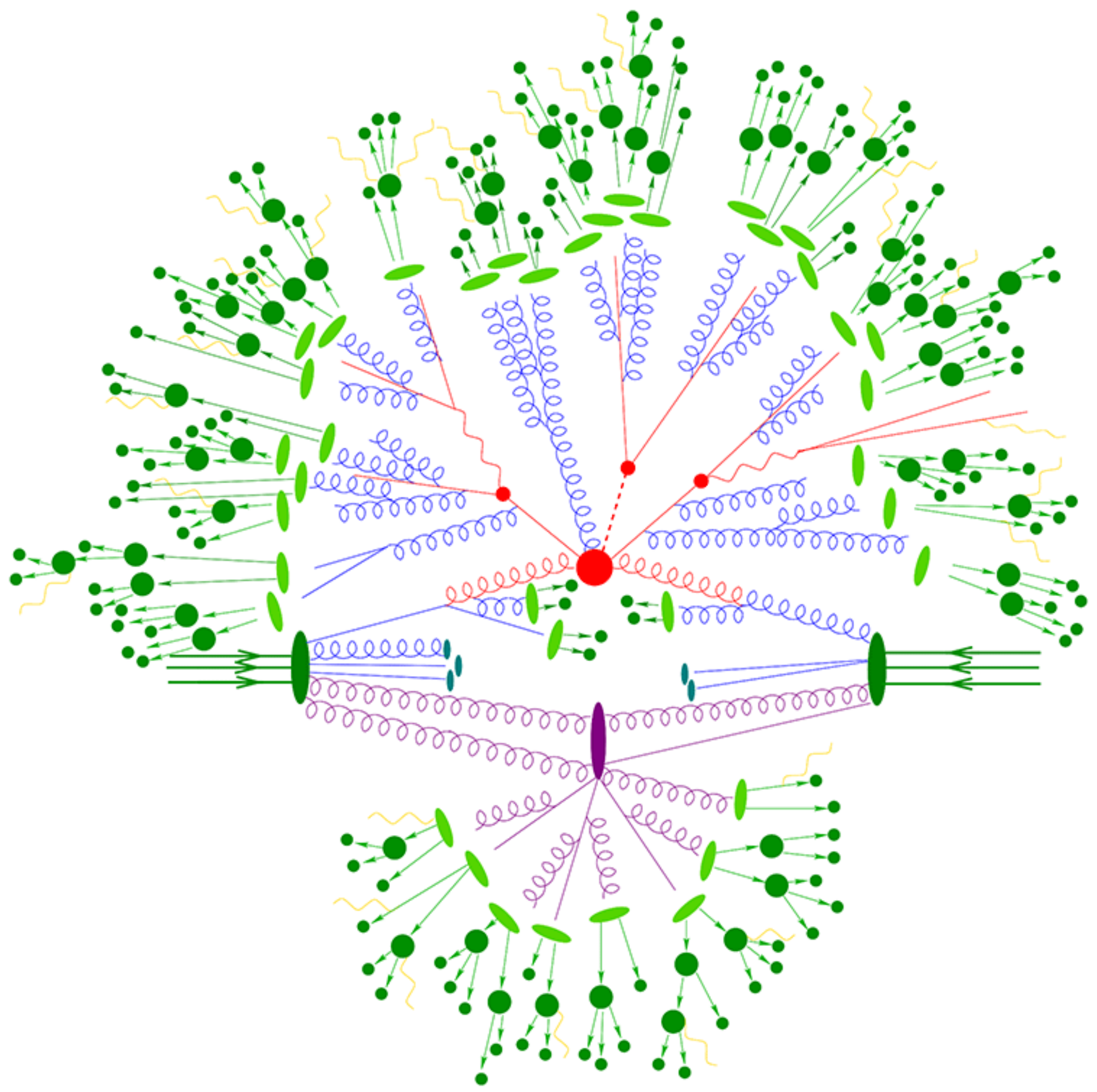

Evolution

# Modelling LHC processes

Latent variables

| Shower splittings | Parton-level momenta | Theory parameters |
| --- | --- | --- |
| $z_s$ | $z_p$ | $\theta$ |

$z_s \longleftarrow z_p \longleftarrow \theta$



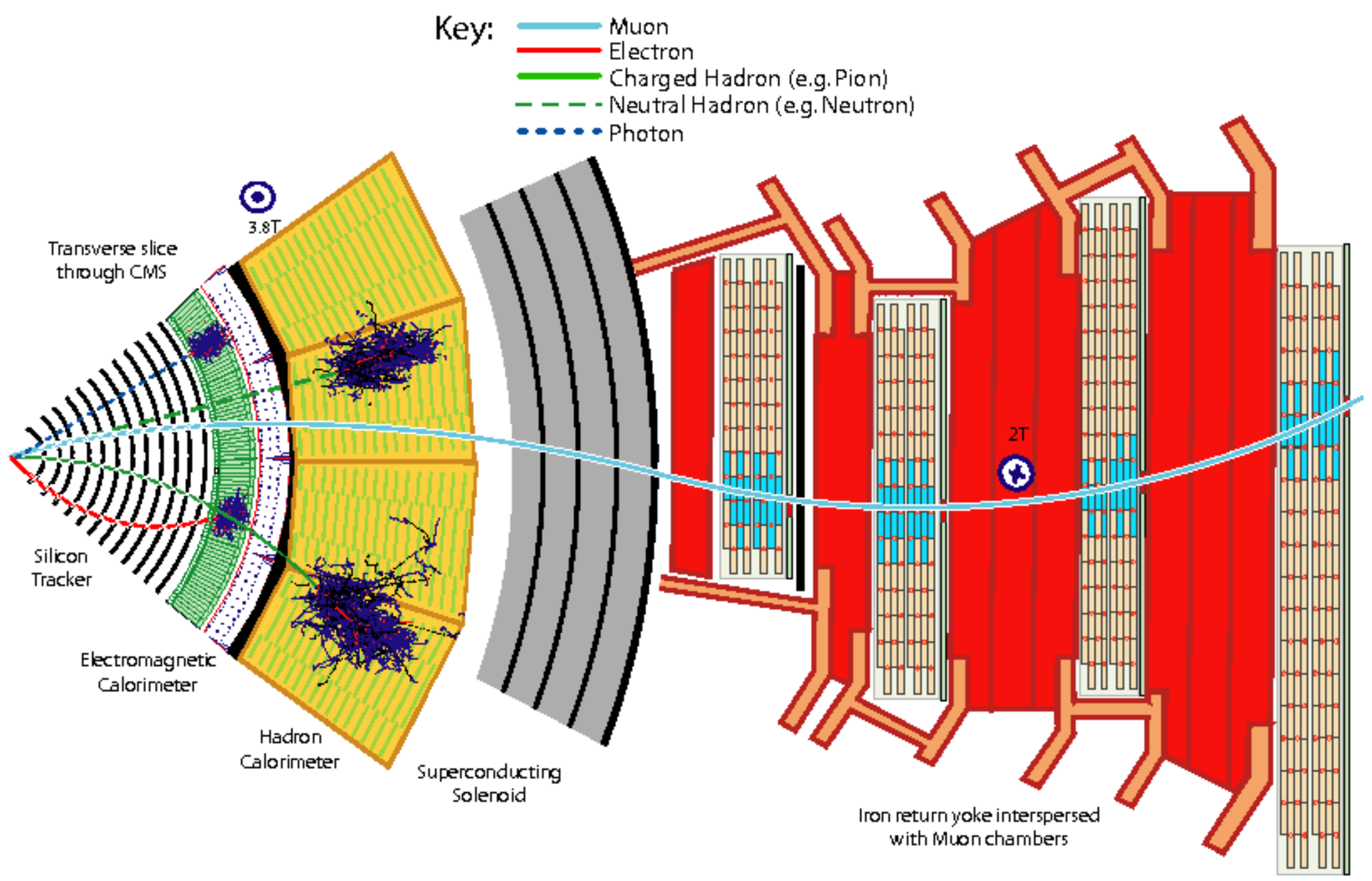
[F. Krauss]

Evolution

# Modelling LHC processes

Latent variables

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




[CMS]

$\longleftarrow$

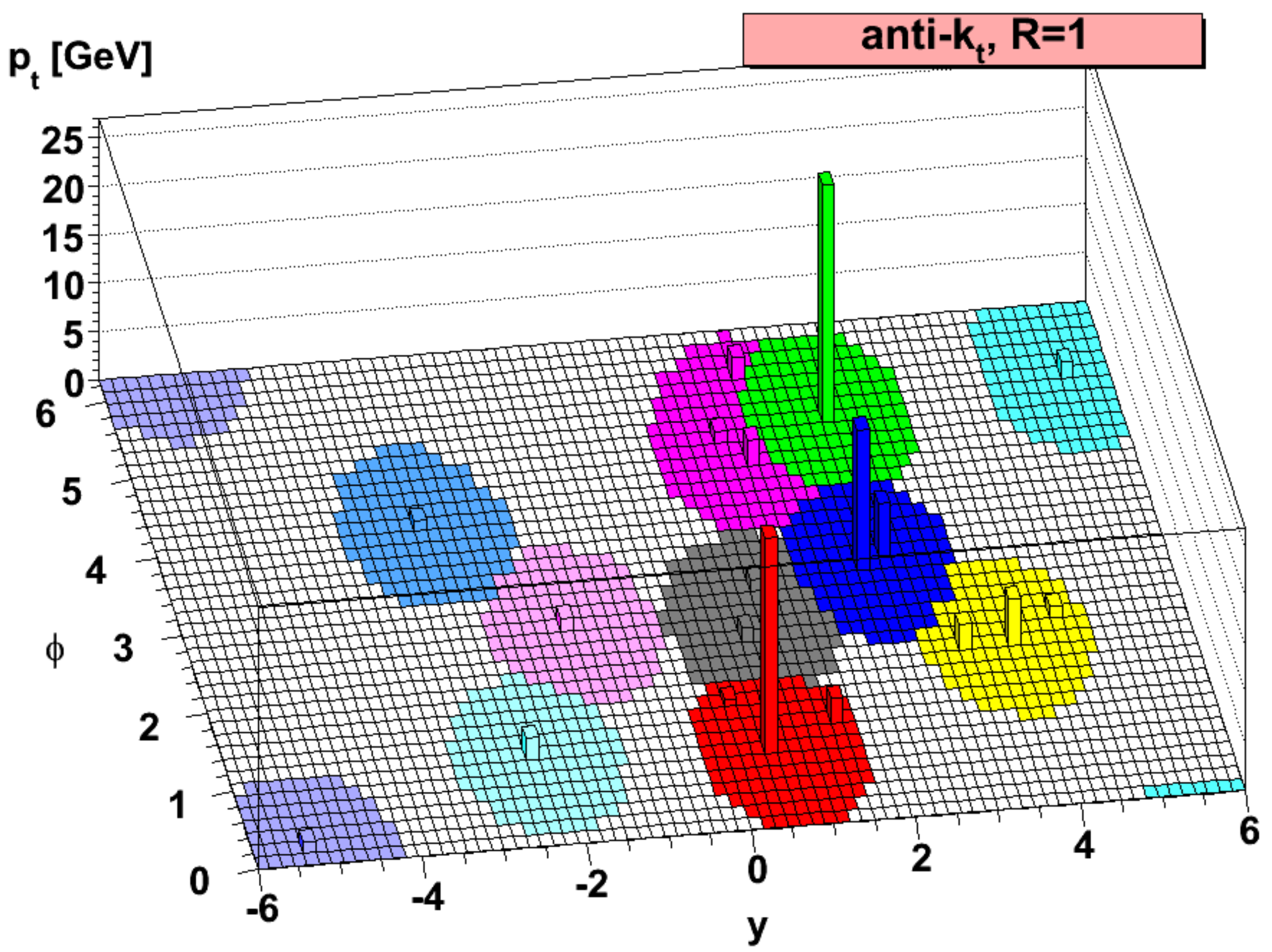
Evolution

# Modelling LHC processes

Latent variables

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

$$x \longleftarrow z_d \longleftarrow z_s \longleftarrow z_p \longleftarrow \theta$$




[M. Cacciari, G. Salam, G. Soyez 0802.1189]

$\longleftarrow$

Evolution

# Modelling LHC processes

Latent variables

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

$$x \longleftarrow z_d \longleftarrow z_s \longleftarrow z_p \longleftarrow \theta$$

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

Prediction (simulation)

# Modelling LHC processes

Latent variables

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

$$x \longleftarrow z_d \longleftarrow z_s \longleftarrow z_p \longleftarrow \theta$$

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

Inference

# Modelling LHC processes

Latent variables

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

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

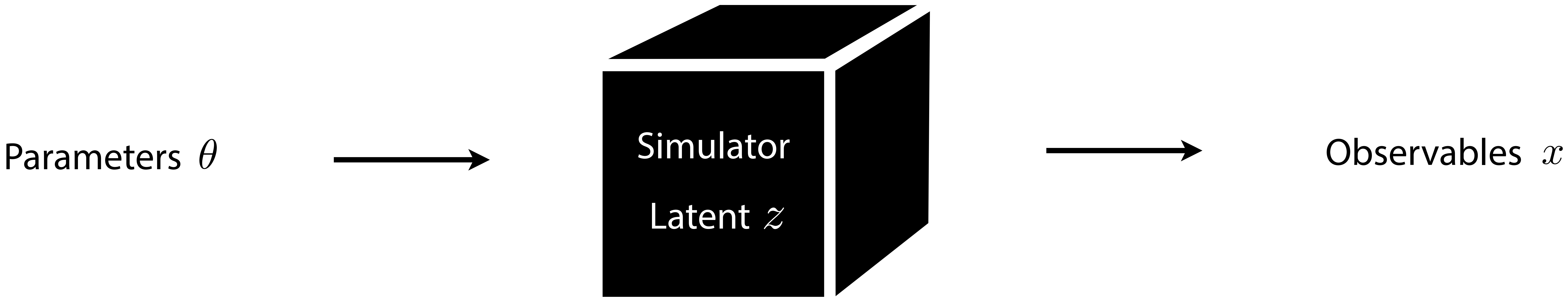
It's infeasible to calculate the integral over this enormous space!

(More subtle: We cannot sample from $p(z|x,\theta)$ efficiently.)

$\longrightarrow$

Inference

# The problem of simulation-based ("likelihood-free") inference



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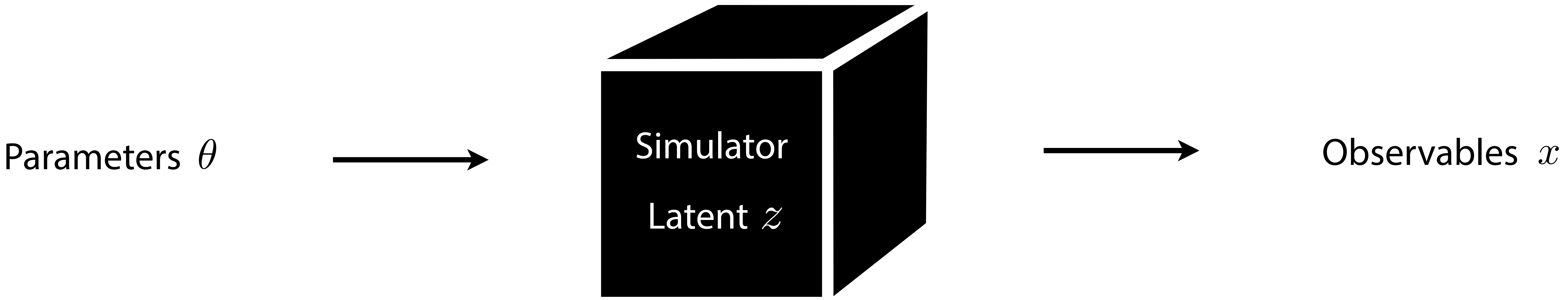
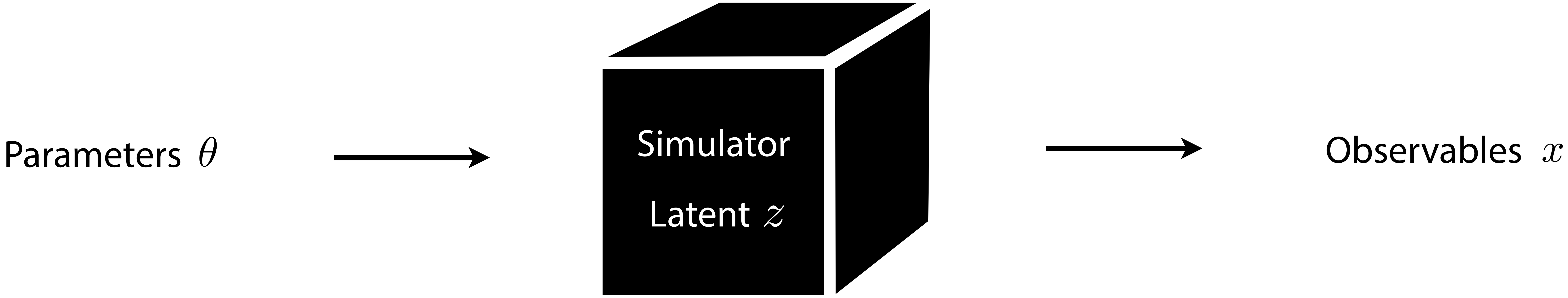



Prediction:
- Well-motivated mechanistic, causal model
- Simulator can generate samples $x \sim p(x|\theta)$

# The problem of simulation-based ("likelihood-free") inference




Prediction:
- Well-motivated mechanistic, causal model
- Simulator can generate samples $x \sim p(x|\theta)$

Inference:
- Interactions between low-level components lead to challenging inverse problems
- Likelihood $p(x|\theta) = \int \mathrm{d}z \; p(x, z|\theta)$ is intractable

# Three problem statements

Given

- a simulator that lets you generate $N$ samples $x_i \sim p(x_i|\theta_i)$ (for parameters $\theta_i$ of our choice),
- observed data $x_{\mathrm{obs}} \sim p(x_{\mathrm{obs}}|\theta_{\mathrm{true}})$, and
- a prior $p(\theta)$,

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Given

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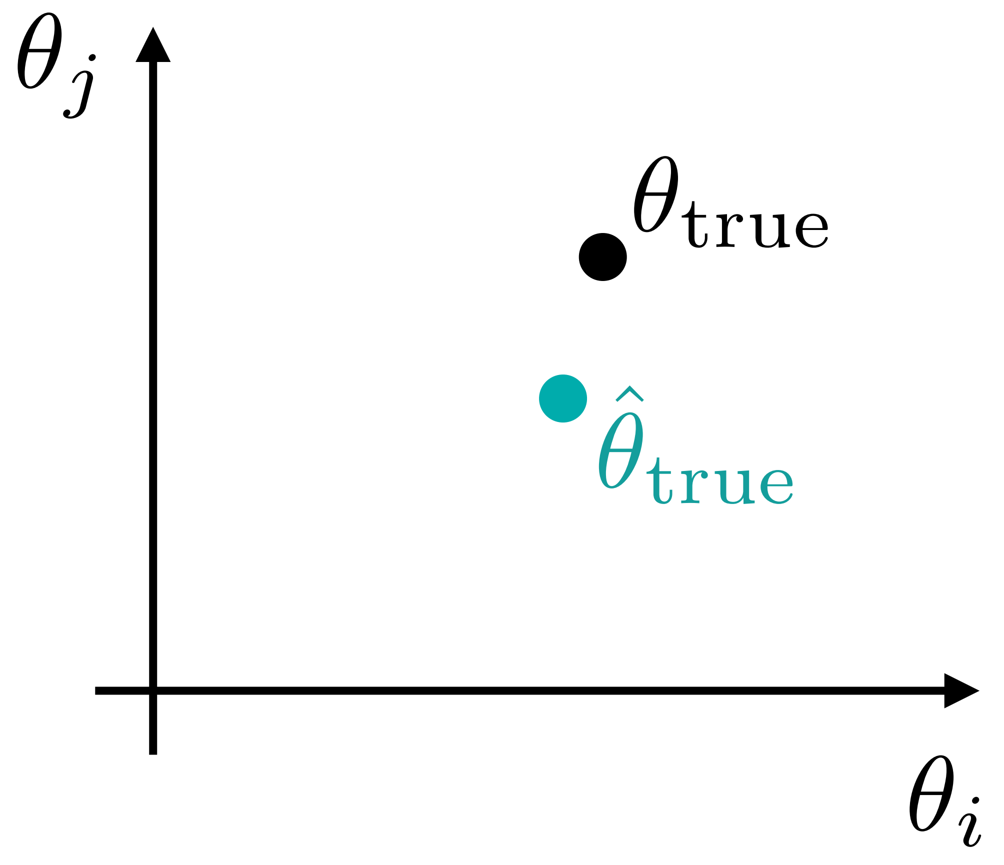
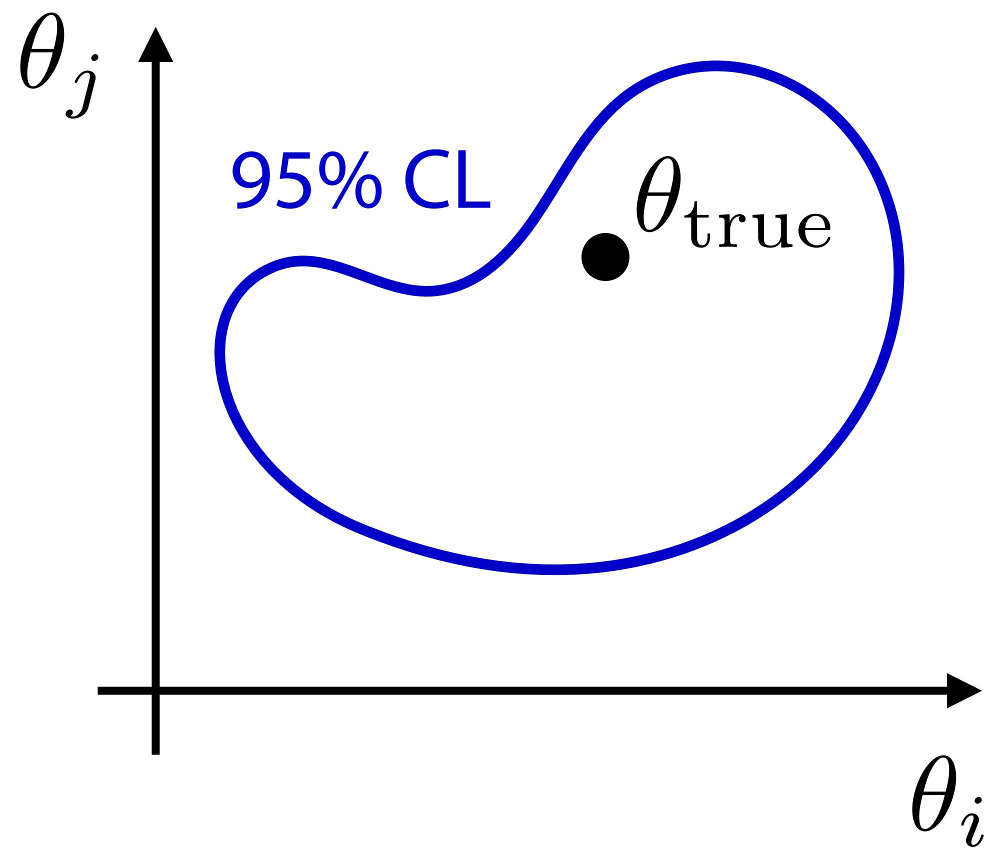
- observed data $x_{\text{obs}} \sim p(x_{\text{obs}}|\theta_{\text{true}})$, and
- a prior $p(\theta)$,

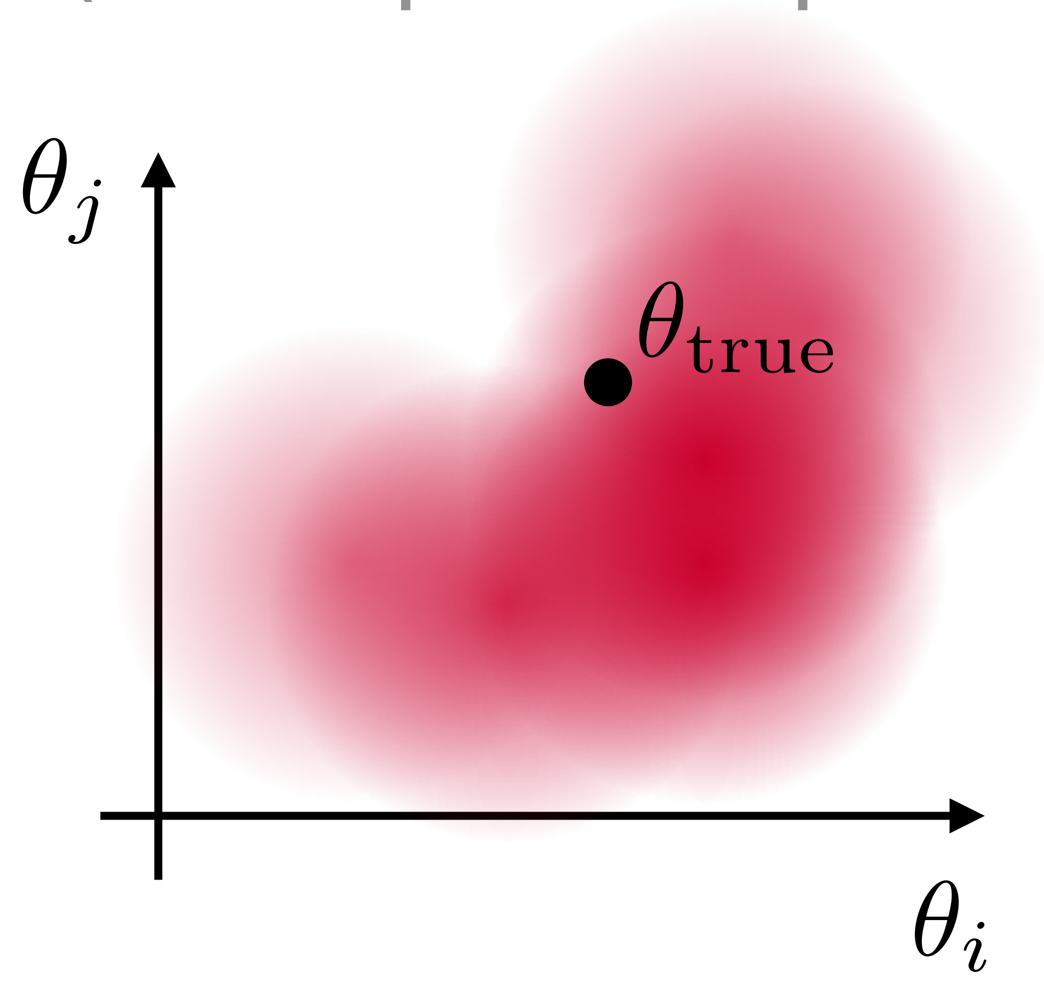
a) estimate $\hat{\theta}_{\text{true}}$
(e.g. MLE)

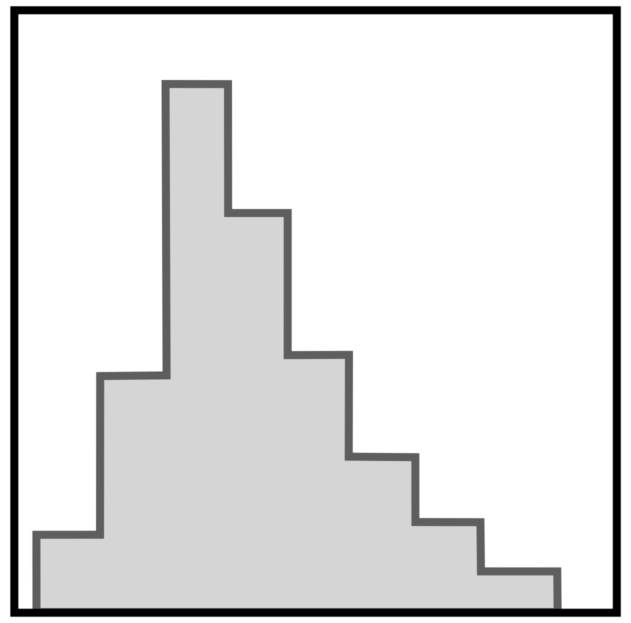



b) construct confidence sets
(e.g. likelihood ratio tests)



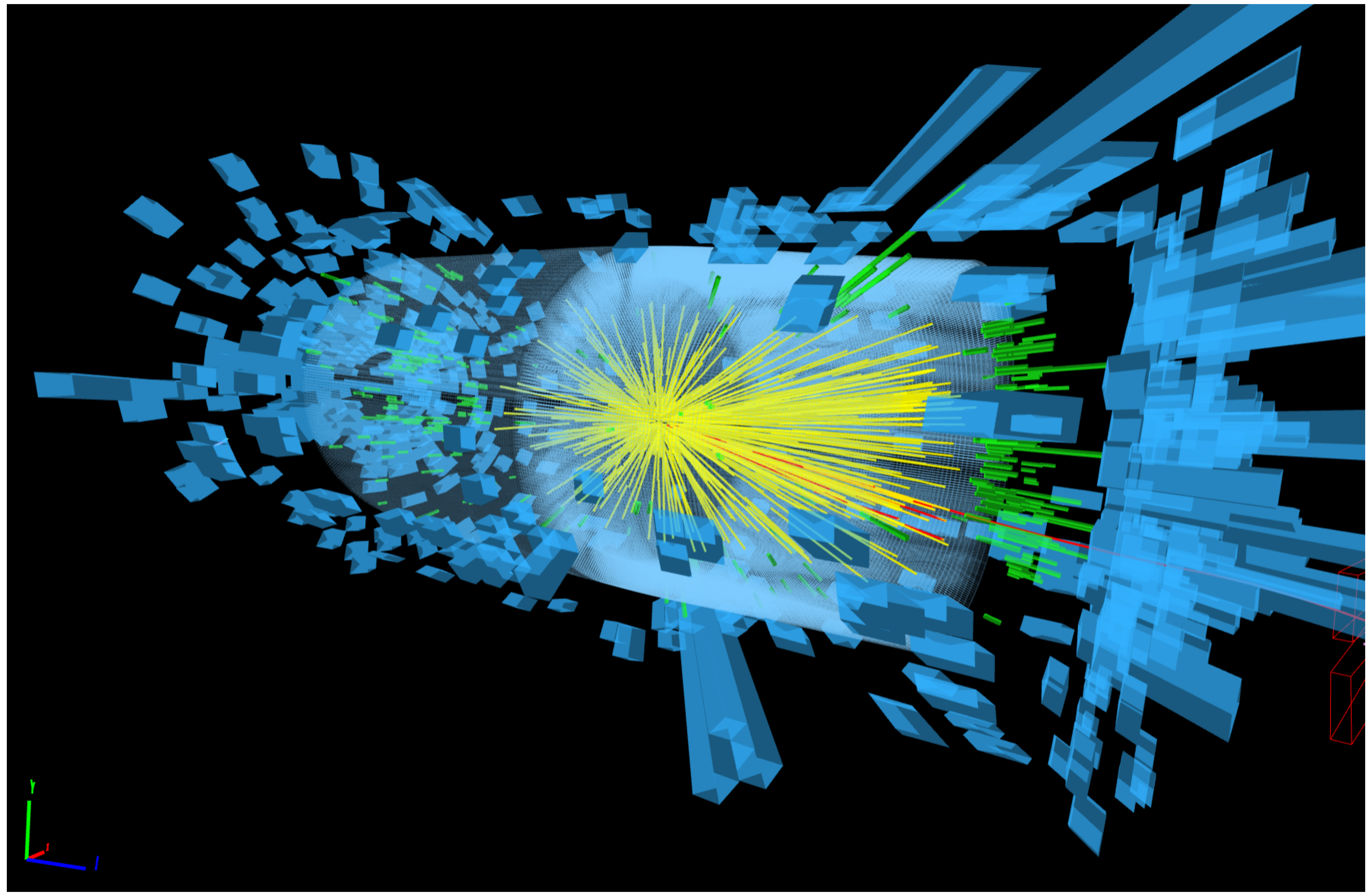

c) estimate the posterior
(or sample from posterior)





## 2. Why has that not stopped us before?

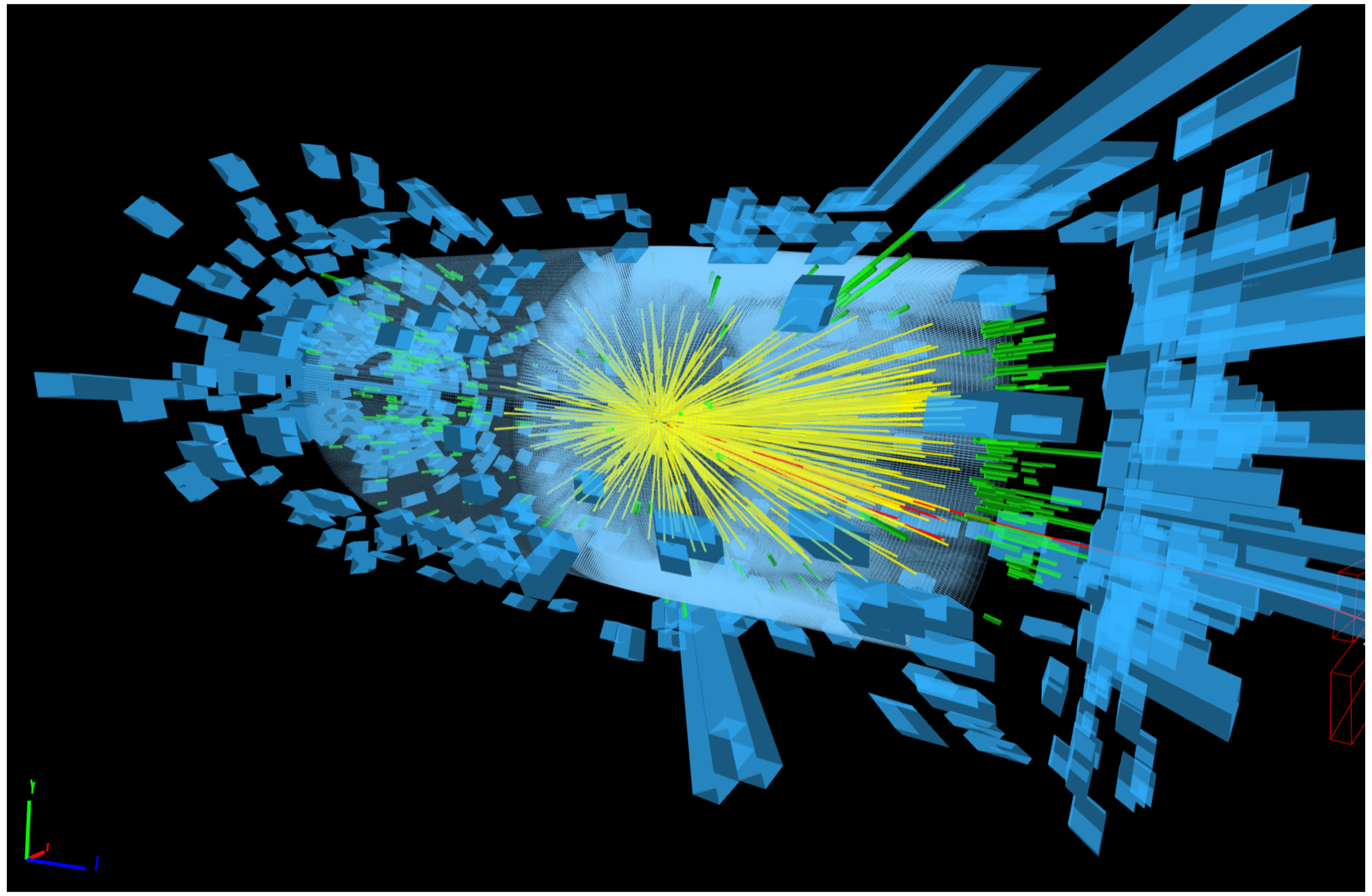
# Solve it with summary statistics

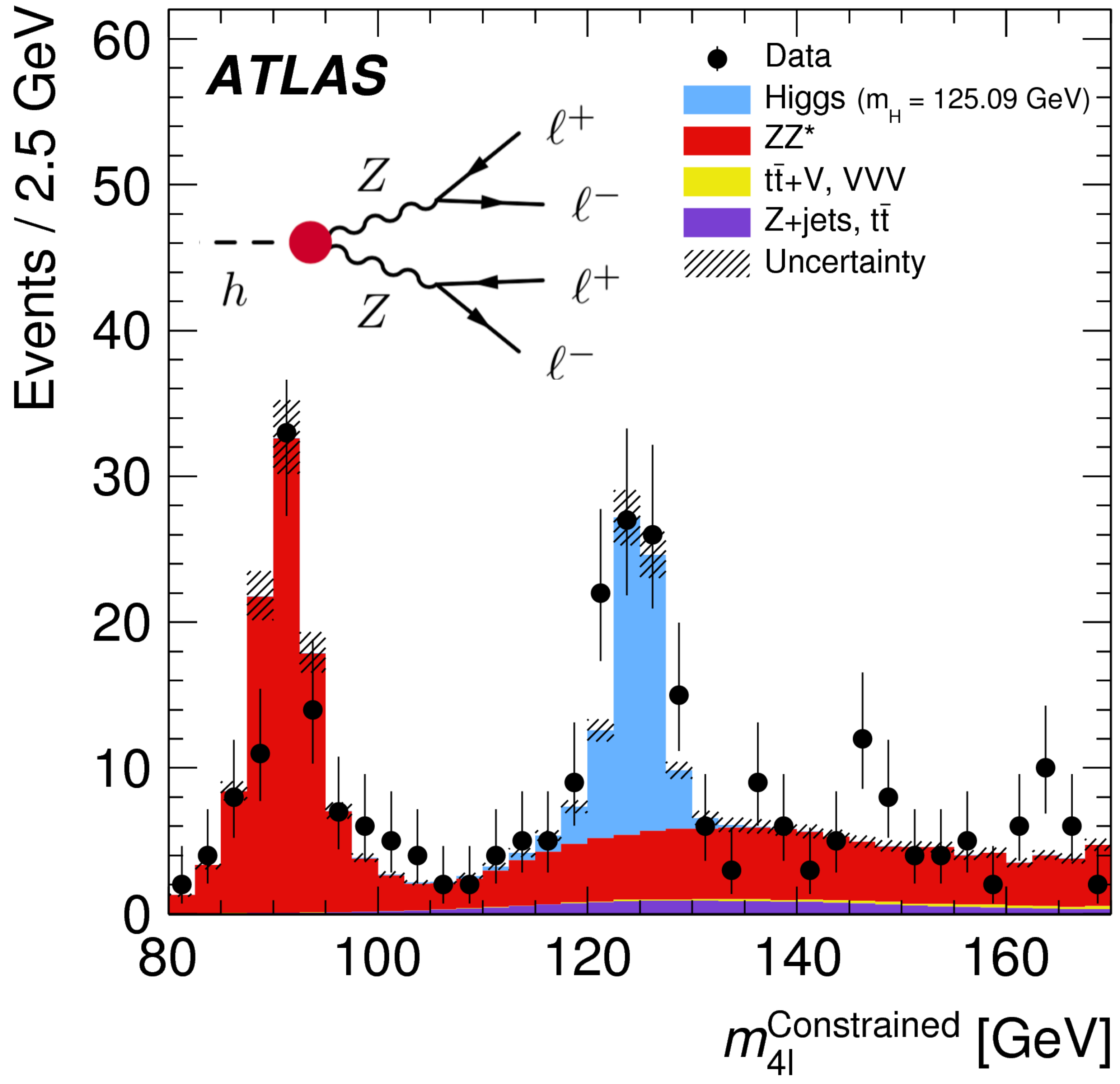


High-dimensional event data $x$

$p(x|\theta)$ cannot be calculated

# Solve it with summary statistics






[ATLAS 1712.02304]

High-dimensional event data $x$

$p(x|\theta)$ cannot be calculated

One or two summary statistics $x'$

$p(x'|\theta)$ can be estimated with histograms, KDE, …

# Summary statistics for LHC measurements?

- In many LHC problems there is no single good summary statistics: compressing to any $x'$ loses information!
  [JB, K. Cranmer, F. Kling, T. Plehn 1612.05261; JB, F. Kling, T. Plehn, T. Tait 1712.02350]

- Ideally: analyze all trustworthy high-level features (reconstructed four-momenta…), or some form of low-level features, including correlations
  (“fully differential cross section”)

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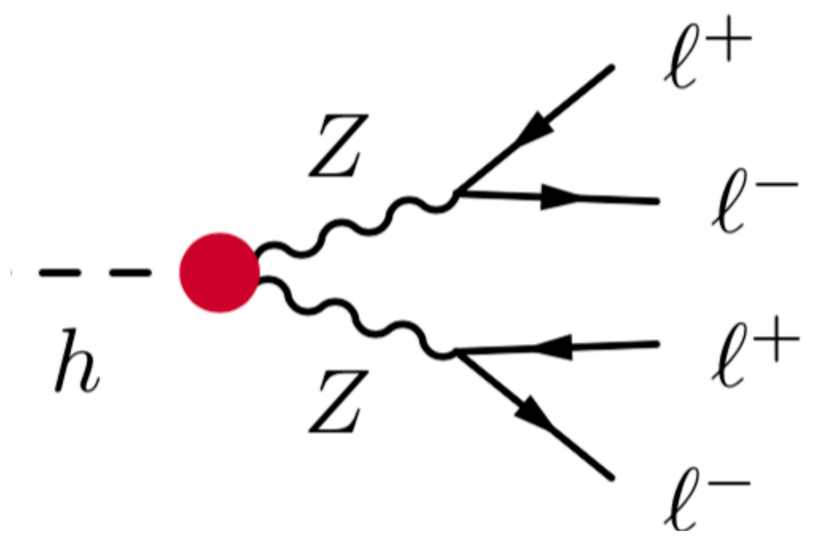
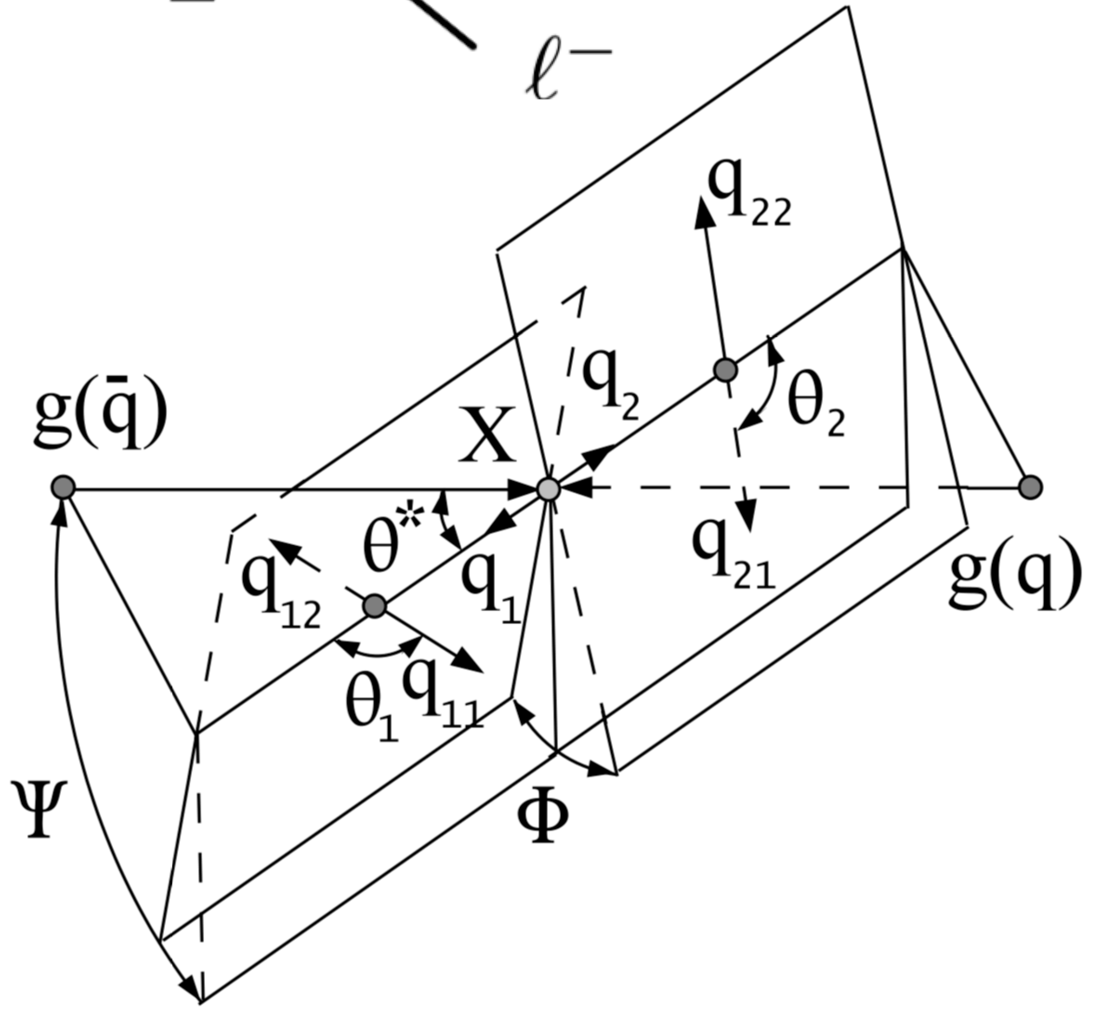
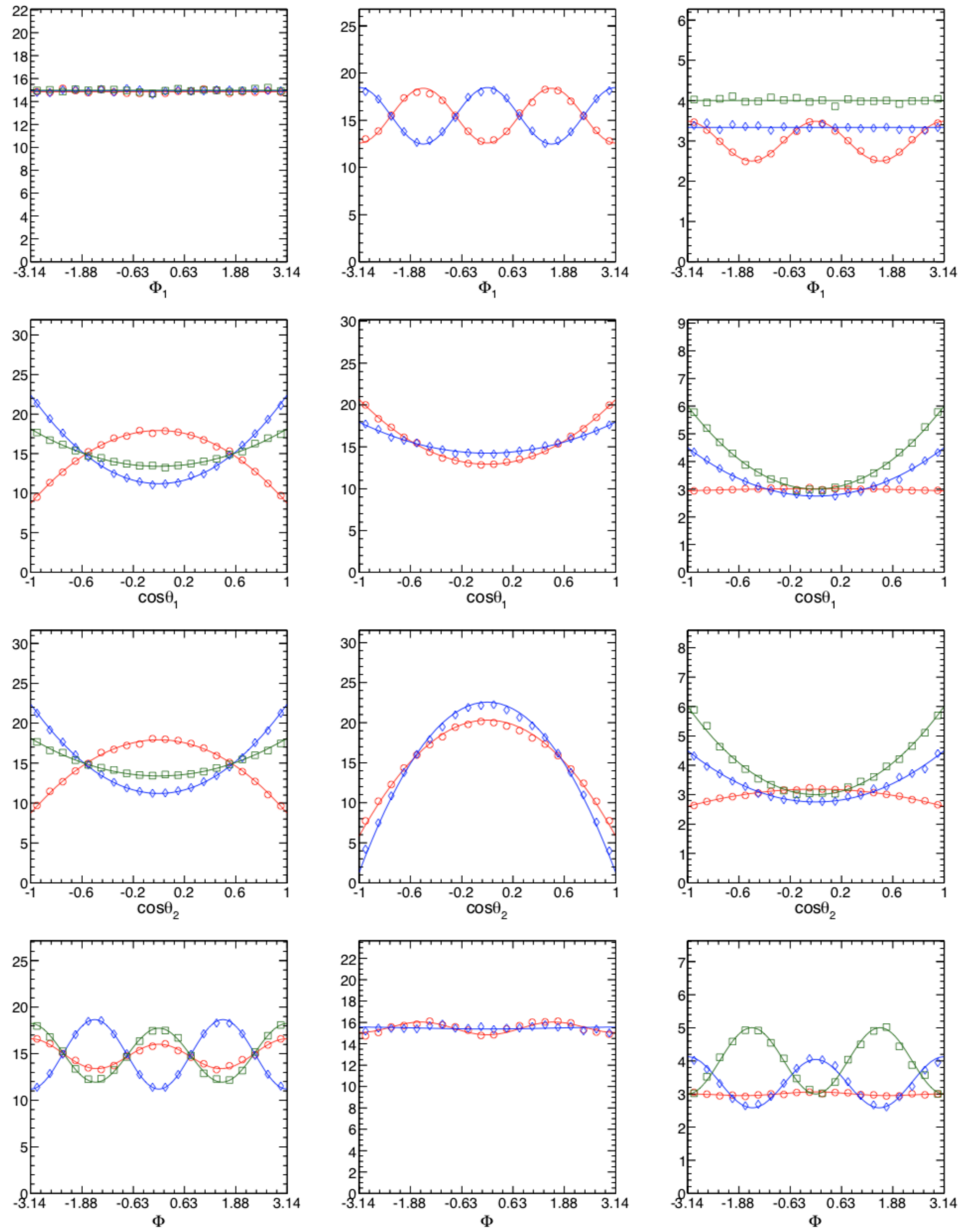


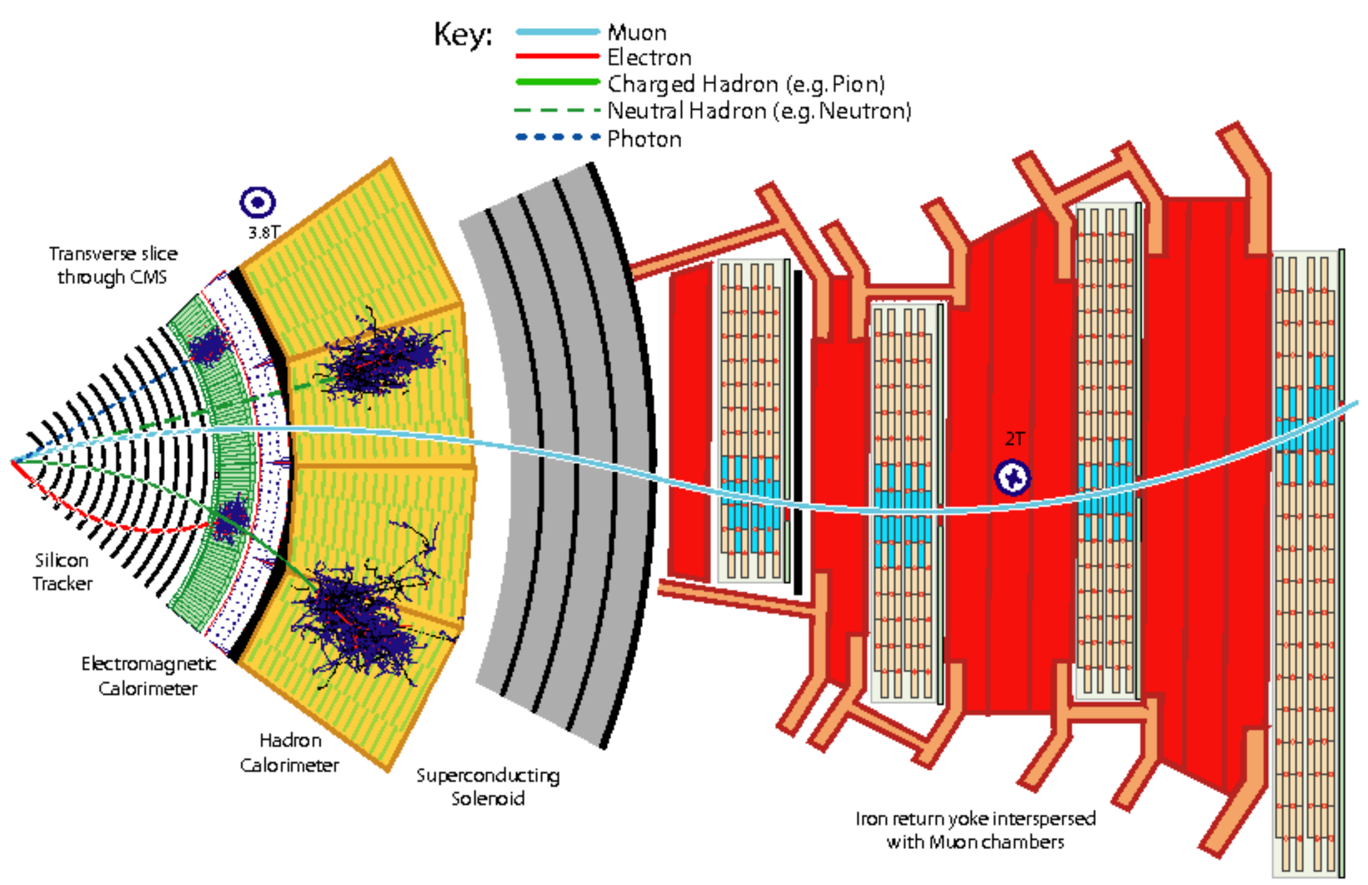

[Bolognesi et al. 1208.4018]

- Ideally: analyze all trustworthy high-level features (reconstructed four-momenta…), or some form of low-level features, including correlations
  ("fully differential cross section")

# Solve it by approximating the integral

- Problem: high-dim. integral over shower / detector trajectories

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




[CMS]

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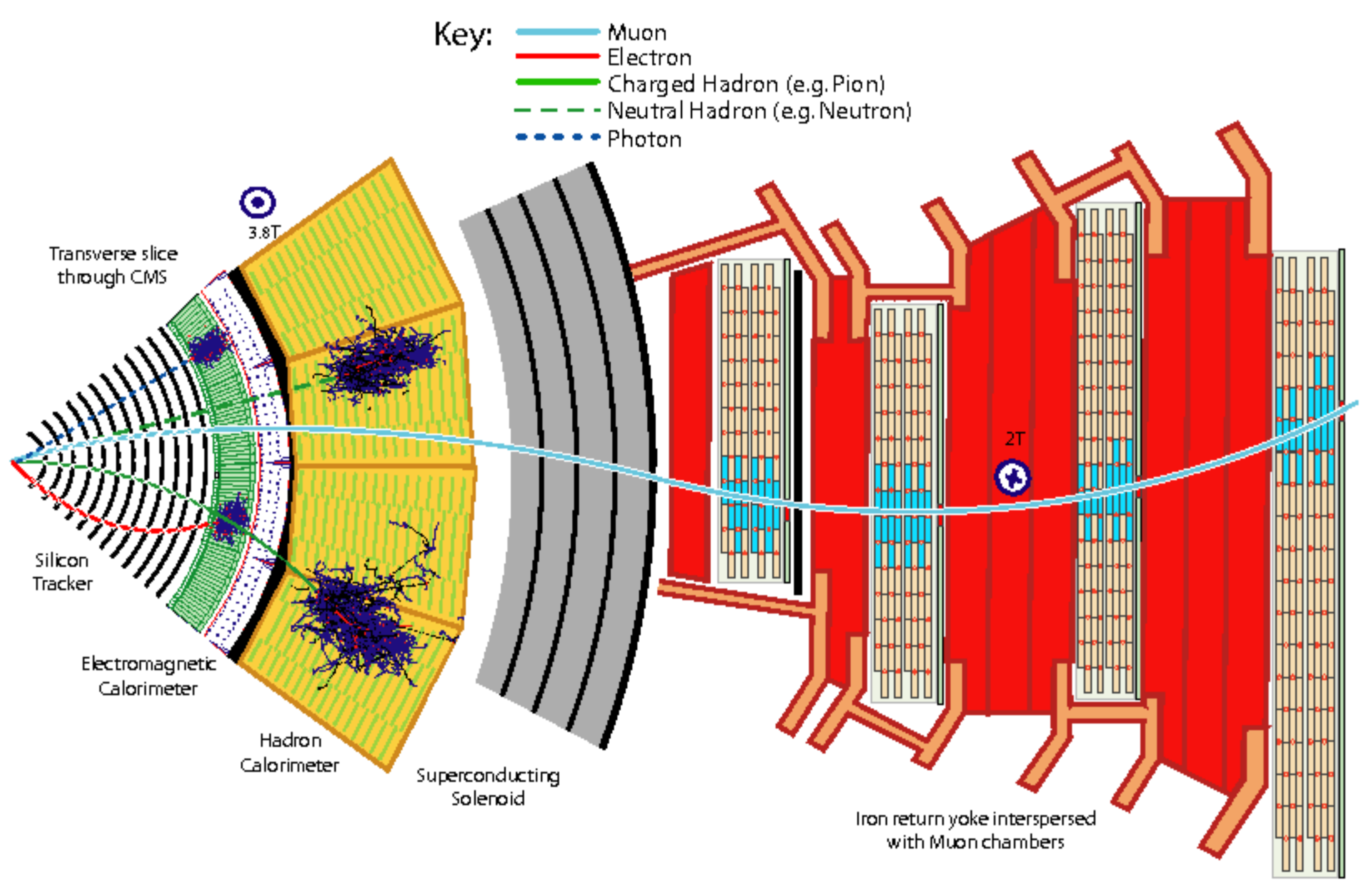
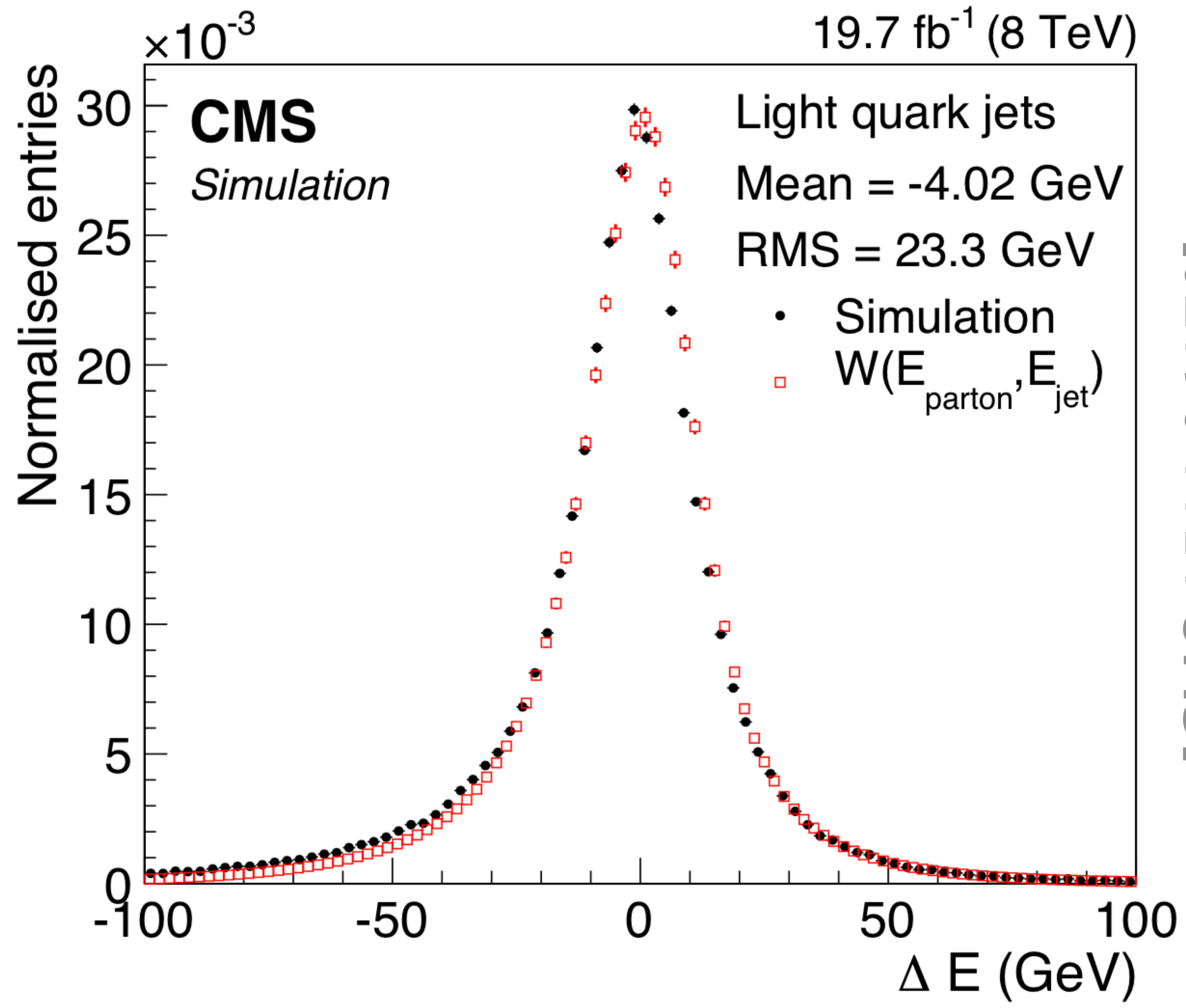



[CMS]

- Matrix Element Method (and similarly Optimal Observables): [K. Kondo 1988]
  - approximate shower + detector effects into transfer function $\hat{p}(x|z_p)$
  - explicitly calculate remaining integral

$$\hat{p}(x|\theta) = \int \mathrm{d}z_p \; \hat{p}(x|z_p)\, p(z_p|\theta)$$




[CMS 1511.06170]

# Solve it by approximating the integral

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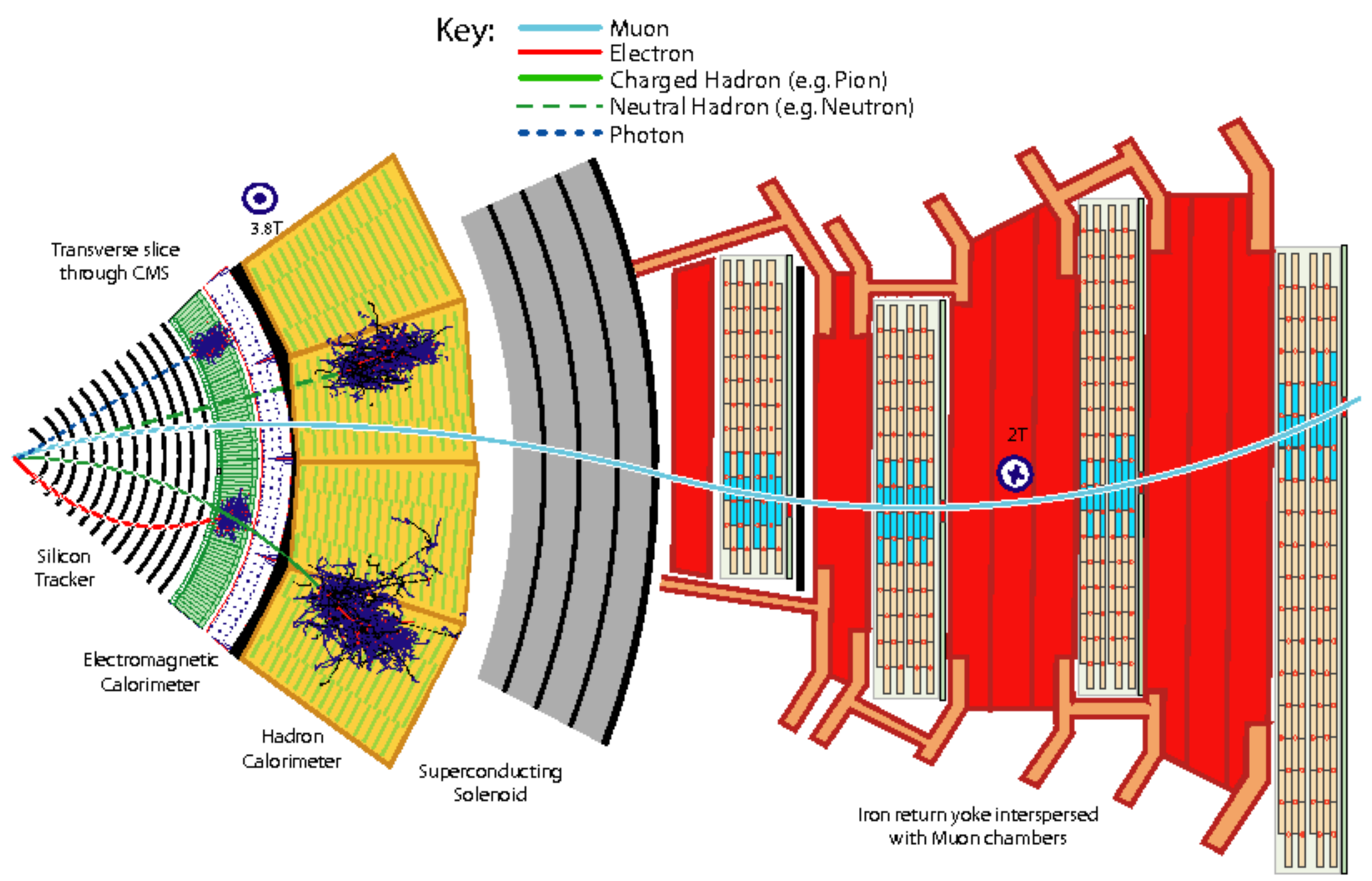


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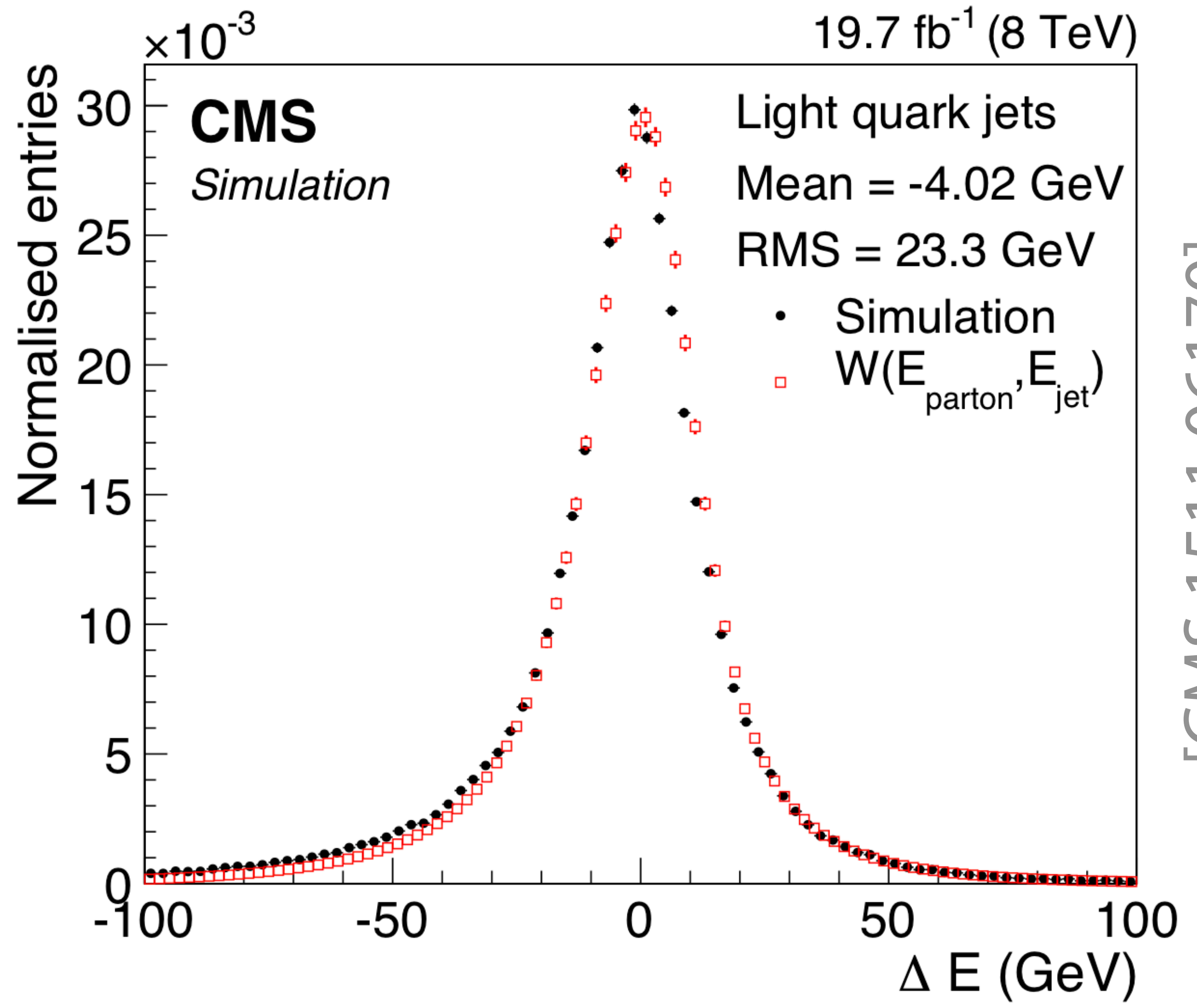
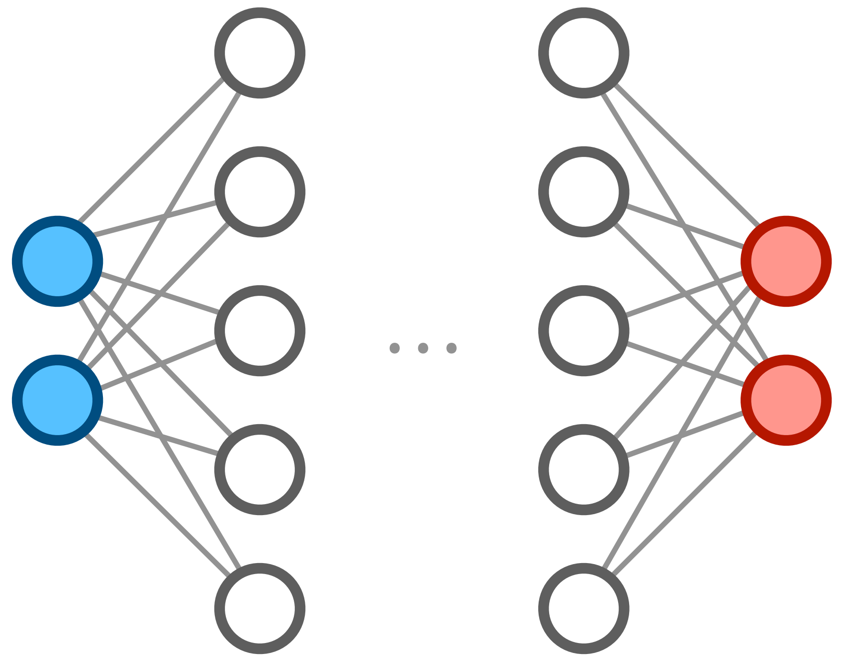



[CMS 1511.06170]

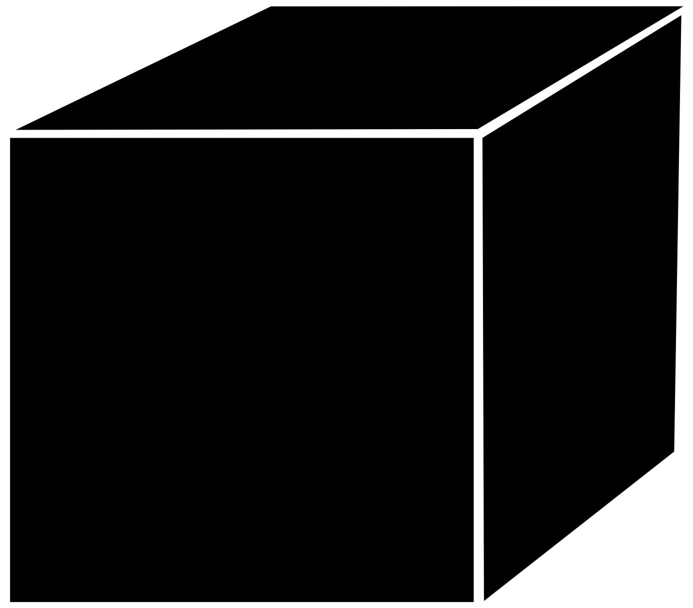
⇒ Uses matrix-element information, no summary statistics necessary, but:

- ad-hoc transfer functions (what about extra radiation?)
- evaluation still requires calculating an expensive integral



# 3. Machine learning solutions

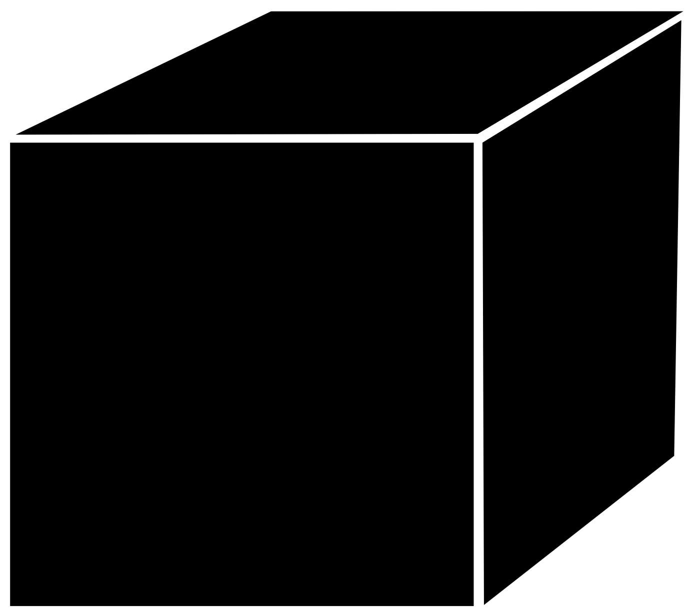
# Get the best of two worlds



Simulators: focus on understanding

- based on mechanistic, causal model
- interpretable parameters

# Get the best of two worlds



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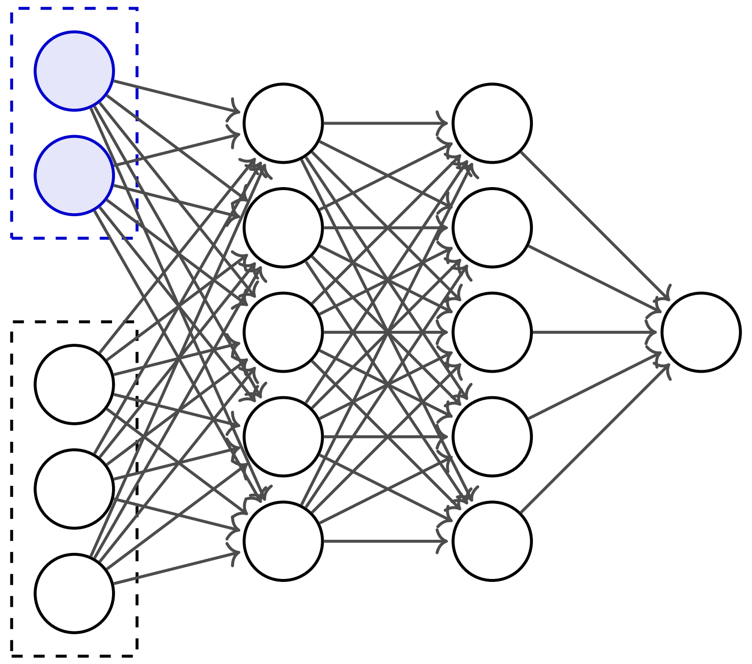
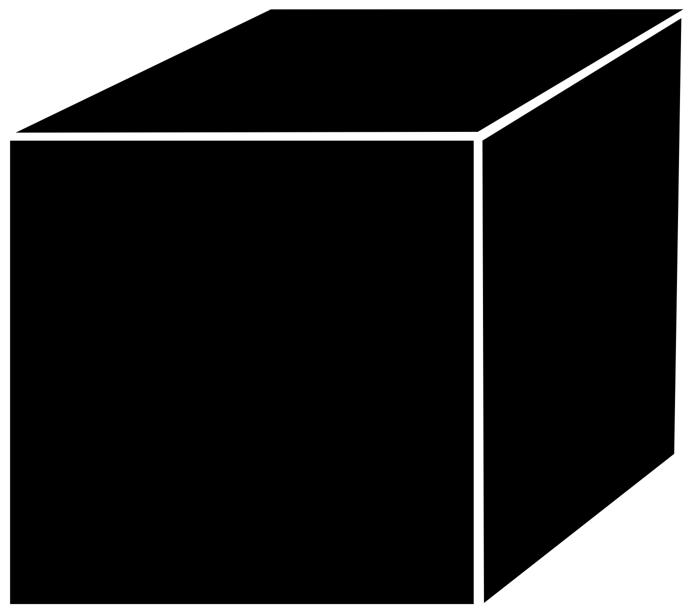
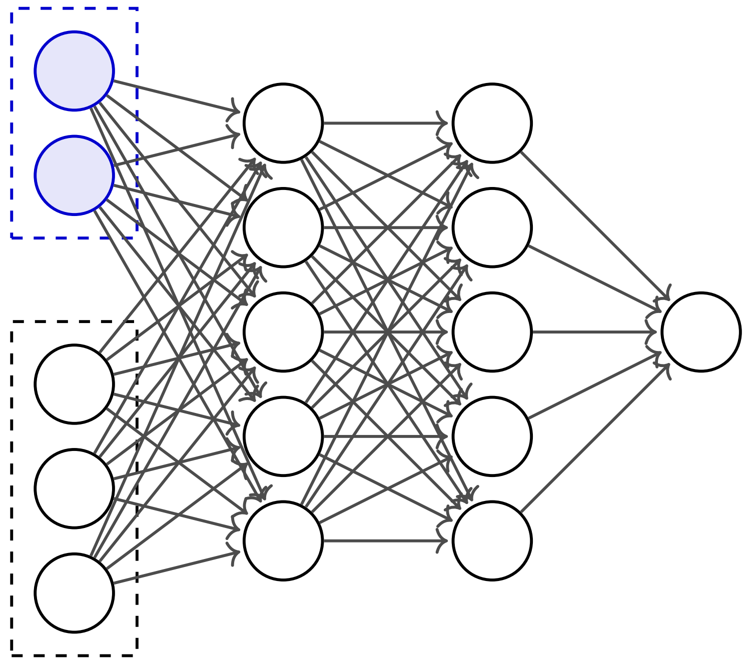


Machine learning models: focus on performance

- good at learning representations from data
- good inductive biases (images, sequences, graphs, symmetries, hierarchical structures…)
- differentiable, often invertible, probabilistic: well-suited for inference / fitting

# Get the best of two worlds





Can we use ML models to fit simulators to data?

Simulators: focus on understanding

- based on mechanistic, causal model
- interpretable parameters

Machine learning models: focus on performance

- good at learning representations from data
- good inductive biases (images, sequences, graphs, symmetries, hierarchical structures…)
- differentiable, often invertible, probabilistic: well-suited for inference / fitting

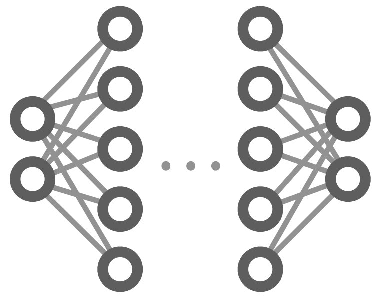
Can we inject domain knowledge into ML models?

# Idea 1: the likelihood ratio trick

- Generative Adversarial Networks (GANs):

[I. Goodfellow et al. 1406.2661]

Generator
(intractable likelihood $p_{\text{gen}}(x)$)



Examples
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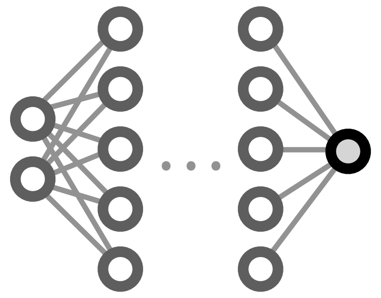

Discriminator

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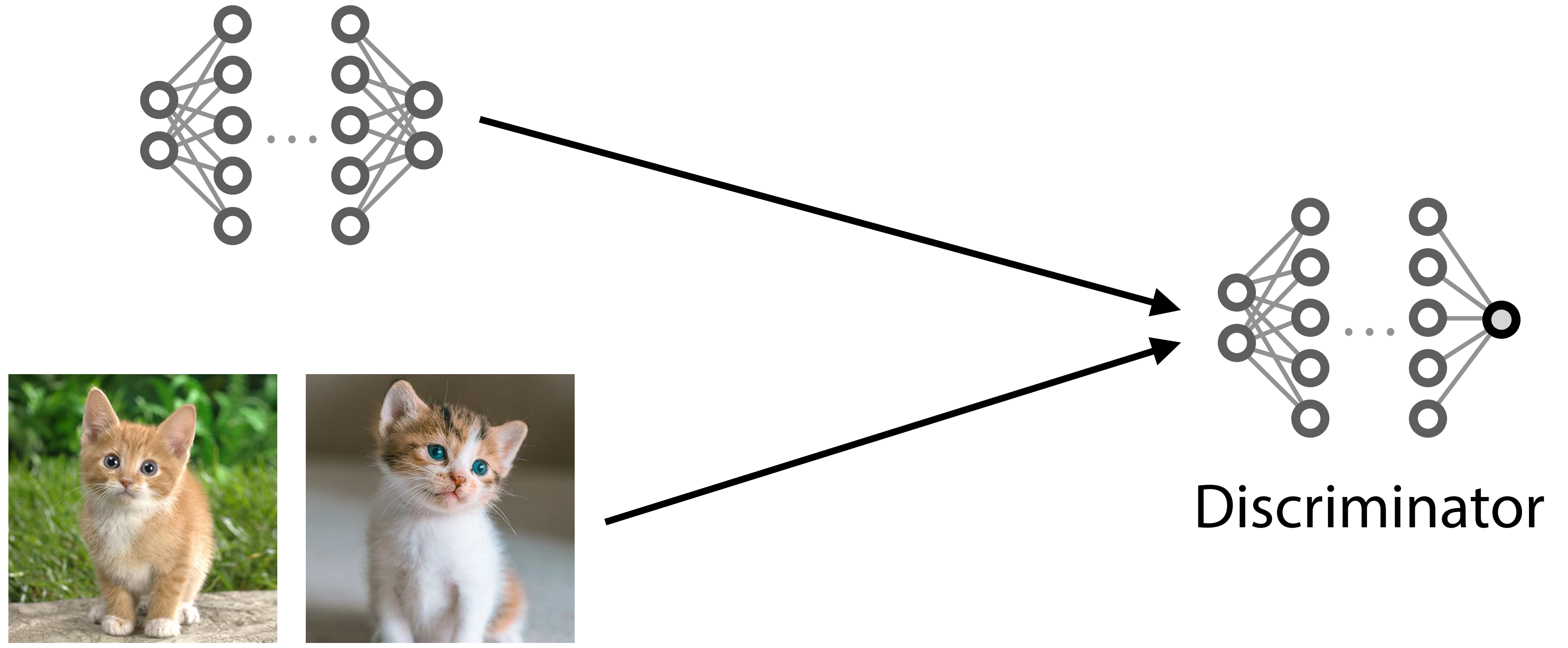



Discriminator learns decision function

$$s(x) \to \frac{p_{\mathrm{true}}(x)}{p_{\mathrm{gen}}(x) + p_{\mathrm{true}}(x)}$$

# Idea 1: the likelihood ratio trick

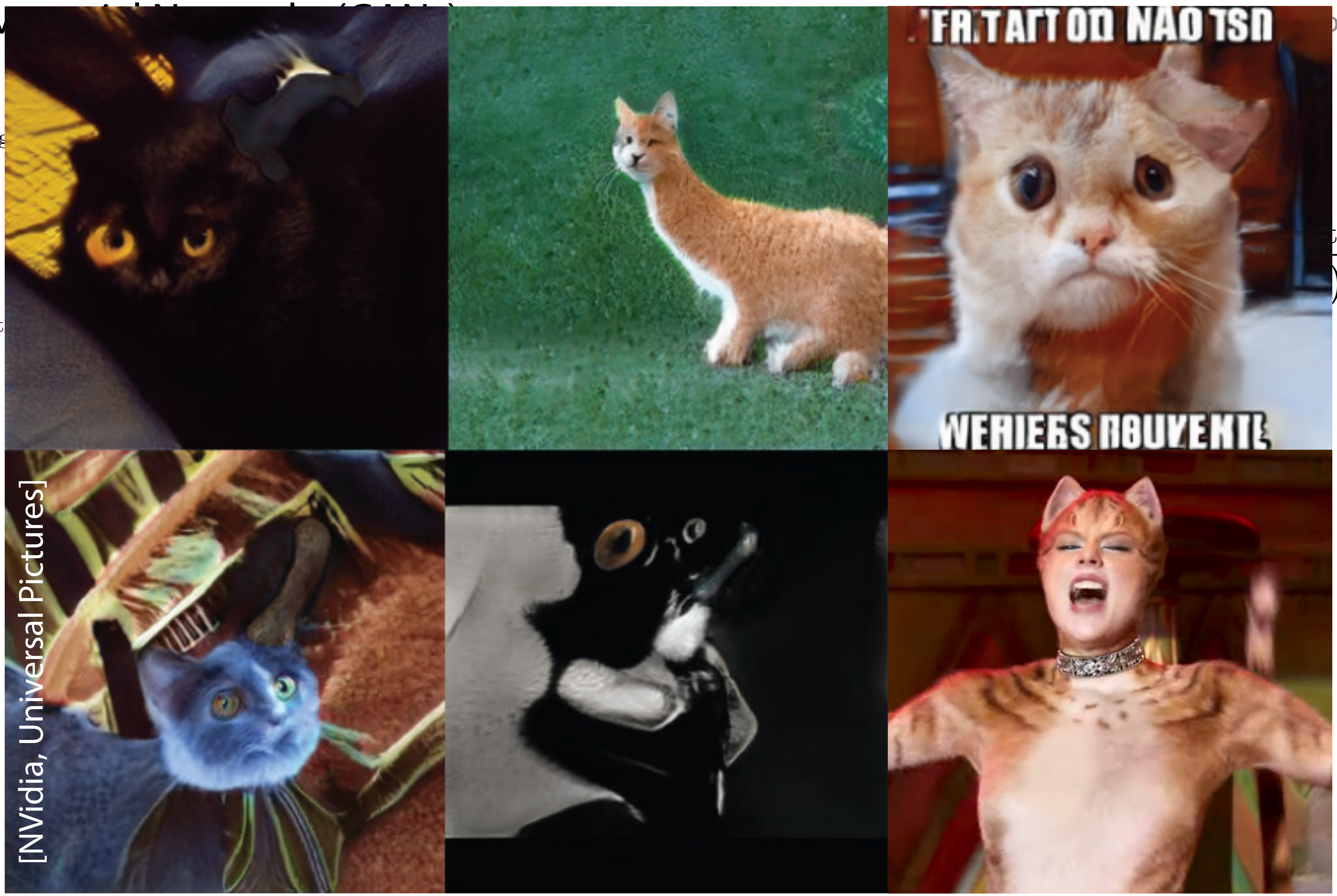
- Generative Adv odfellow et al. 1406.2661]

Generator
(intractable likelihood $p_g$

Examples
(intractable likelihood $p_t$

decision function

$$\ldots_{\mathrm{true}}(x) \,/\, \ldots) + p_{\mathrm{true}}(x)$$



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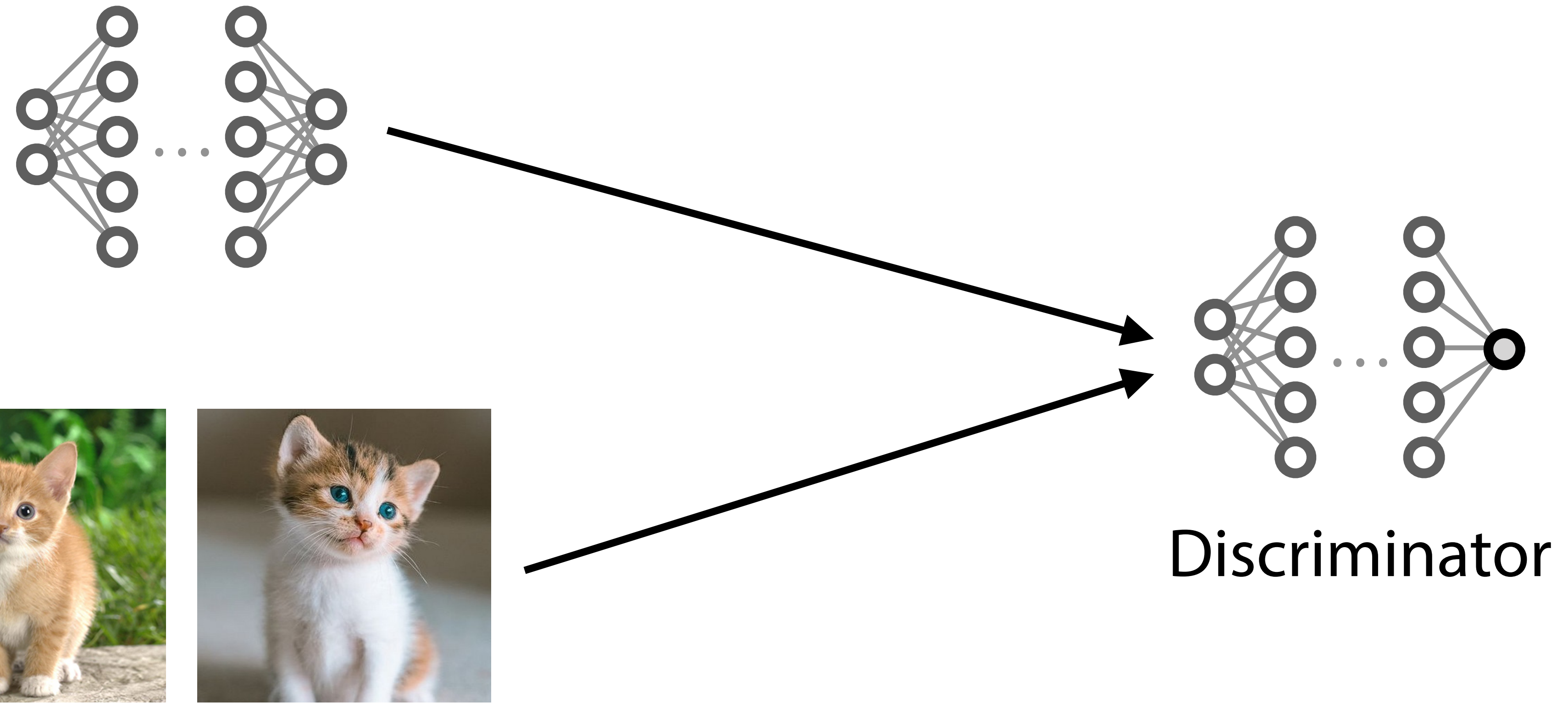


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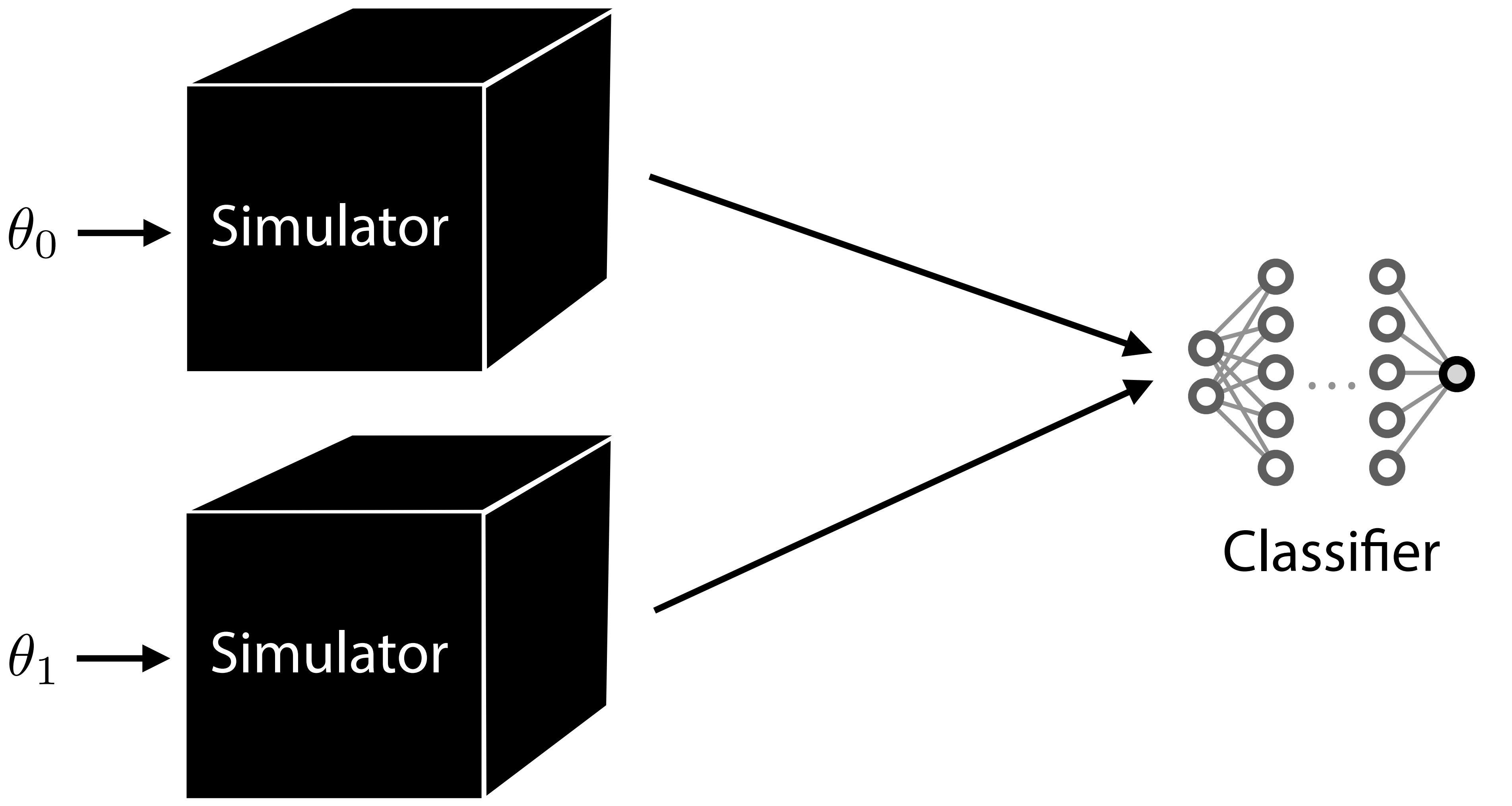
- Similarly, we can train a classifier between two sets of simulated samples [K. Cranmer, J. Pavez, G. Louppe 1506.02169]

Simulator
(intractable likelihood $p(x|\theta_0)$)

Simulator
(intractable likelihood $p(x|\theta_1)$)



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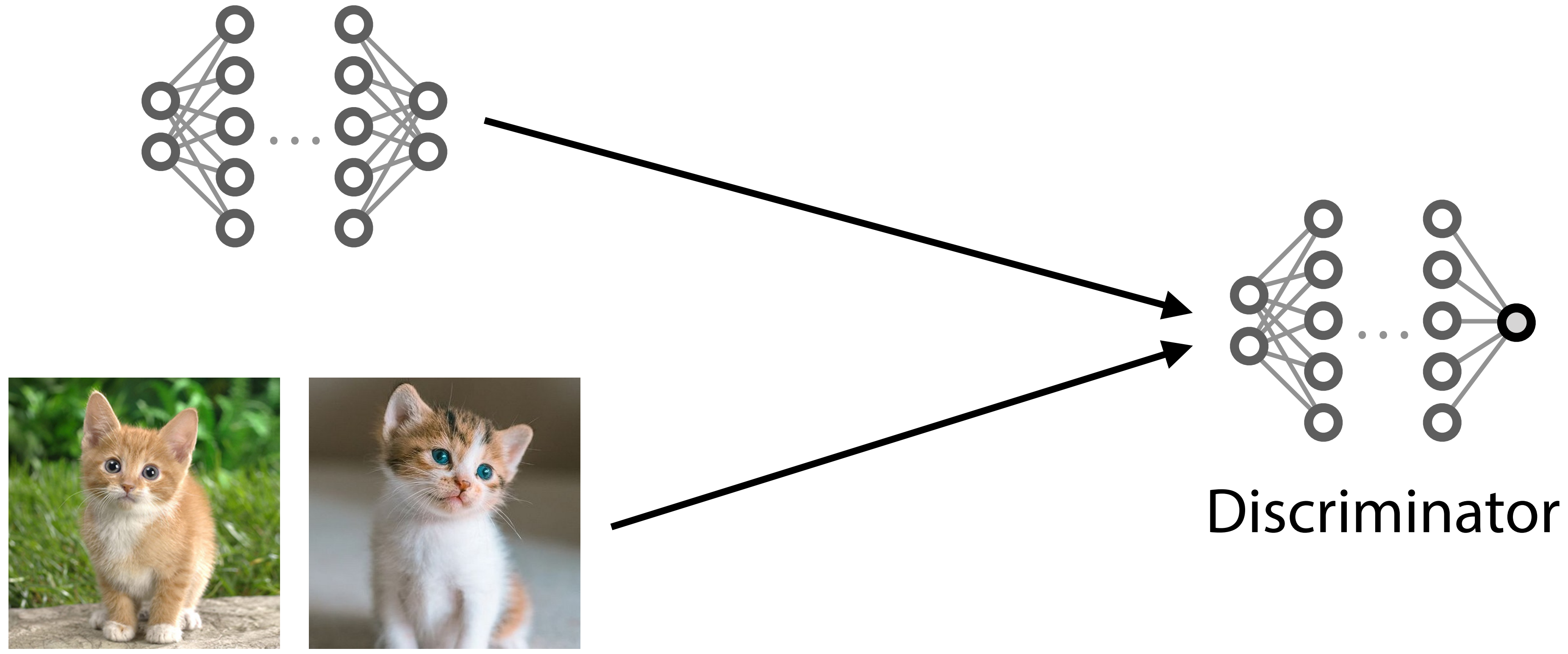

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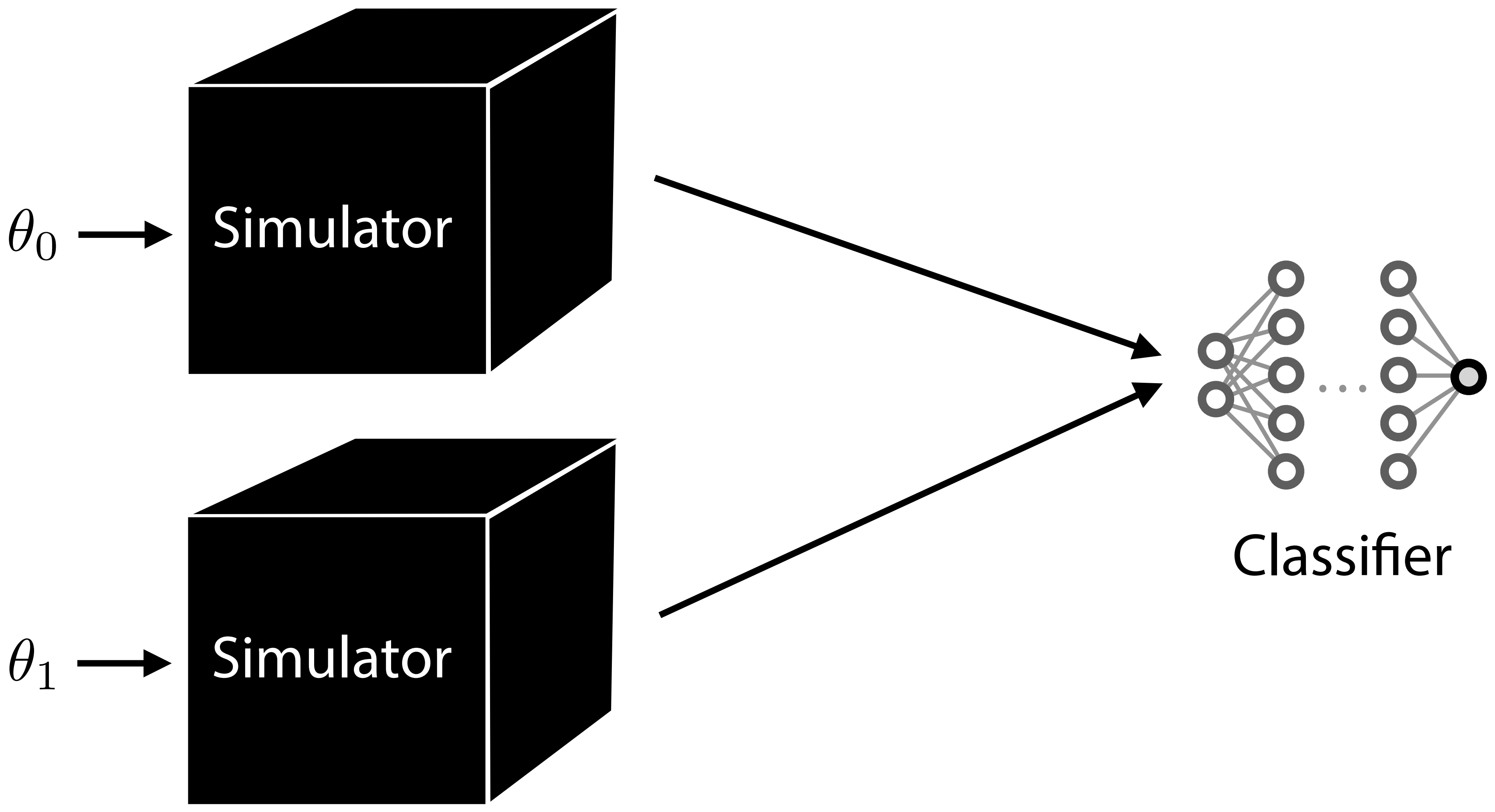



Classifier

Classifier learns decision function

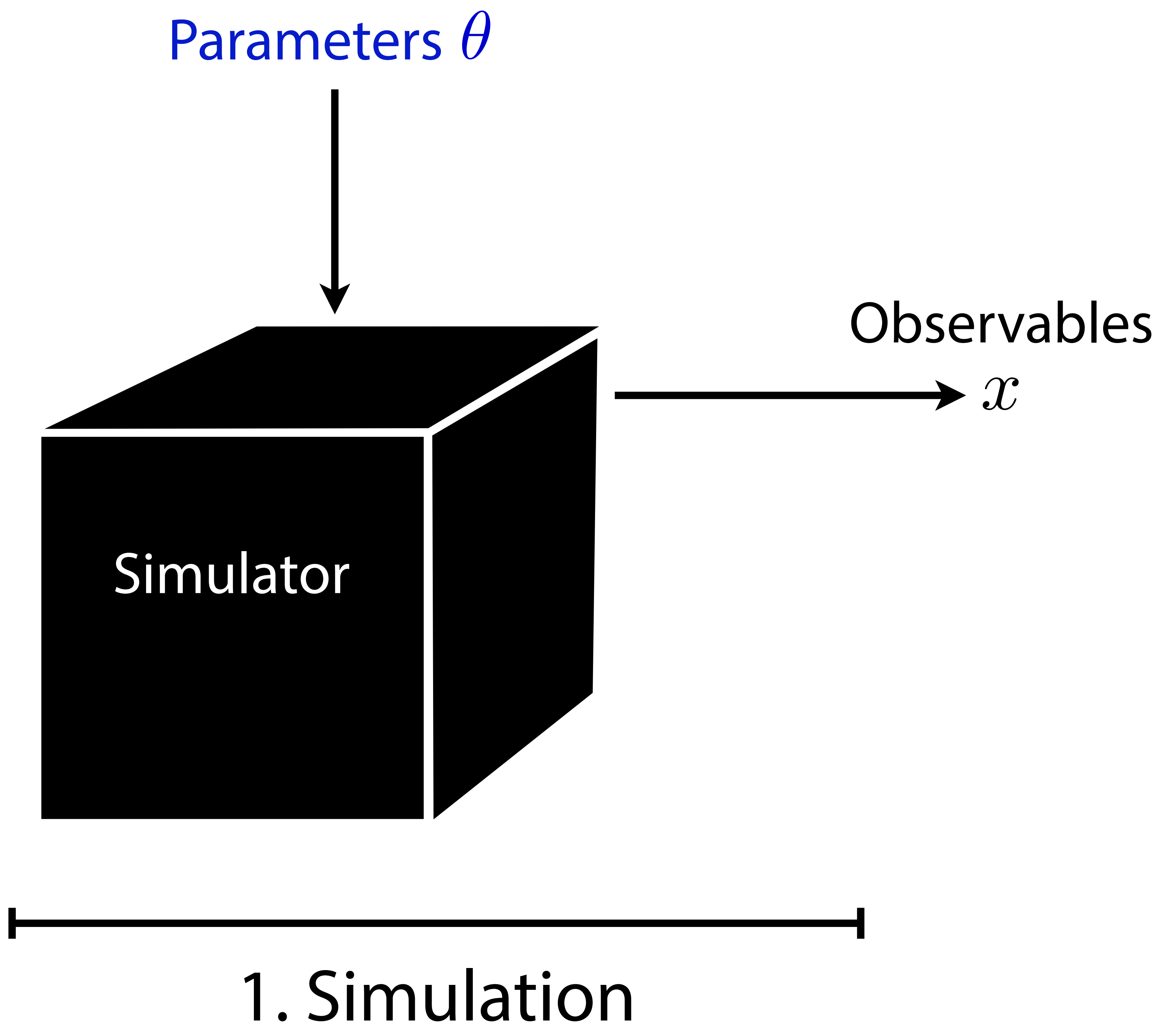
$$s(x) \to \frac{p(x|\theta_1)}{p(x|\theta_0) + p(x|\theta_1)}$$

$\Rightarrow$ Estimator for likelihood ratio

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

# Inference by likelihood ratio trick

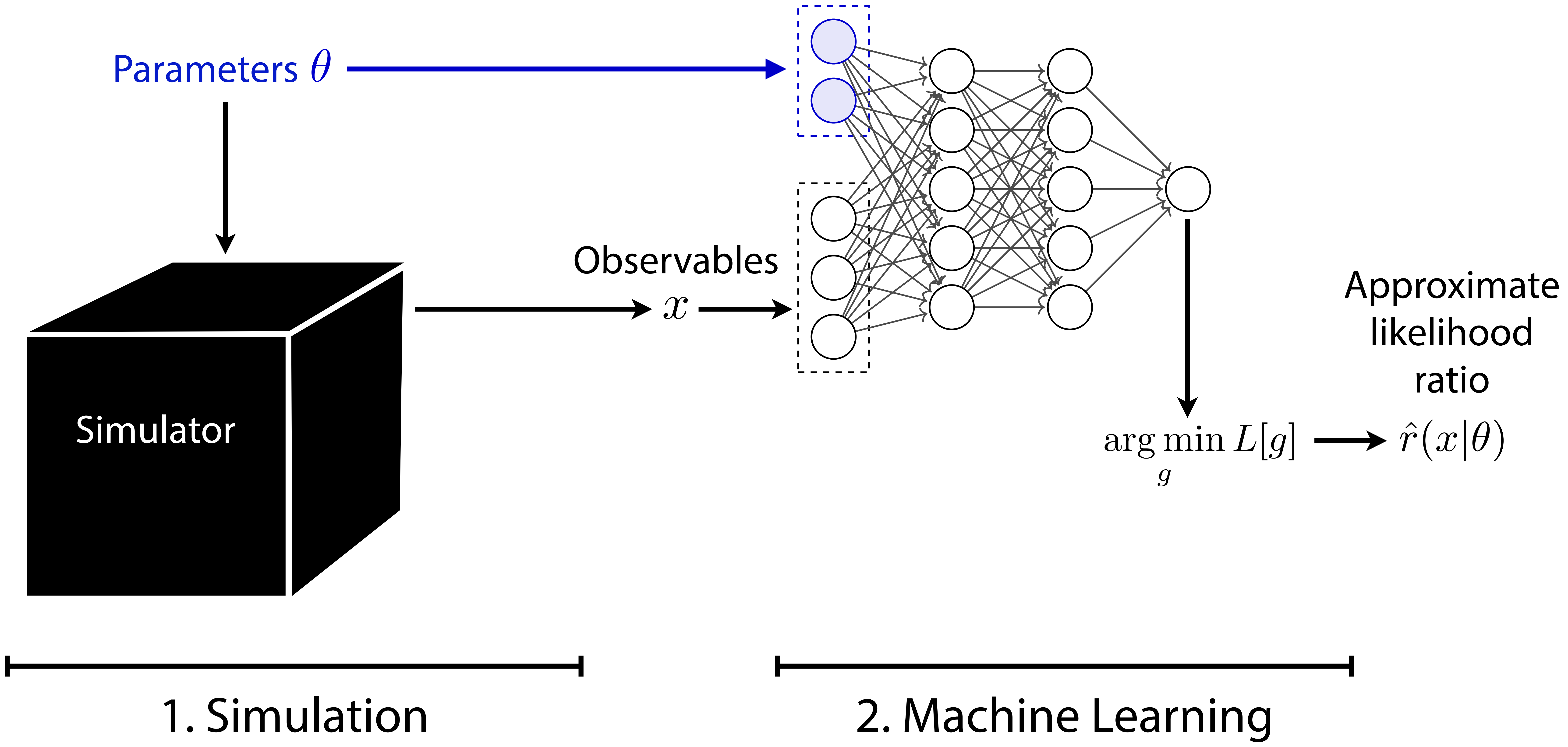
[K. Cranmer, J. Pavez, G. Louppe 1506.02169]




Run simulator and save data

# Inference by likelihood ratio trick

[K. Cranmer, J. Pavez, G. Louppe 1506.02169]




Run simulator and save data

Train NN classifier, interpret as likelihood ratio estimator

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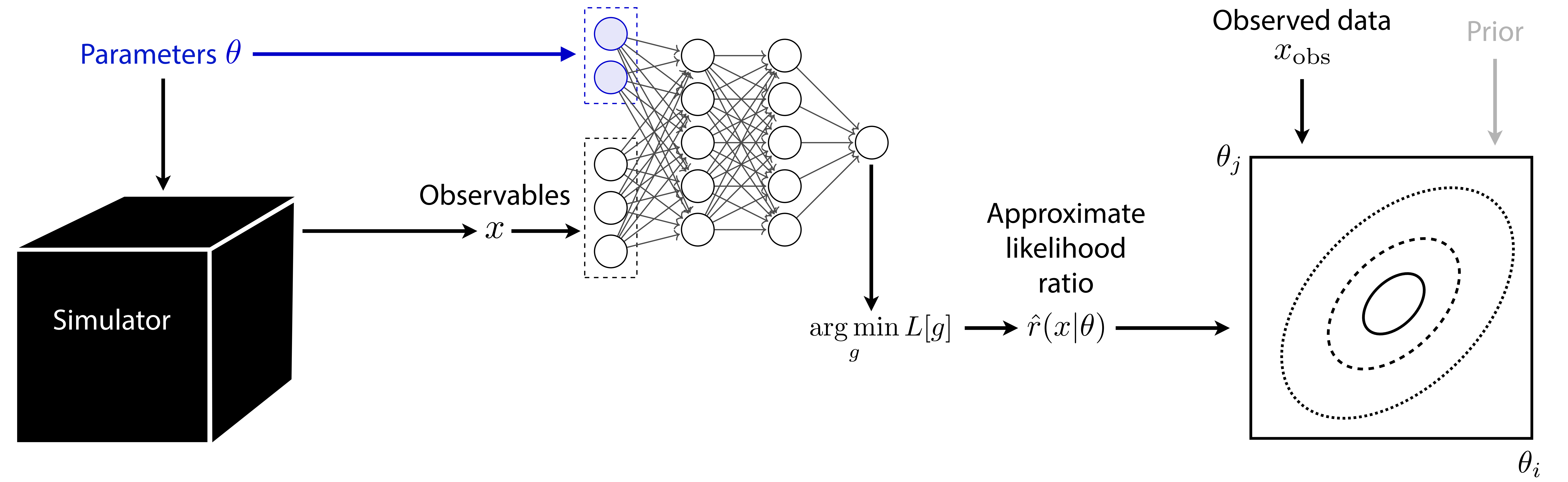



1. Simulation

2. Machine Learning

3. Inference

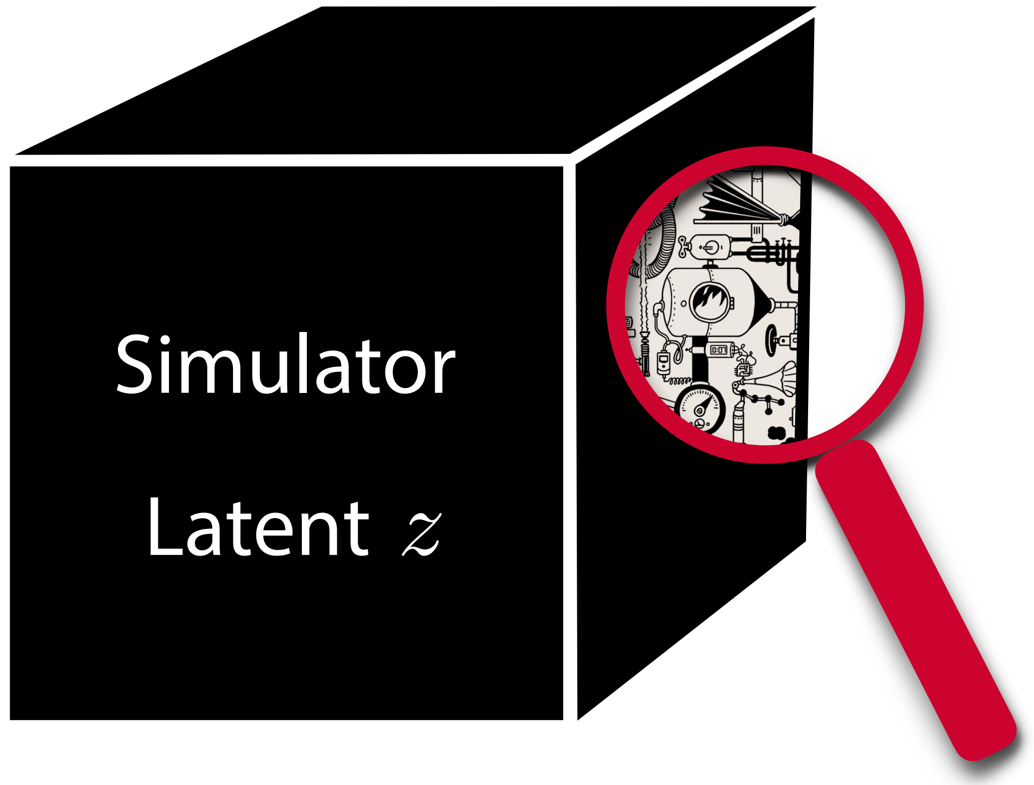
Run simulator and save data

Train NN classifier, interpret as likelihood ratio estimator

Amortized: cheap to repeat for new data

# Idea 2: “mining gold”

[JB, G. Louppe, J. Pavez, K. Cranmer 1805.12244, 1805.00013, 1805.00020]




We cannot compute $p(x|\theta) = \int dz\, p(x,z|\theta)$ ,

but for each simulated event we can compute

- the joint likelihood ratio

$$r(x,z|\theta) = \frac{p(x,z|\theta)}{p_{\text{ref}}(x,z)} \sim \frac{|\mathcal{M}|^2(z|\theta)}{|\mathcal{M}|^2_{\text{ref}}(z)}$$

- the joint score

$$t(x,z|\theta) = \nabla_\theta \log p(x,z|\theta) \sim \frac{\nabla_\theta |\mathcal{M}|^2(z|\theta)}{|\mathcal{M}|^2(z|\theta)}$$

(Both depend on the truth-level four-momenta $z$)

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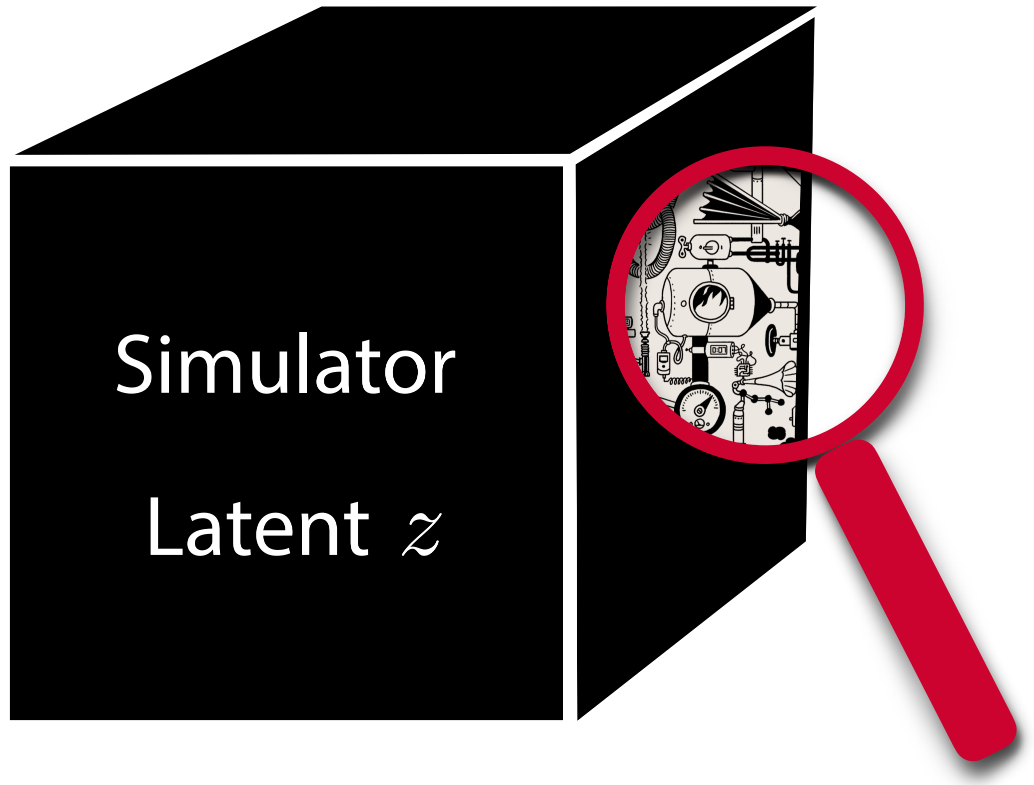


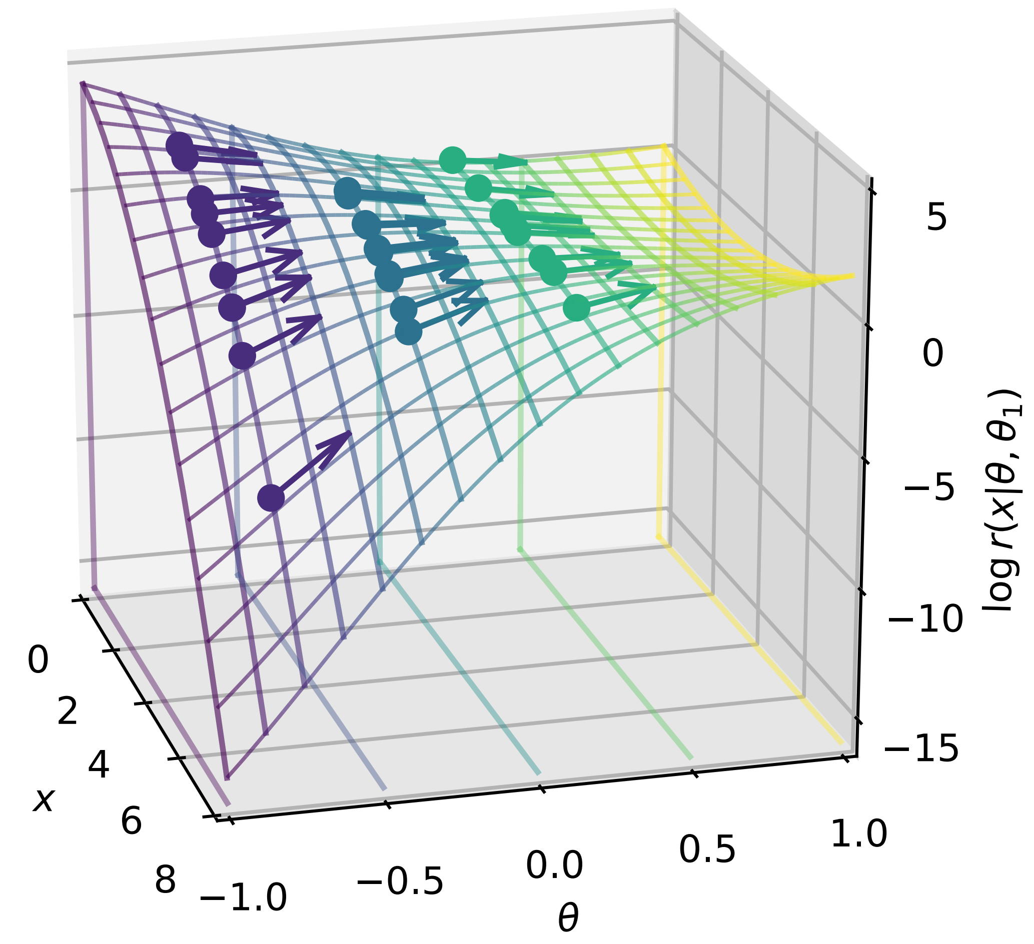


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(Both depend on the truth-level four-momenta $z$)

Why are they useful? One can show that

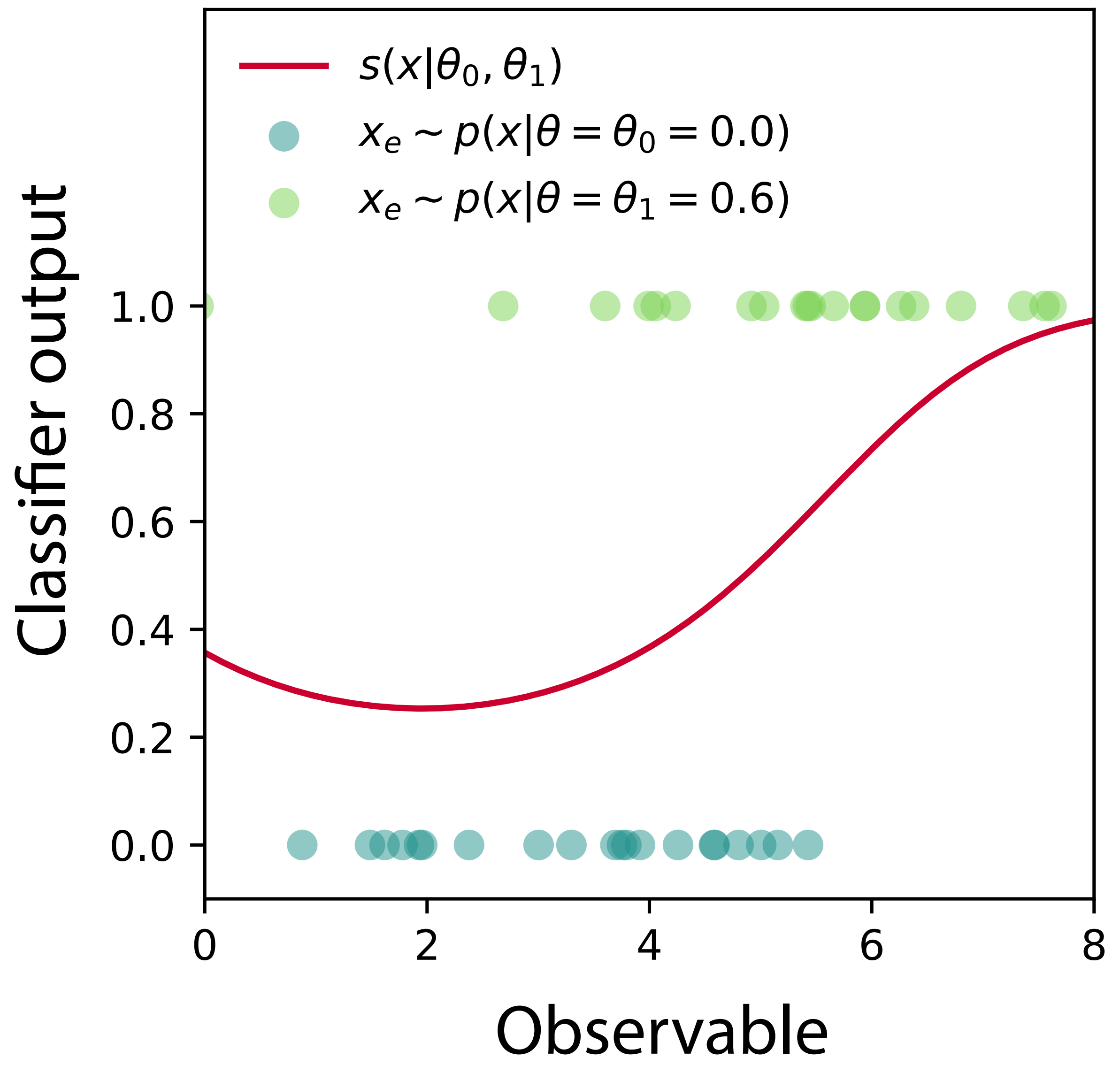
- the joint likelihood ratio is an unbiased estimator of the likelihood ratio
- the joint score provides unbiased gradient information

⇒ use them as labels in supervised NN training!

# Mining gold adds information

[JB, G. Louppe, J. Pavez, K. Cranmer
1805.12244, 1805.00013, 1805.00020]

Likelihood ratio trick



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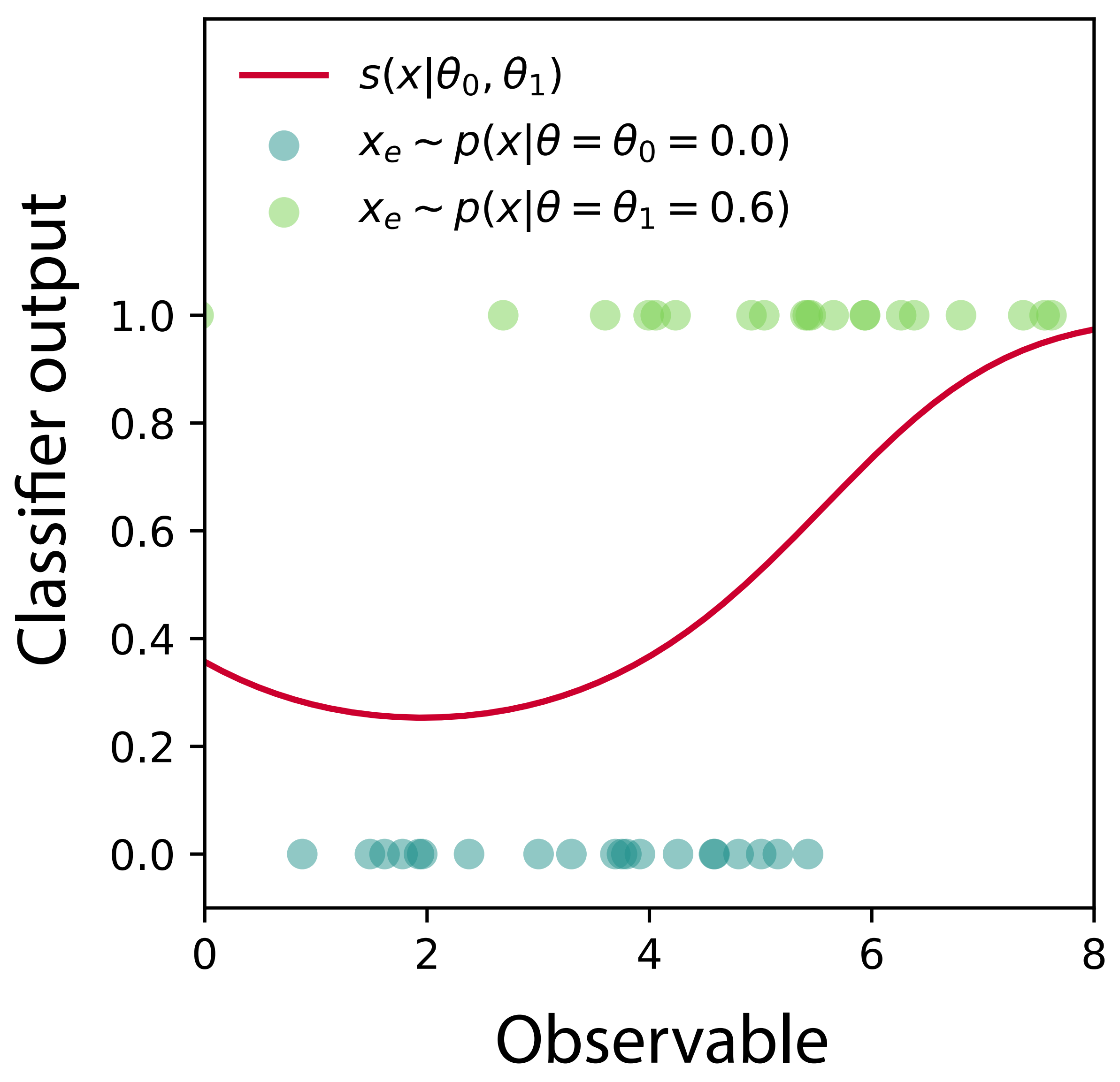
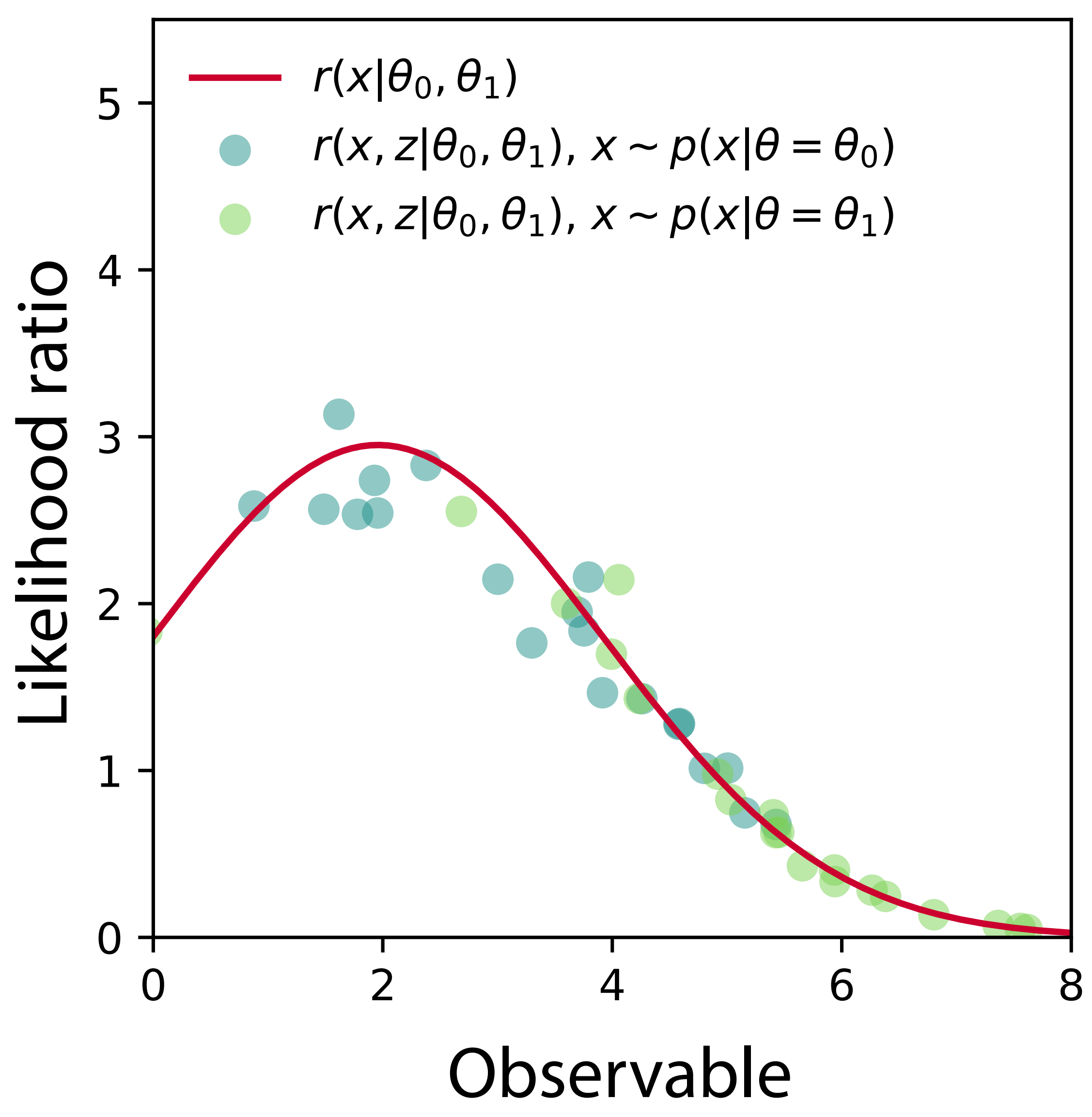



+ joint likelihood ratio



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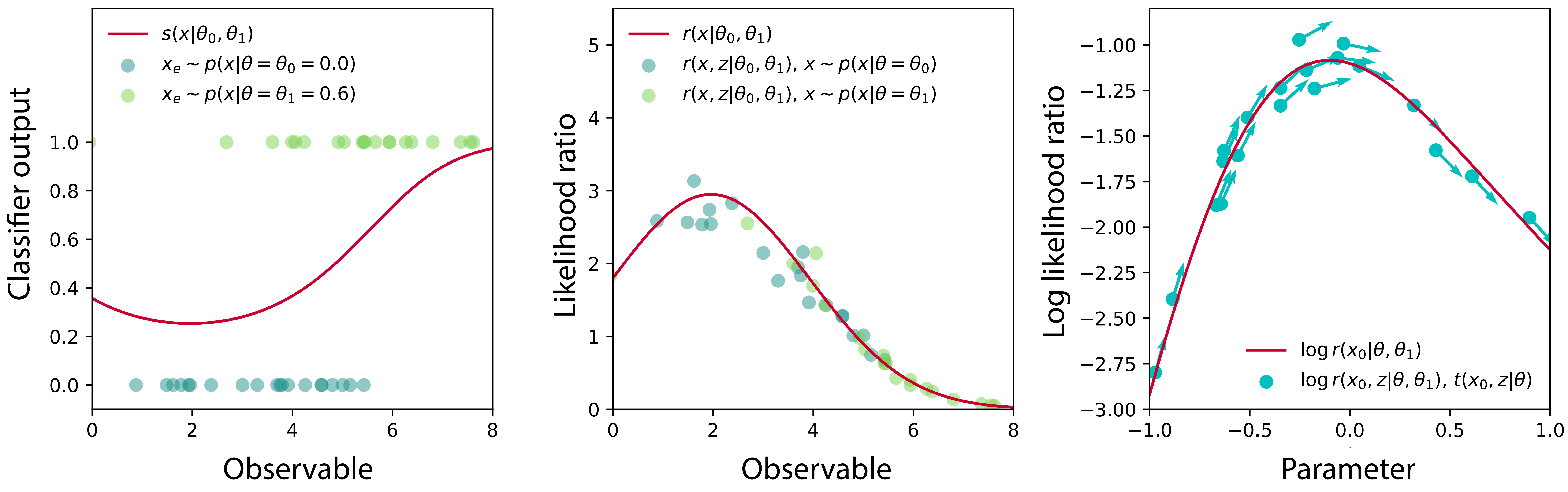
Likelihood ratio trick

+ joint likelihood ratio

+ joint score



# Mining gold adds information

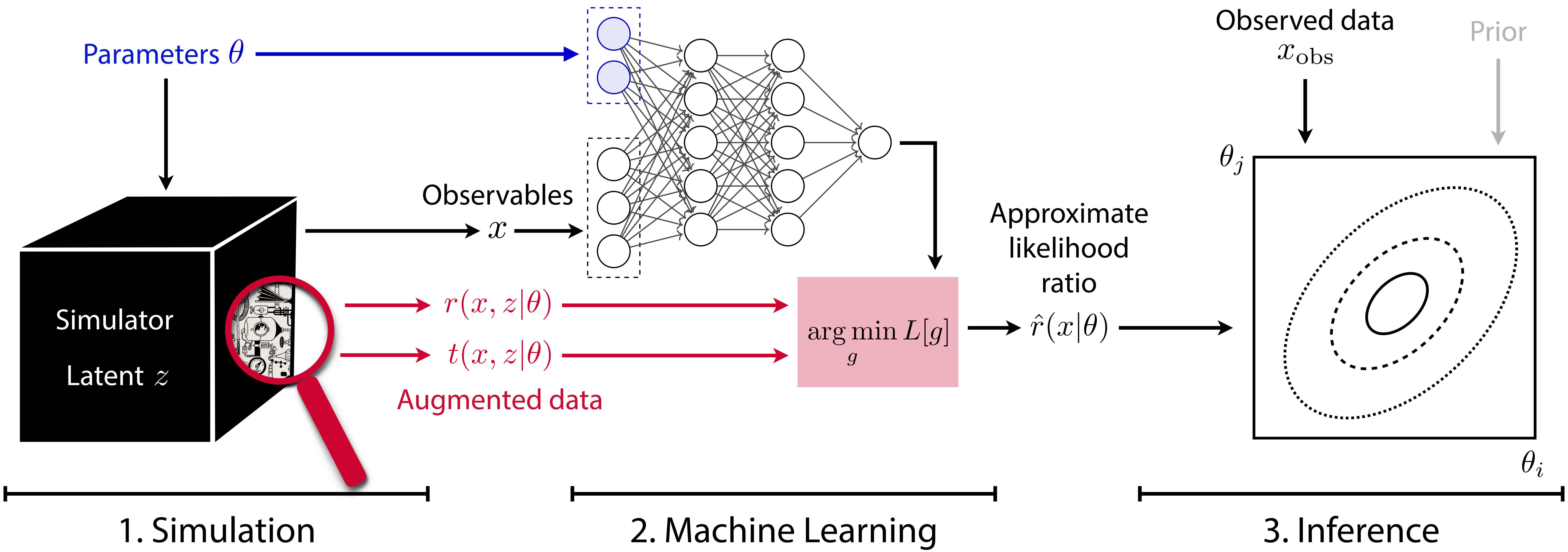
[JB, G. Louppe, J. Pavez, K. Cranmer
1805.12244, 1805.00013, 1805.00020]

Likelihood ratio trick | + joint likelihood ratio | + joint score | = RASCAL


Using more information = more sample-efficient inference

# RASCAL

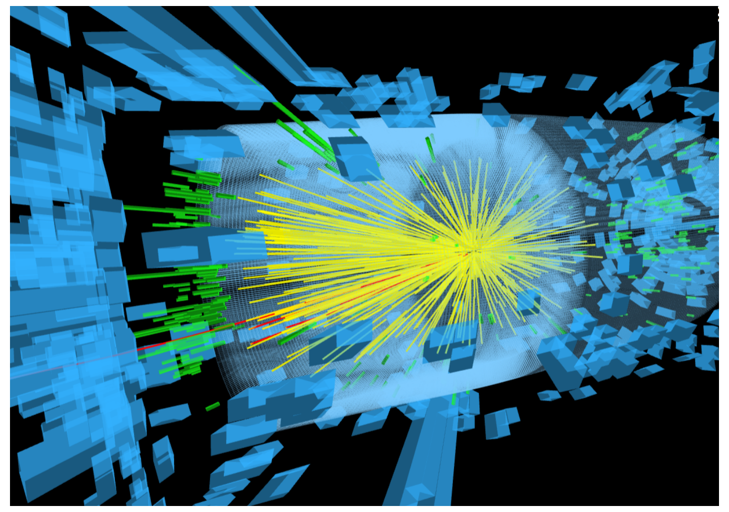
[JB, G. Louppe, J. Pavez, K. Cranmer
1805.12244, 1805.00013, 1805.00020]



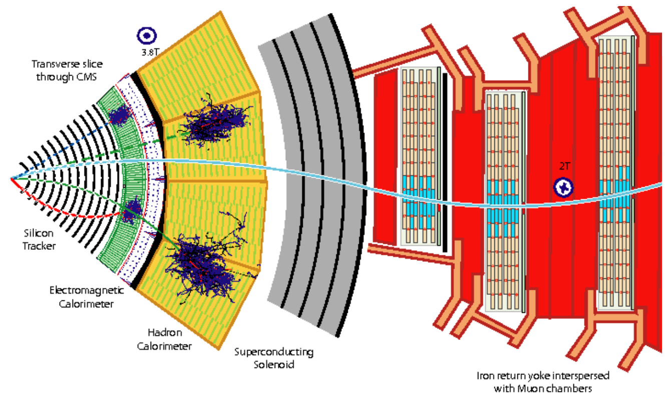

Extract joint likelihood ratio
and joint score from simulator

Augment training data &
use as labels in new loss functions
⇒ improve training efficiency

# Sales pitch



Get all the information in high-dimensional data (no need for summary statistics)

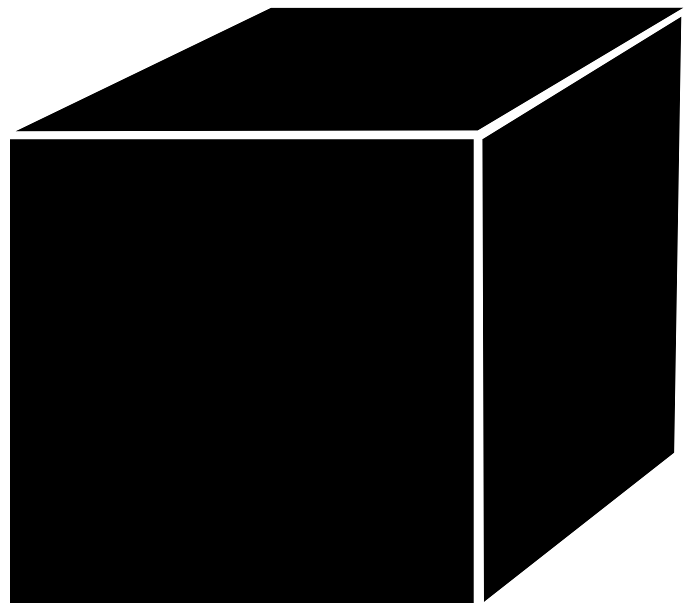


Use state-of-the-art shower and detector models (no transfer fns)

Evaluate events in microseconds (amortized inference)

Need less training data than black-box ML methods (using matrix-element information)

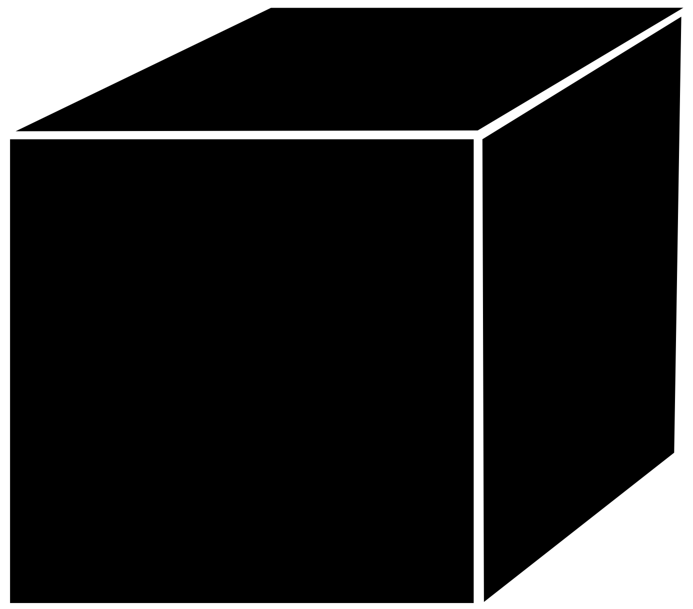
# Systematics



Can you trust the simulator?

- Model uncertainties explicitly:
  nuisance parameters + profiling / marginalization
- Make analysis robust:
  ideas from domain adaptation, algorithmic fairness
  [G. Louppe, M. Kagan, K. Cranmer 1611.01046; J. Alsing, B. Wandelt 1903.01473; P. de Castro, T. Dorigo 1806.04743]

# Systematics



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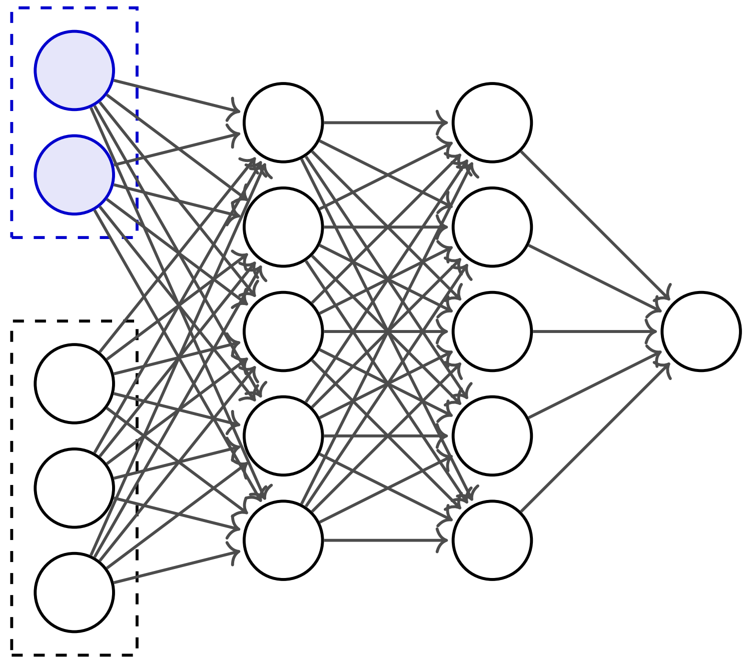
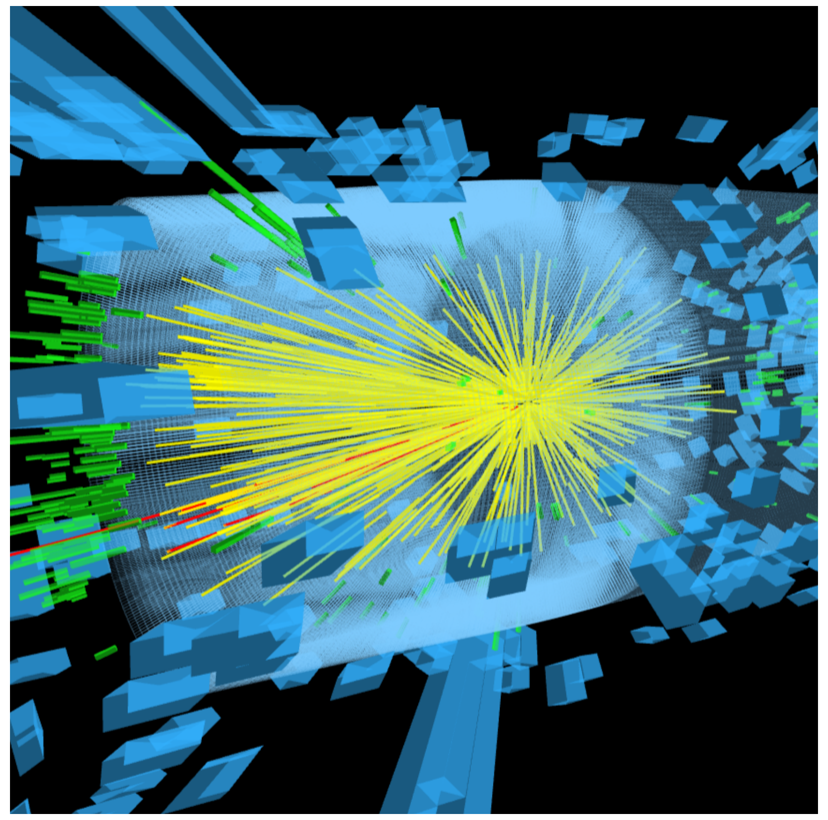


Can you trust the neural network?

- Sanity checks: expectation values, “critic” tests
- Calibrate NN output
- Neyman construction with toys
  (badly trained network can lead to suboptimal limits, but not to wrong limits)
  [JB, G. Louppe, J. Pavez, K. Cranmer 1805.00020]

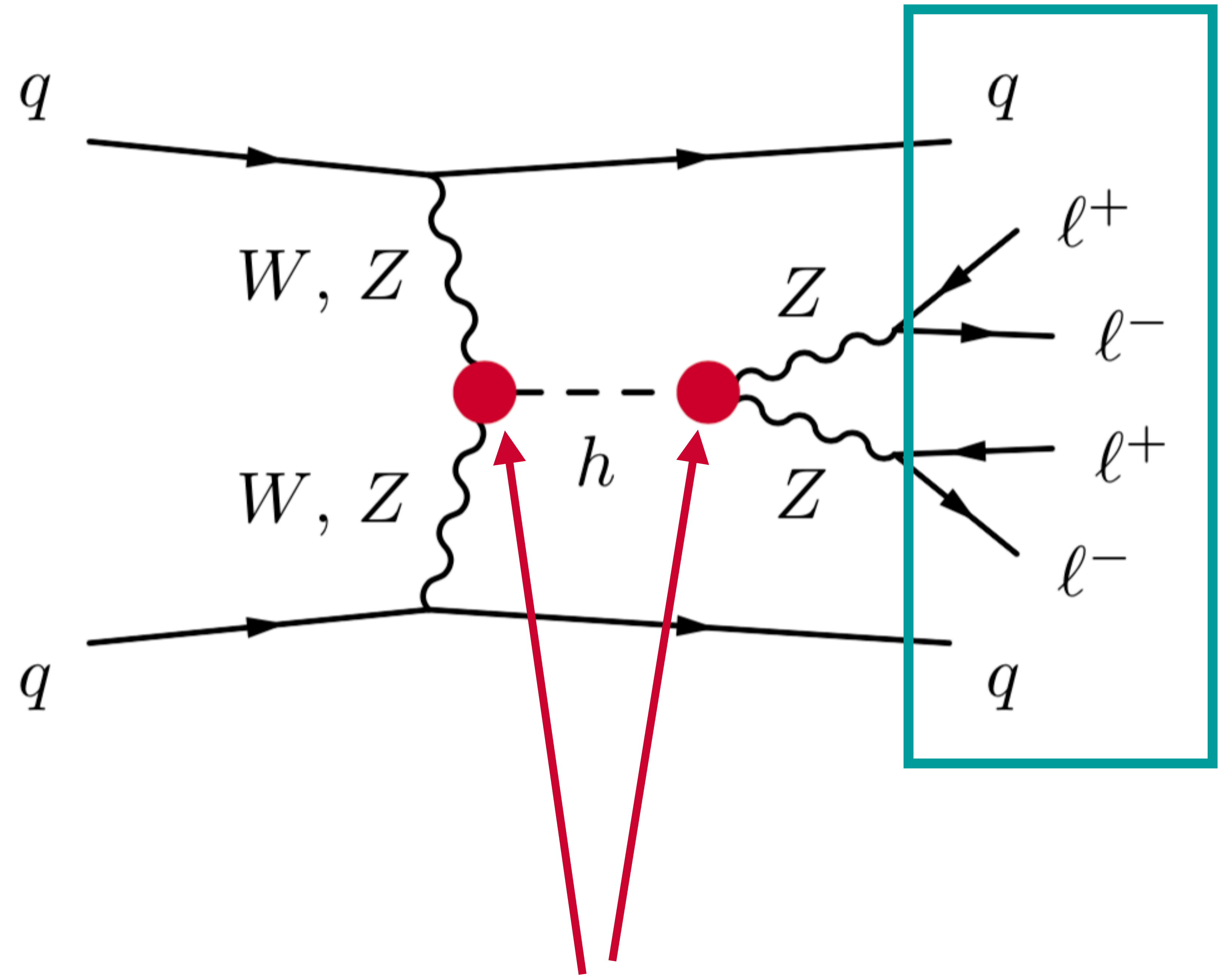


# 4. Examples

# Proof of concept: Higgs production in weak boson fusion

[JB, K. Cranmer, G. Louppe, J. Pavez
1805.00013, 1805.00020]

at least 16-dimensional
observable space




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

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

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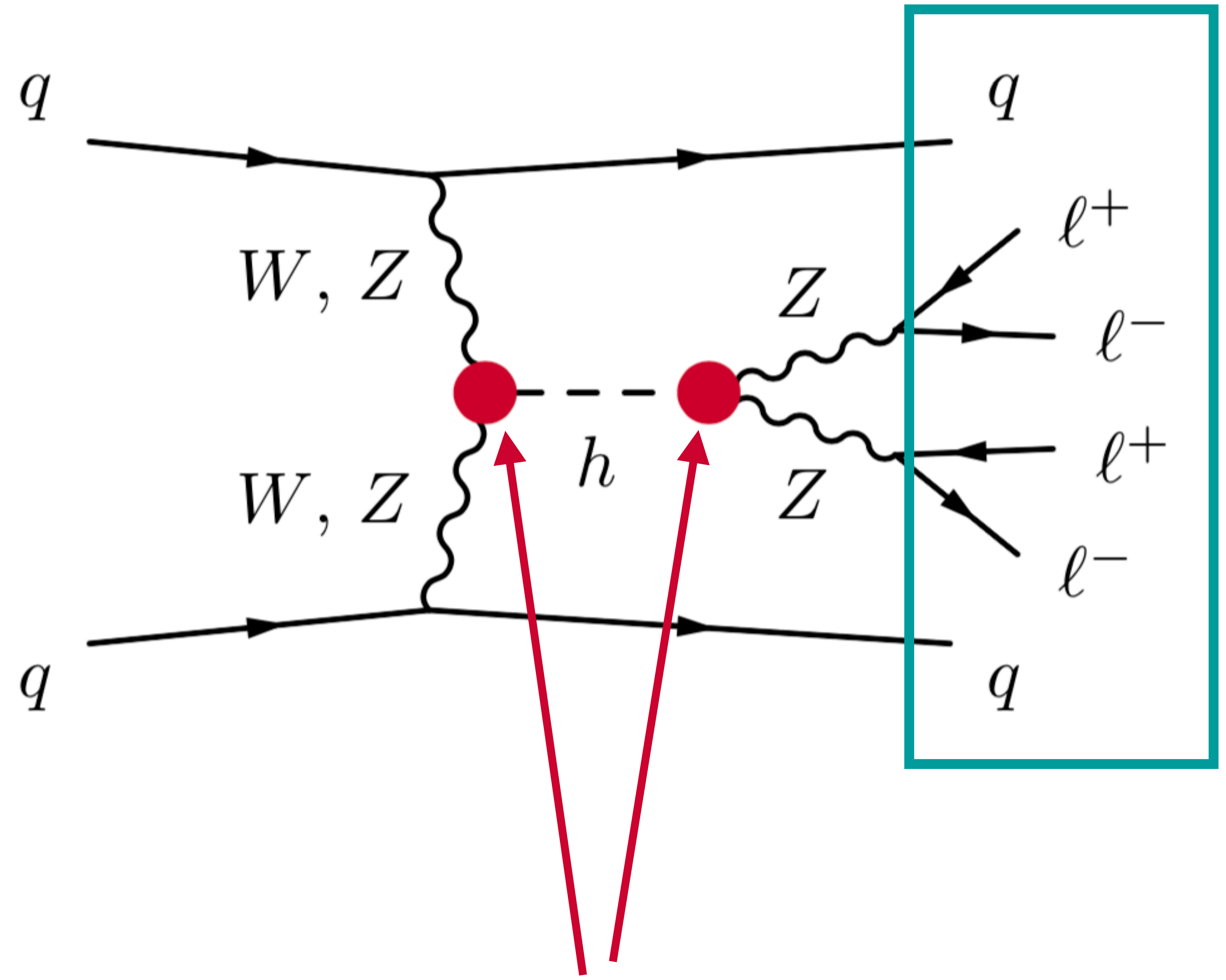


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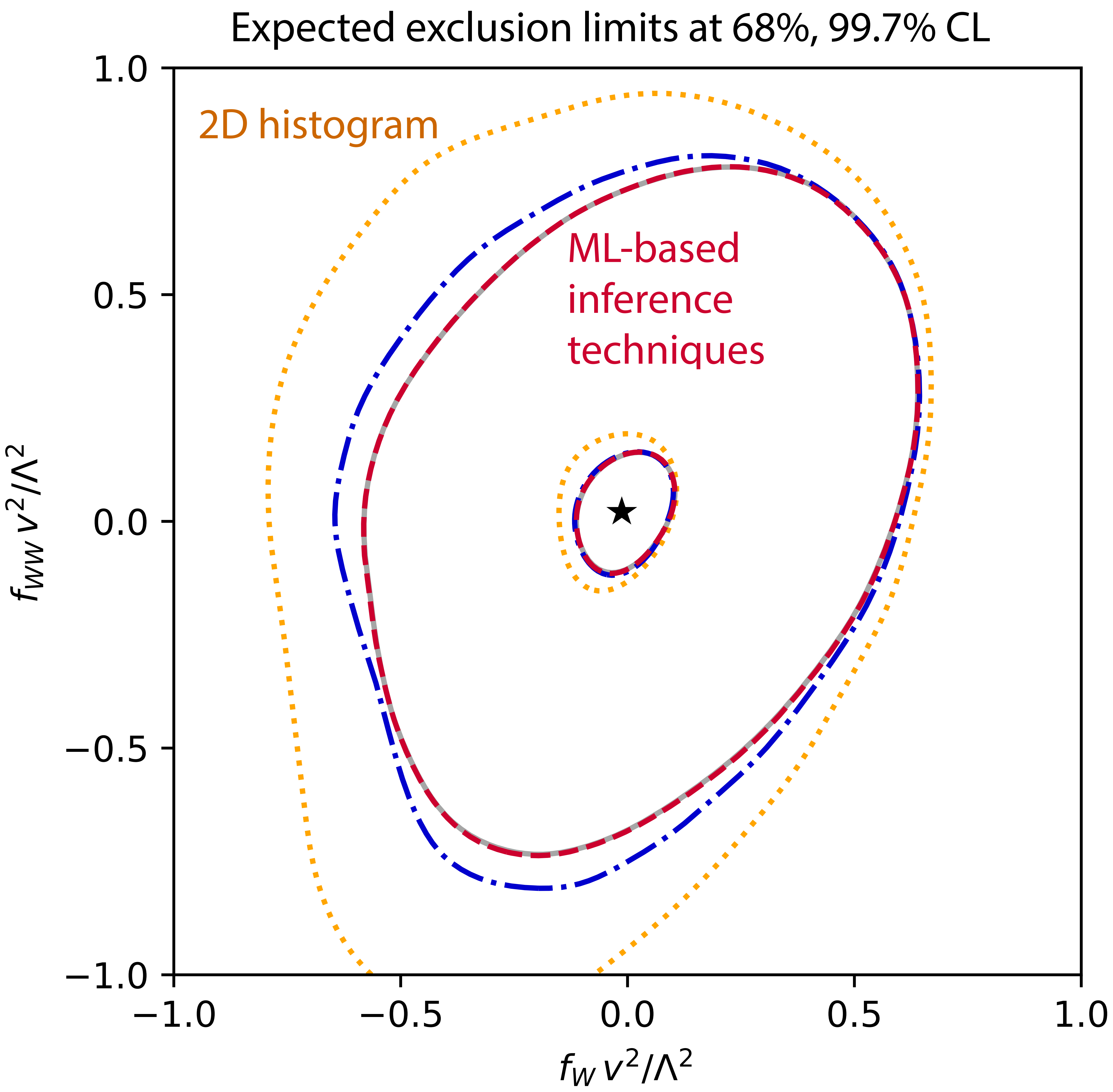
Goal: constrain the two EFT parameters

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

Two scenarios:

- Simplified setup in which we can compare to true likelihood
- "Realistic" simulation with approximate detector effects

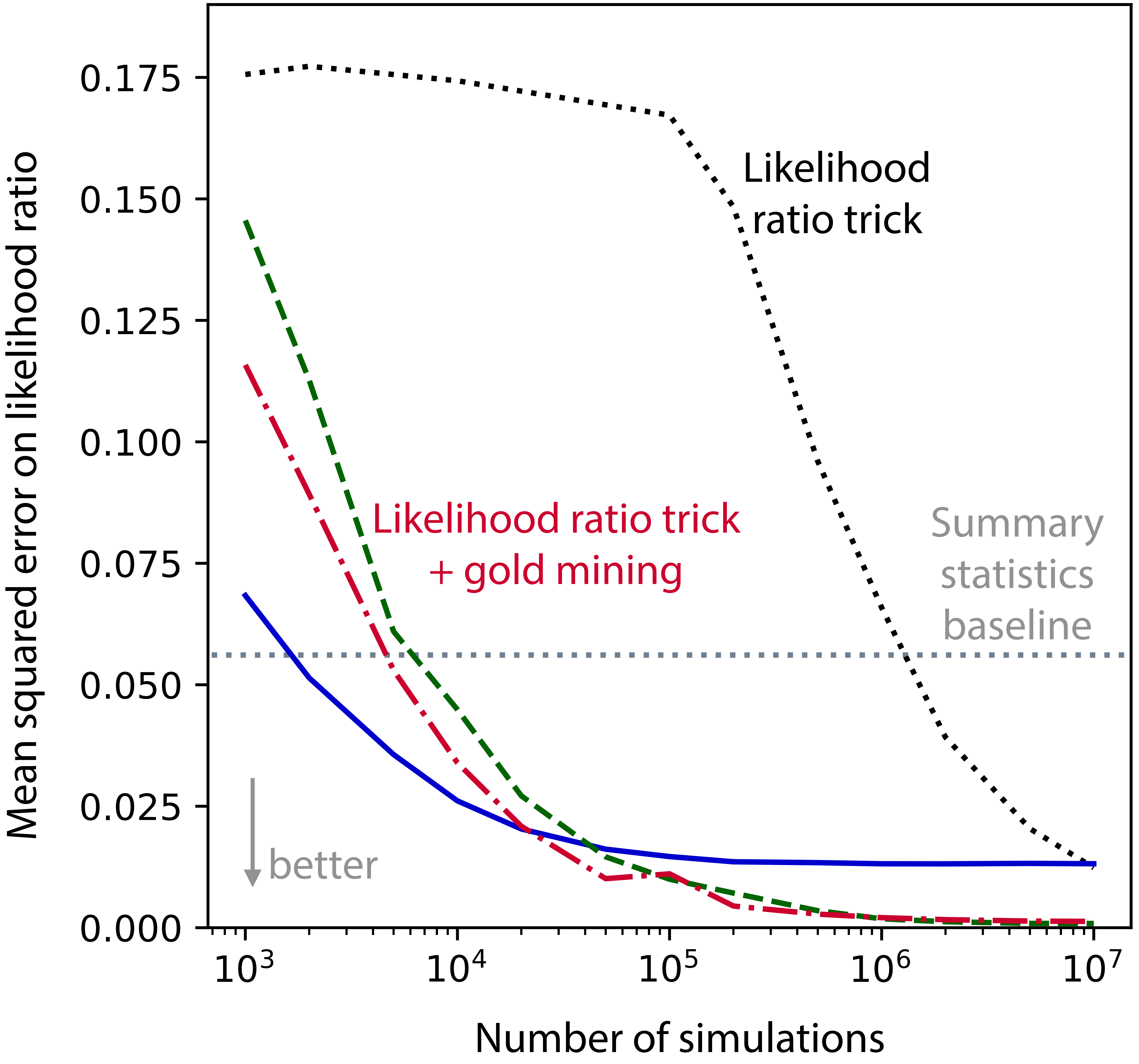
# Stronger limits…




In some regions of parameter space, the ML-based inference techniques improve the sensitivity as much as taking 90% more data would!

[JB, K. Cranmer, G. Louppe, J. Pavez 1805.00013; 1805.00020; M. Stoye, JB, K. Cranmer, G. Louppe, J. Pavez 1808.00973]

# …with less training data




With enough training data, the ML algorithms get the likelihood function right.

Using more information from the simulator improves sample efficiency substantially.

[JB, K. Cranmer, G. Louppe, J. Pavez 1805.00013; 1805.00020; M. Stoye, JB, K. Cranmer, G. Louppe, J. Pavez 1808.00973]

# Constraining operators in ttH effectively

[JB, F. Kling, I. Espejo, K. Cranmer 1907.10621]

- Pheno-level analysis of

  $$pp \to t\bar{t}\,h \to (b\ell^+)\,(\bar{b}\ell^-)\,(\gamma\gamma)\,E_T^{\text{miss}}$$

  with MadGraph + Pythia + Delphes

- Inference on three EFT operators:

$$\mathcal{O}_u = -\frac{1}{v^2}(H^\dagger H)(H^\dagger \bar{Q}_L)u_R\,,\ \mathcal{O}_G = \frac{g_s^2}{m_W^2}(H^\dagger H)G^a_{\mu\nu}G_a^{\mu\nu}\,,$$

$$\mathcal{O}_{uG} = -\frac{4g_s}{m_W^2}y_u(H^\dagger \bar{Q}_L)\gamma^{\mu\nu}T_a u_R G^a_{\mu\nu}$$

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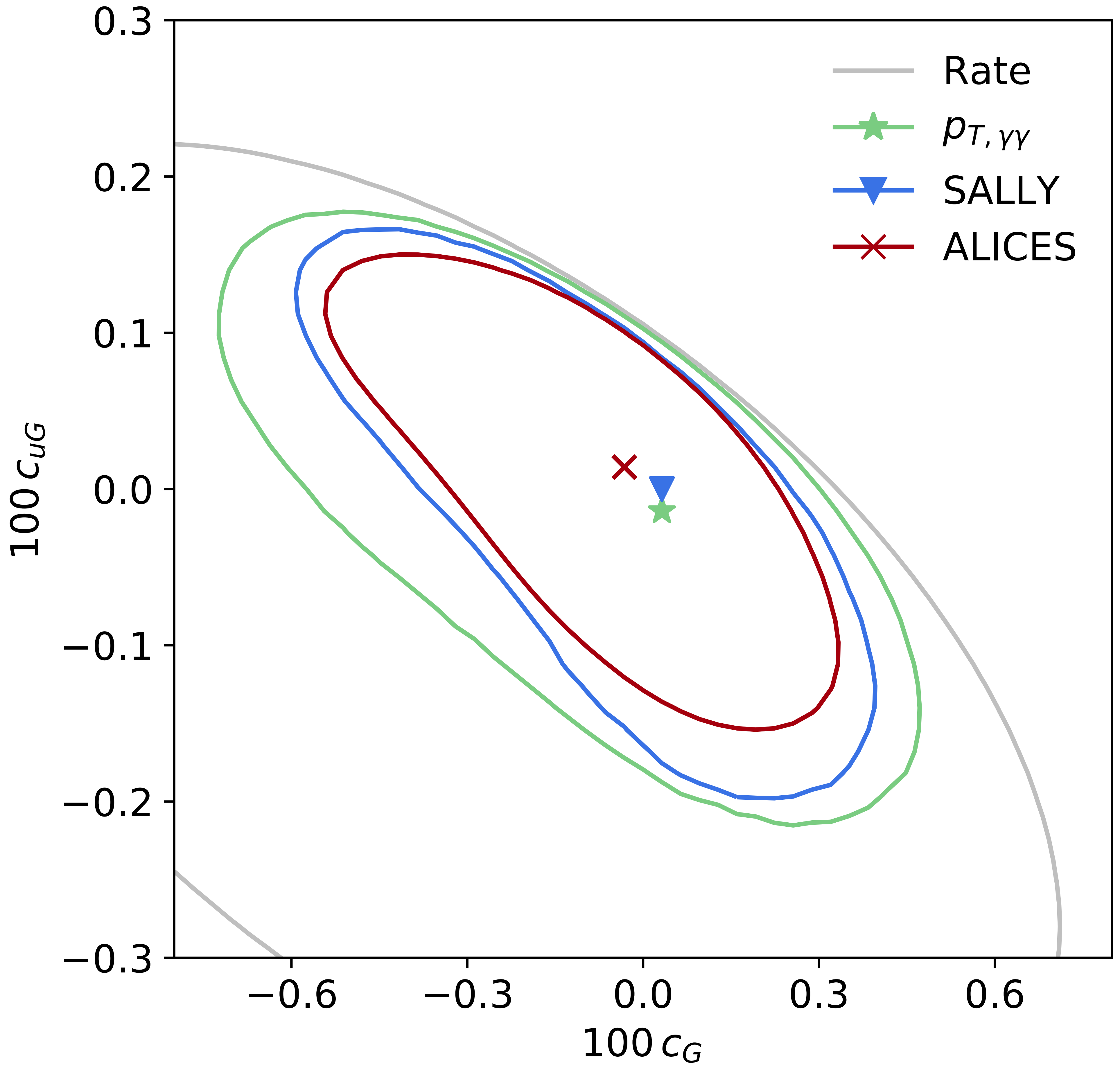
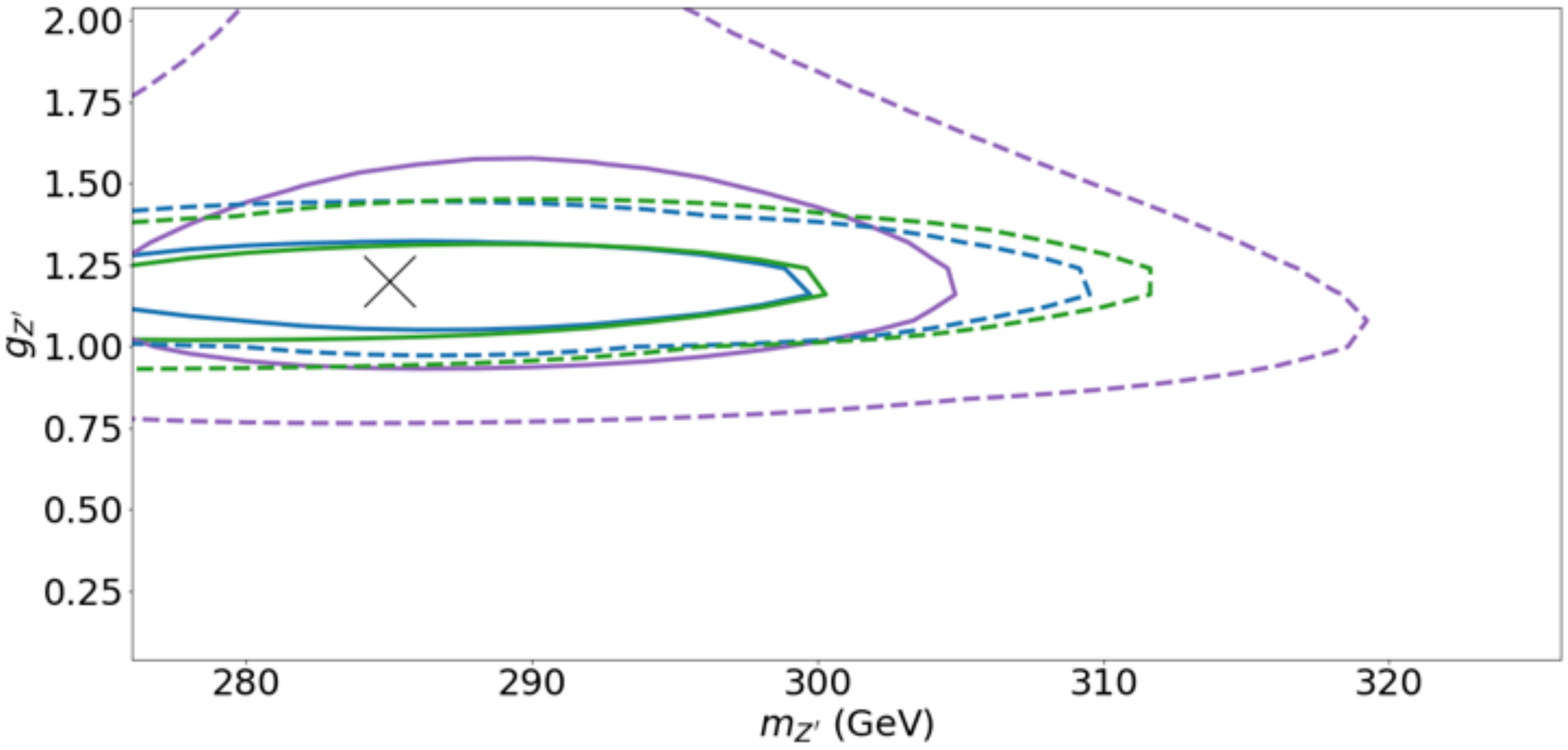
$$\mathcal{O}_{uG} = -\frac{4g_s}{m_W^2}y_u(H^\dagger \bar{Q}_L)\gamma^{\mu\nu}T_a u_R G^a_{\mu\nu}$$

- New inference techniques improve expected HL-LHC limits compared to histogram baseline:



# Hunting $Z' \to jj$

[J. Hollingworth, D. Whiteson 2002.04699]

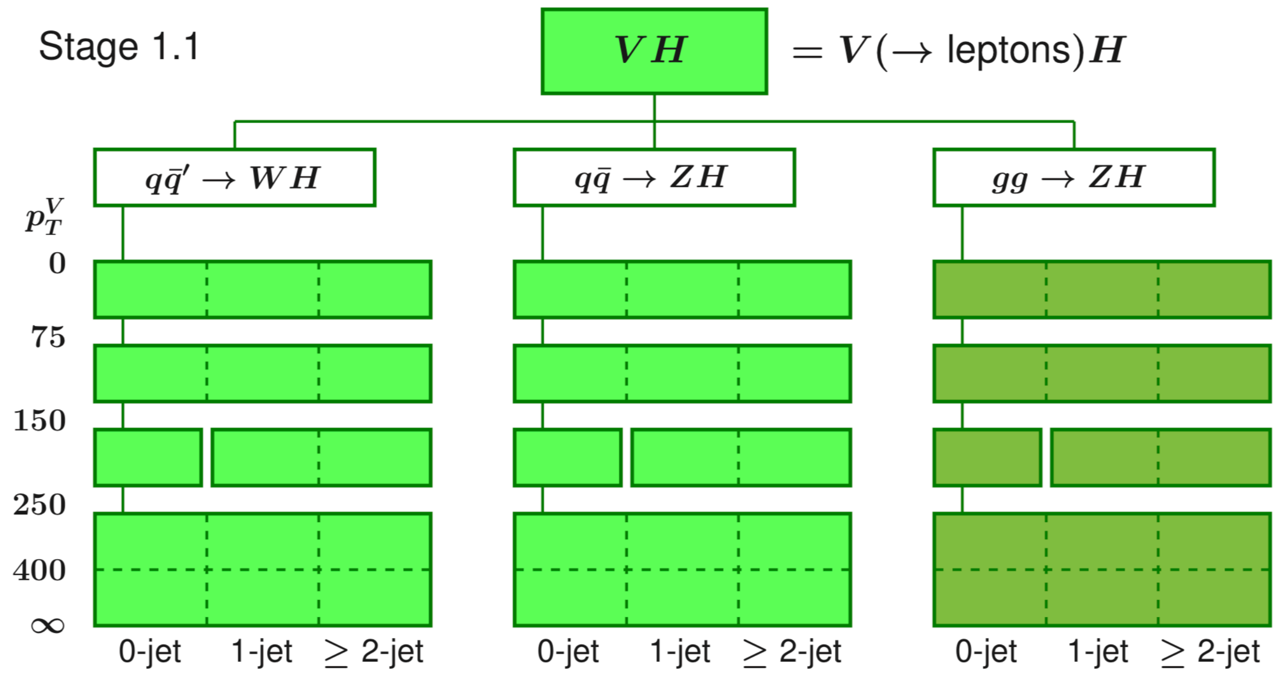



Multivariate analysis with new ML-based inference techniques leads to better expected limits than $m_{jj}$ analysis

# Benchmarking STXS in WH

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

- Simplified Template Cross-Sections (STXS) define observable bins that are supposed to capture as much information on NP as possible
  [N. Berger et al. 1906.02754; HXSWG YR4]




- Let's check! How much information on

$$\tilde{\mathcal{O}}_{HD} = \mathcal{O}_{H\Box} - \frac{\mathcal{O}_{HD}}{4} = (\phi^\dagger\phi)\Box(\phi^\dagger\phi) - \frac{1}{4}(\phi^\dagger D^\mu\phi)^*(\phi^\dagger D_\mu\phi)$$

$$\mathcal{O}_{HW} = \phi^\dagger\phi W^a_{\mu\nu}W^{\mu\nu a}$$

$$\mathcal{O}^{(3)}_{Hq} = (\phi^\dagger i\overleftrightarrow{D}^a_\mu\phi)(\overline{Q}_L\sigma^a\gamma^\mu Q_L)\ ,$$

can we extract from $pp \to WH \to \ell\nu\, b\bar{b}$ ?

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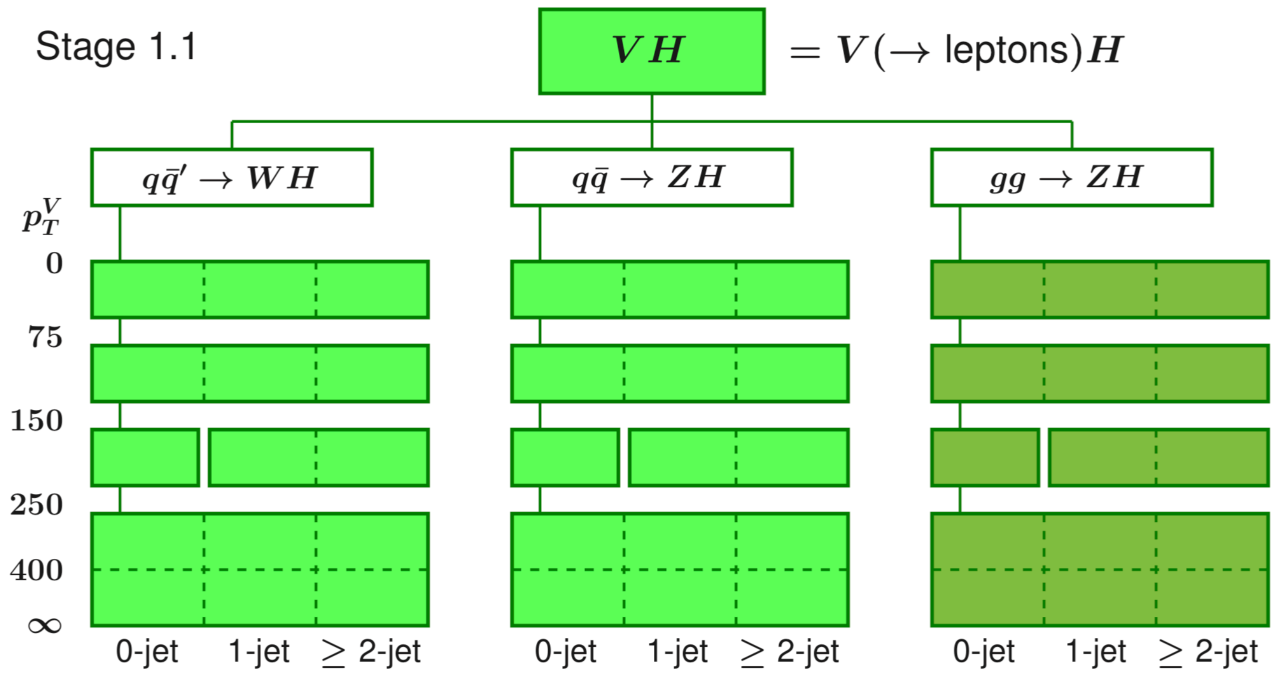


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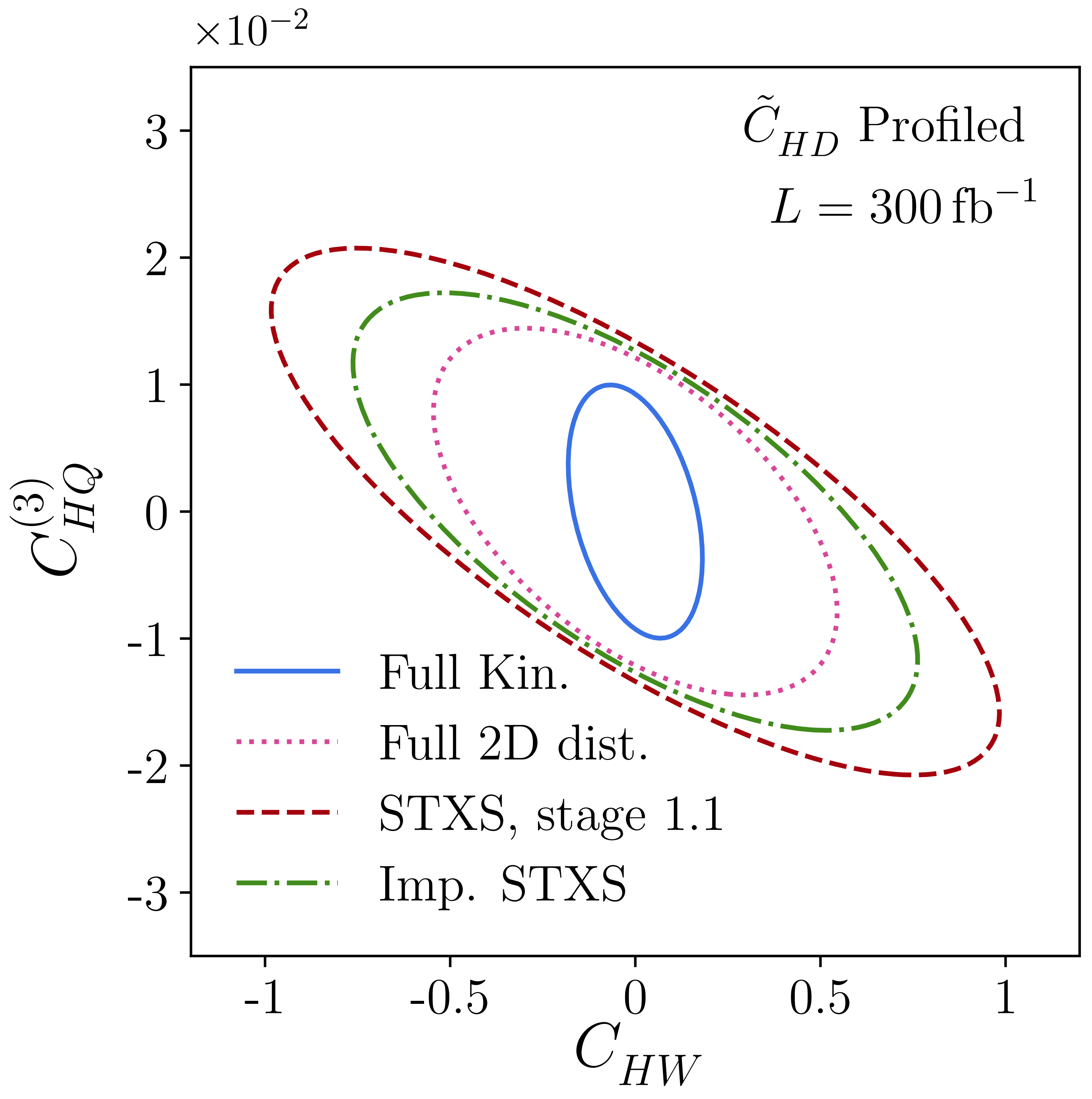
- Results: STXS are indeed sensitive to operators, adding a few more bins improve them, but a multivariate analysis is still stronger



# Automation

[JB, F. Kling, I. Espejo, K. Cranmer 1907.10621]

Our open-source Python package MadMiner makes it straightforward to apply these ML-based inference techniques

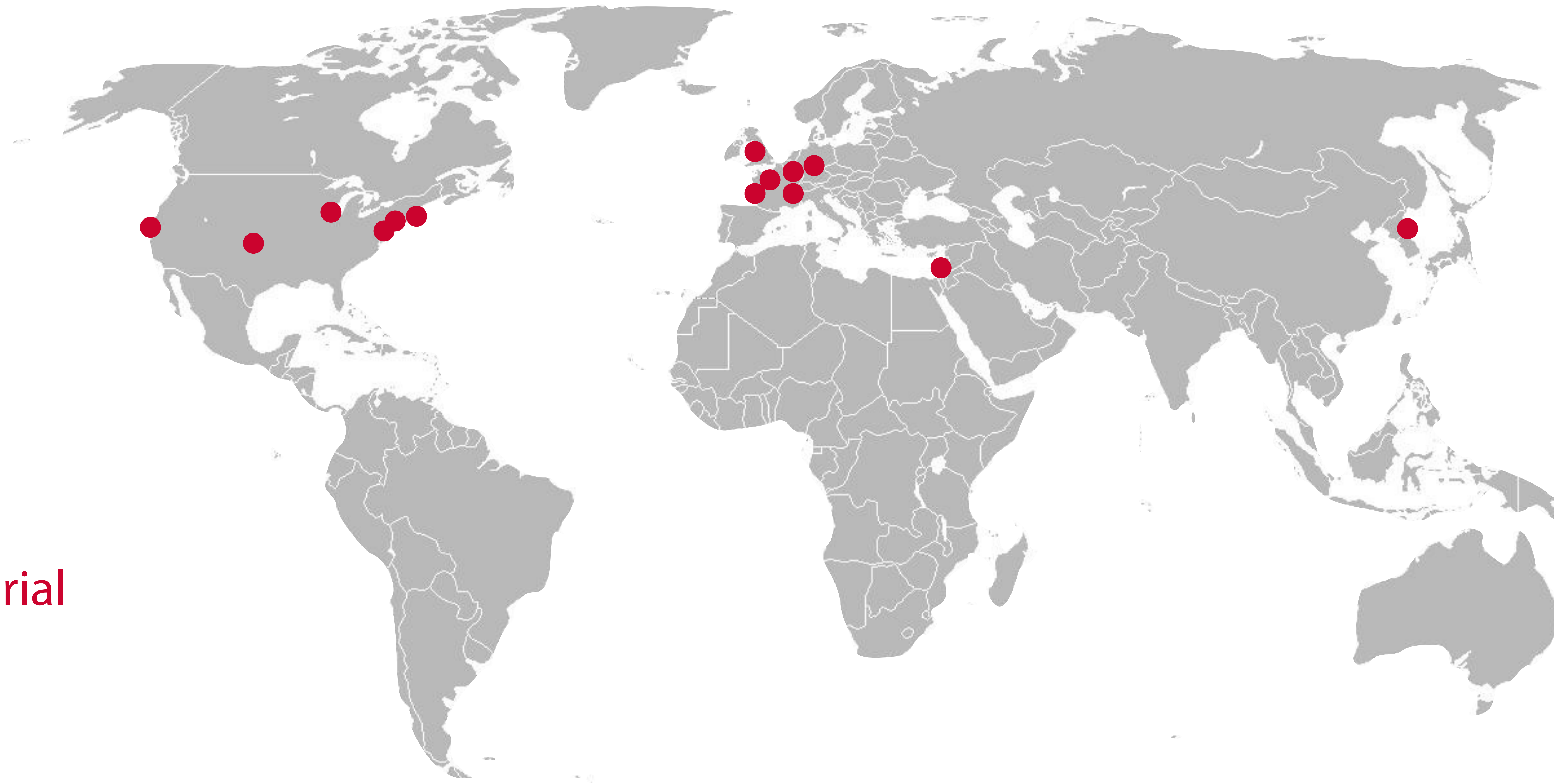
github.com/diana-hep/madminer

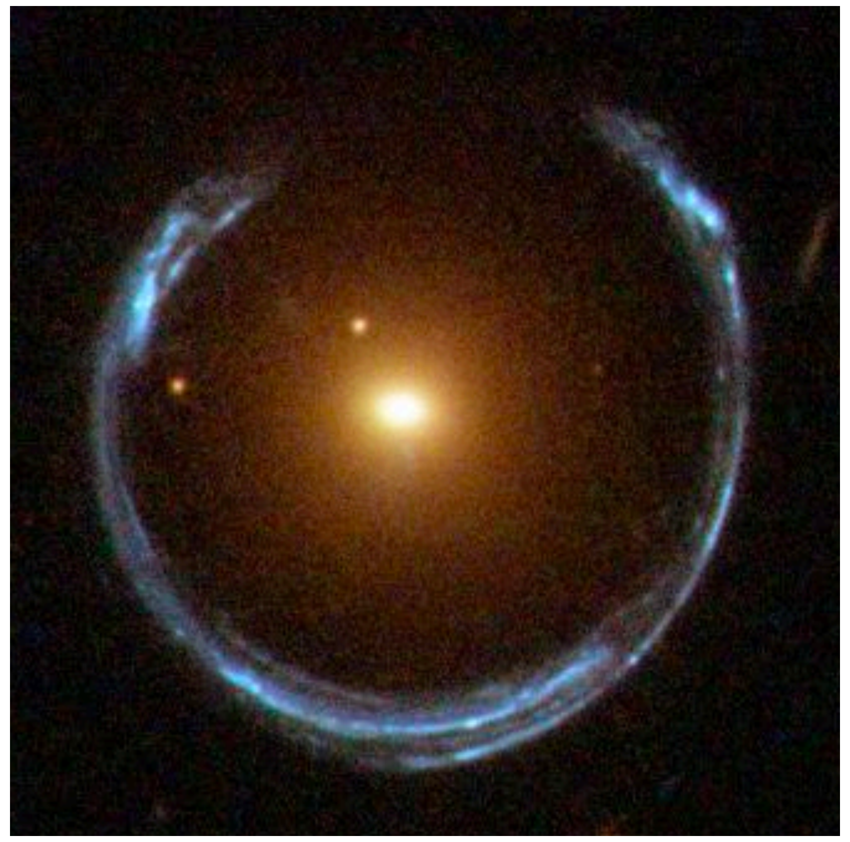
`pip install madminer`

hub.docker.com/u/madminertool

cranmer.github.io/madminer-tutorial

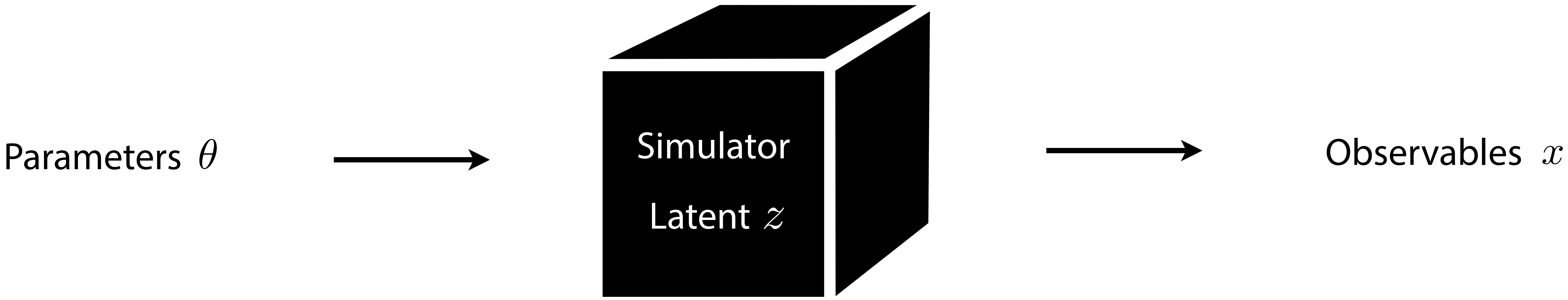
madminer.readthedocs.io





# 5. Beyond the LHC

# Simulation-based ("likelihood-free") inference problems…



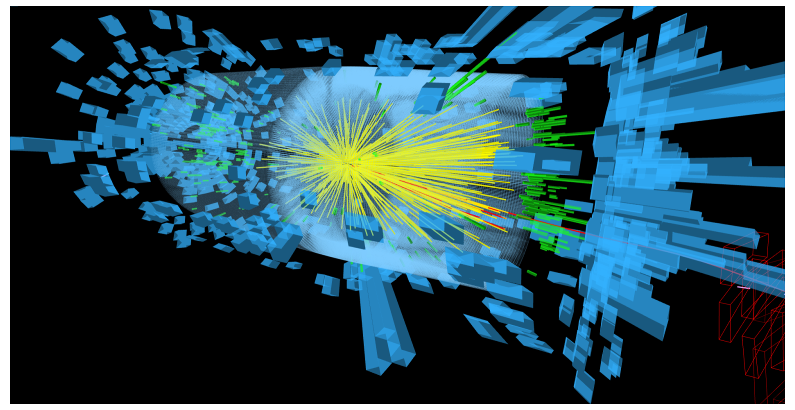

**Prediction:**

- Well-motivated mechanistic, causal model
- Simulator can generate samples $x \sim p(x|\theta)$

**Inference:**

- Interactions between low-level components lead to challenging inverse problems
- Likelihood $p(x|\theta) = \int \mathrm{d}z \; p(x, z|\theta)$ is intractable

# … appear in many fields of science



Collider experiments

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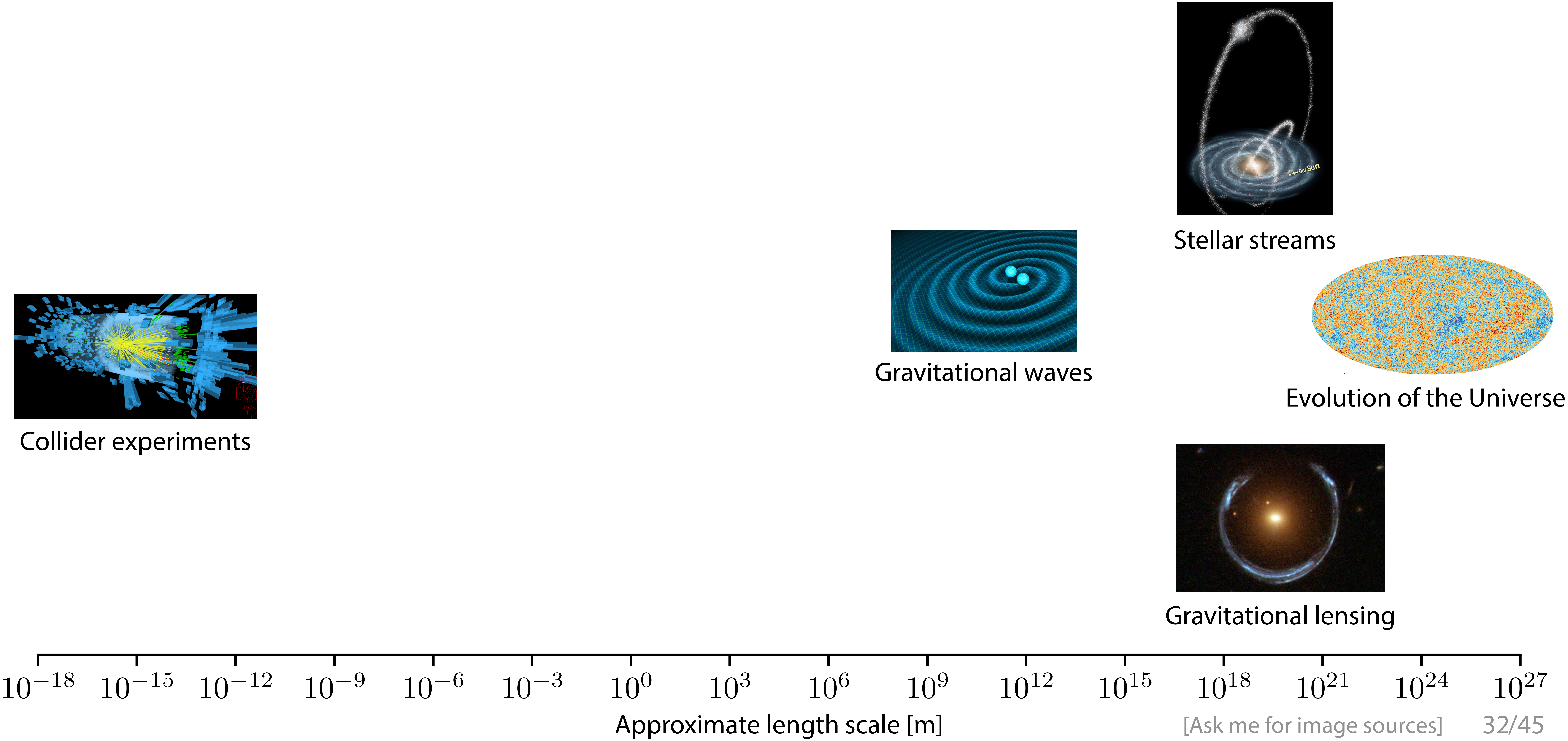
Approximate length scale [m]

[Ask me for image sources]

# … appear in many fields of science

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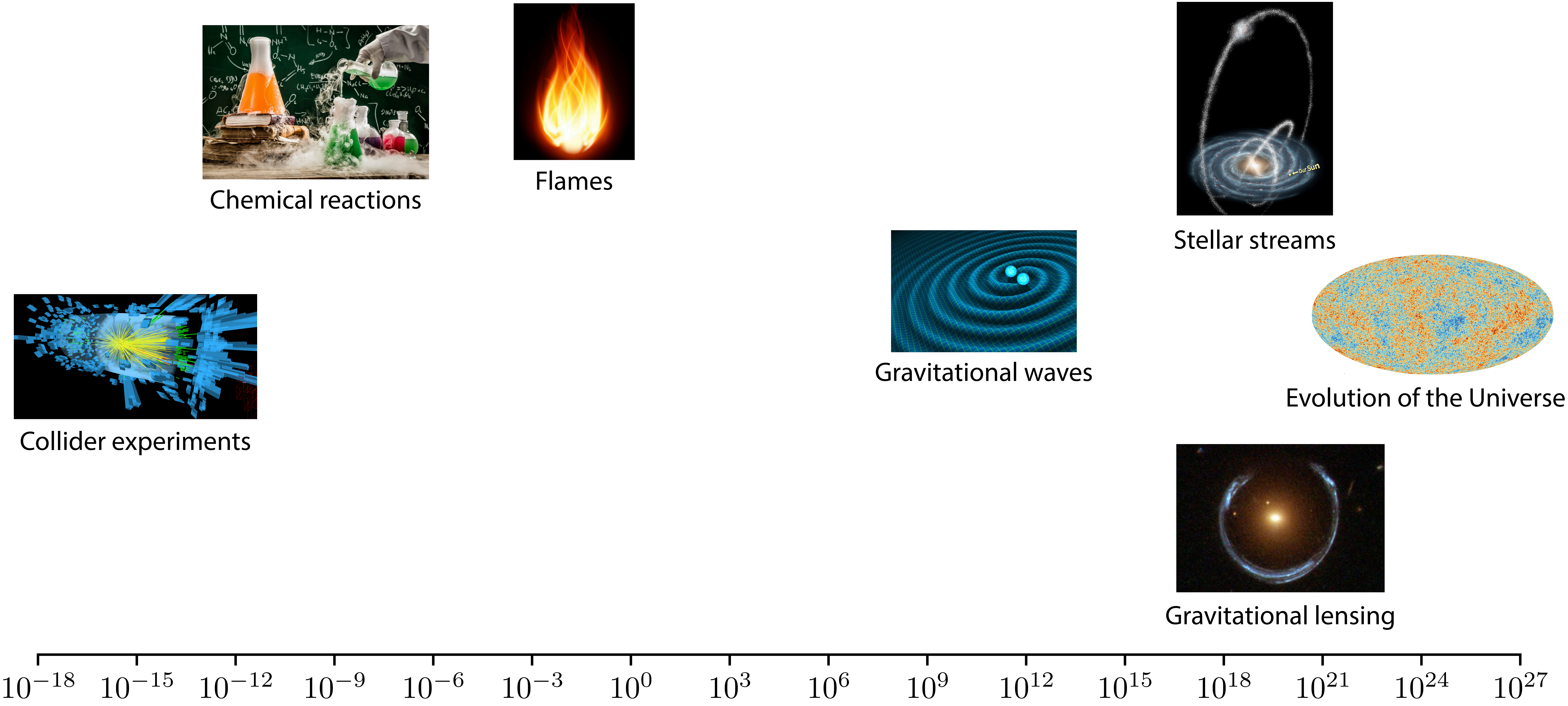
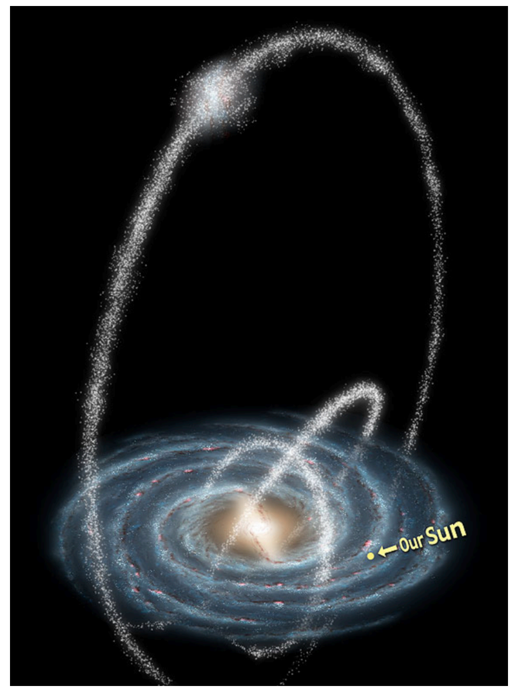



Approximate length scale [m]

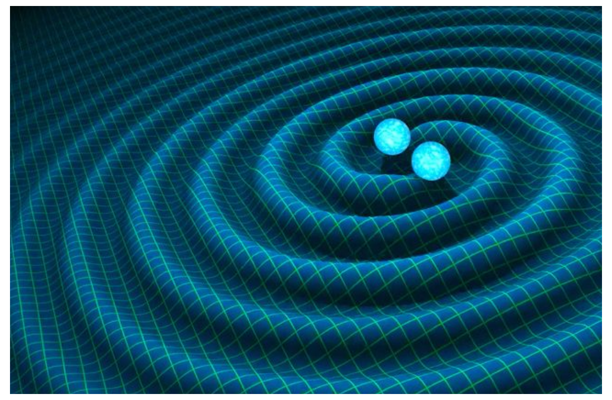
# … appear in many fields of science

Chemical reactions

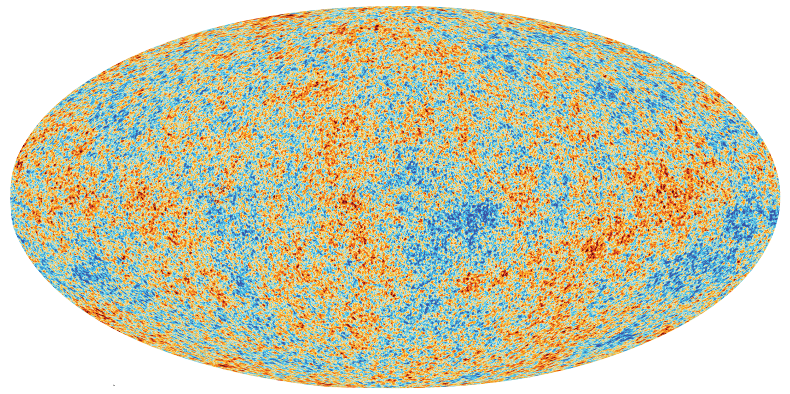
Flames



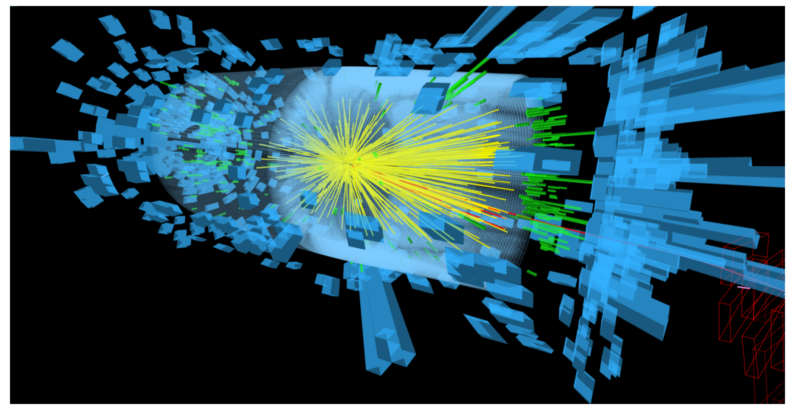

Stellar streams



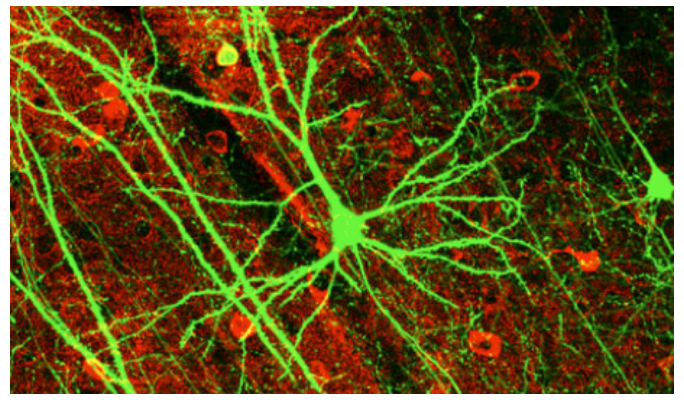
Gravitational waves



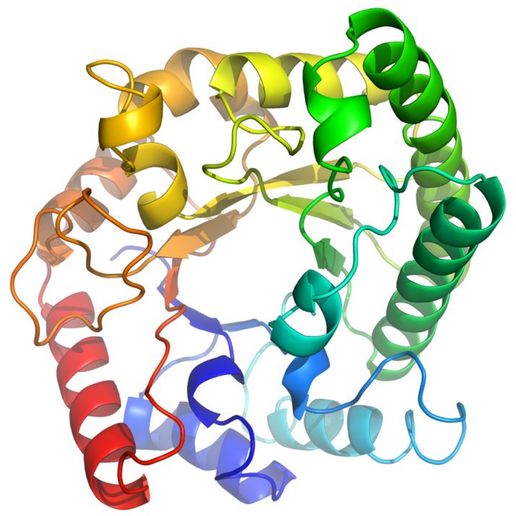
Evolution of the Universe



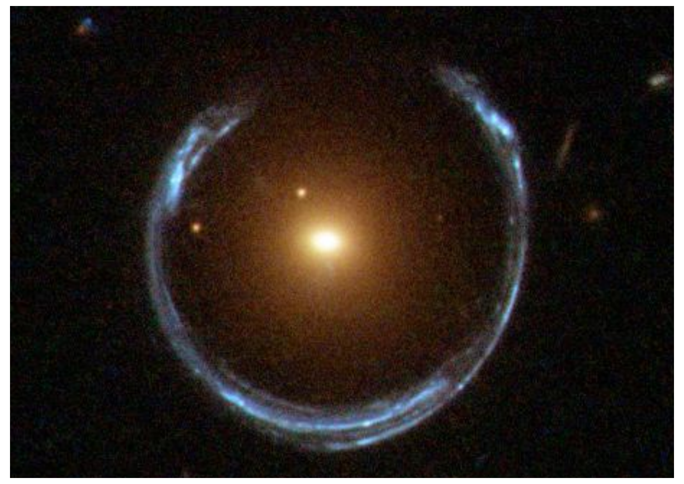
Collider experiments



Neurons



Protein networks



Gravitational lensing

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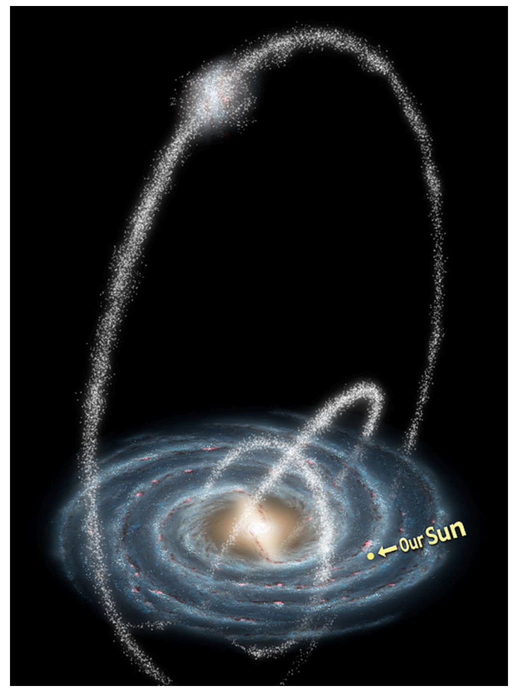
Flames



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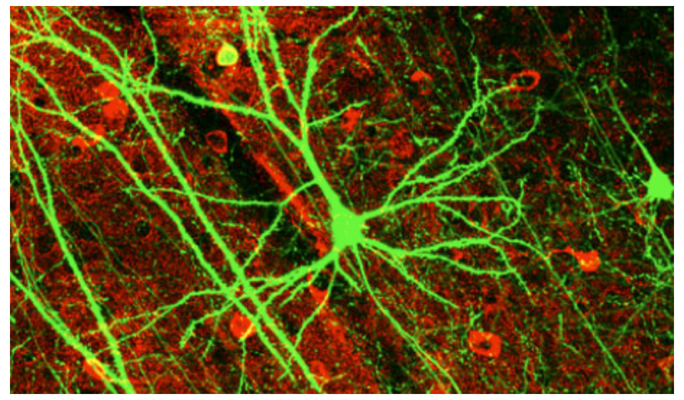
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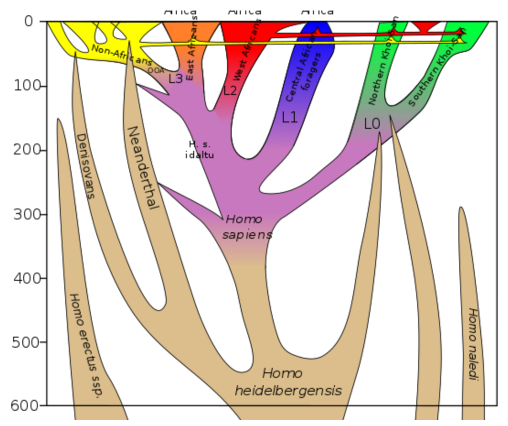
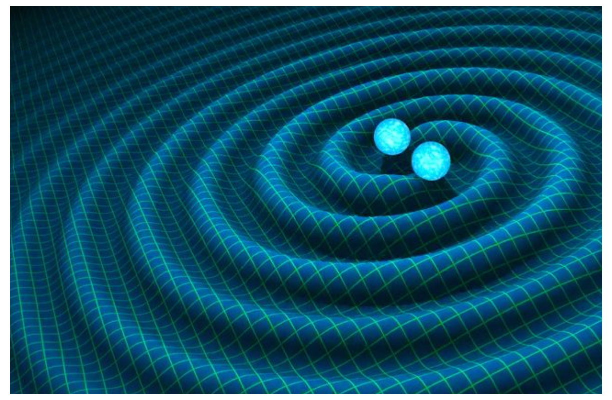

Evolution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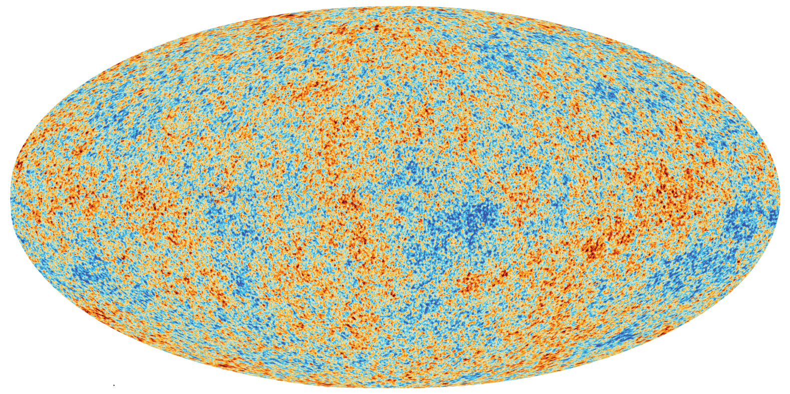
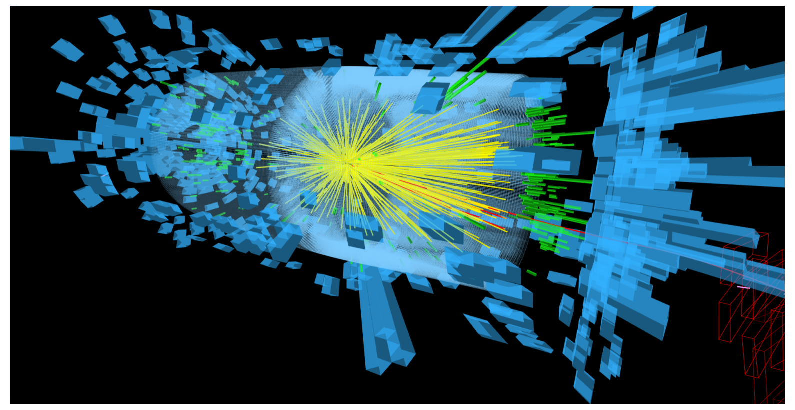
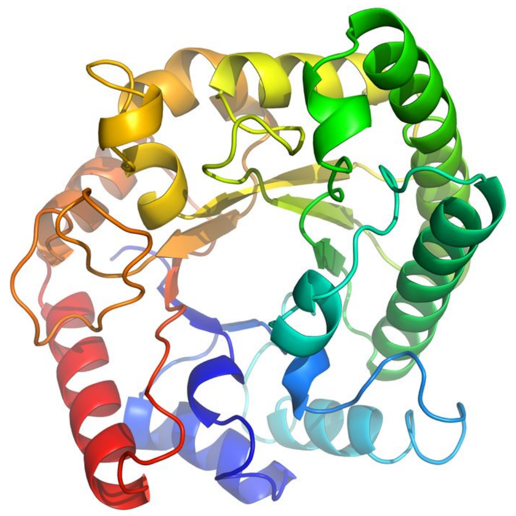
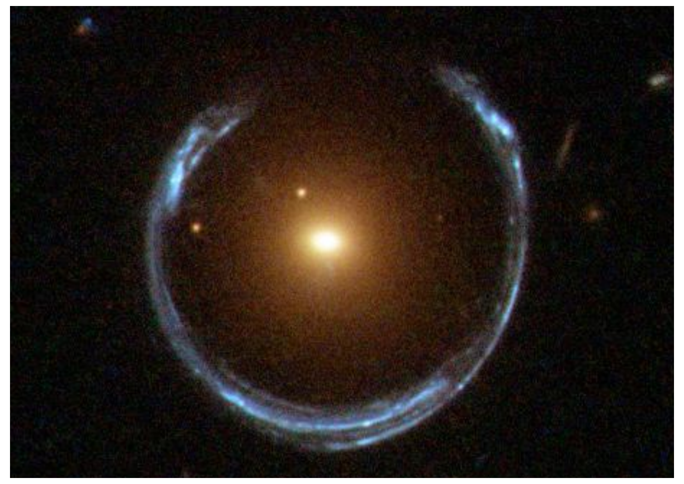

Evolution of the Universe


Collider experiments


Protein networks


Ecological systems


Gravitational lensing

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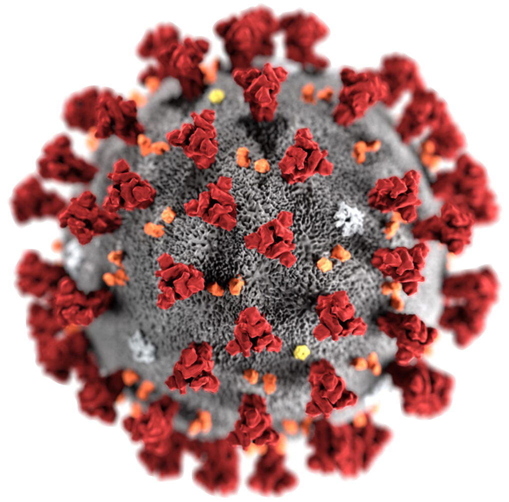
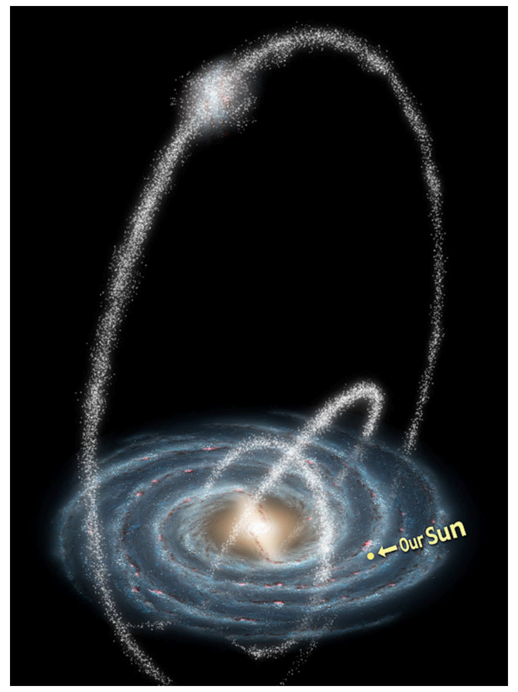
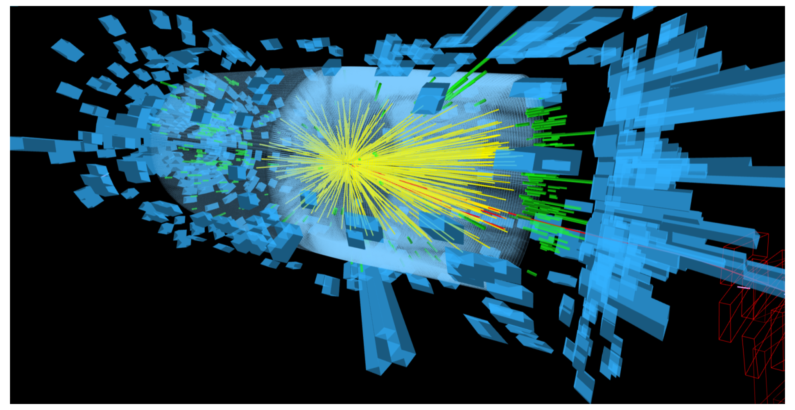
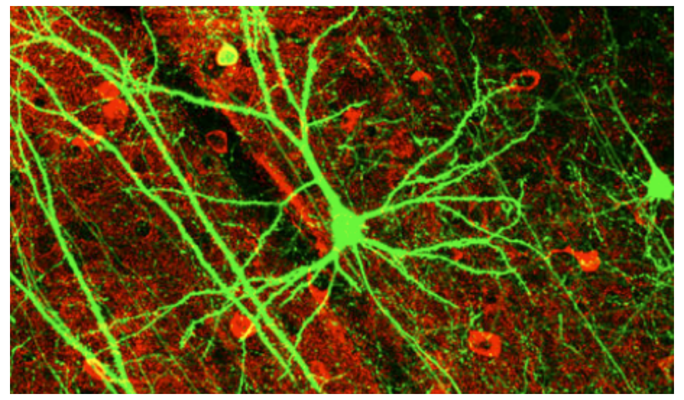

Epidemics

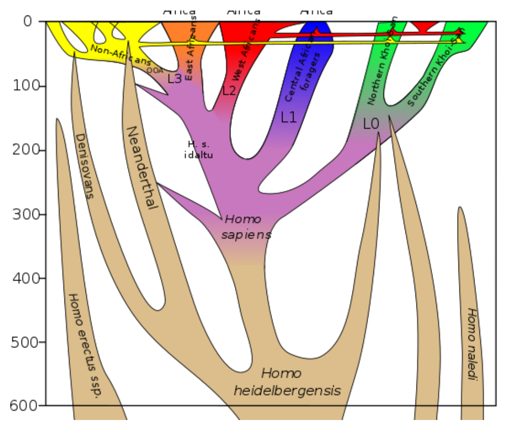


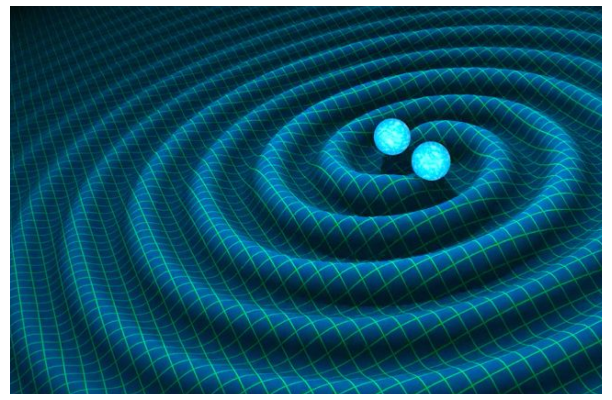
Stellar streams

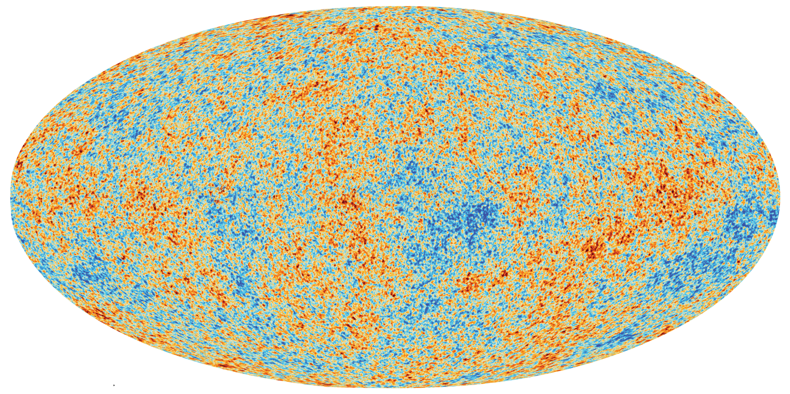

Collider experiments


Neurons


Robotics


Evolution


Gravitational waves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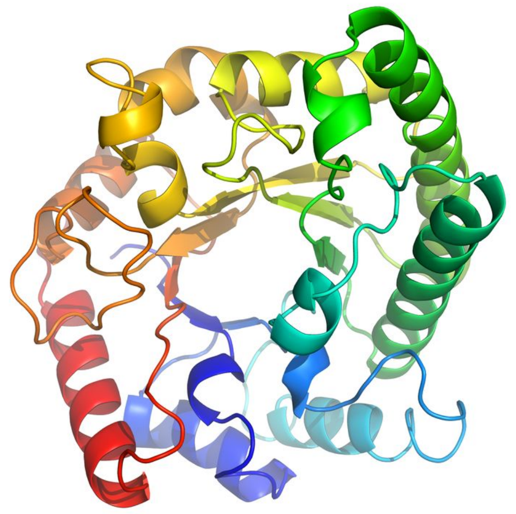
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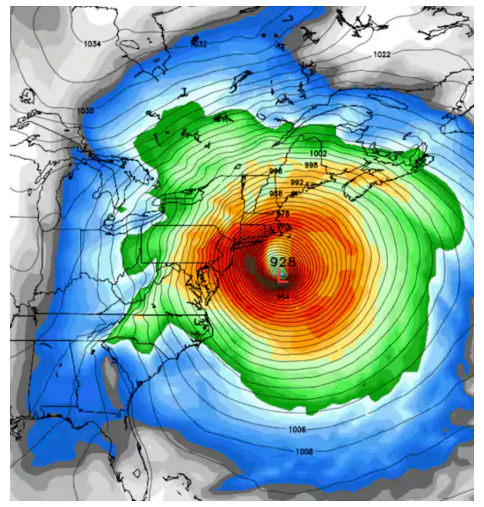
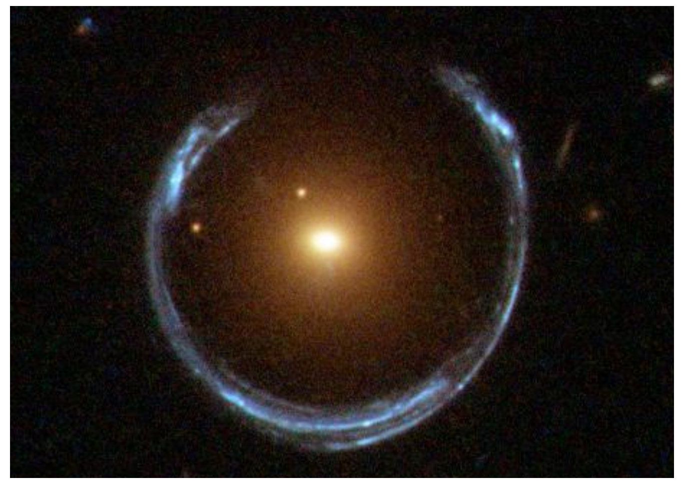

Weather and climate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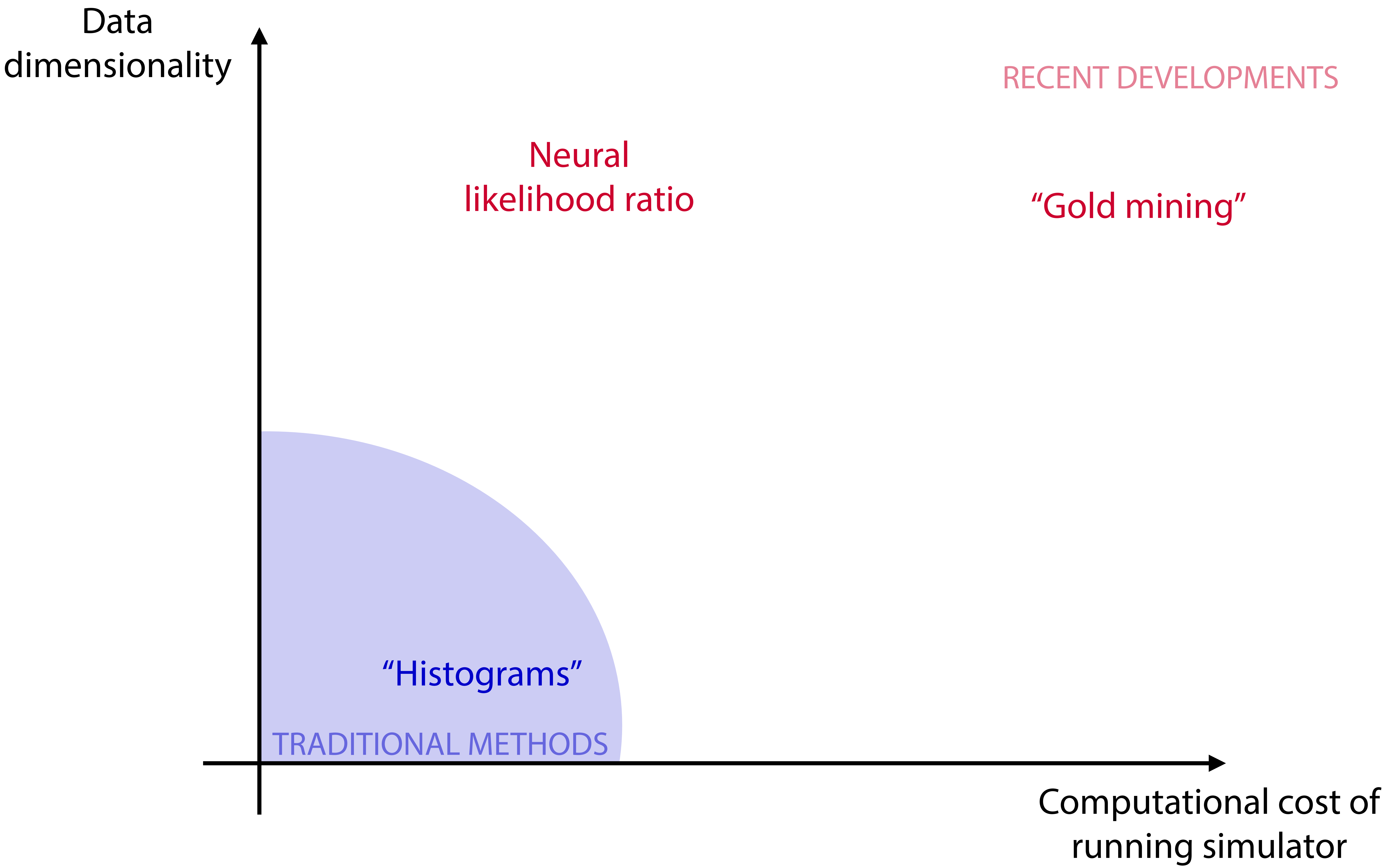
Approximate length scale [m]

[Ask me for image sources]

# The frontier of simulation-based inference

[K. Cranmer, JB, G. Louppe 1911.01429]



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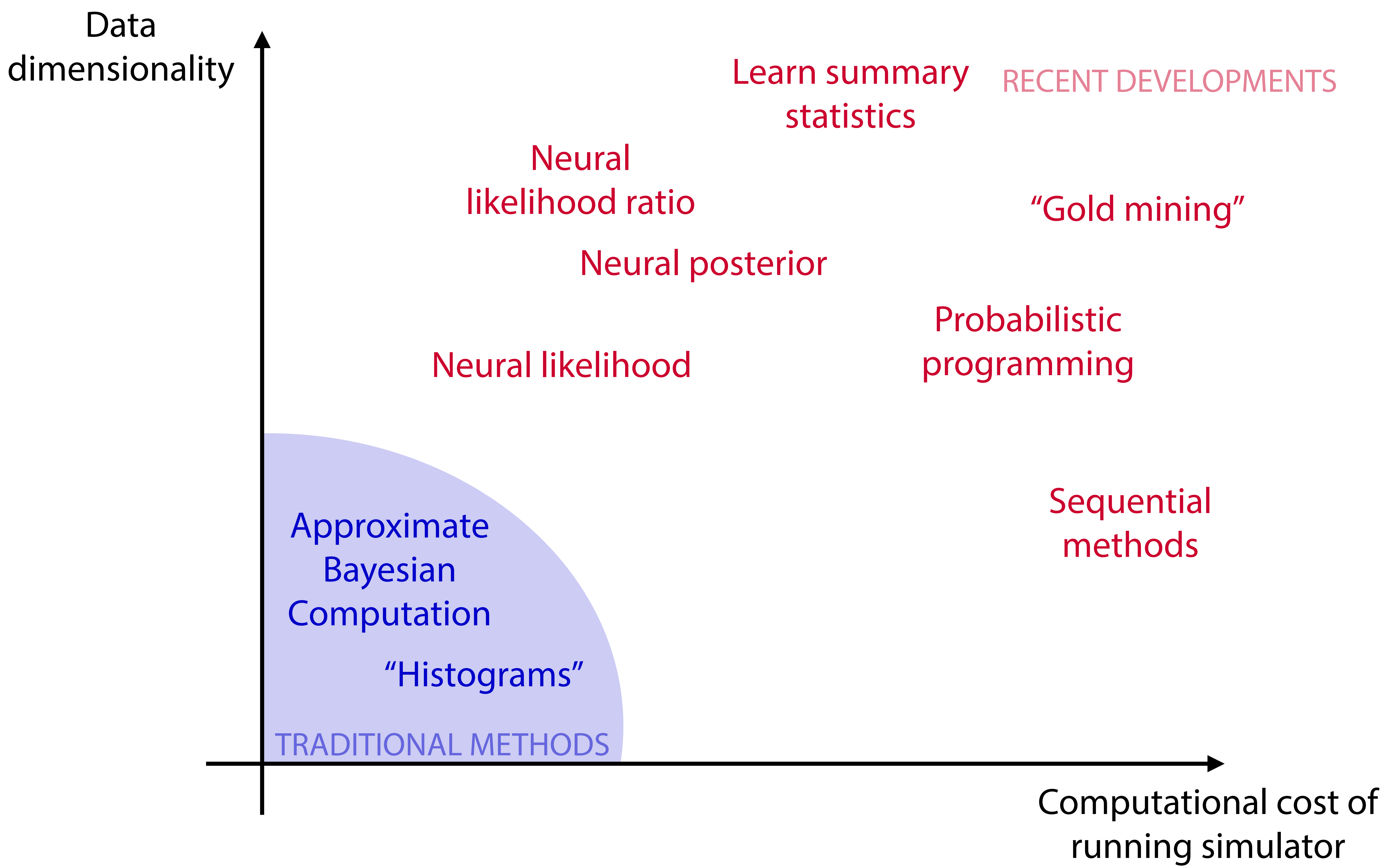

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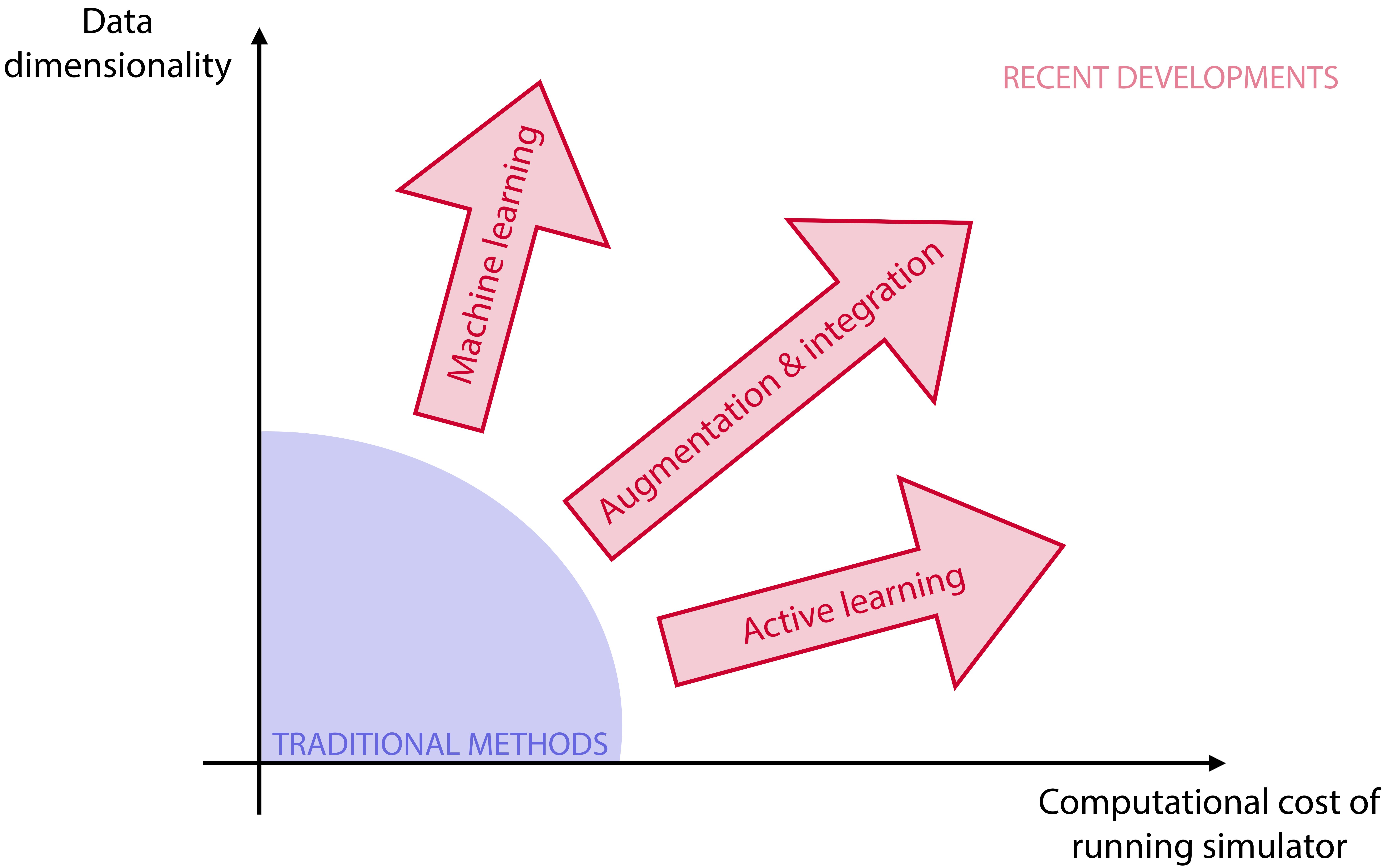

Th… …e

[K. Cranmer, JB, G. Louppe 1911.01429]

Check for updates

COLLOQUIUM PAPER

# 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, New York, NY 10003; [b]Center for Data Science, New York University, New York, NY 10011; and [c]Montefiore Institute, University of Liège, B-4000 Liège, Belgium

Edited by Jitendra Malik, University of California, Berkeley, CA, and approved April 10, 2020 (received for review November 4, 2019)

**Many domains of science have developed complex simulations to describe phenomena of interest. While these simulations provide high-fidelity models, they are poorly suited for inference and lead to challenging inverse problems. We review the rapidly developing field of simulation-based inference and identify the forces giving additional momentum to the field. Finally, we describe how the frontier is expanding so that a broad audience can appreciate the profound influence these developments may have on science.**

statistical inference | implicit models | likelihood-free inference | approximate Bayesian computation | neural density estimation

Mechanistic models can be used to predict how systems will behave in a variety of circumstances. These run the gamut of distance scales, with notable examples including particle physics, molecular dynamics, protein folding, population genetics, neuroscience, epidemiology, economics, ecology, climate science, astrophysics, and cosmology. 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. Unfortunately, these simulators are poorly suited for statistical inference. The source of the challenge is that the probability density (or likelihood) for a given observation—an essential ingredient for both frequentist and Bayesian inference methods—is typically intractable. Such models are often referred to as implicit models and contrasted against prescribed models where the likelihood for an observation can be explicitly calculated (1). The problem setting of statistical inference under intractable likelihoods has been dubbed likelihood-free inference—although it is a bit of a misnomer as typically one attempts to estimate the intractable likelihood, so we feel the term simulation-based inference is more apt.

The intractability of the likelihood is an obstruction for scientific progress as statistical inference is a key component of the scientific method. In areas where this obstruction has appeared, scientists have developed various ad hoc or field-specific methods to overcome it. In particular, two common traditional approaches rely on scientists to use their insight into the system to construct powerful summary statistics and then compare the observed data to the simulated data. In the first one, density estimation methods are used to approximate the distribution of

the simulator—is being recognized as a key idea to improve the sample efficiency of various inference methods. A third direction of research has stopped treating the simulator as a black box and focused on integrations that allow the inference engine to tap into the internal details of the simulator directly.

Amidst this ongoing revolution, the landscape of simulation-based inference is changing rapidly. In this review we aim to provide the reader with a high-level overview of the basic ideas behind both old and new inference techniques. Rather than discussing the algorithms in technical detail, we focus on the current frontiers of research and comment on some ongoing developments that we deem particularly exciting.

## Simulation-Based Inference

**Simulators.** Statistical inference is performed within the context of a statistical model, and in simulation-based inference the simulator itself defines the statistical model. For the purpose of this paper, a simulator is a computer program that takes as input a vector of parameters $\theta$, samples a series of internal states or latent variables $z_i \sim p_i(z_i|\theta, z_{<i})$, and finally produces a data vector $x \sim p(x|\theta, z)$ as output. Programs that involve random samplings and are interpreted as statistical models are known as probabilistic programs, and simulators are an example. Within this general formulation, real-life simulators can vary substantially:

- The parameters $\theta$ describe the underlying mechanistic model and thus affect the transition probabilities $p_i(z_i|\theta, z_{<i})$. Typically the mechanistic model is interpretable by a domain scientist and $\theta$ has relatively few components and a fixed dimensionality. Examples include coefficients found in the Hamiltonian of a physical system, the virulence and incubation rate of a pathogen, or fundamental constants of Nature.
- The latent variables $z$ that appear in the data-generating process may directly or indirectly correspond to a physically meaningful state of a system, but typically this state is unobservable in practice. The structure of the latent space varies substantially between simulators. The latent variables may be continuous or discrete and the dimensionality of the latent space may be fixed or may vary, depending on the control flow of the simulator. The simulation can freely combine deterministic and stochastic steps. The deterministic components of the simulator may be differentiable or may involve discontinuous control

STATISTICS

…CENT DEVELOPMENTS

Computational cost of running simulator

[K. Cranmer, JB, G. Louppe 1911.01429]

# Th… …e

# 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, New York, NY 10003; [b]Center for Data Science, New Yor…
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statistical inference | implicit models | likelihood-free inference | approximate Bayesian computation | neural density estimation


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**Simulation-Based Inference**

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of a statistical model, and in sim…
simulator itself defines the statisti…
of this paper, a simulator is a co…
as input a vector of parameters $\theta$, …
states or latent variables $z_i \sim p_i(z_i$…
a data vector $x \sim p(x|\theta, z)$ as ou…
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known as probabilistic programs, …
ple. Within this general formulation…
substantially:

- The parameters $\theta$ describe the u… and thus affect the transition pro… ically the mechanistic model is… scientist and $\theta$ has relatively fe… dimensionality. Examples includ… Hamiltonian of a physical system,… rate of a pathogen, or fundament…
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# Likelihood-Free Inference Workshop

18-22 March 2019 @ Flatiron Institute, NYC

Home Schedule Hackathon Logistics Participants Registration

## Rationale

The goal of this interdisciplinary meeting is to gather developers and users of Likelihood-Free Inference methods to share latest techniques, use cases and applications across different fields, and discuss open challenges.

The first two days of the workshop will be focused on talks and discussions, while the remaining of the week will be dedicated to a hackathon with the goal of seeding the development of a common probabilistic programming framework for Likelihood-Free Inference as well as collaboratively working on LFI-related hack projects.

## News

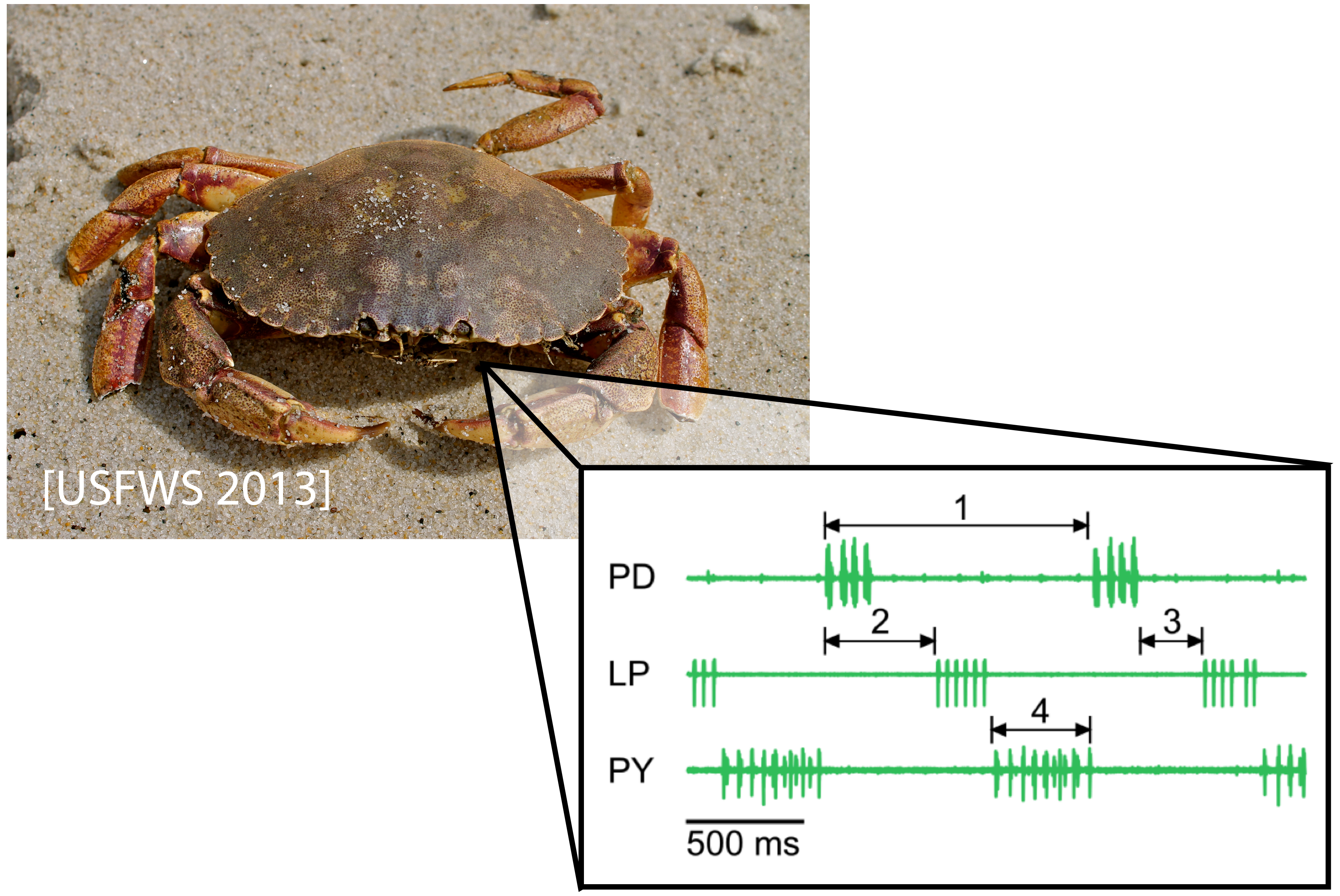
- *March 4th, 2019* : Preliminary schedule available, new Gitter channel chat on gitter, new Hackathon page
- *February 19th, 2019* : Main registration is closed, contact organizers for late registration
- *February 19th, 2019* : Travel funding application deadline
- *February 6th, 2019* : Opening registration

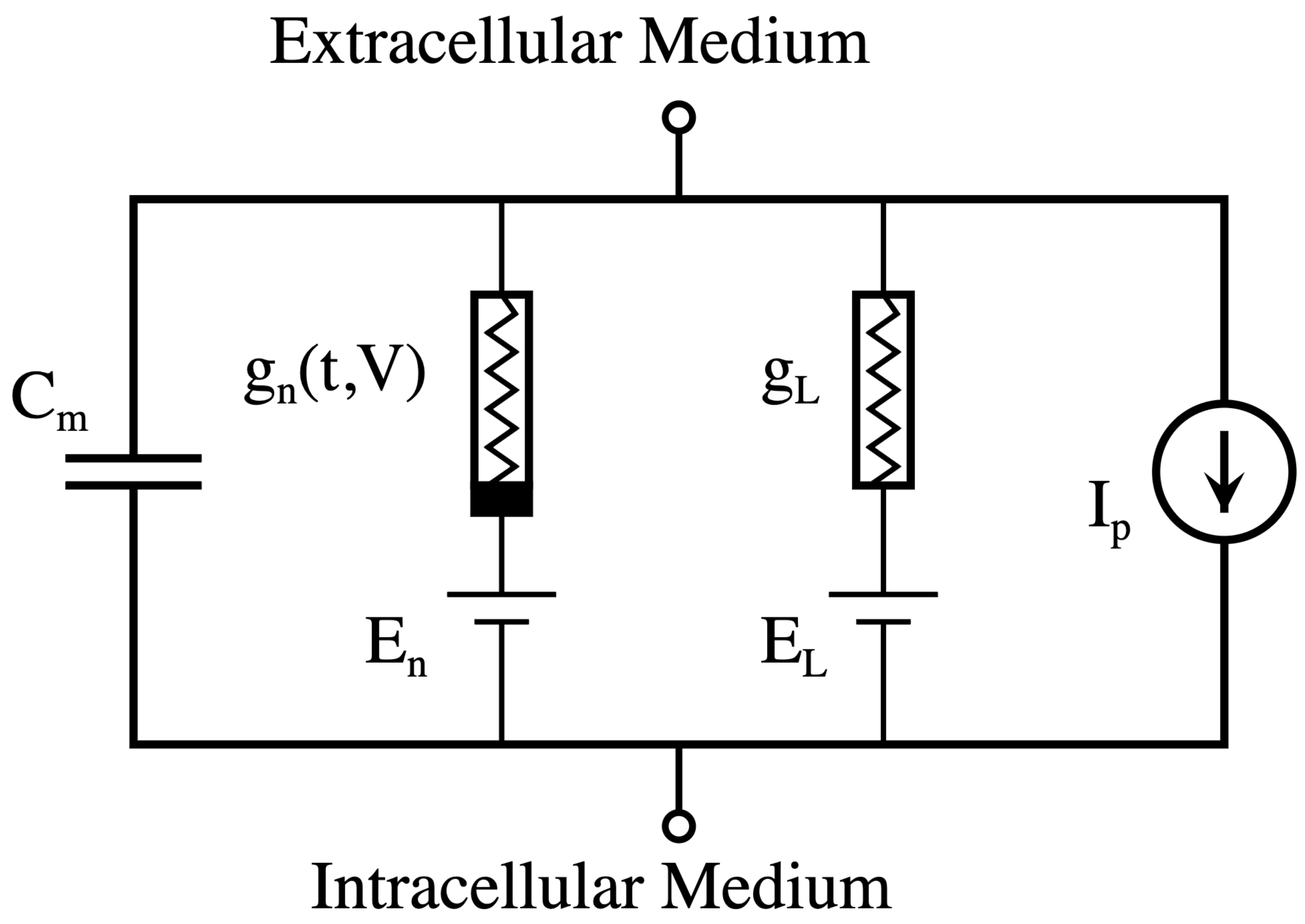
## Organizing Committee

- Justin Alsing, Oskar Klein Center, Stockholm University
- Johann Brehmer, Center for Data Science, New York University
- Stephen Feeney, Center for Computational Astrophysics, Flatiron Institute

# Neuroscience example

[P. Gonçalves et al., bioRxiv:10.1101.838383]



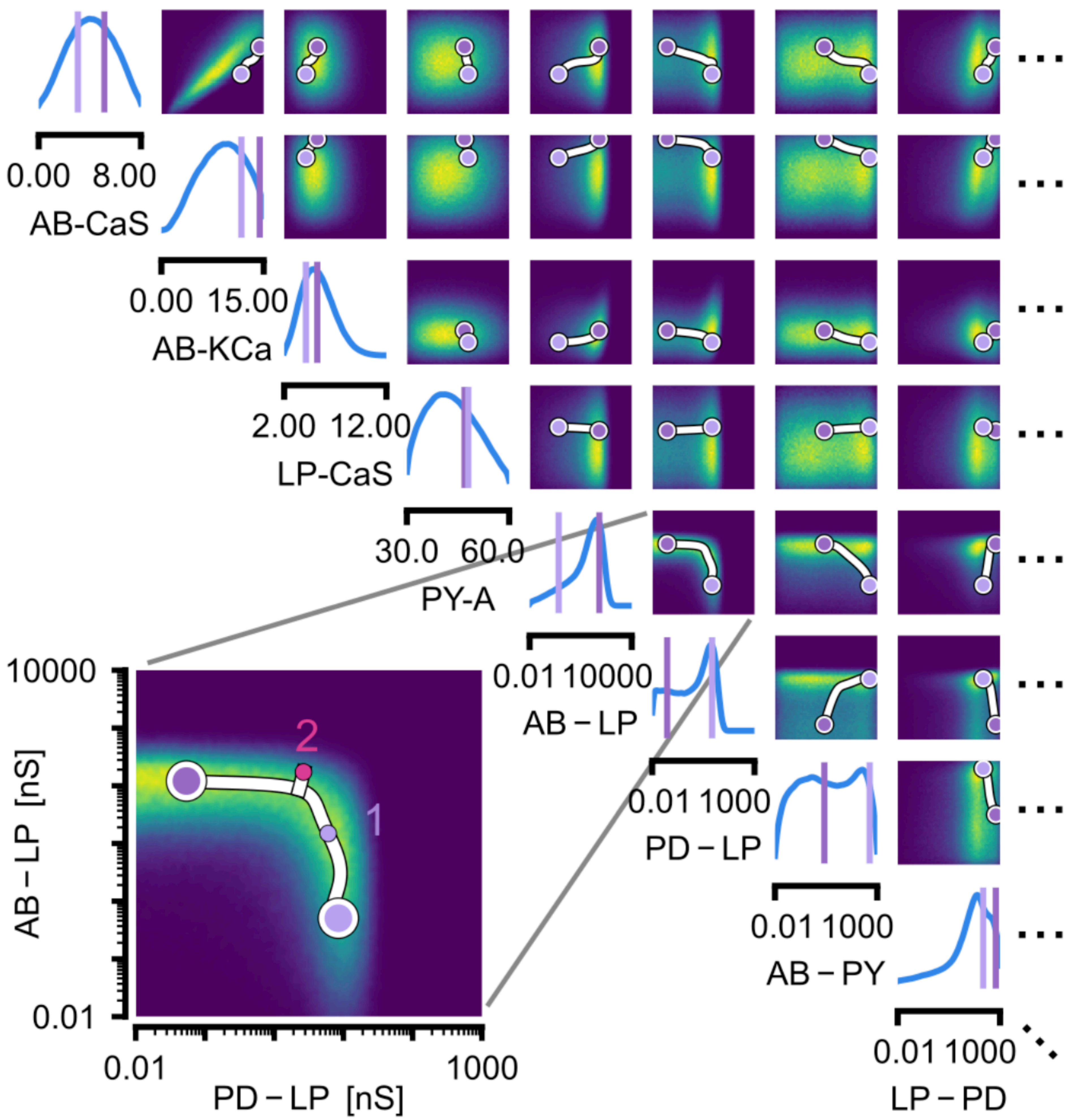

Activity recordings in stomatogastric ganglion nerve cells in Jonah Crabs

Goal: infer 31 parameters of Hodgkin-Huxley model of neuron dynamics

# Crab results

[P. Gonçalves et al., bioRxiv:10.1101.838383]

Bayesian posterior



# Gravitational lensing example

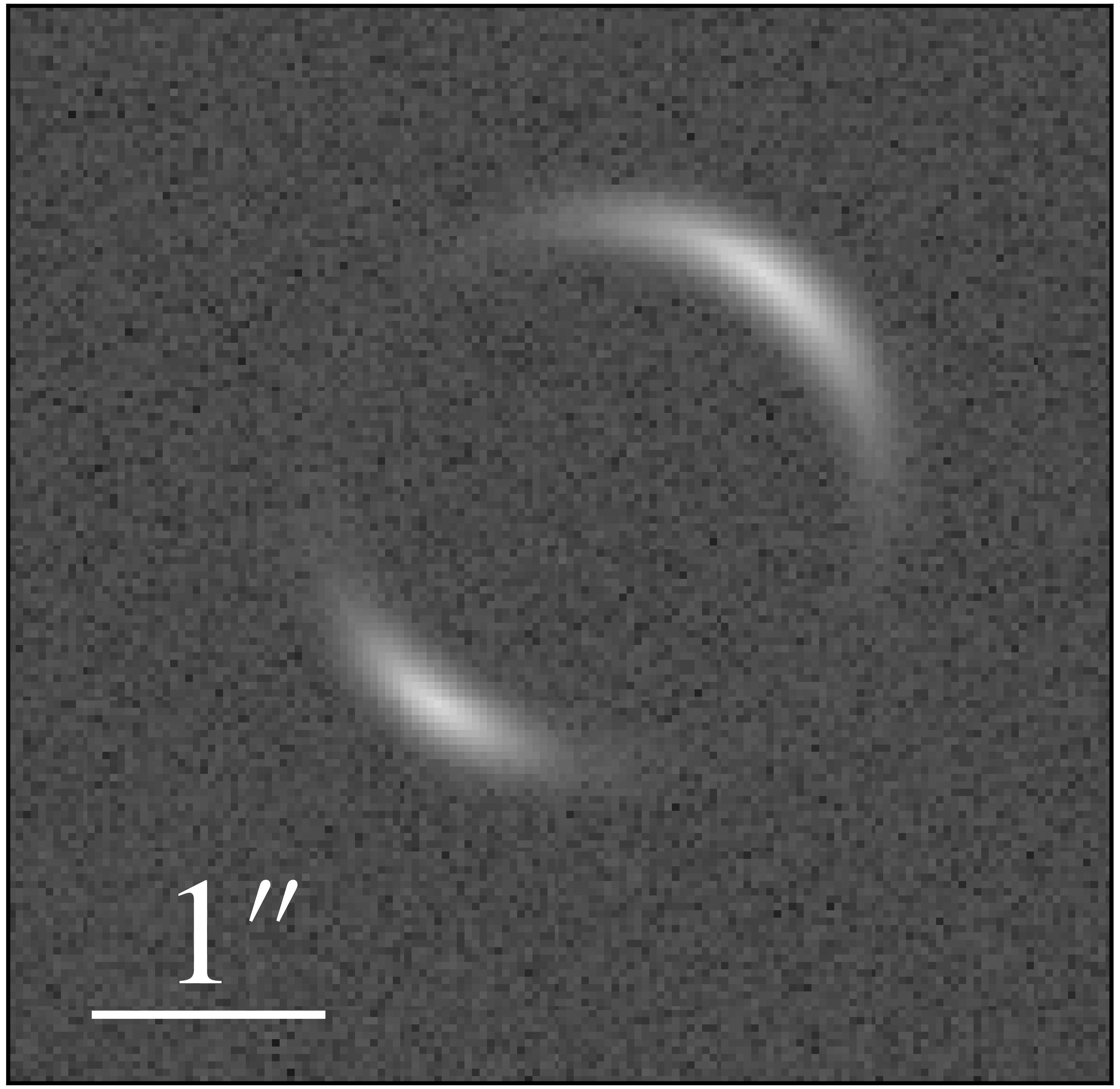
[T. Brown, J.Tumlinson]

[NASA/ESA; Abe Books]


[Hubble Space Telescope]

# Subhalos affect strong lensing

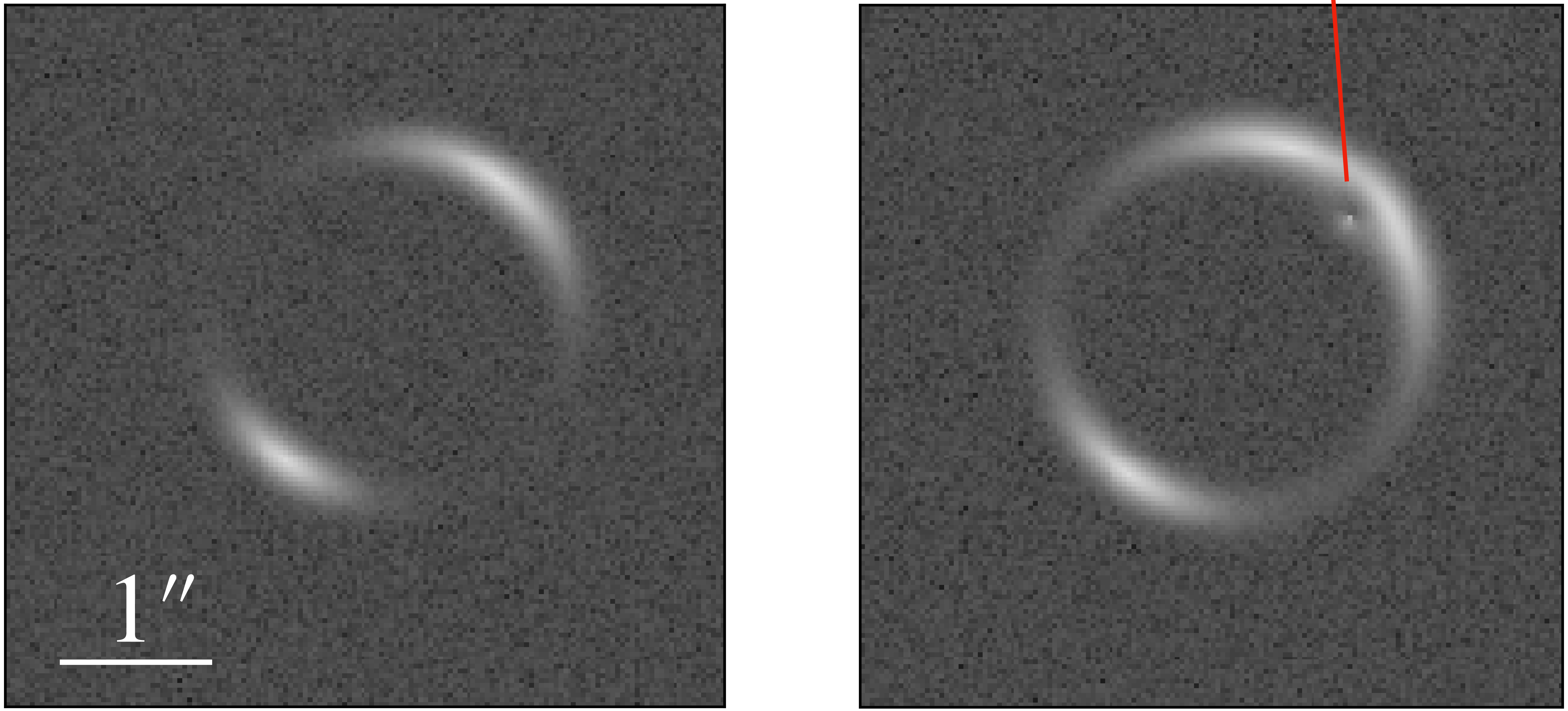
Smooth halo only



# Subhalos affect strong lensing

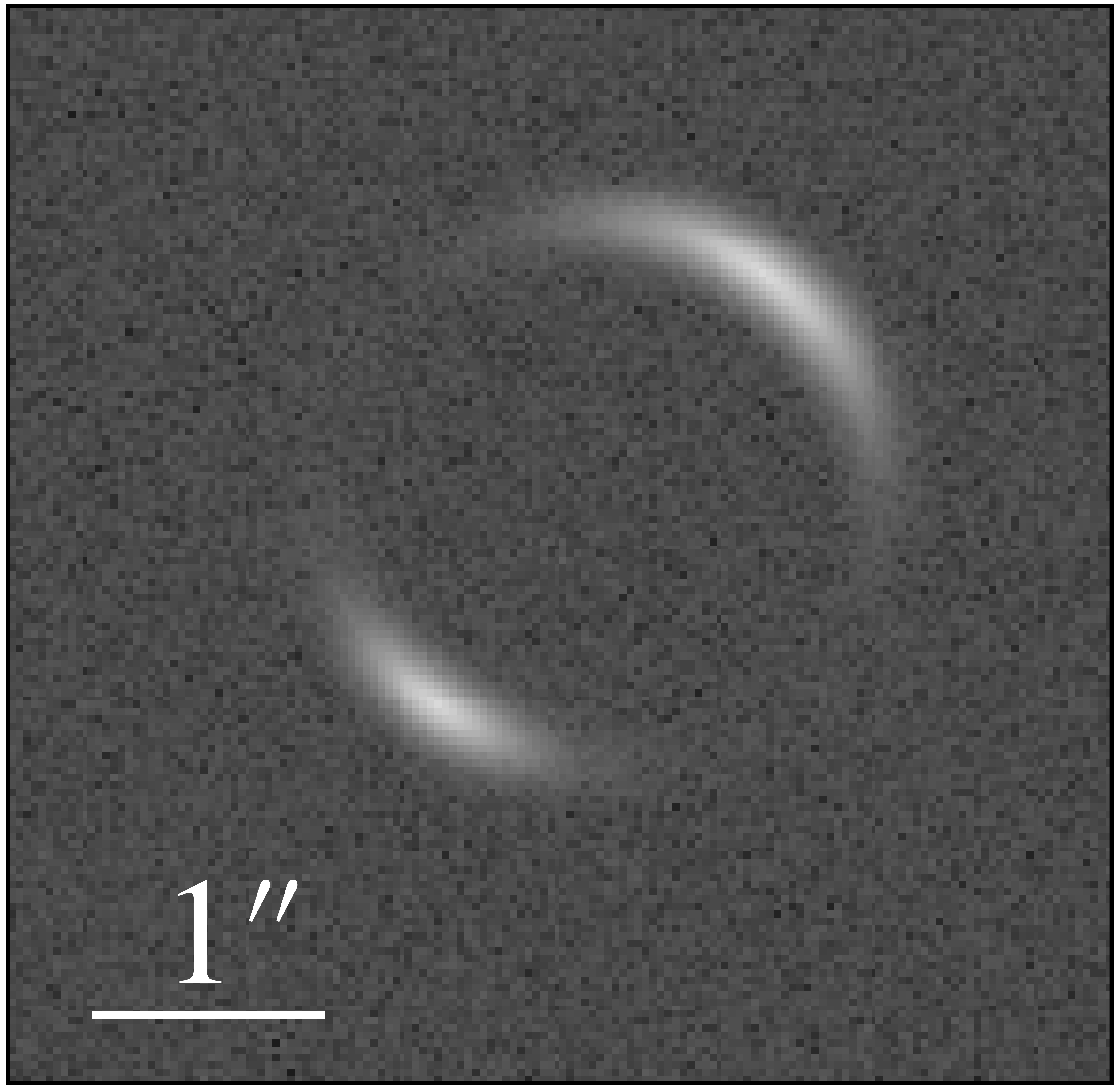
Smooth halo only

Smooth halo + subhalo

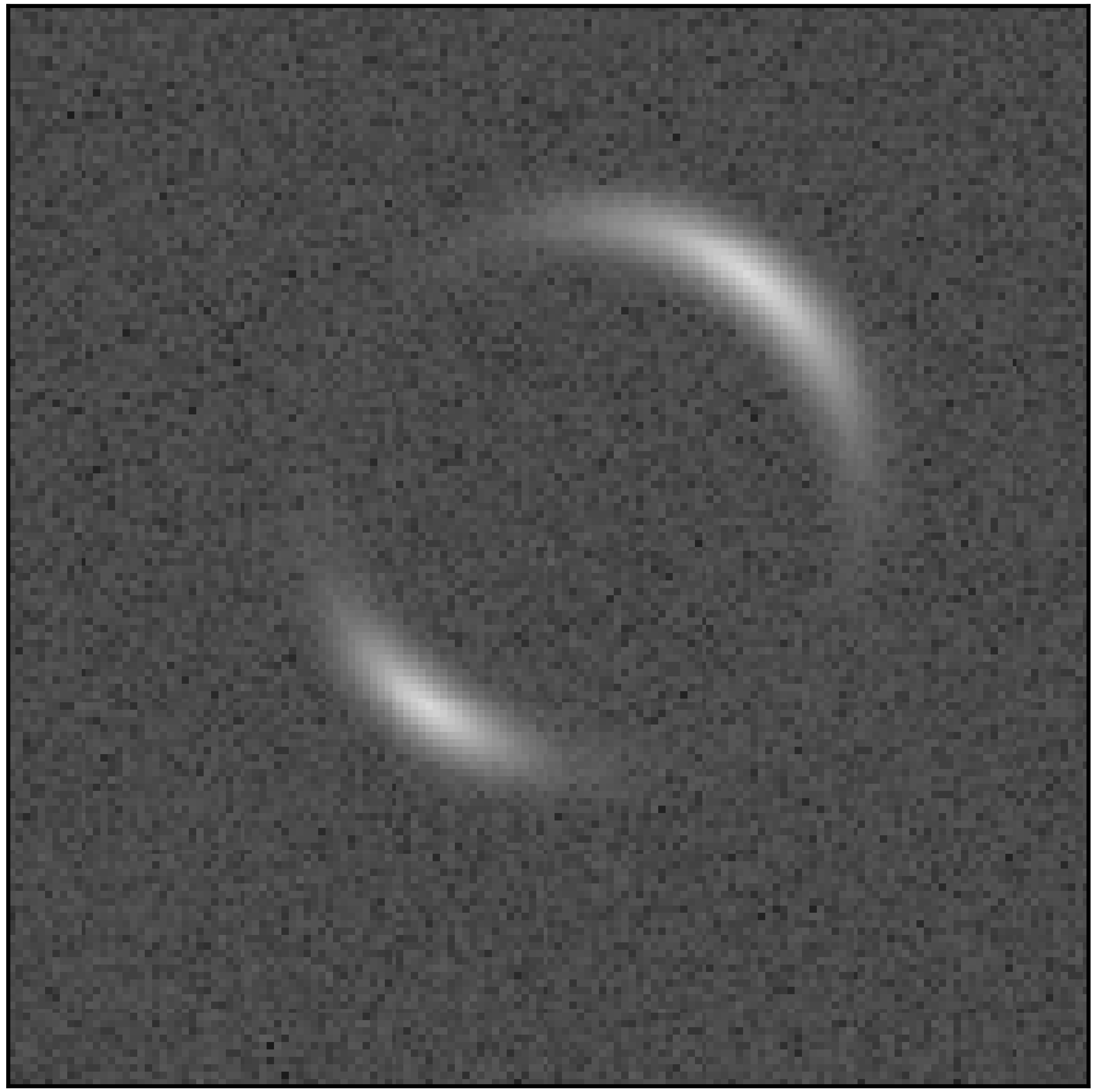


# Subhalos affect strong lensing… realistically

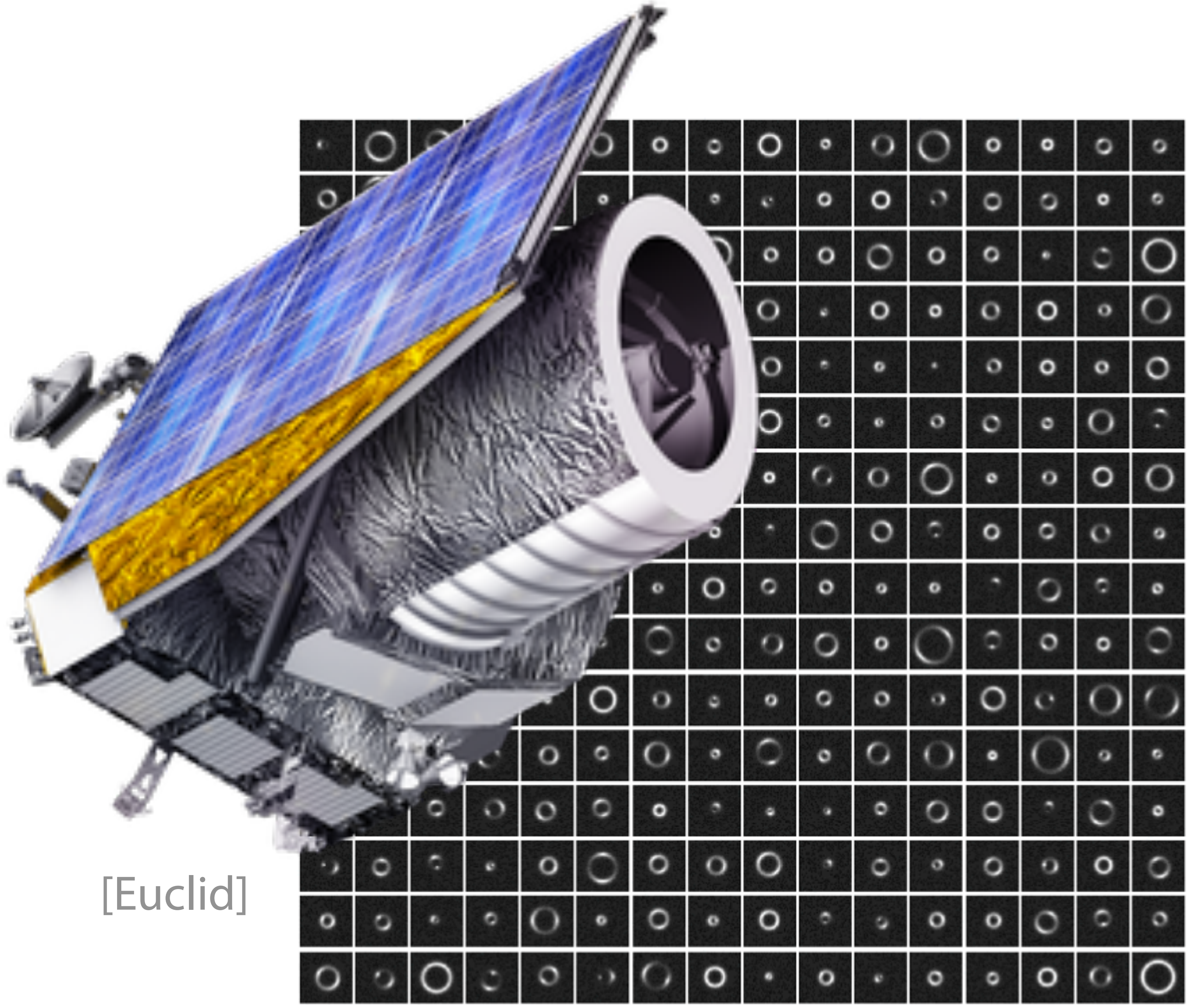
Smooth halo only

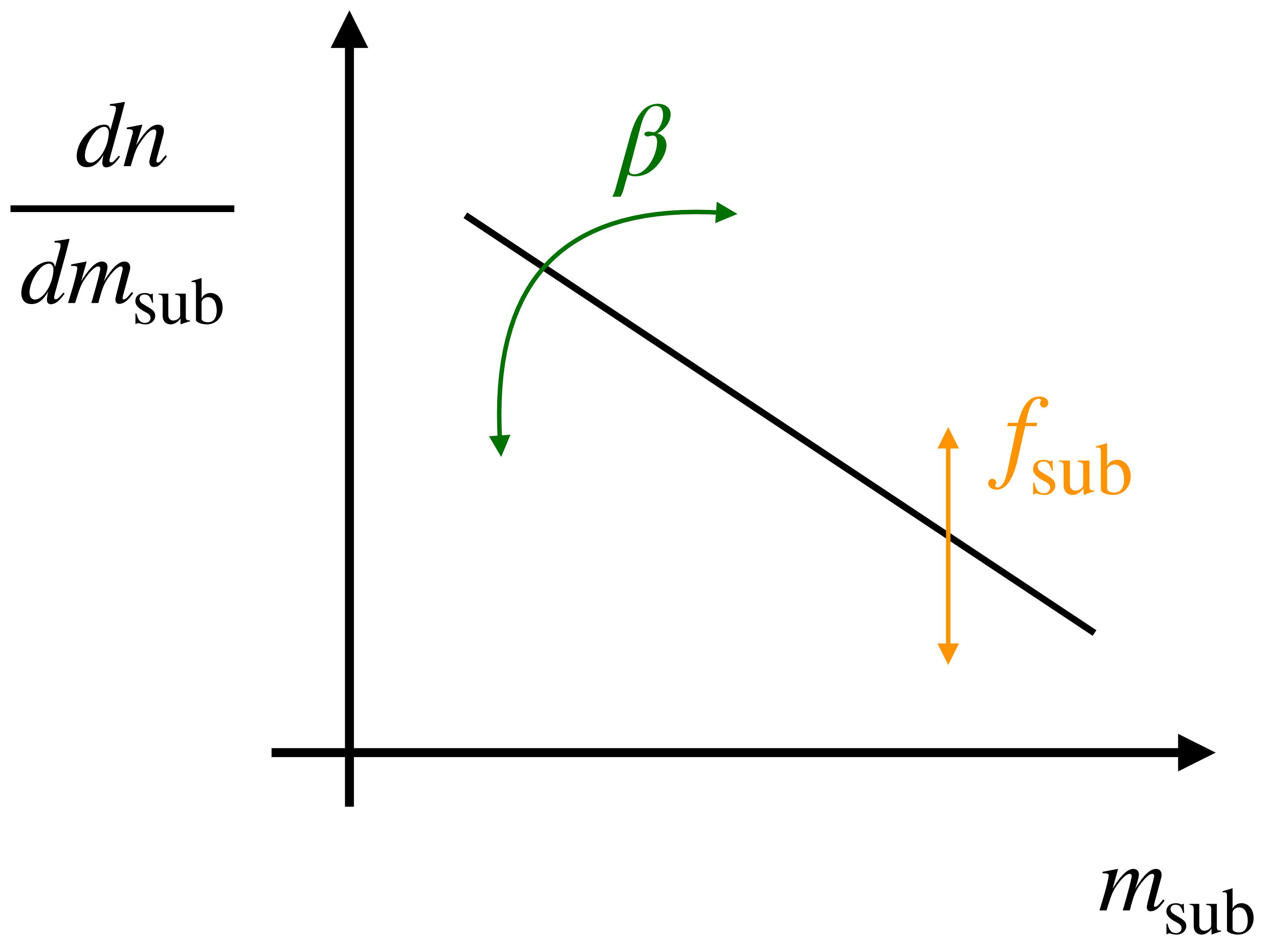



Smooth halo + subhalos



# Scalable inference for small subhalos



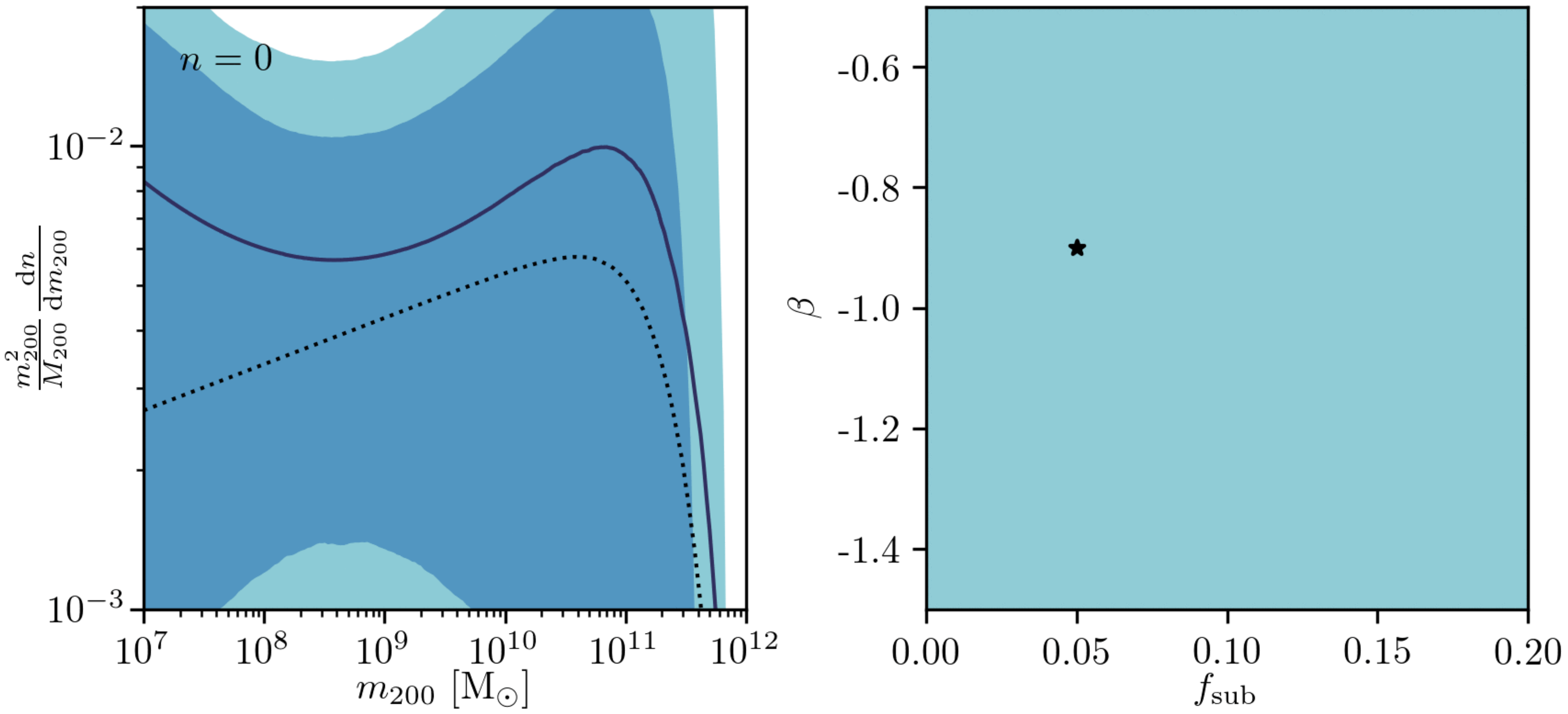




Near-future telescopes and satellites will collect hundreds of lensing images [Collett et al 1507.02657]

Goal: infer DM properties from all images and all clumps at once

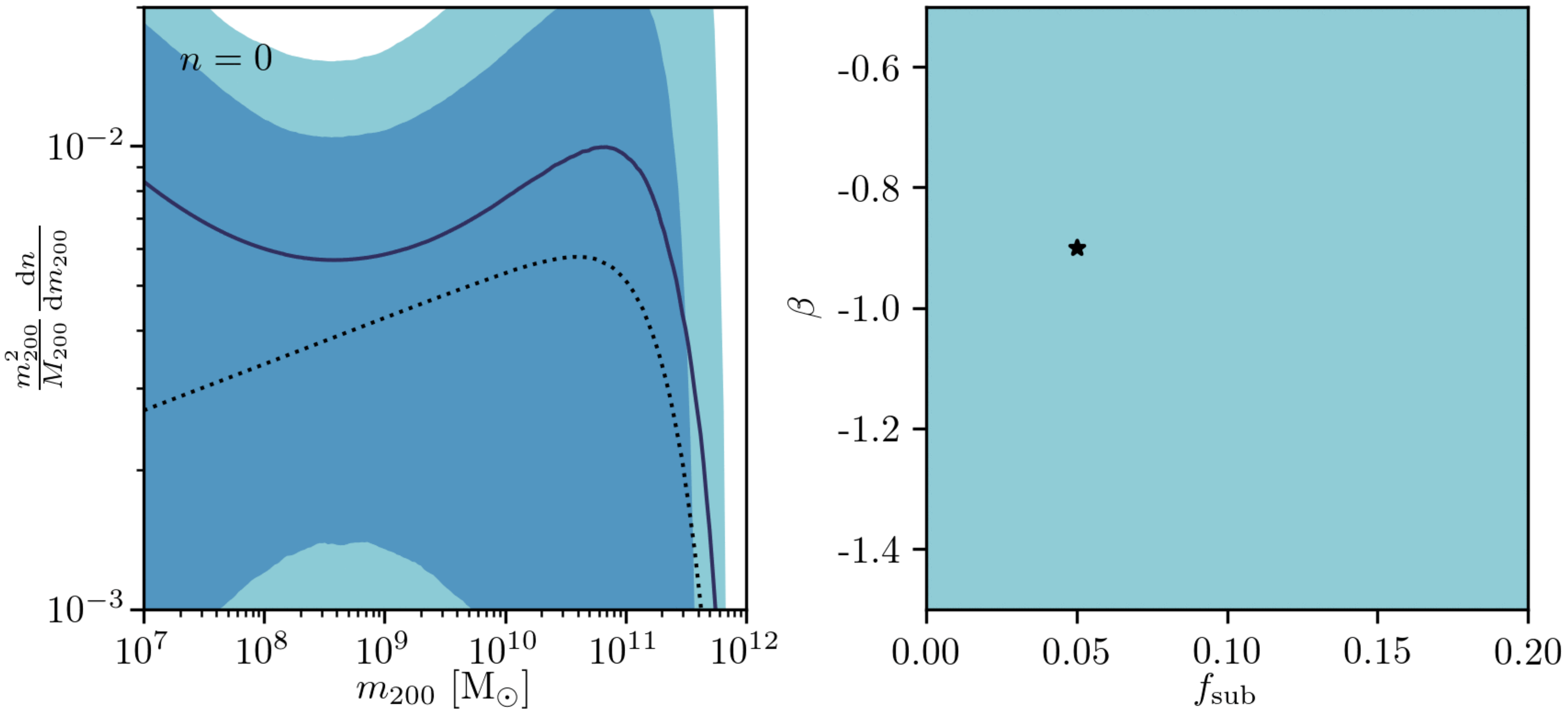
# ML-based Bayesian inference

[JB, S. Mishra-Sharma, J. Hermans, G. Louppe, K. Cranmer 1909.02005]



# ML-based Bayesian inference

[JB, S. Mishra-Sharma, J. Hermans, G. Louppe, K. Cranmer 1909.02005]




Kyle Cranmer


Gilles Louppe


Juan Pavez

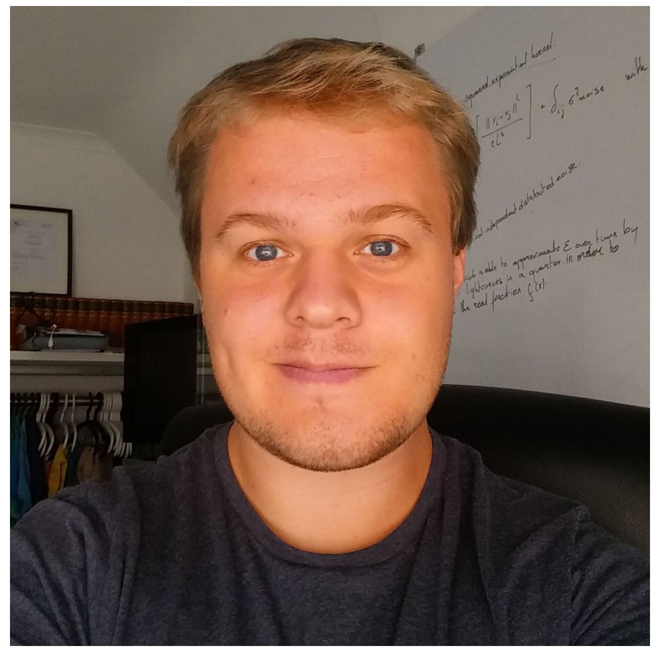

Markus Stoye


Felix Kling

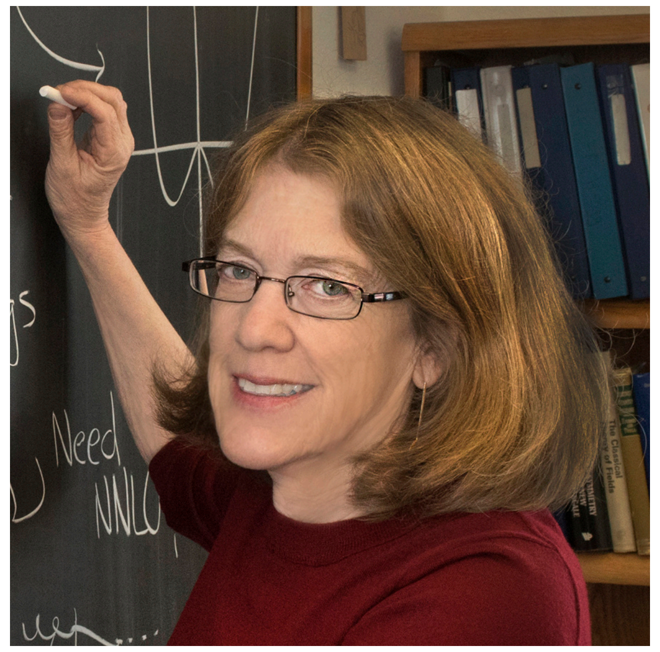

Irina Espejo


Sinclert Perez


Sid Mishra-Sharma


Joeri Hermans


Tilman Plehn


Sally Dawson


Sam Homiller


Zubair Bhatti

Parts of this talk were inspired by great presentations by Kyle Cranmer, Gilles Louppe, Sid Mishra-Sharma, and Jakob Macke

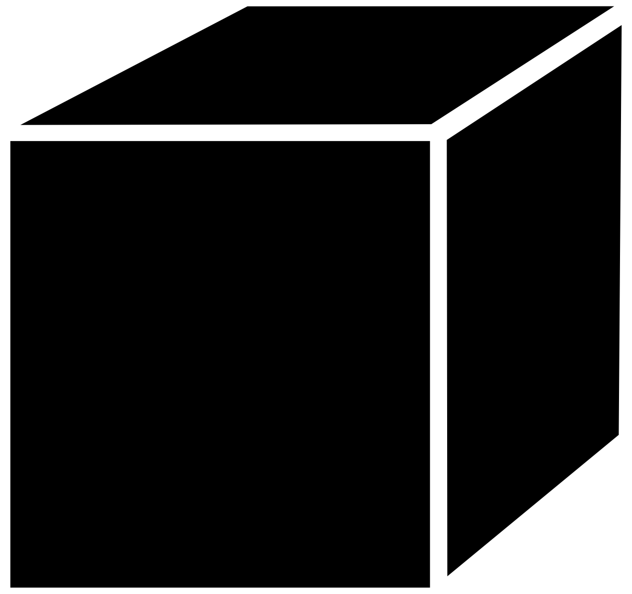
NYU

MSDSE
Moore - Sloan
Data Science Environments

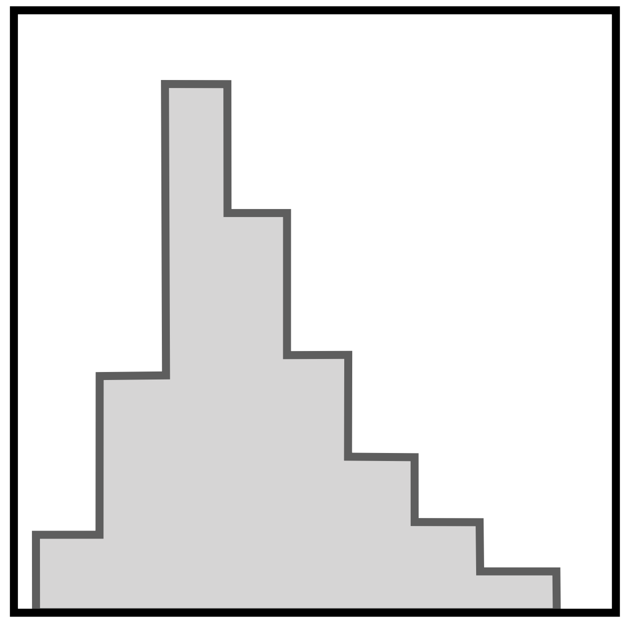
dianahep

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

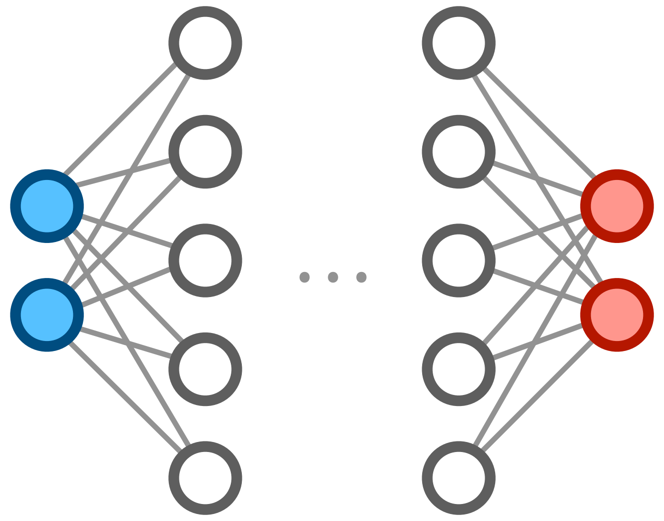
**The SCAILFIN Project**
scailfin.github.io



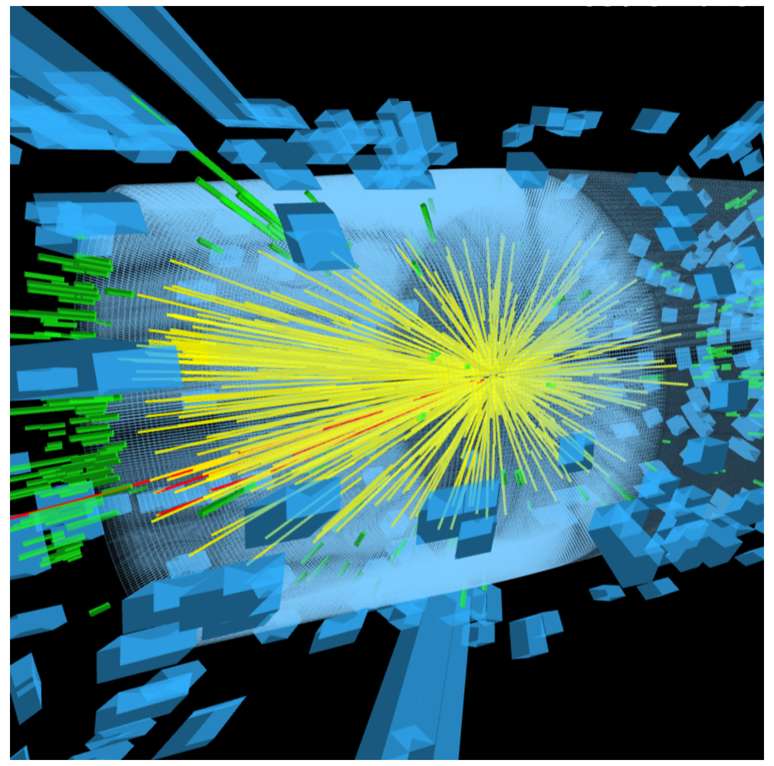
Simulators make precise predictions, but inference is challenging.



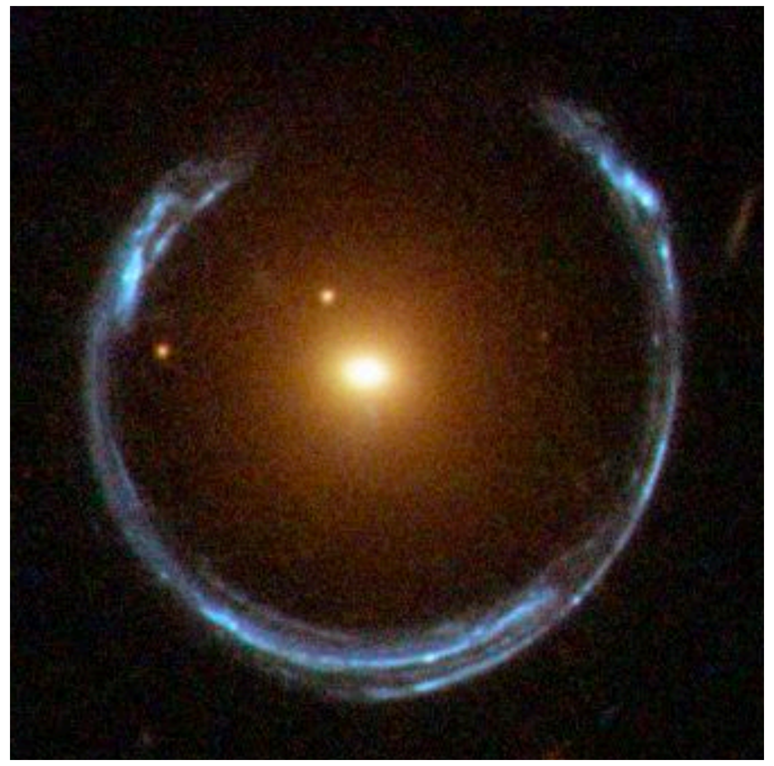
Scientists have side-stepped this problem with summary statistics.




Machine learning enables powerful inference methods, especially when we inject domain information.



They work in problems from the smallest…



… to the largest scales.

# Selected references


**Reviews**

K. Cranmer, **J. Brehmer**, G. Louppe:
"The frontier of simulation-based inference"
PNAS, 1911.01429

**J. Brehmer** and K. Cranmer:
"Simulation-based inference methods for particle physics"
2010.06439

**Simulation–based inference methods**

**J. Brehmer**, G. Louppe, J. Pavez, K. Cranmer:
"Mining gold from implicit models to improve likelihood-free inference"
PNAS, 1805.12244

M. Stoye, **J. Brehmer**, K. Cranmer, G. Louppe, J. Pavez:
"Likelihood-free inference with an improved cross-entropy estimator"
NeurIPS workshop, 1808.00973

**Particle physics**

**J. Brehmer**, K. Cranmer, G. Louppe, J. Pavez:
"Constraining Effective Field Theories with machine learning"
PRL, 1805.00013

**J. Brehmer**, K. Cranmer, G. Louppe, J. Pavez:
"A guide to constraining Effective Field Theories with machine learning"
PRD, 1805.00020

**J. Brehmer**, F. Kling, I. Espejo, K. Cranmer:
"MadMiner: Machine learning–based inference for particle physics"
CSBS, 1907.10621, https://github.com/diana-hep/madminer

**J. Brehmer**, K. Cranmer, F. Kling, and T. Plehn:
"Better Higgs Measurements Through Information Geometry"
PRD, 1612.05261

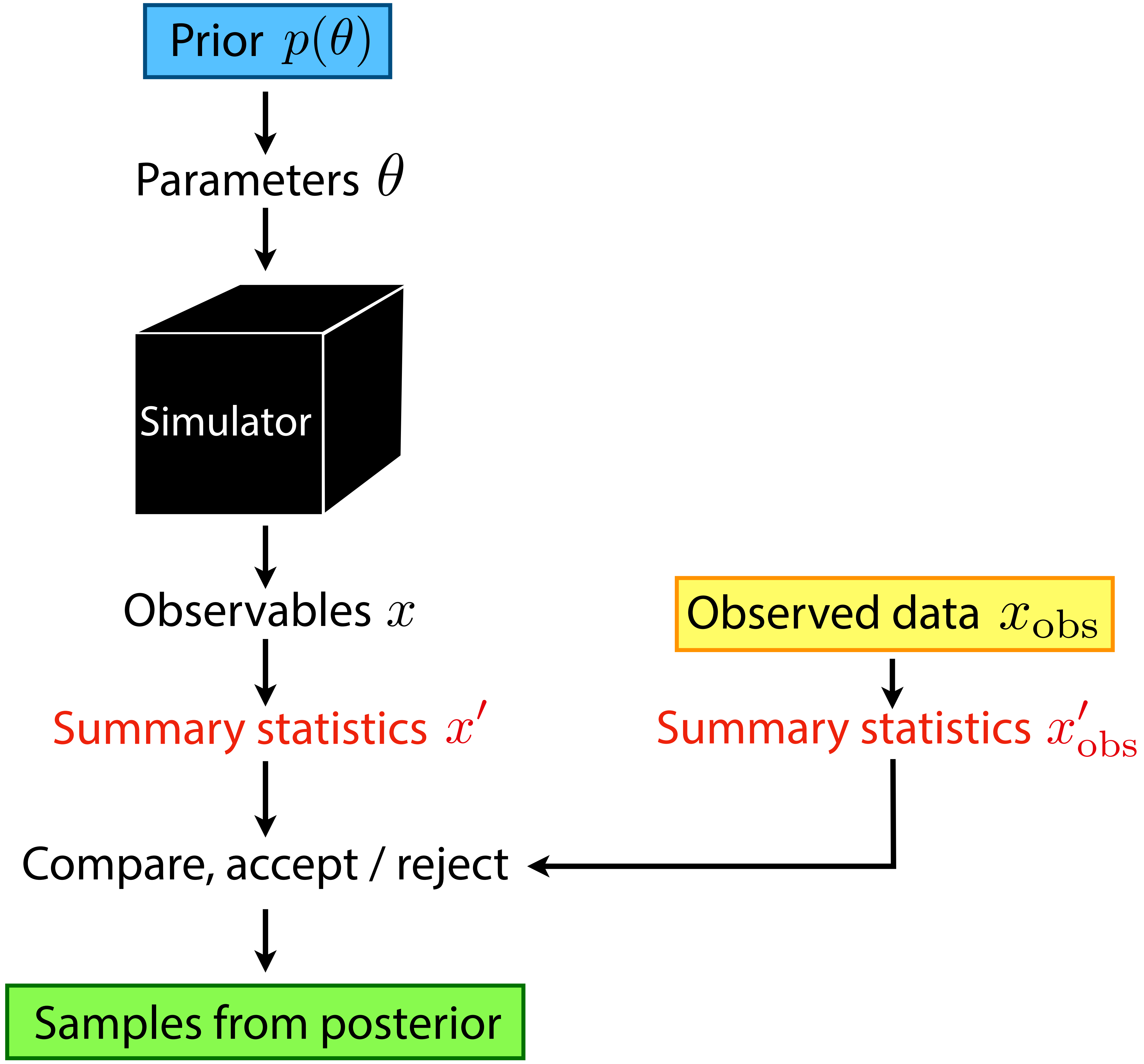
**Astrophysics**

**J. Brehmer**, S. Mishra-Sharma, J. Hermans, G. Louppe, K. Cranmer
"Mining for Dark Matter Substructure: Inferring subhalo population properties from strong lenses with machine learning"
ApJ, 1909.02005

# Bonus material: simulation-based inference

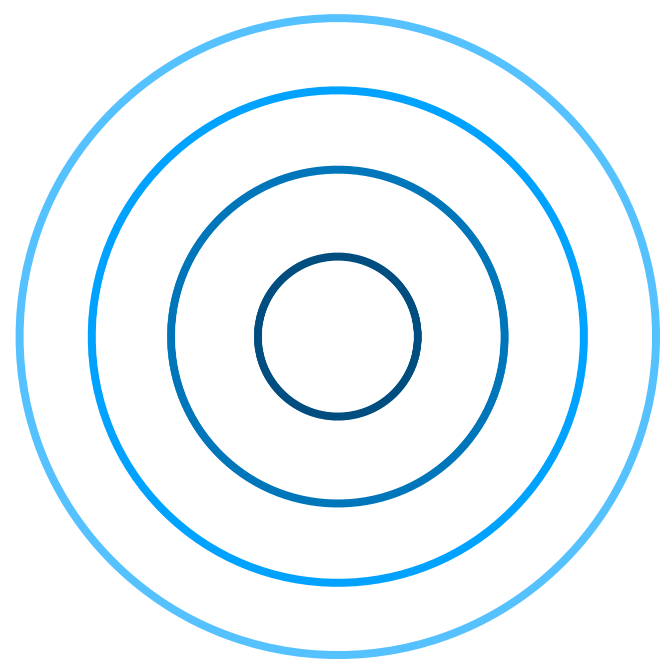
# Approximate Bayesian Computation (ABC)

[D. Rubin 1984]



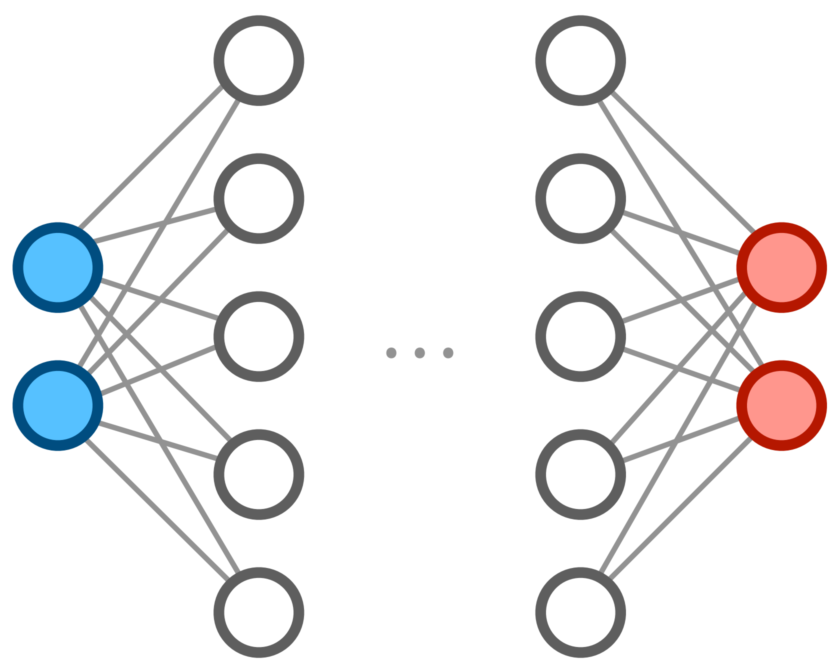

- Compression to summary statistics and acceptance threshold reduce quality of inference
- Rejection algorithm can be very sample inefficient

# High-dimensional density estimation with normalizing flows



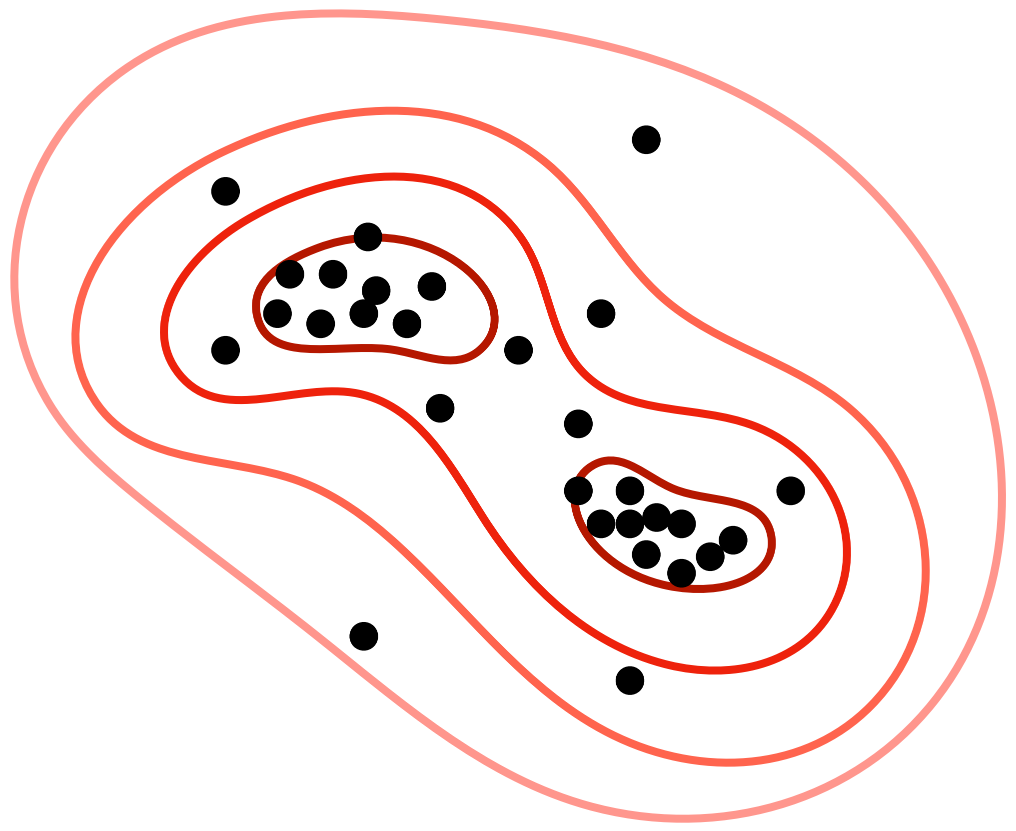
Simple base density

$u \sim \pi(u)$



NN: transformation $x = f(u)$

- one-to-one and invertible
- differentiable
- $f^{-1}$ and $\det \nabla f$ are tractable



Target density is given by

$$\hat{p}(x) = \pi(f^{-1}(x)) \, |\det \nabla f|^{-1}$$

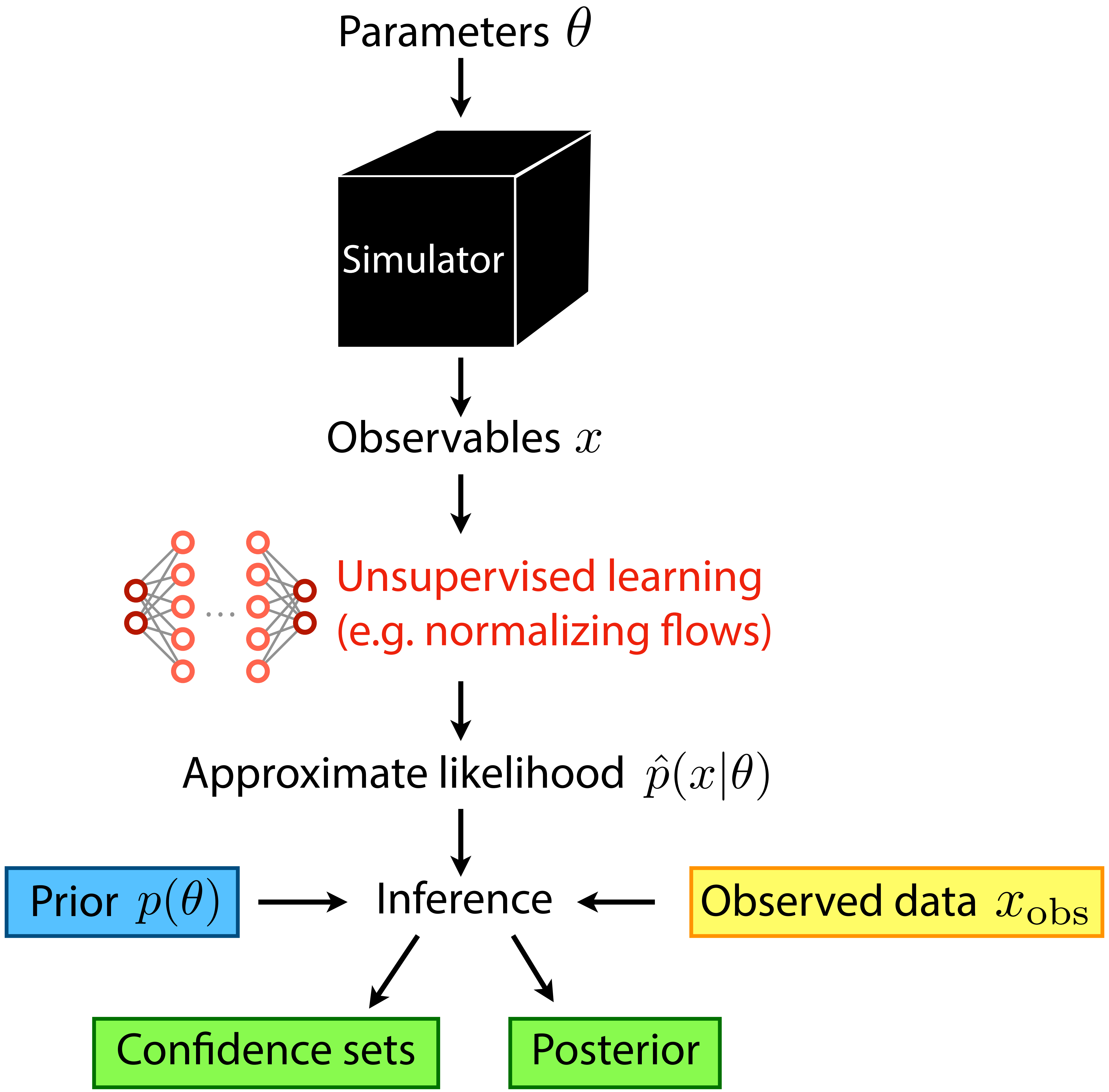
Train transformation by maximizing $\log \hat{p}(x)$

Transformation can depend on $\theta$ to model conditional density $\log \hat{p}(x|\theta)$

[lots of great work recently; see G. Papamakarios et al 1912.02762 for a review]

# Inference with neural likelihood estimation

[G. Papamakarios, D. Sterrart, I. Murray 1805.07226;
J.-M. Lueckmann, G. Bassetto, T. Karaletsos, J. Macke 1805.09294]

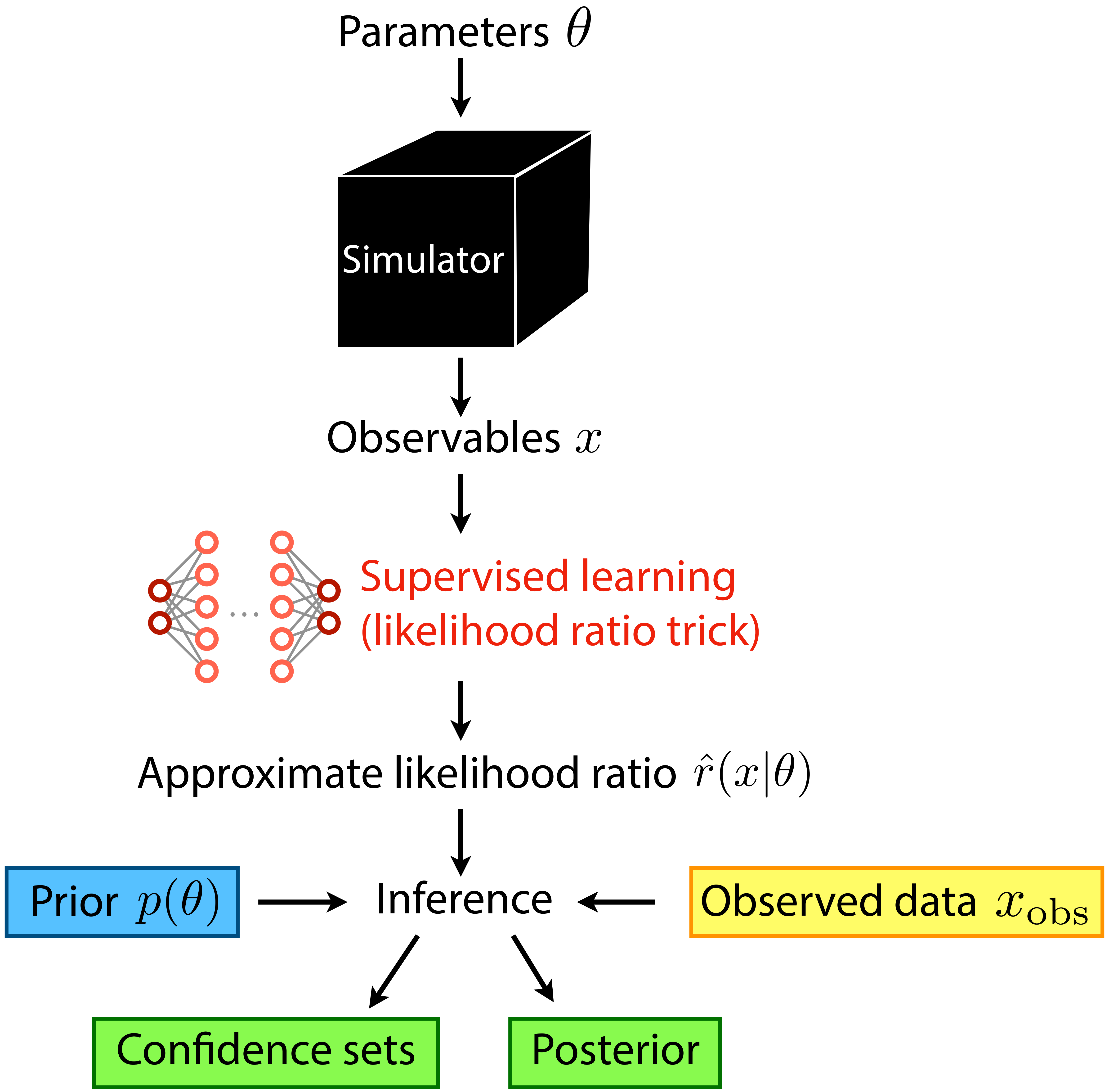



- Conditional neural density estimator (e.g. normalizing flow) as tractable surrogate for simulator likelihood
- Scales well to high-dimensional data (no compression to summary stats necessary)
- Amortized: After upfront simulation + training phase, inference is efficient for new data or prior
- Related alternative: learn posterior $\hat{p}(\theta|x_{\mathrm{obs}})$

[G. Papamakarios et al 1605.06376;
J.-M. Lueckmann et al 1711.01861]

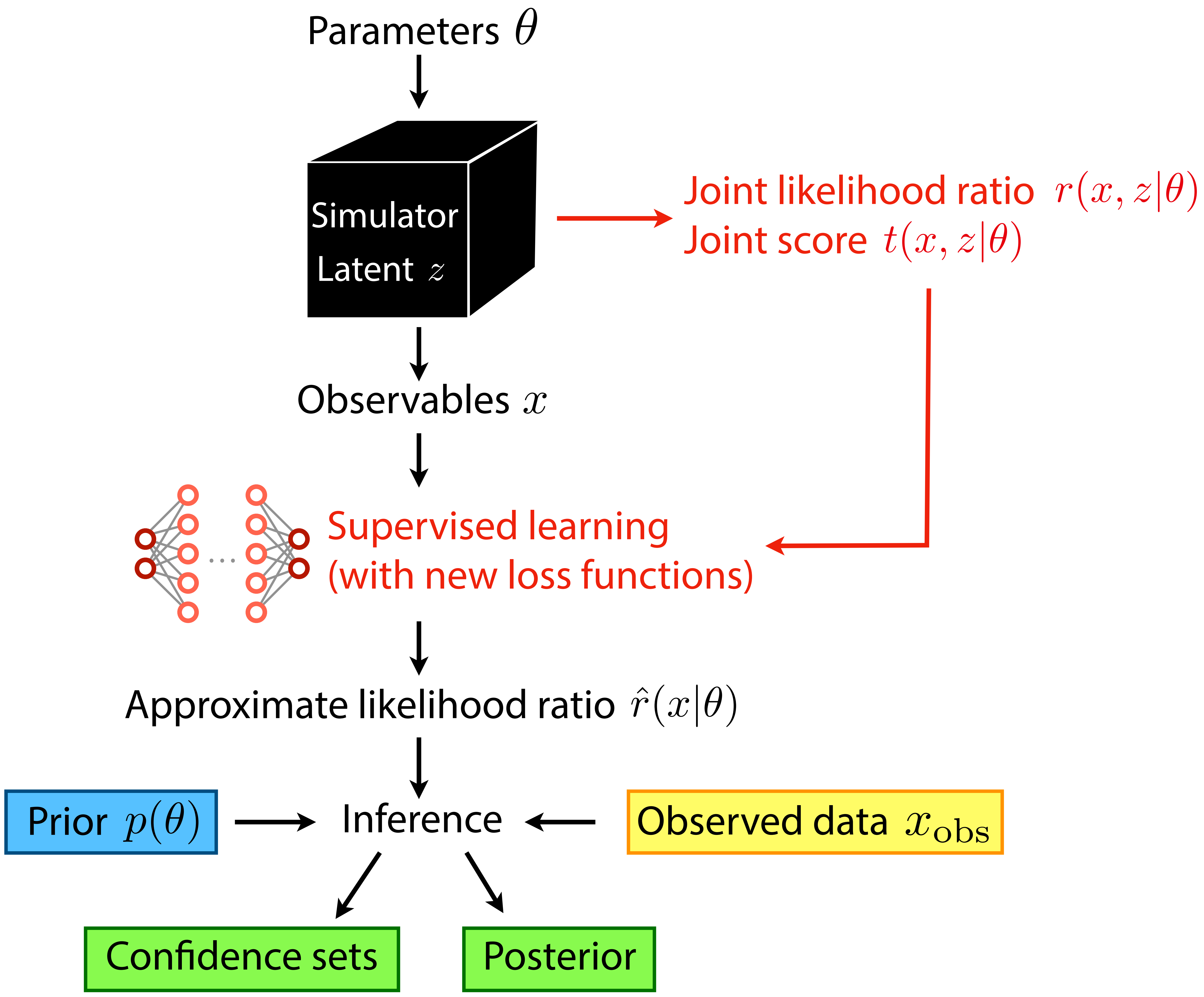
# Inference by likelihood ratio trick

[K. Cranmer J. Pavez, G. Louppe 1506.02169]

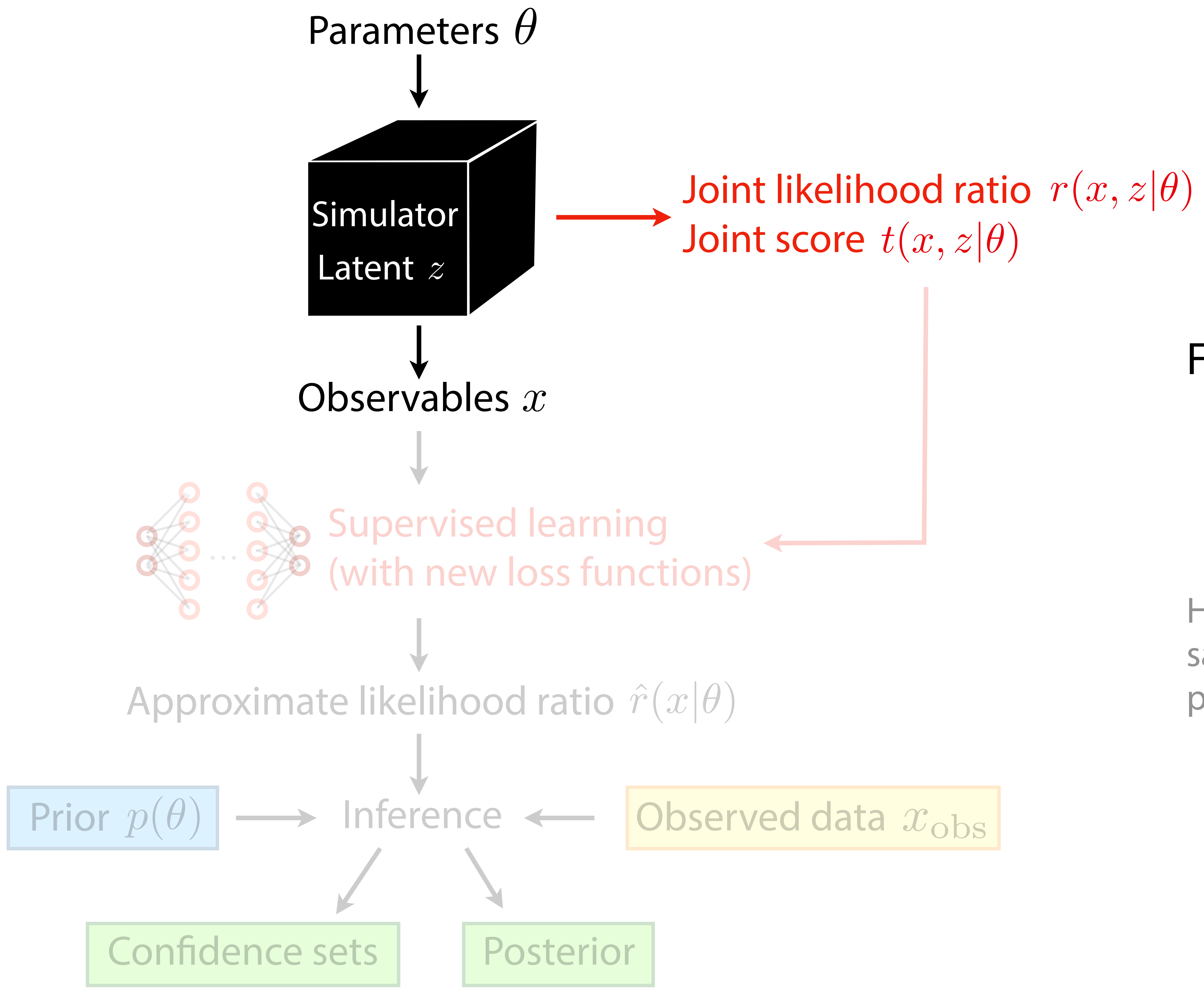



- For inference, likelihood and likelihood ratio are interchangeable
- Advantage: Learning the likelihood ratio can be a simpler task than learning the likelihood
- Disadvantage: Cannot sample from likelihood ratio

# Mining gold


Parameters $\theta$
Simulator
Latent $z$
Joint likelihood ratio $r(x, z|\theta)$
Joint score $t(x, z|\theta)$
Observables $x$
Supervised learning
(with new loss functions)
Approximate likelihood ratio $\hat{r}(x|\theta)$
Prior $p(\theta)$
Inference
Observed data $x_{\text{obs}}$
Confidence sets
Posterior

# Step 1: Extracting more information from simulations

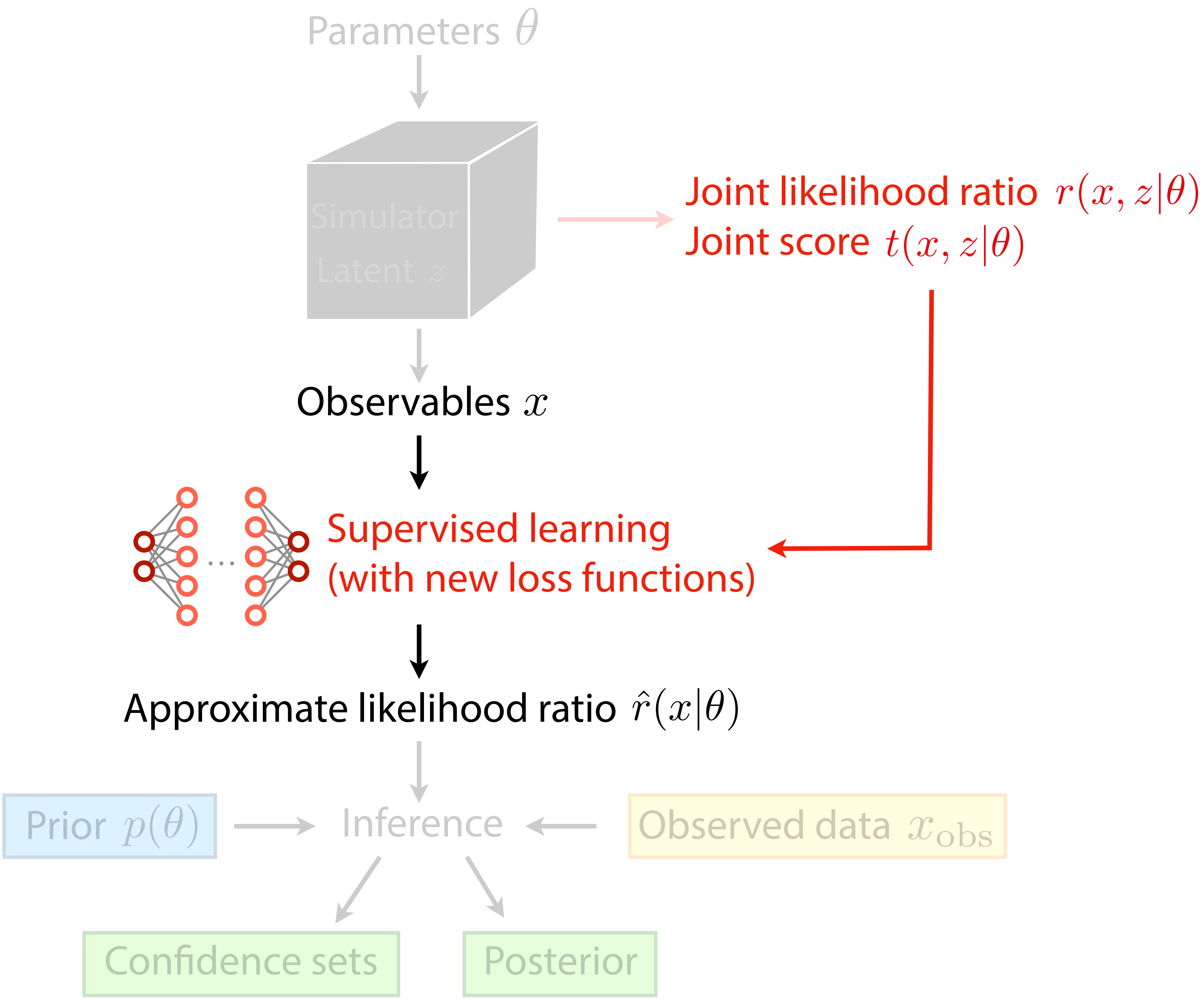



For each simulated event, calculate

- joint likelihood ratio $r(x, z|\theta) = \dfrac{p(x, z|\theta)}{p_{\text{ref}}(x, z)}$
- joint score $t(x, z|\theta) = \nabla_\theta \log p(x, z|\theta)$

How much more or less likely would this simulated sample (fixing all latent variables) be when changing the parameters?

# Step 2: Machine learning




- Train a neural network $g(x, \theta)$ on loss functionals like

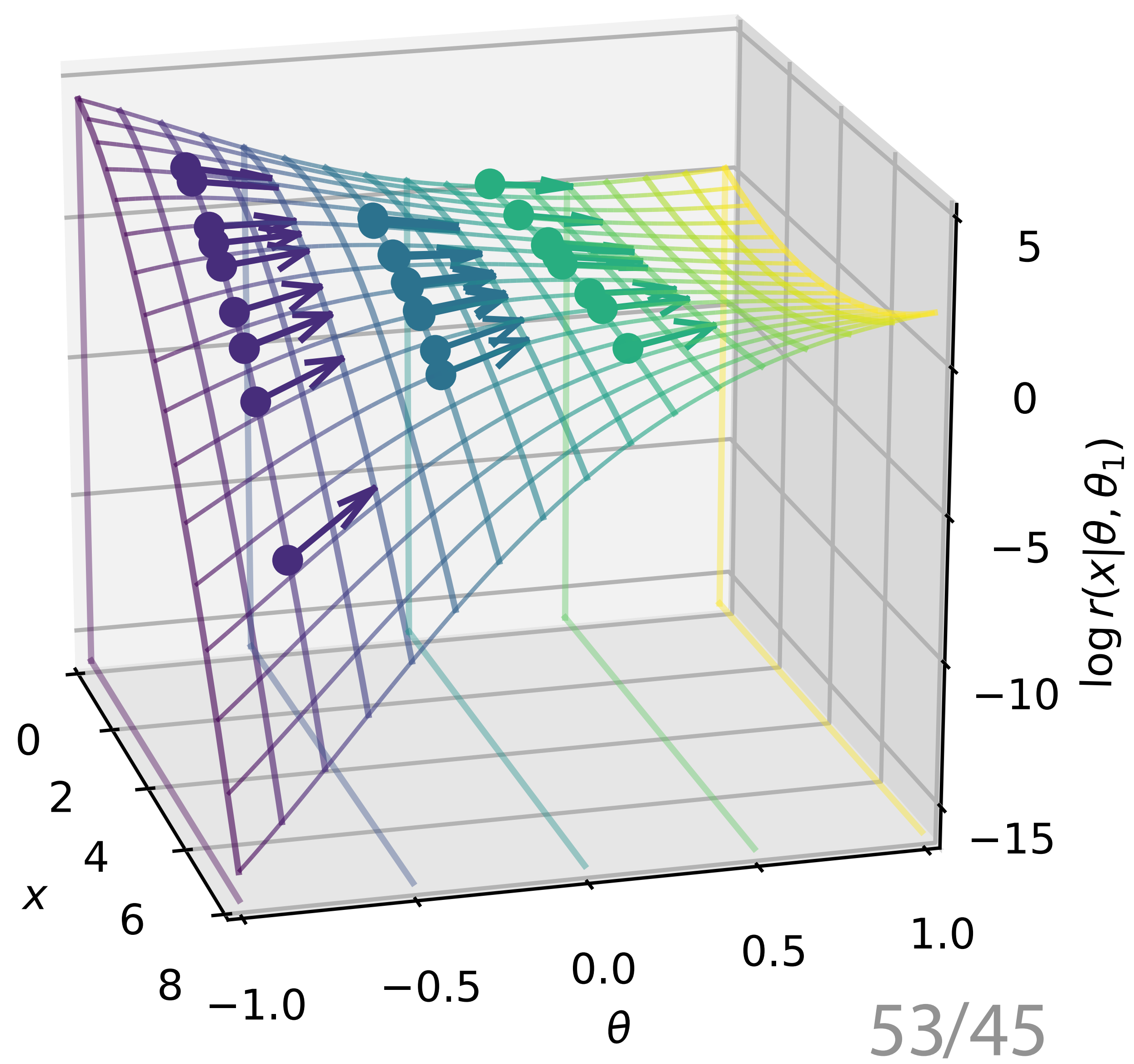
$$L[g] = \frac{1}{N} \sum_i |g(x_i, \theta_i) - r(x_i, z_i|\theta_i)|^2$$

- The network will converge to

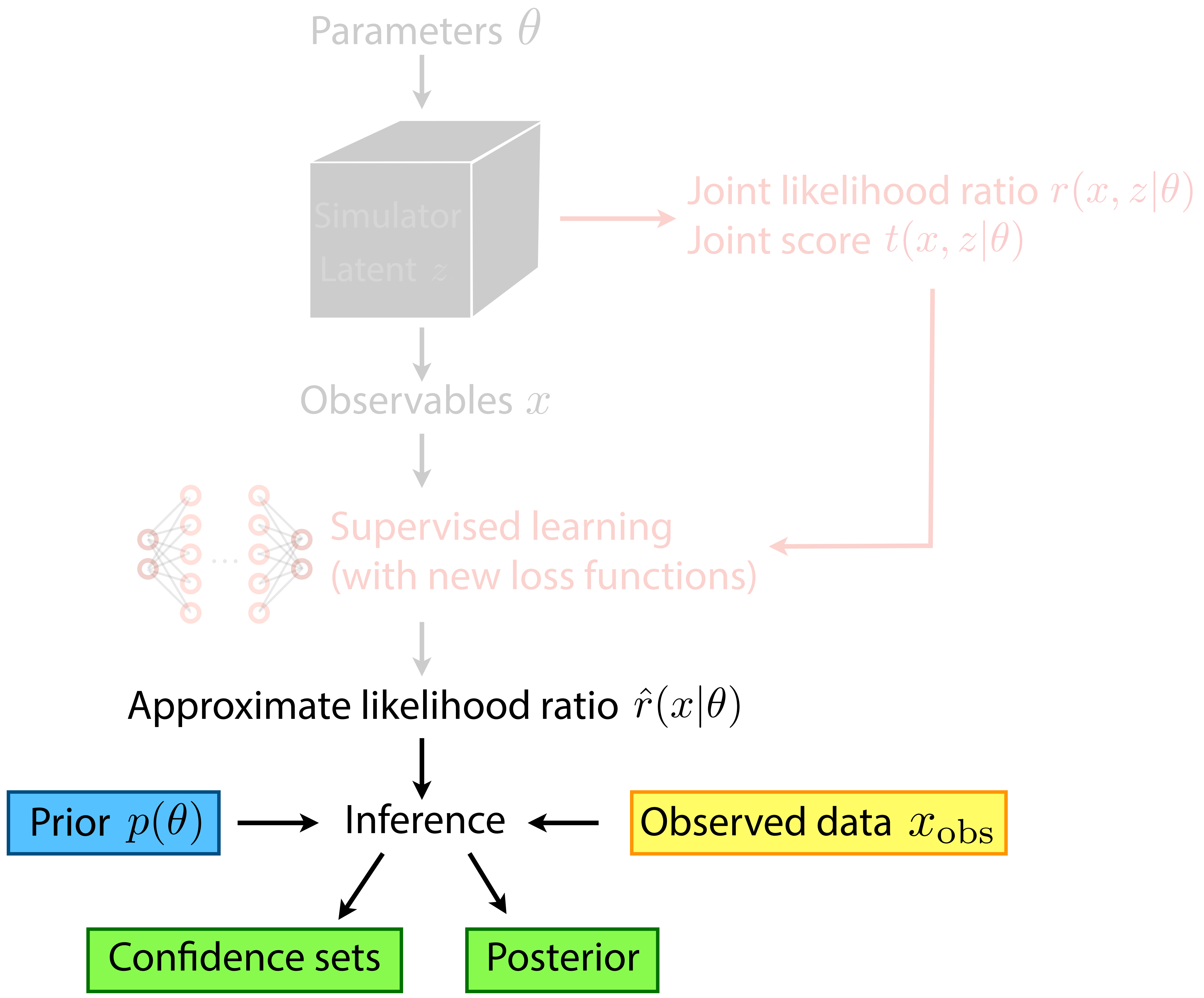
$$g(x, \theta) \to \arg\min L[g] = r(x|\theta) = \frac{p(x|\theta)}{p_{\text{ref}}(x)} \;!$$

(for sufficient training data, NN capacity, efficient optimization)

- RASCAL:
  Joint score adds gradient information
  $\Rightarrow$ three orthogonal pieces of information



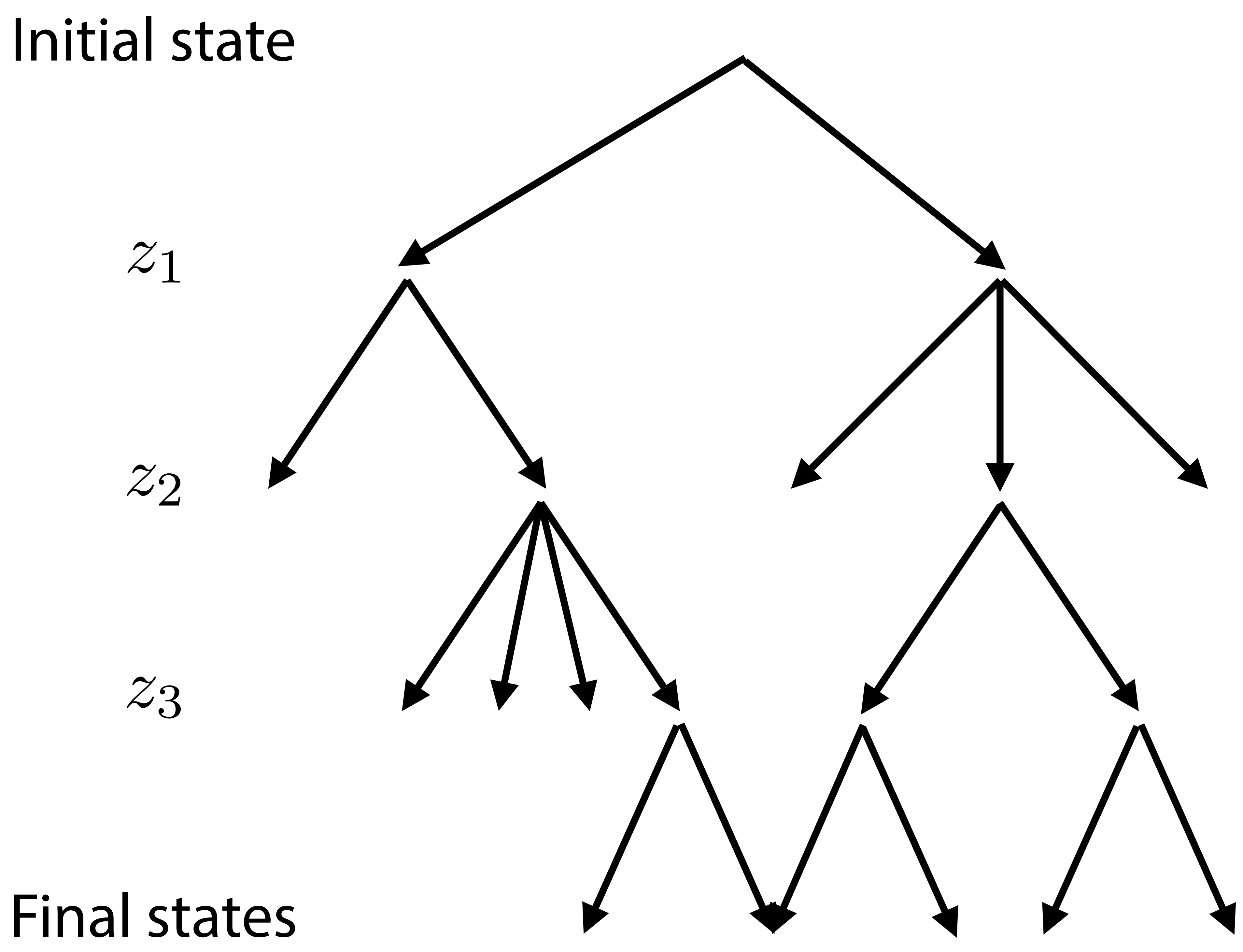
# Step 3: Inference



# Mining gold from any simulation

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

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



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else:
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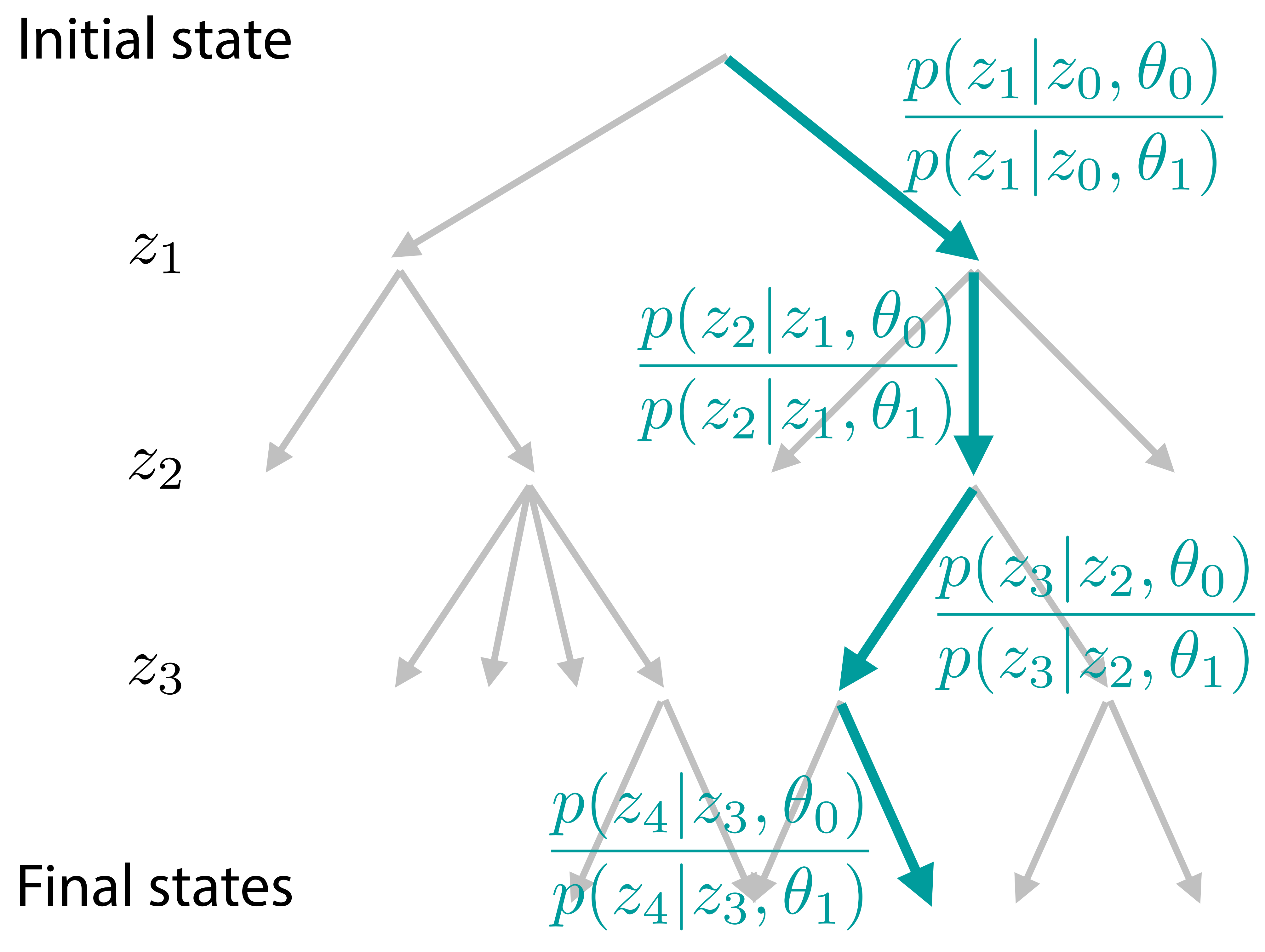
```

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

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



# The value of gold

Expectation value of the joint likelihood ratio:

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

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

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

It is minimized by

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

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

# Machine learning = applied calculus of variatios

So to get a good estimator of the likelihood ratio,
we need to mimimize a functional numerically:

Variational family

Extremization

Functional with integral

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

A sufficiently expressive neural network
efficiently trained in this way
with enough data will learn
the likelihood ratio function $r(x|\theta_0, \theta_1)$!

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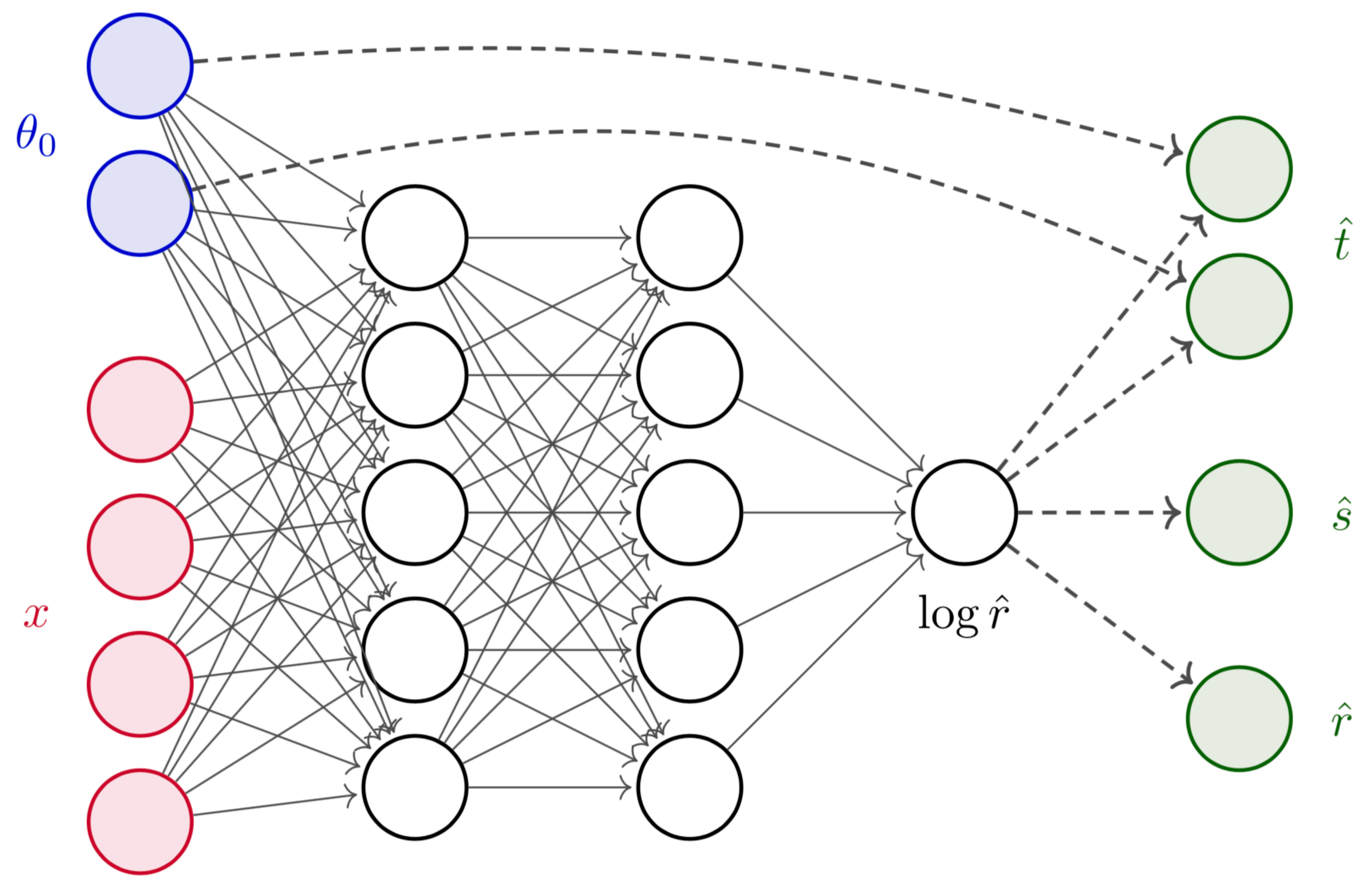
This is where machine learning comes in!

Loss function with
finite sum over samples

Neural network

Stochastic gradient descent




A sufficiently expressive neural network
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with enough data will learn
the likelihood ratio function $r(x|\theta_0, \theta_1)$!

# The local model

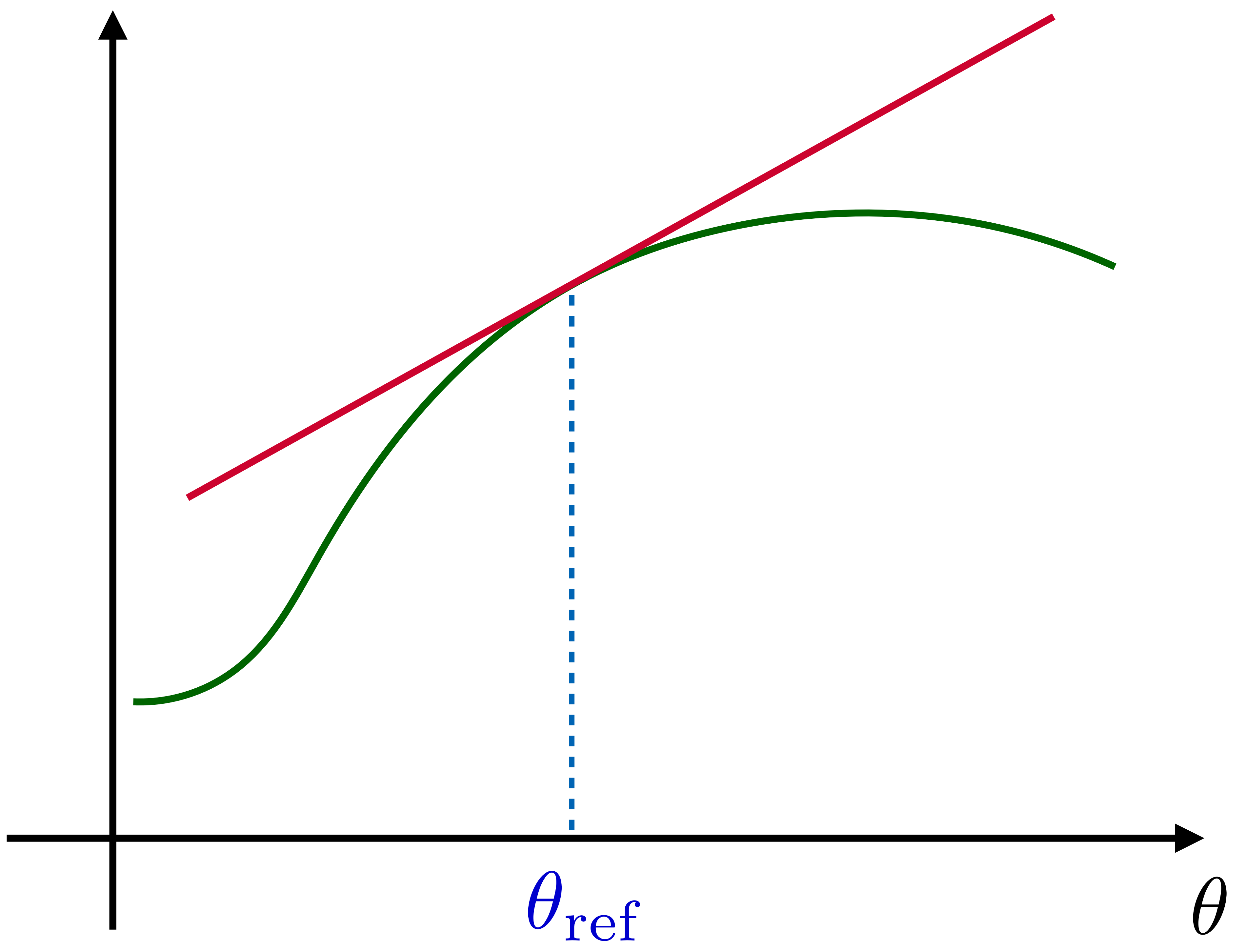
[see also J. Alsing, B. Wandelt 1712.00012; J. Alsing, B. Wandelt. S. Freeney 1801.01497; P. de Castro, T. Dorigo 1806.04743; J. Alsing, B. Wandelt 1903.01473]

Taylor expansion of $\log p(x|\theta)$ around $\theta_{\mathrm{ref}}$:

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

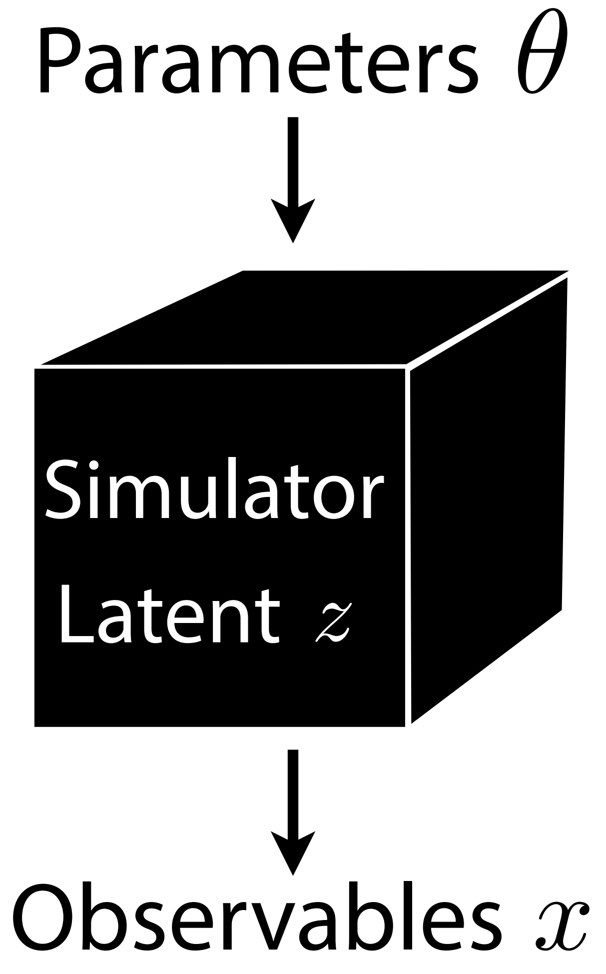
In the neighborhood of $\theta_{\mathrm{ref}}$:

- the score vector $t(x|\theta_{\mathrm{ref}})$ is the sufficient statistics
- knowing $t(x|\theta_{\mathrm{ref}})$ is just as powerful as knowing the full function $\log p(x|\theta)$
- $t(x|\theta_{\mathrm{ref}})$ is the most powerful observable




The score itself is intractable. But we can use the same trick as for the likelihood ratio!

# Neural optimal observables (SALLY)



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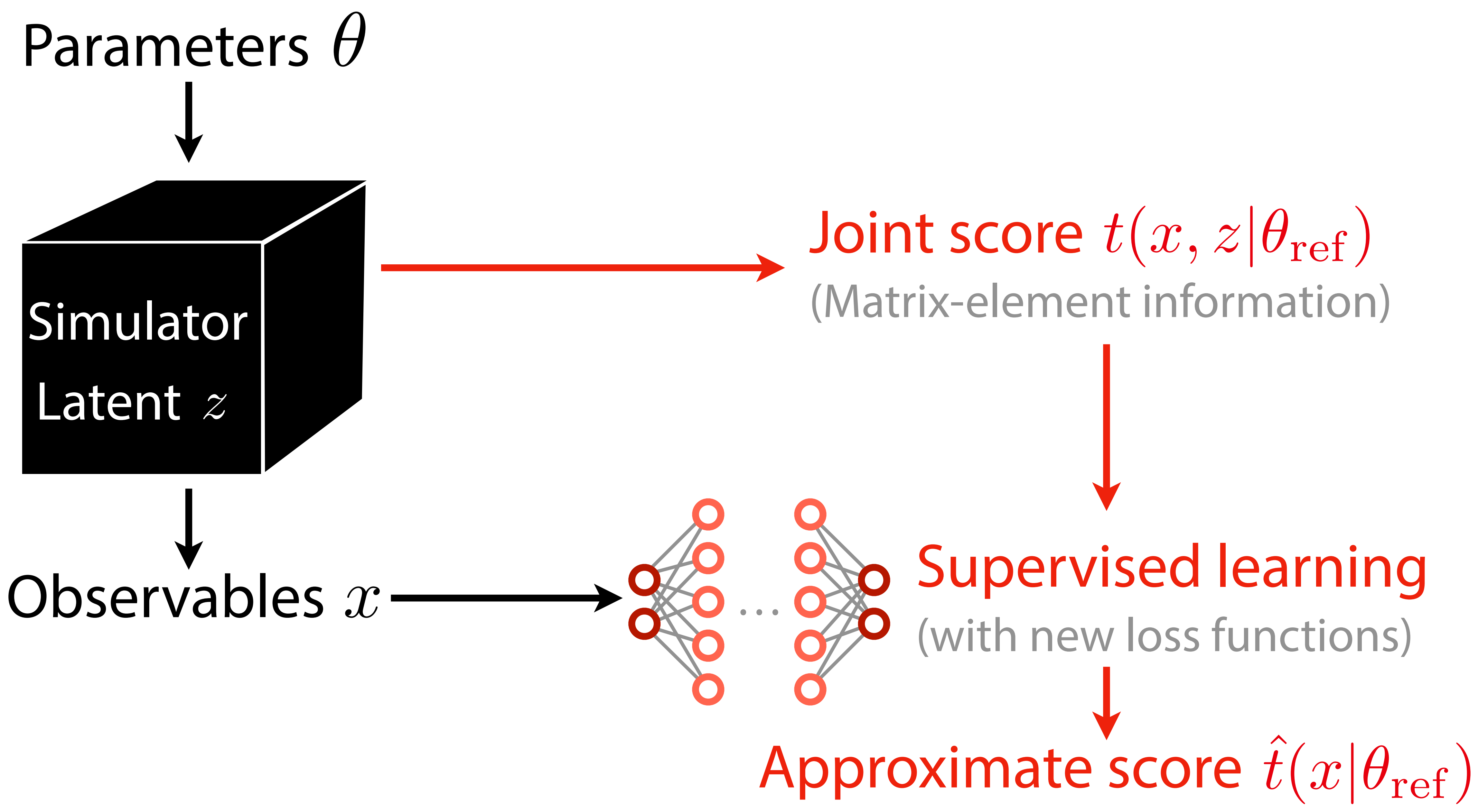

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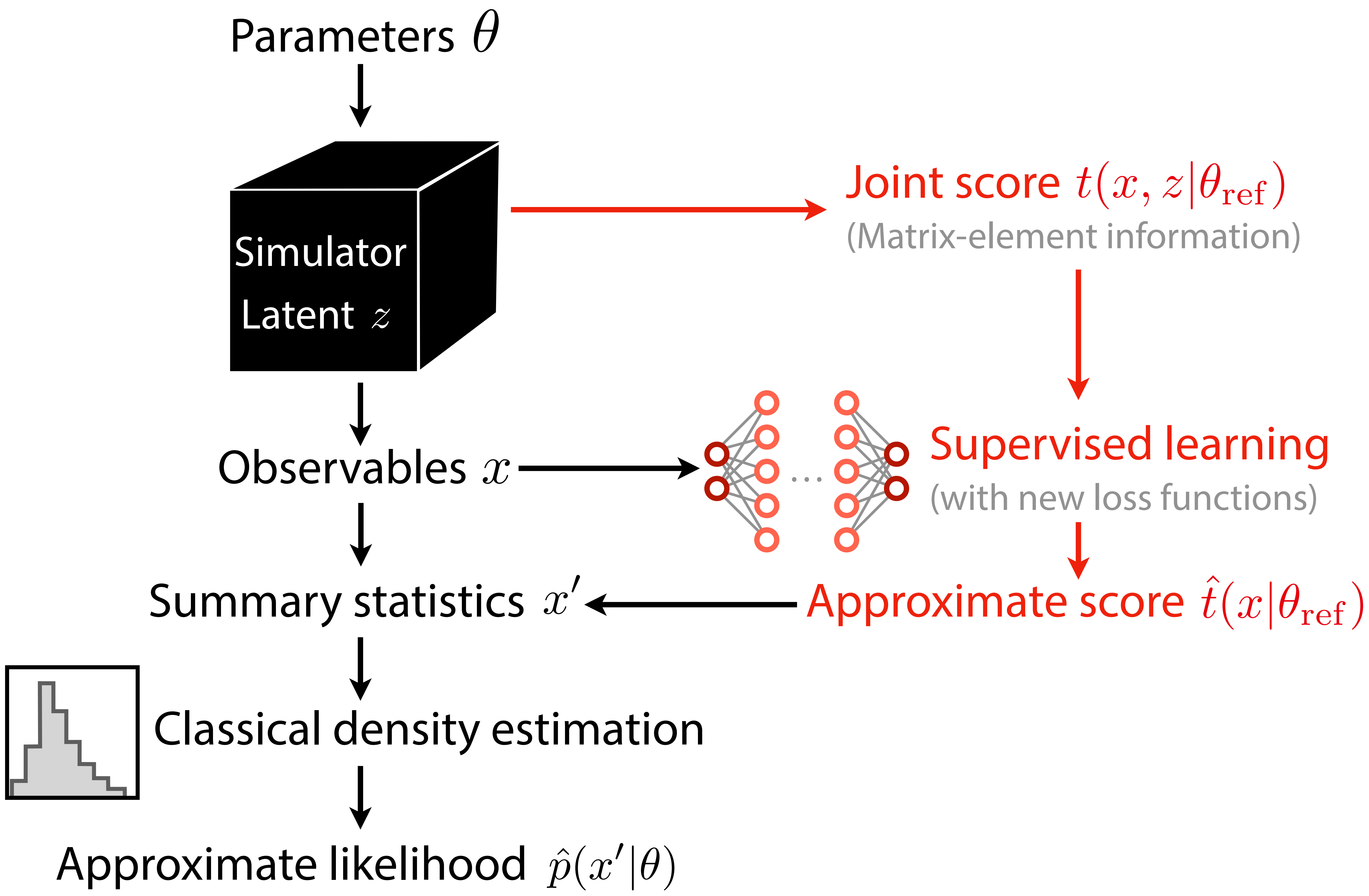

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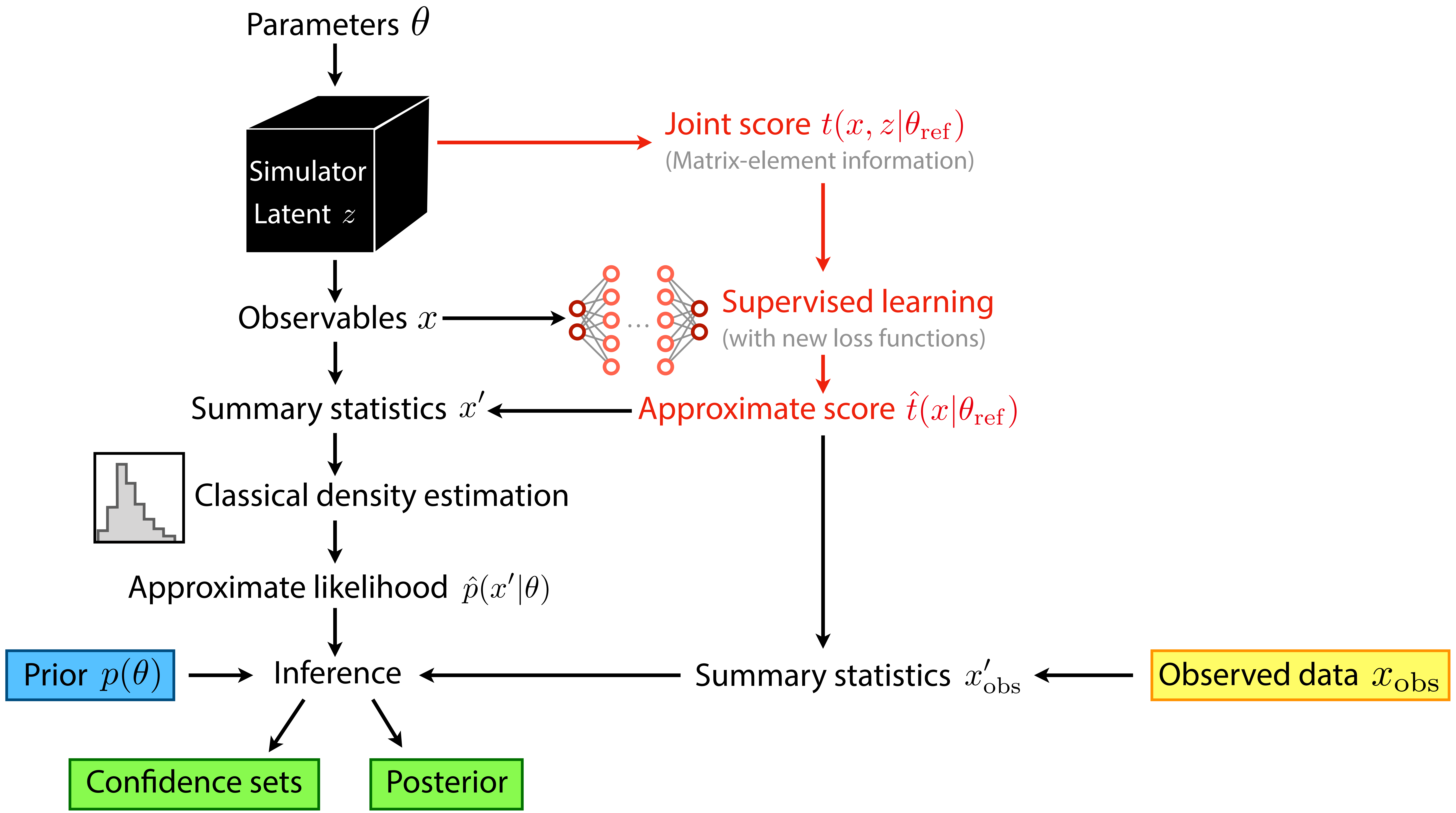
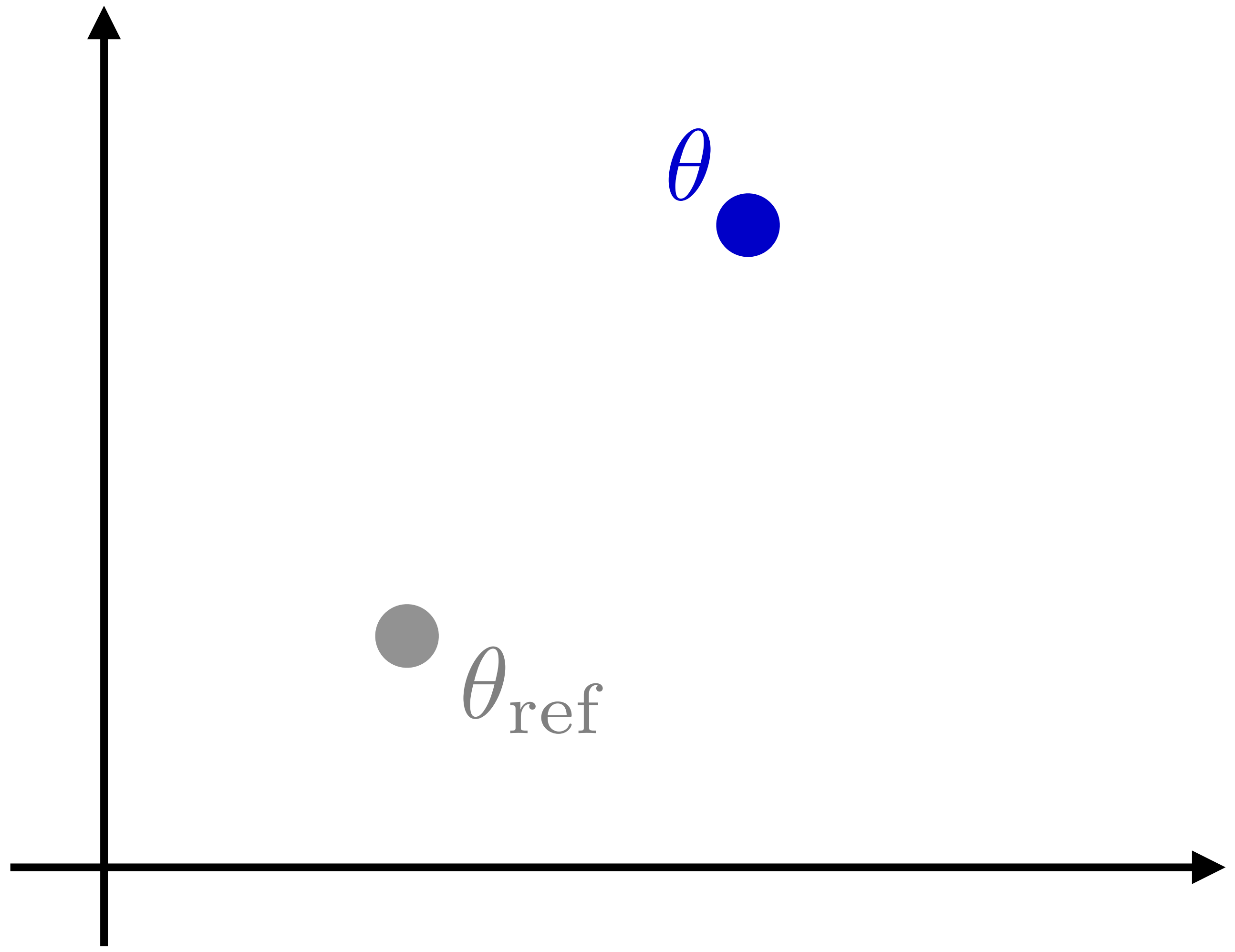


# Frequentist inference

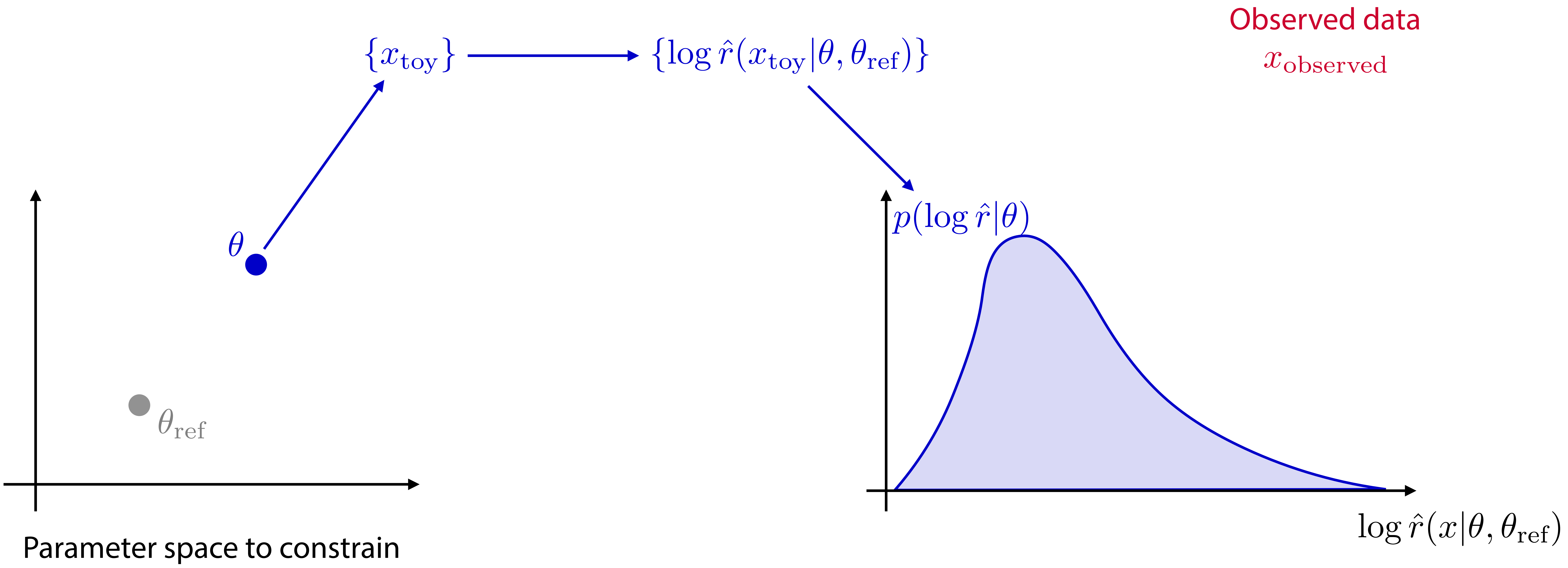
Observed data

$x_{\text{observed}}$




Parameter space to constrain

# Frequentist inference



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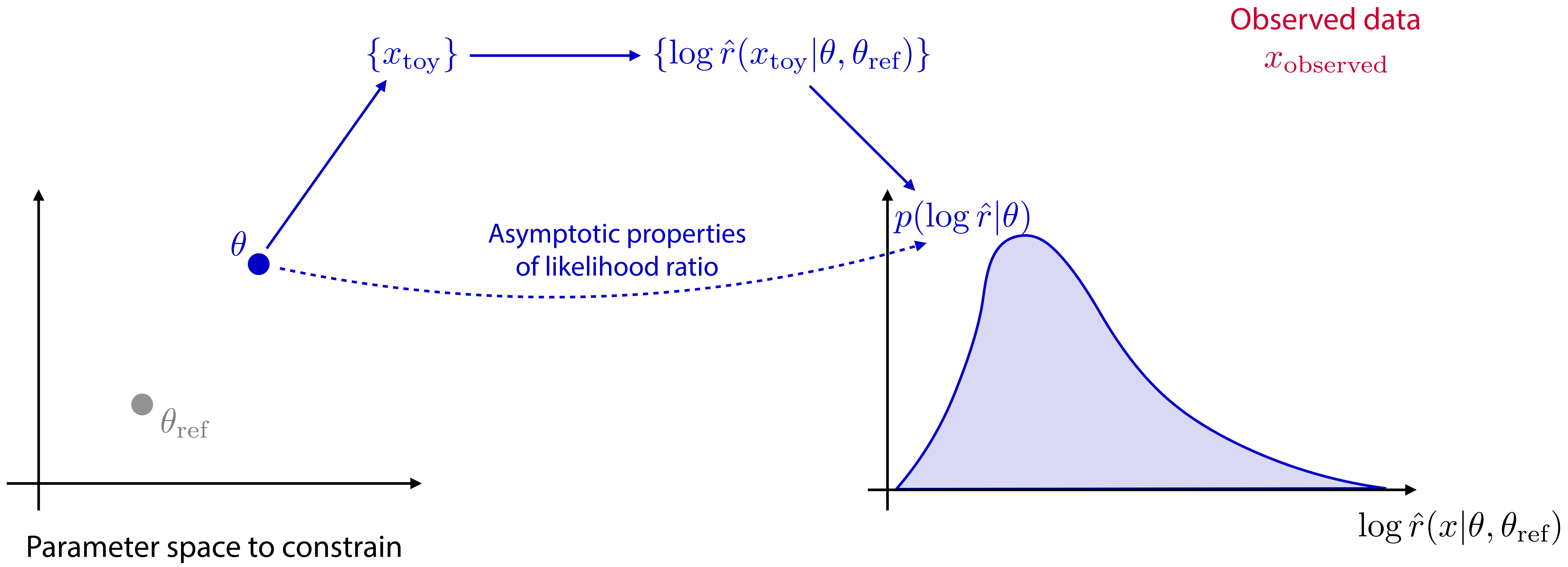

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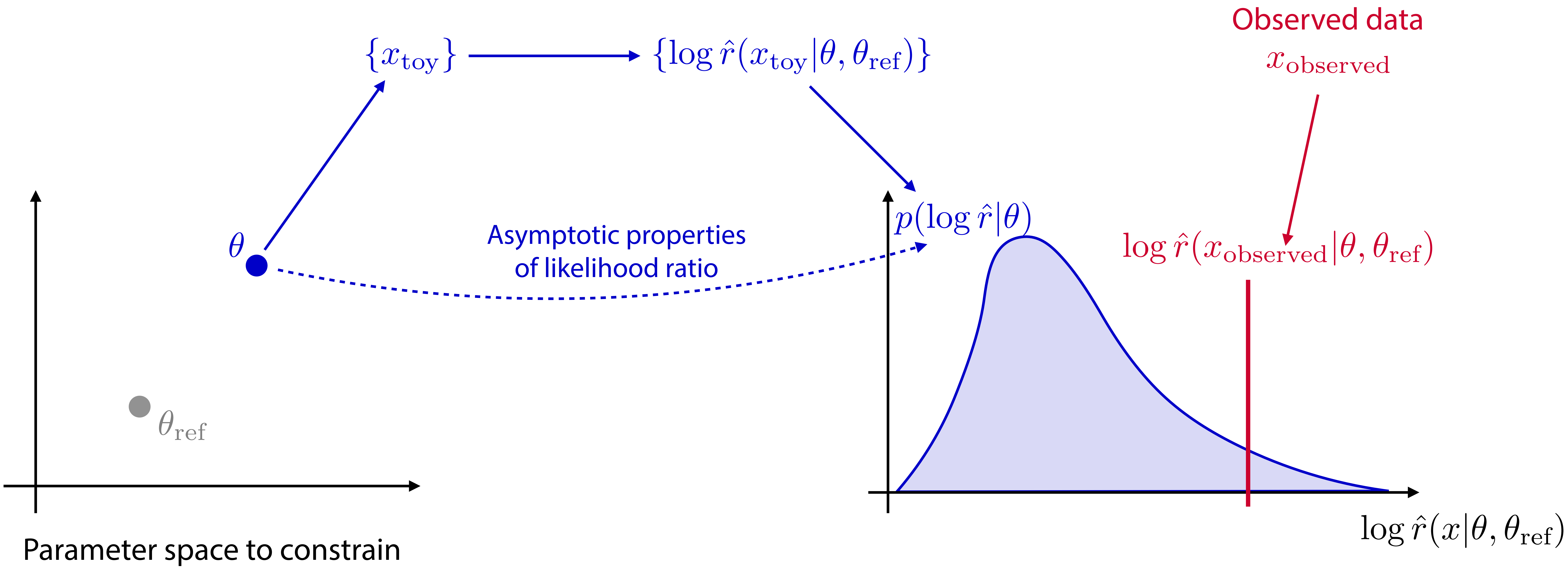

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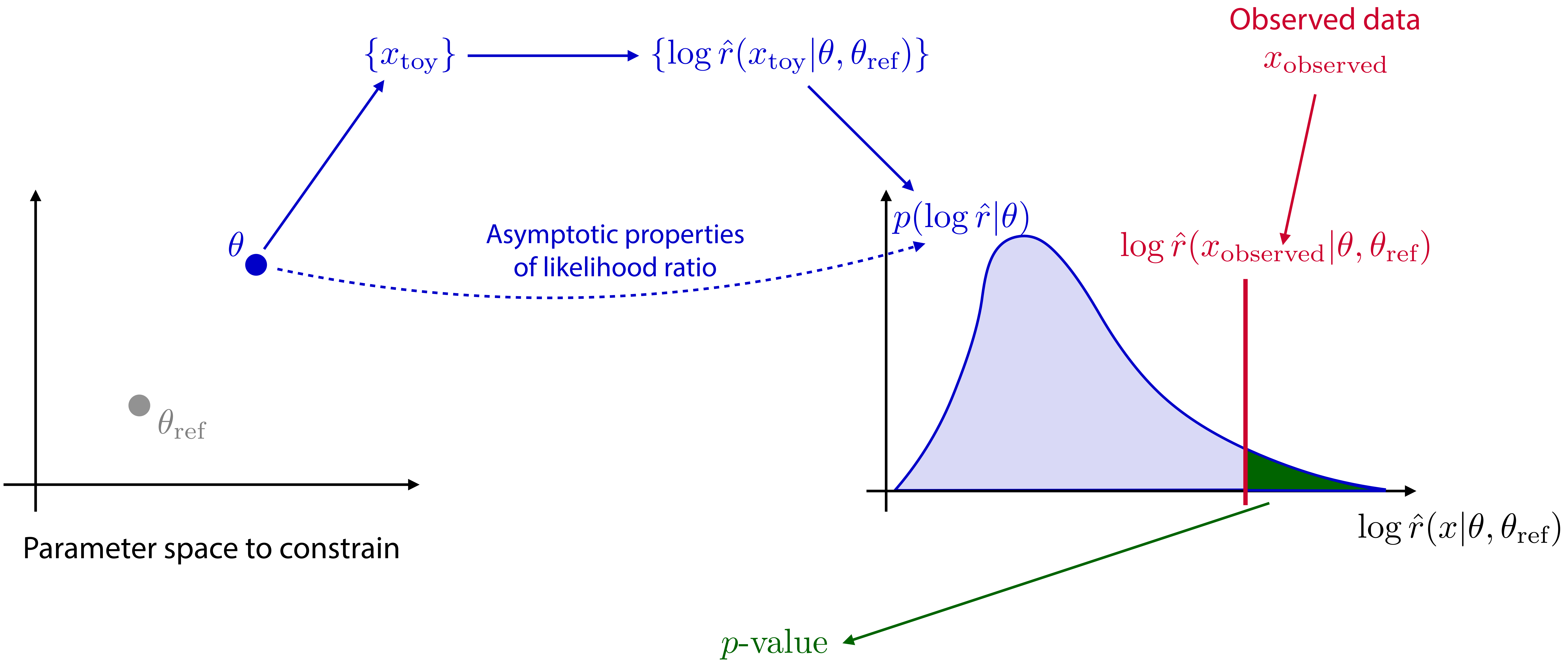

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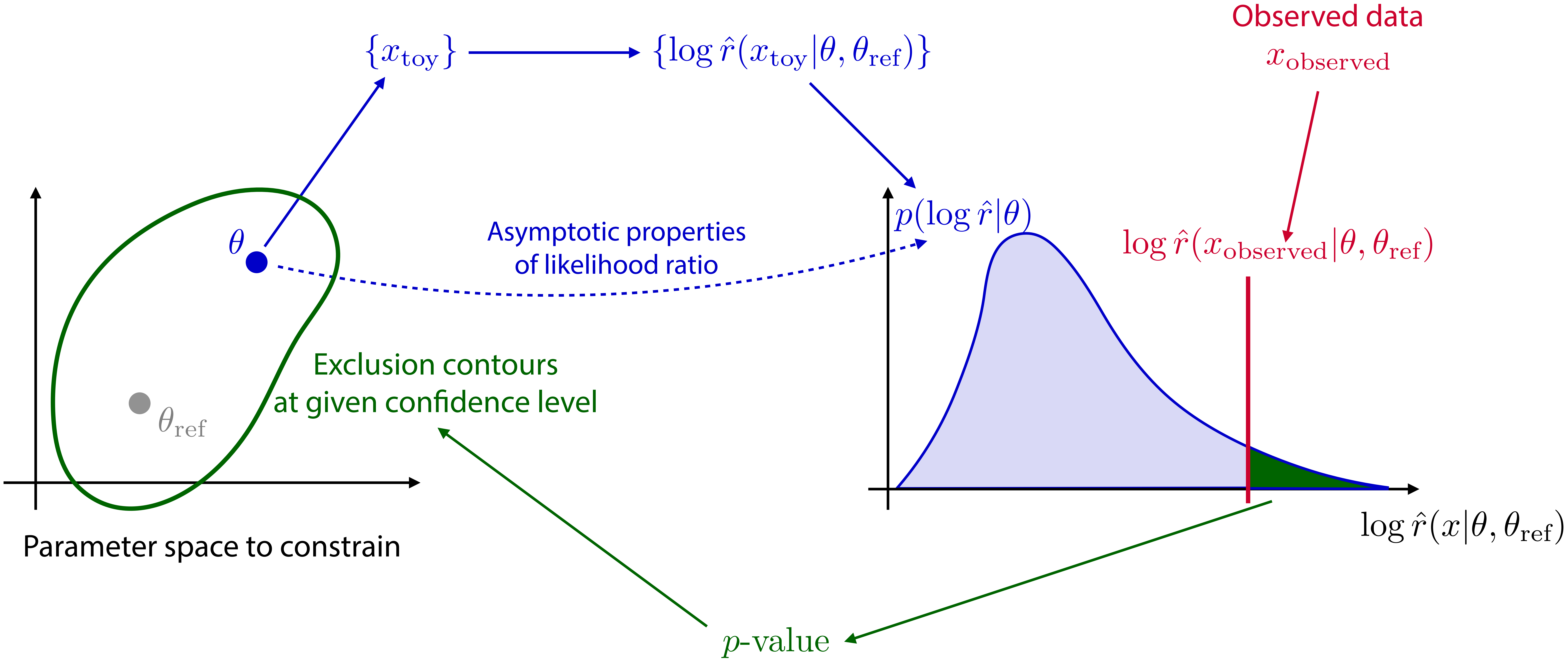
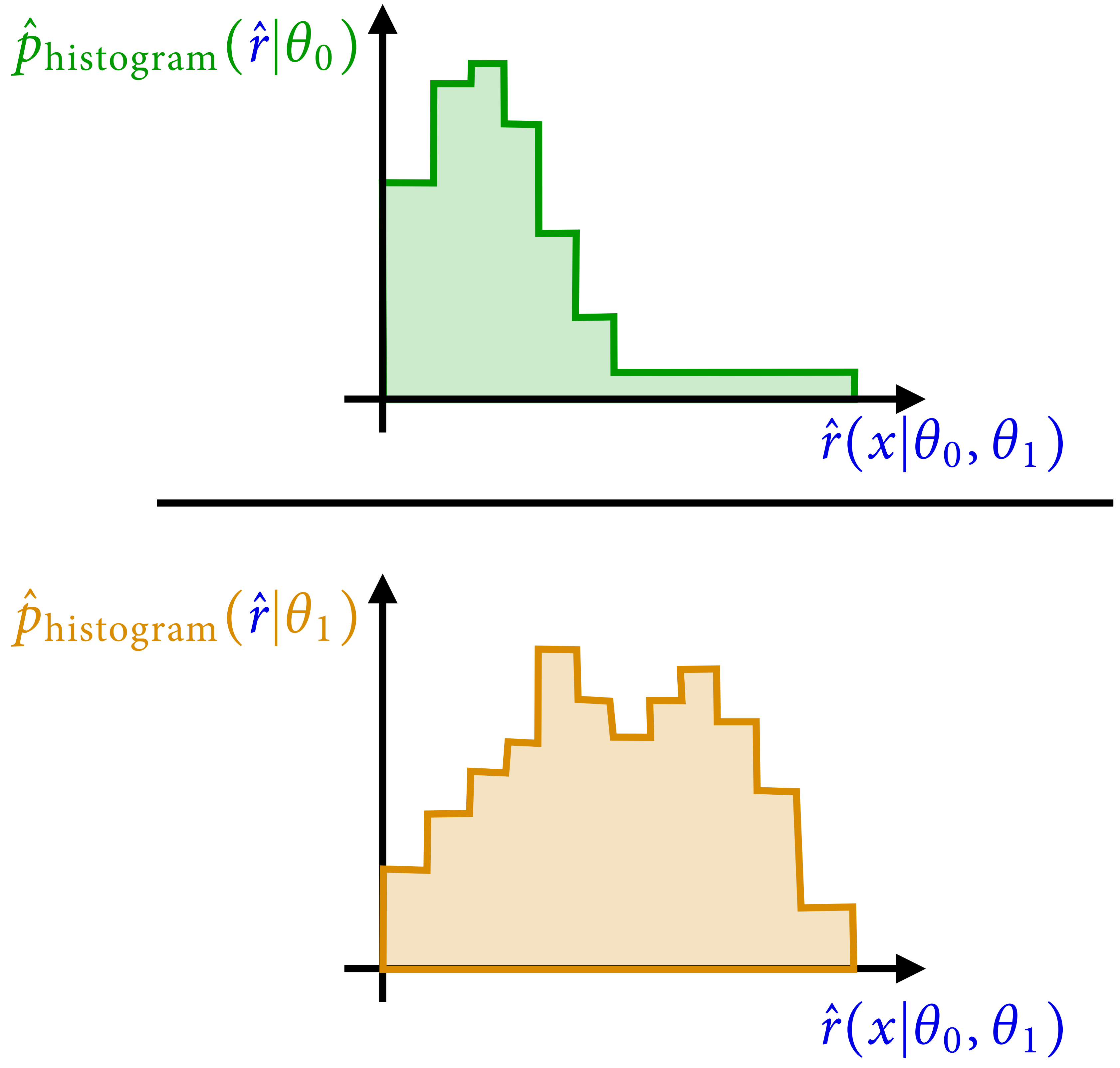


# Calibration

[K. Cranmer J. Pavez, G. Louppe 1506.02169]

What if the NN likelihood ratio estimator $\hat{r}(x|\theta_0, \theta_1)$ is off? Calibrate!

$$\hat{r}_{\text{calibrated}}(x|\theta_0, \theta_1) = \frac{\hat{p}_{\text{histogram}}(\hat{r}(x|\theta_0, \theta_1)|\theta_0)}{\hat{p}_{\text{histogram}}(\hat{r}(x|\theta_0, \theta_1)|\theta_1)}$$



# Bonus material: particle physics

# LHC footnotes

- Full LHC likelihood: $$p_{\text{full}}(\{x\}|\theta) = \text{Pois}(n|L\sigma(\theta)) \prod_{\text{events } x} p(x|\theta)$$

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Total rate term:

- How likely is it to observe $n$ events after cuts?
- “Easy” to compute
- For simplicity, we ignore this part in this talk

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- ~ normalized differential xsec
- This is the intractable part of the likelihood
- Focus of this talk

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- Event selection:
  - Choice of cuts shifts information between rate and kinematic part
  - "Good" cuts depend on inference strategy
  - This talk: assume fixed event selection

# Modelling particle physics processes

Theory
parameters
$\theta$

Evolution

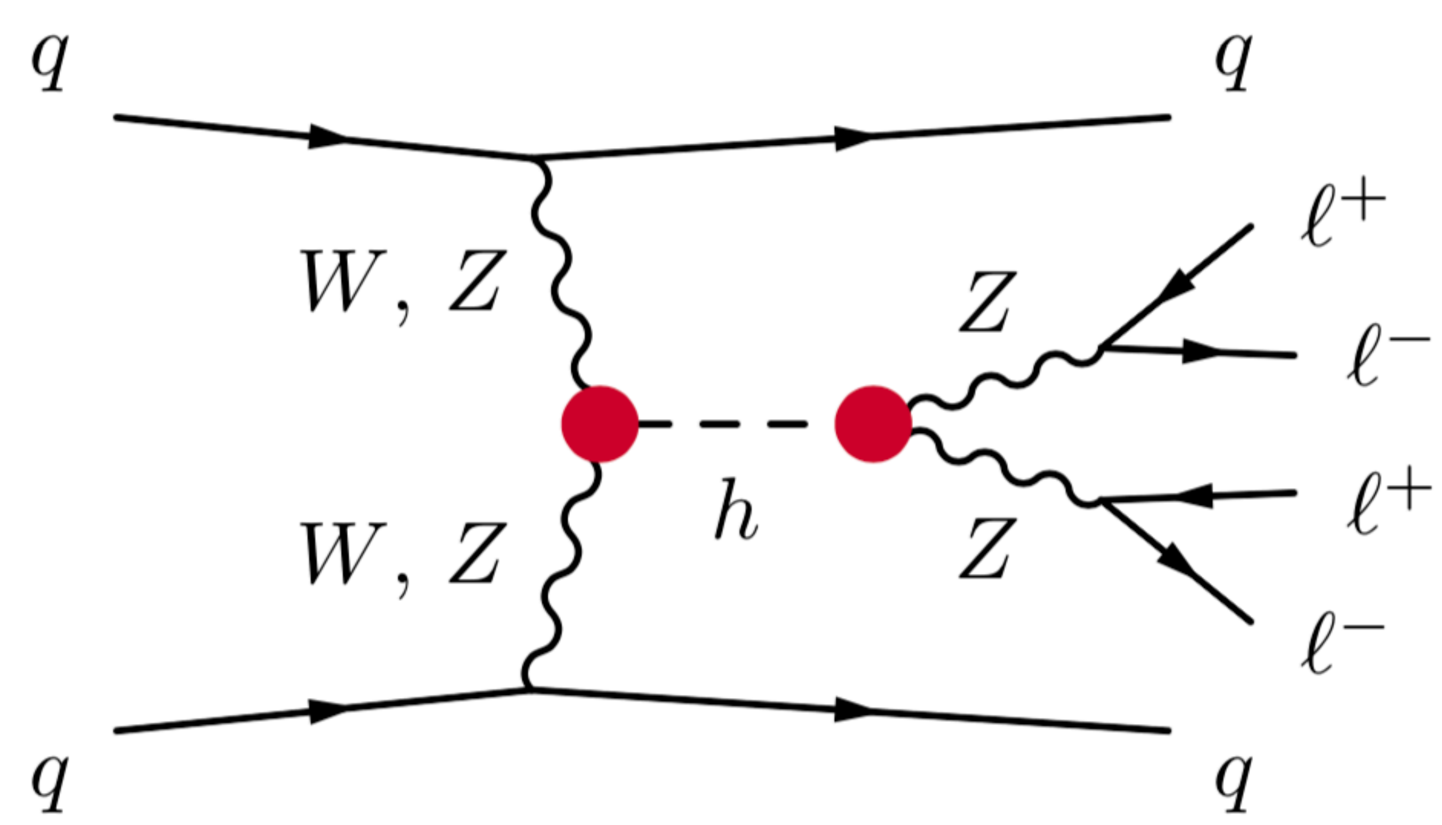
# Modelling particle physics processes

Latent variables

Parton-level momenta

Theory parameters

$z_p \longleftarrow \theta$

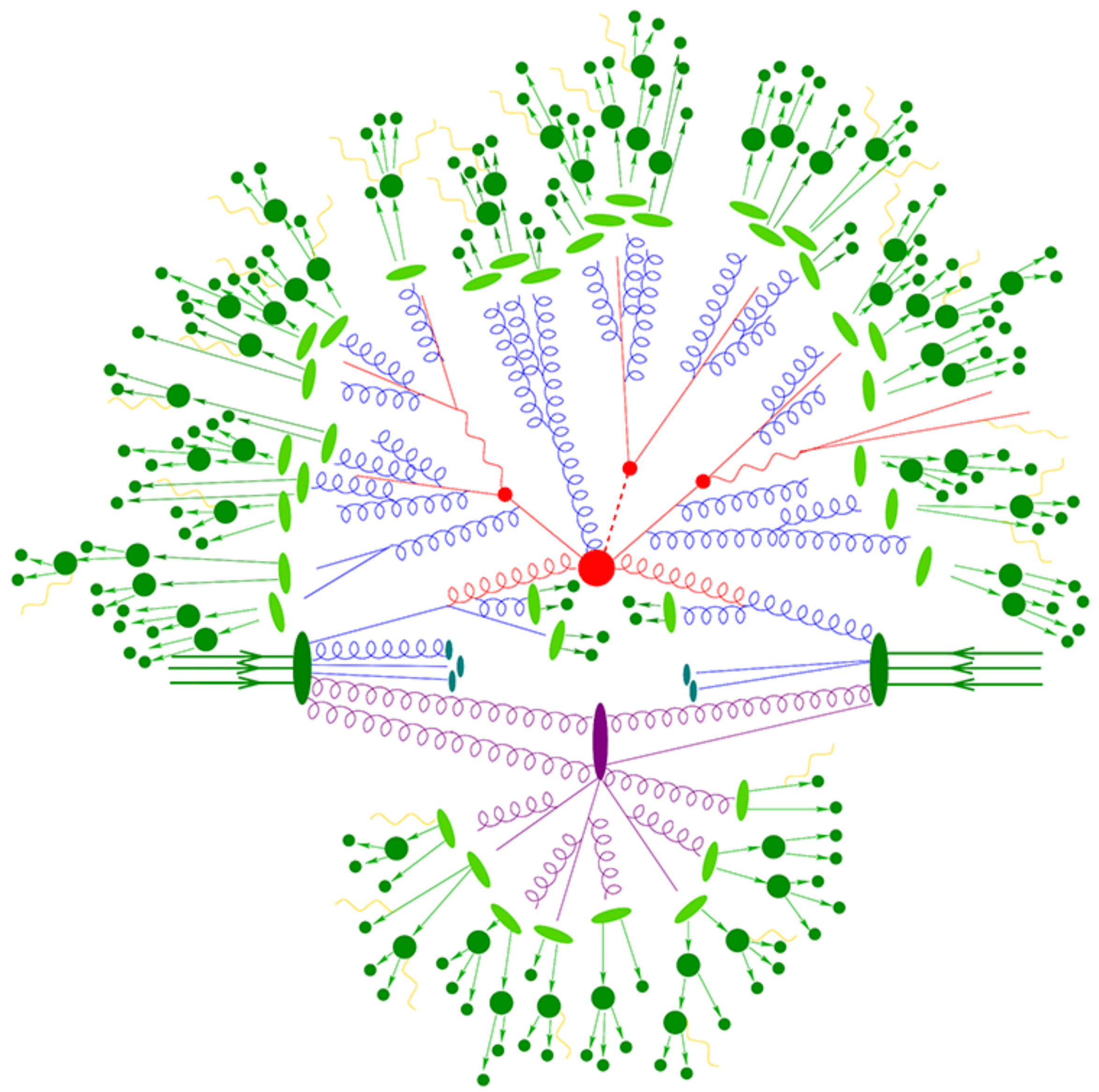



Evolution

# Modelling particle physics processes

Latent variables

| Shower splittings | | Parton-level momenta | | Theory parameters |
|---|---|---|---|---|
| $z_s$ | $\longleftarrow$ | $z_p$ | $\longleftarrow$ | $\theta$ |



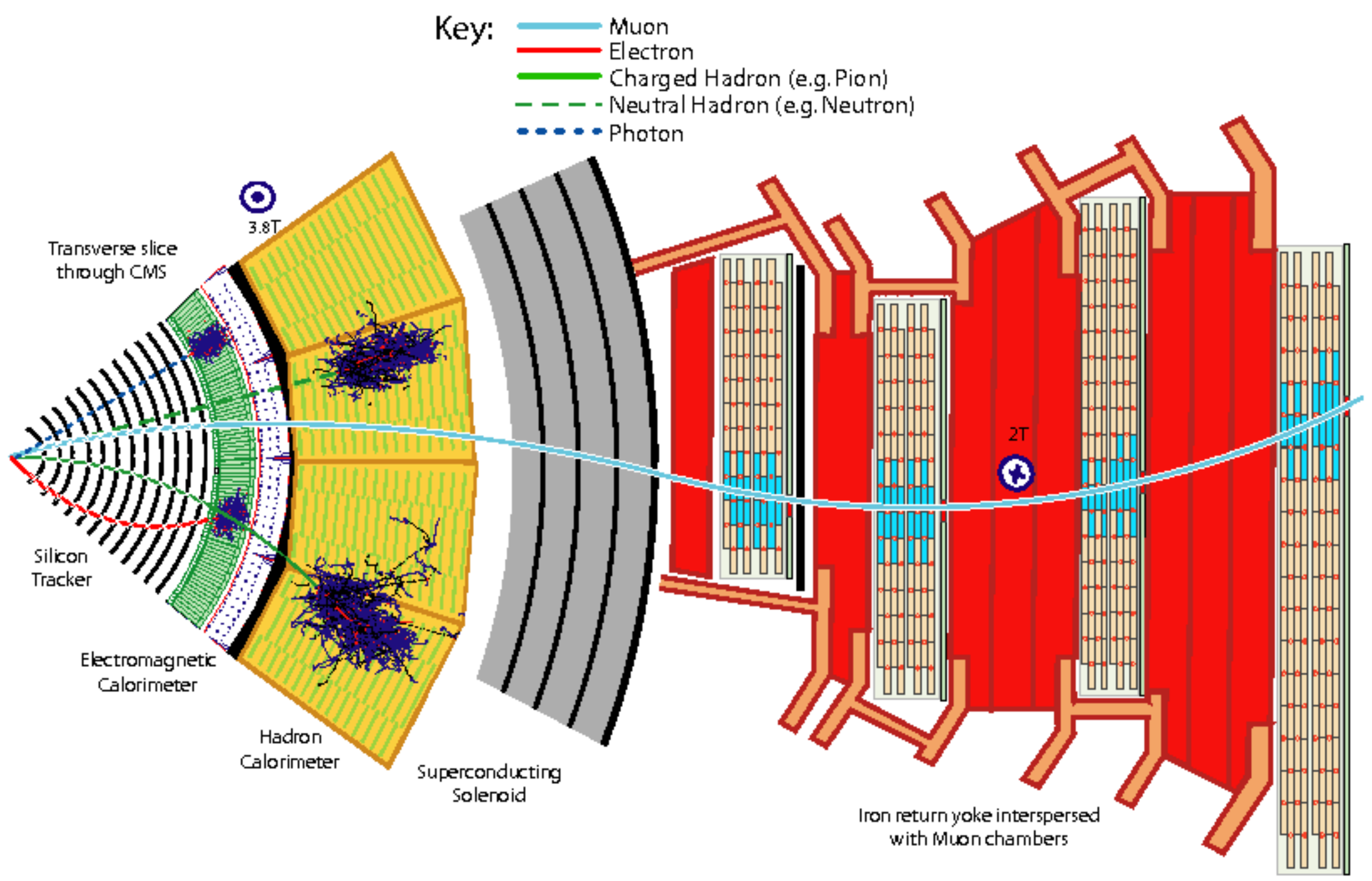
[F. Krauss]

$\longleftarrow$ Evolution

# Modelling particle physics processes

Latent variables

| Detector interactions | Shower splittings | Parton-level momenta | Theory parameters |
|---|---|---|---|
| $z_d$ ← | $z_s$ ← | $z_p$ ← | $\theta$ |




[CMS]

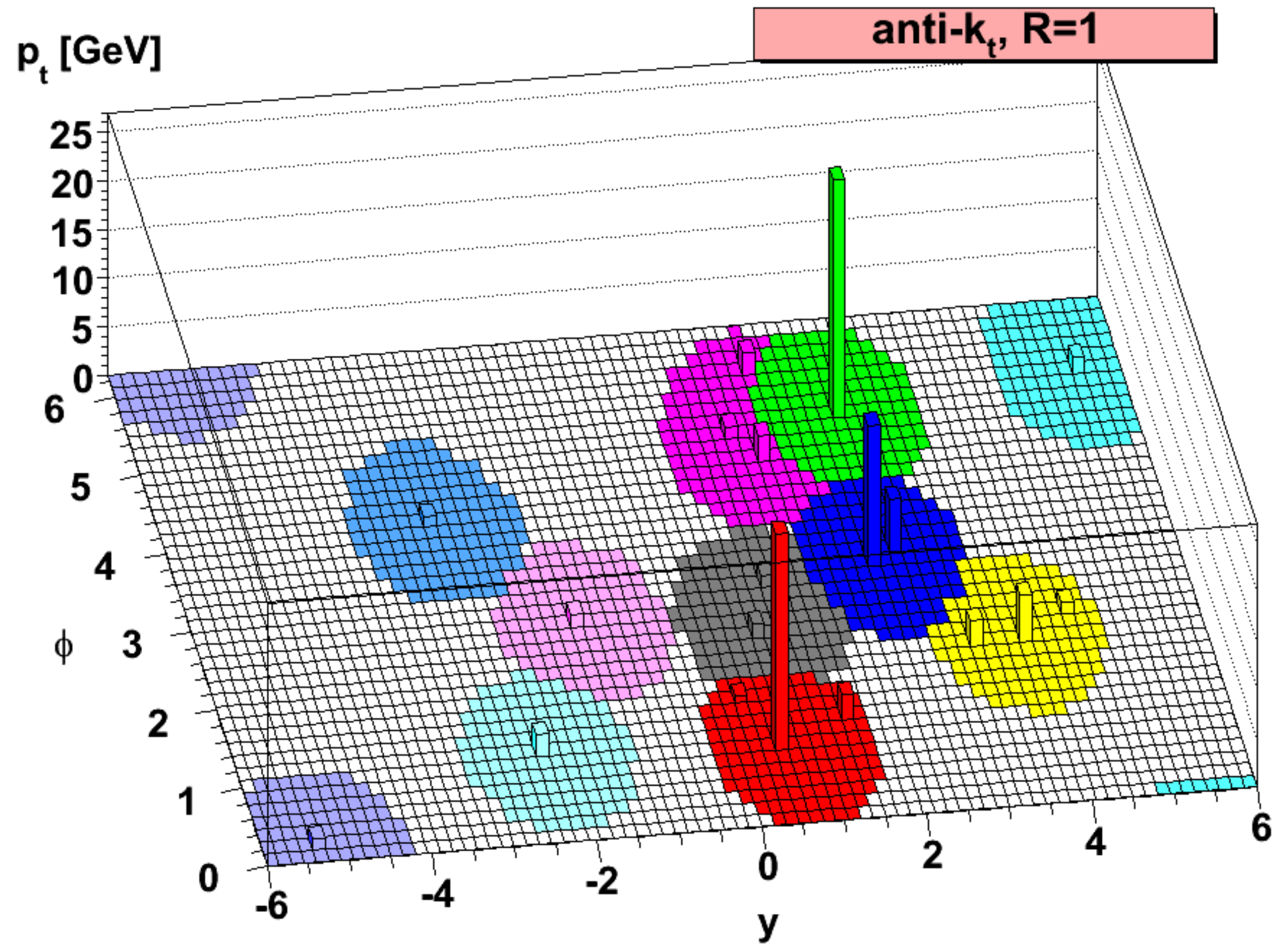
← Evolution

# Modelling particle physics processes

Latent variables

| Observables | | Detector interactions | Shower splittings | Parton-level momenta | Theory parameters |
|---|---|---|---|---|---|

$$x \longleftarrow z_d \longleftarrow z_s \longleftarrow z_p \longleftarrow \theta$$




[M. Cacciari, G. Salam, G. Soyez 0802.1189]

$\longleftarrow$

Evolution

# Modelling particle physics processes

Latent variables

| Observables | | Detector interactions | Shower splittings | Parton-level momenta | Theory parameters |
|---|---|---|---|---|---|
| $x$ | $\longleftarrow$ | $z_d$ $\longleftarrow$ | $z_s$ $\longleftarrow$ | $z_p$ $\longleftarrow$ | $\theta$ |
| Sample from | $p(x\|z_d)$ | $p(z_d\|z_s)$ | $p(z_s\|z_p)$ | $p(z_p\|\theta)$ | |

$\longleftarrow$ Prediction (simulation)

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|---|---|---|---|---|---|

$$x \longleftarrow z_d \longleftarrow z_s \longleftarrow z_p \longleftarrow \theta$$

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

Inference

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

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

(More subtle: We cannot sample from $p(z|x, \theta)$ efficiently.)

$\longrightarrow$

Inference

# Mining gold from the simulator

Latent variables

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

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Intractable integrals

# Mining gold from the simulator

Latent variables

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| $x$ | $\longleftarrow$ | $z_d$ $\longleftarrow$ | $z_s$ $\longleftarrow$ | $z_p$ $\longleftarrow$ | $\theta$ |

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

Parton-level likelihood
is given by matrix element
and can be evaluated!

⇒ For each simulated event, we can calculate the joint likelihood ratio which depends on the specific evolution of the simulation:

$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)} = \frac{p(x|z_d)}{p(x|z_d)} \frac{p(z_d|z_s)}{p(z_d|z_s)} \frac{p(z_s|z_p)}{p(z_s|z_p)} \boxed{\frac{p(z_p|\theta_0)}{p(z_p|\theta_1)} \sim \frac{|\mathcal{M}(z_p|\theta_0)|^2}{|\mathcal{M}(z_p|\theta_1)|^2}}$$

# 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 $\theta_0$ compared to $\theta_1$?")

$$\downarrow$$

We want the likelihood ratio function

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

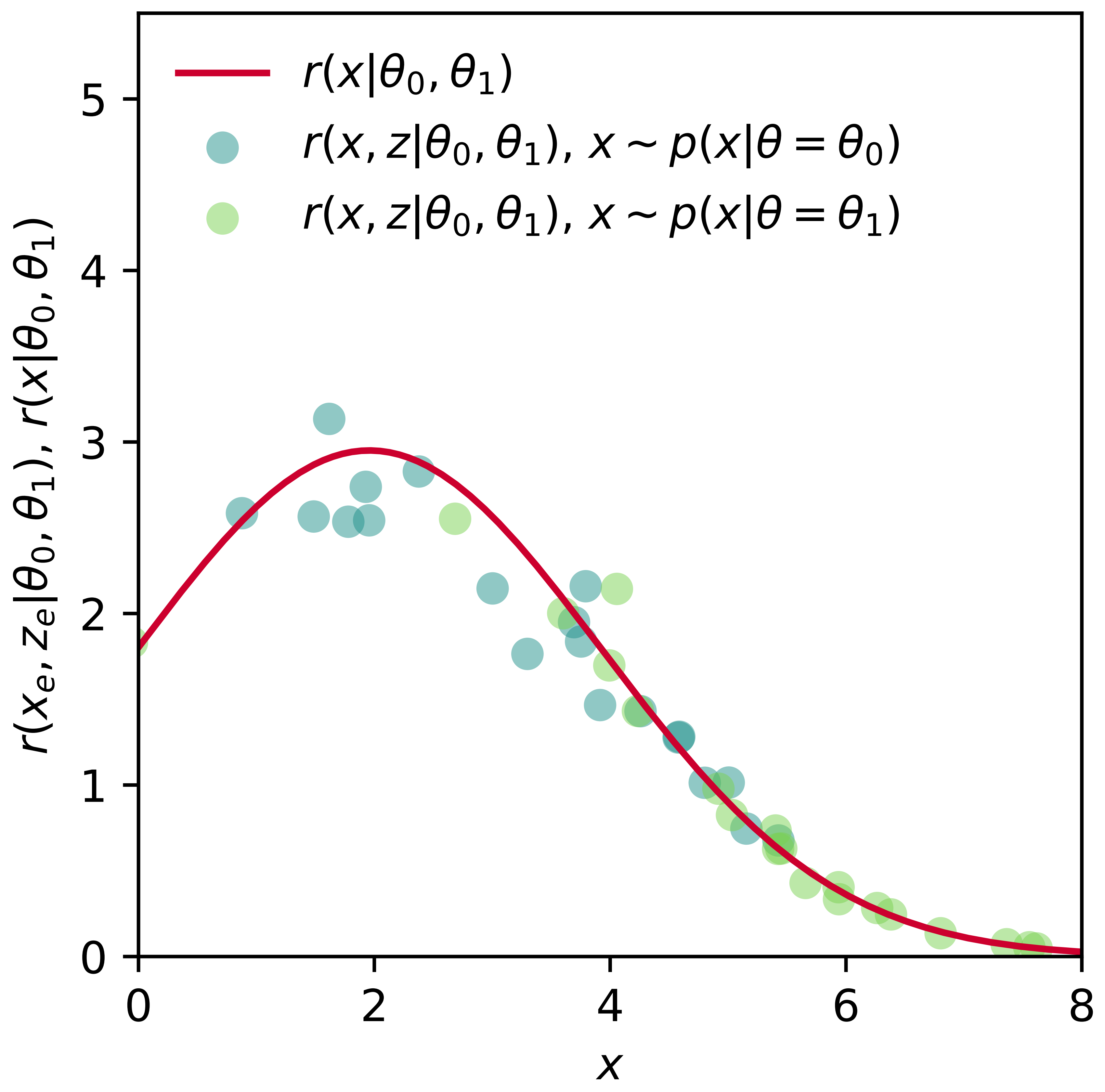
("How much more likely is the observation $x$ for $\theta_0$ compared to $\theta_1$?")

# The value of gold

We can calculate the joint likelihood ratio

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

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

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# The value of gold

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

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

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

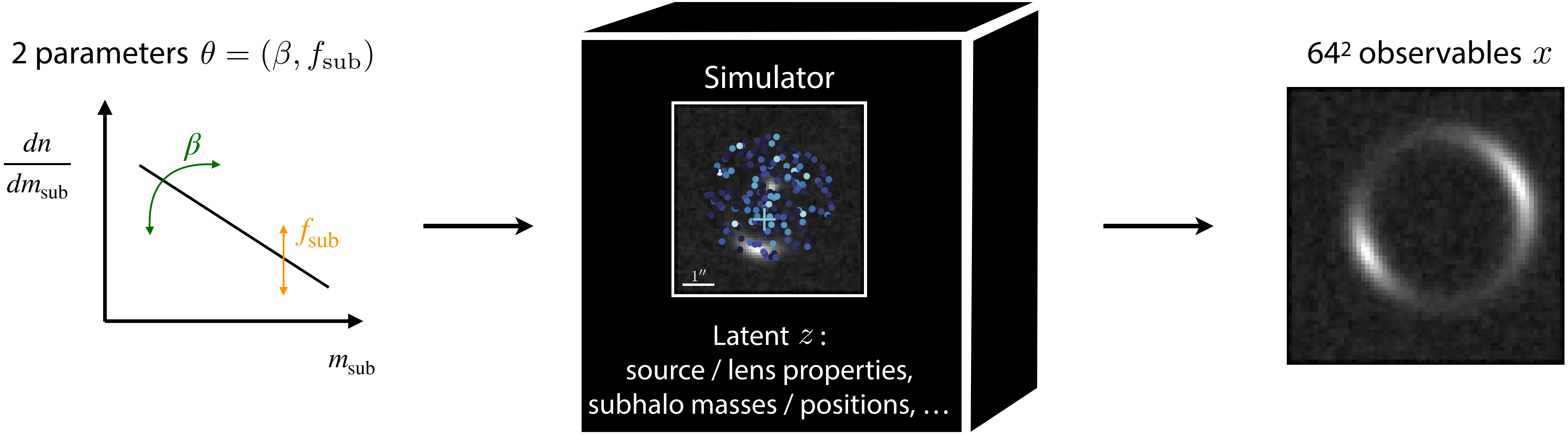
(And we can sample from $p(x, z|\theta)$ by running the simulator.)

We want the likelihood ratio function

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

# Bonus material: gravitational lensing

# Overview




Prediction: We construct a simulator that can sample $x \sim p(x|\theta)$

Inference: We train neural likelihood ratio estimators $\hat{r}(x|\theta)$

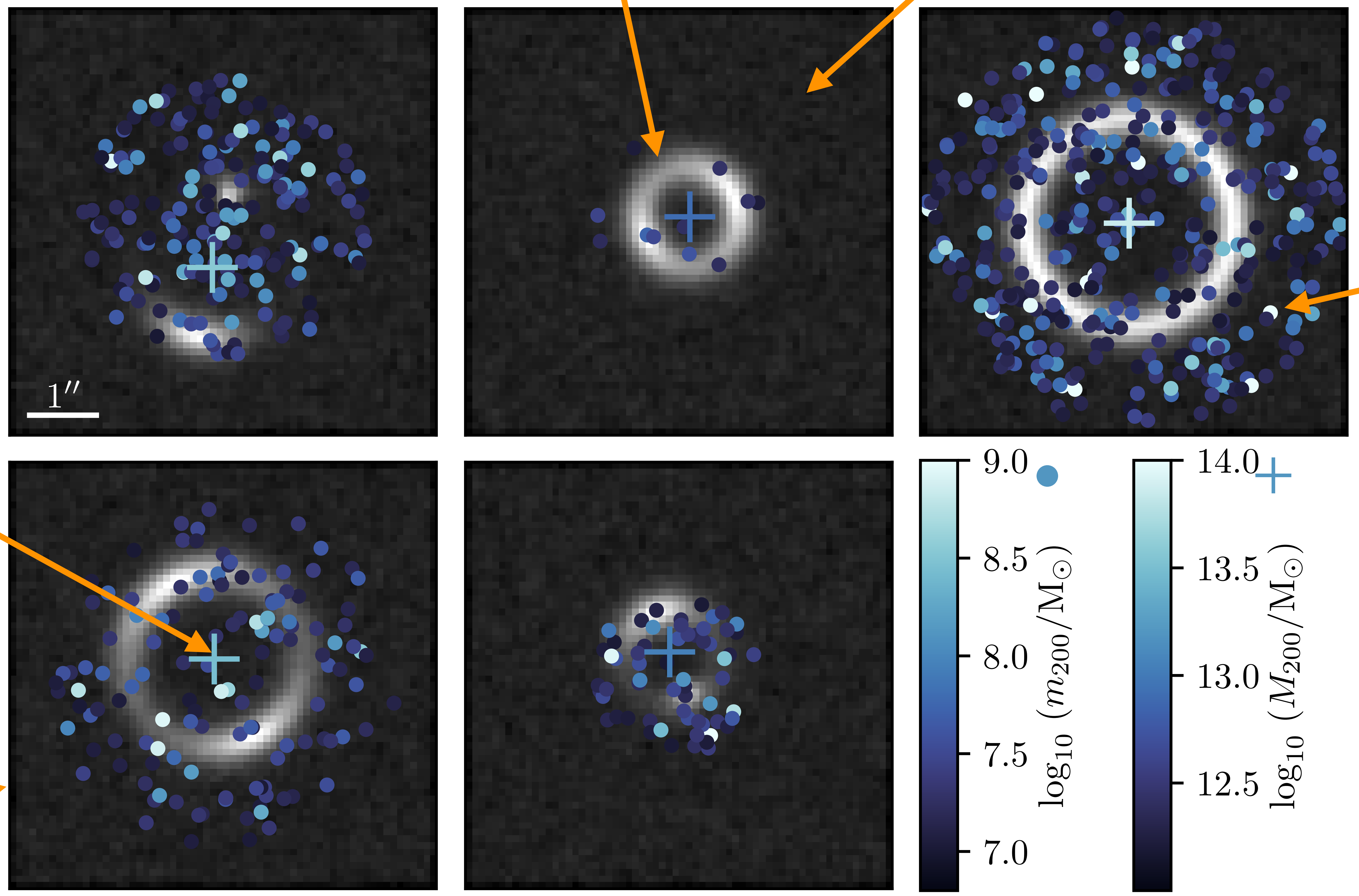
# Proof-of-principle simulator

[following T. Collett 1507.02657]

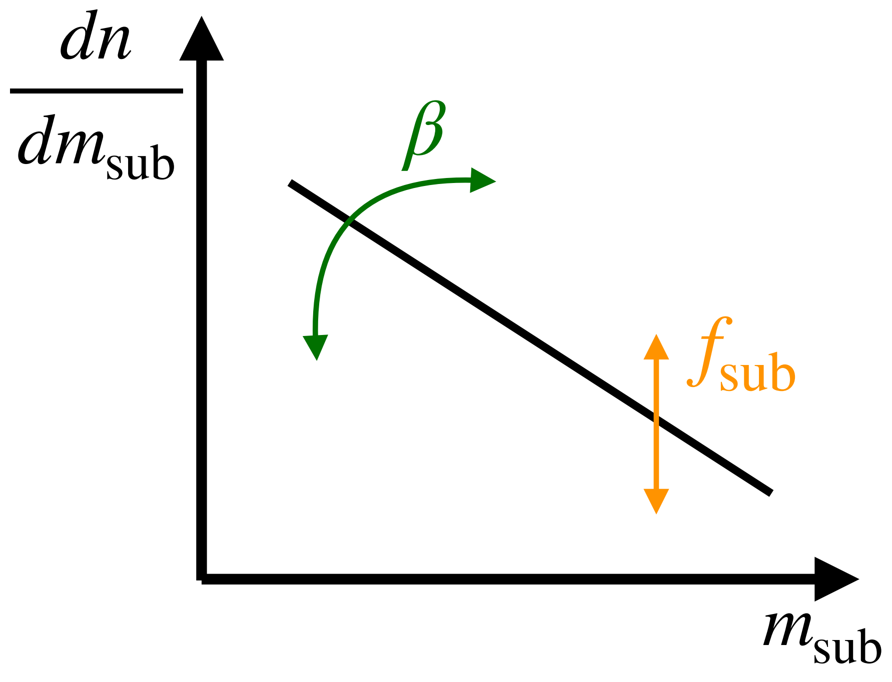
Spherical lensing host galaxies
at redshift ~0.5…1

Poisson fluctuations

Extended galaxy sources
at redshift 1.5

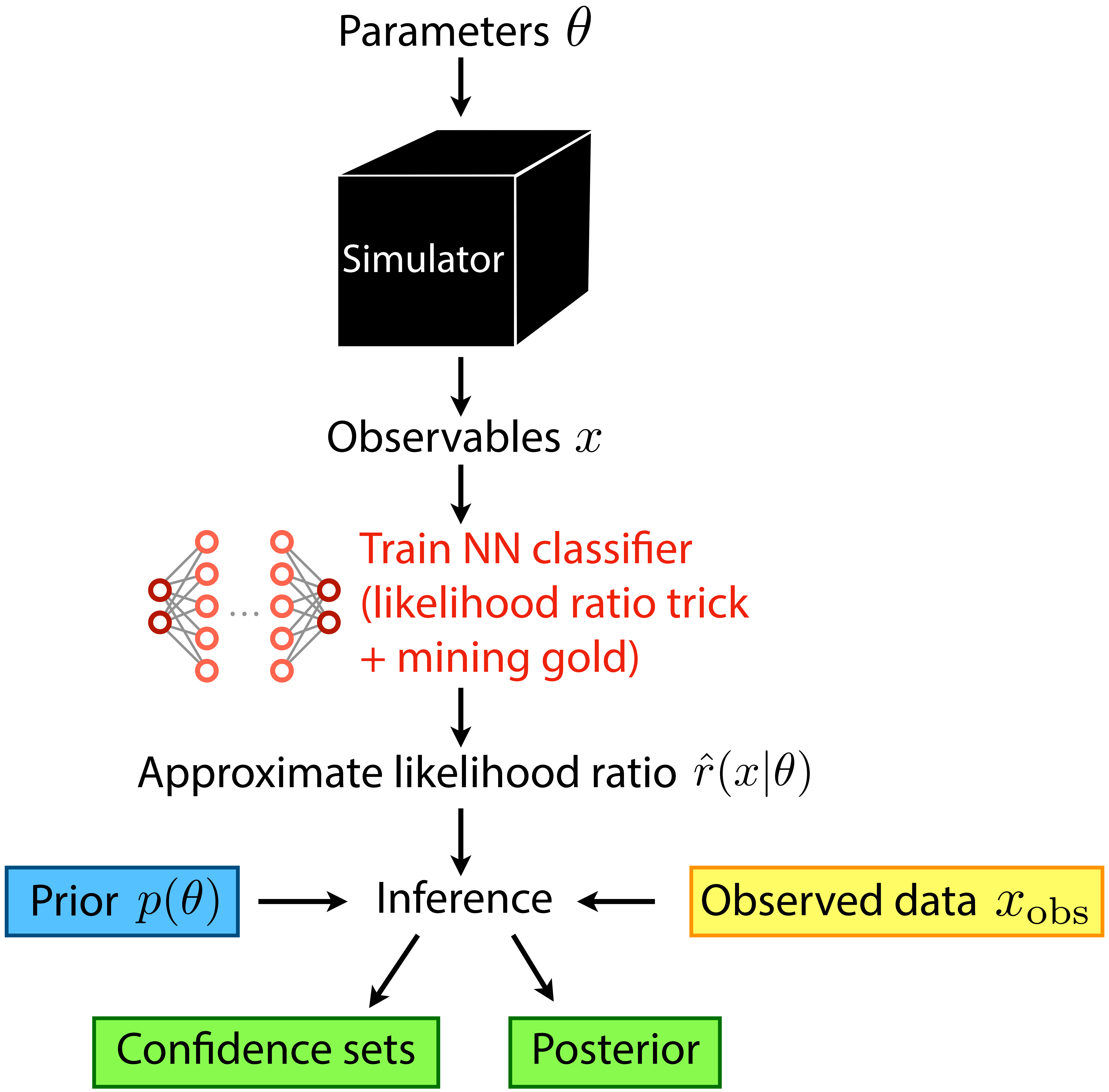



Subhalos follow mass distribution with two parameters




Euclid detector model
(single optical band,
$64^2$ pixel, Gaussian PSF)

# Inference setup




Training data: $10^6$ lensed images with $0 \leq f_{\text{sub}} \leq 0.2, -1.5 \leq \beta \leq -0.5$

Convolutional neural network (modified ResNet-18) trained on ALICES loss

[M. Stoye, JB, J. Pavez, G, Louppe, K. Cranmer 1808.00973]

Calibration of network output

Synthetic "observed" data set: $f_{\text{sub}} = 0.05, \beta = -0.9$

Bayesian & frequentist inference

# LHC footnotes

- Full LHC likelihood: $$p_{\text{full}}(\{x\}|\theta) = \text{Pois}(n|L\sigma(\theta)) \prod_{\text{events } x} p(x|\theta)$$

Total rate term:

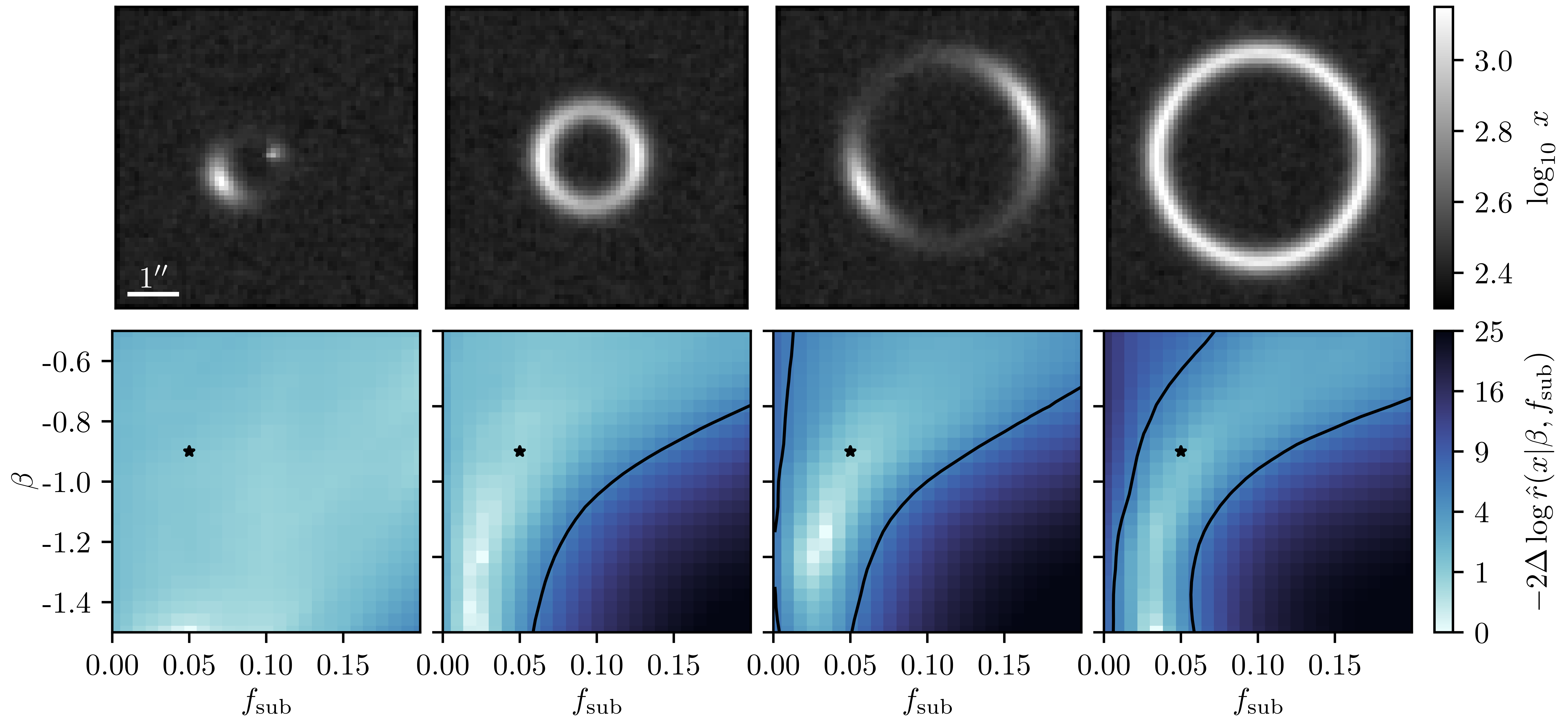
- How likely is it to observe $n$ events after cuts?
- "Easy" to compute
- For simplicity, we ignore this part in this talk

Kinematic term for each event:

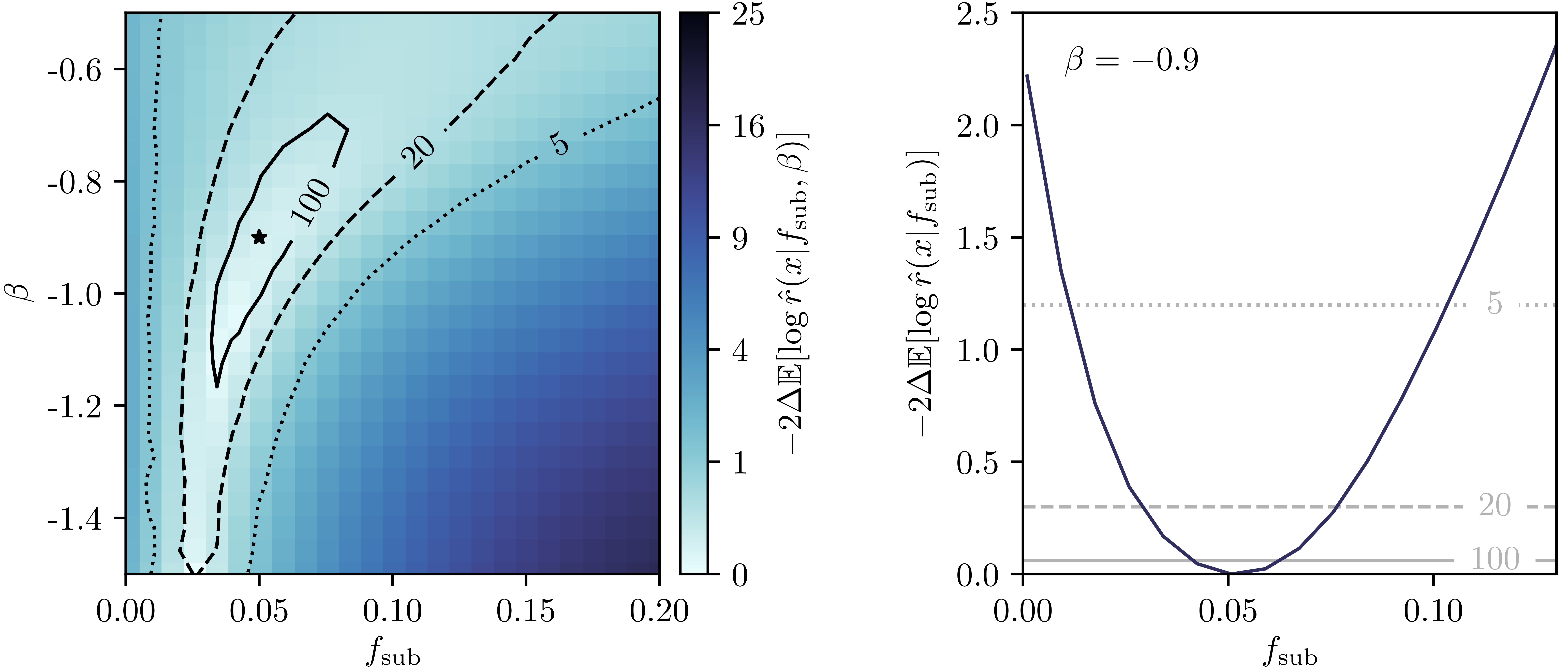
- How likely is it that an event looks like it does?
- ~ normalized differential xsec
- This is the intractable part of the likelihood
- Focus of this talk

- Event selection:
  - Choice of cuts shifts information between rate and kinematic part
  - "Good" cuts depend on inference strategy
  - This talk: assume fixed event selection

# Inferring parameters from individual images



# Expected likelihood ratio map



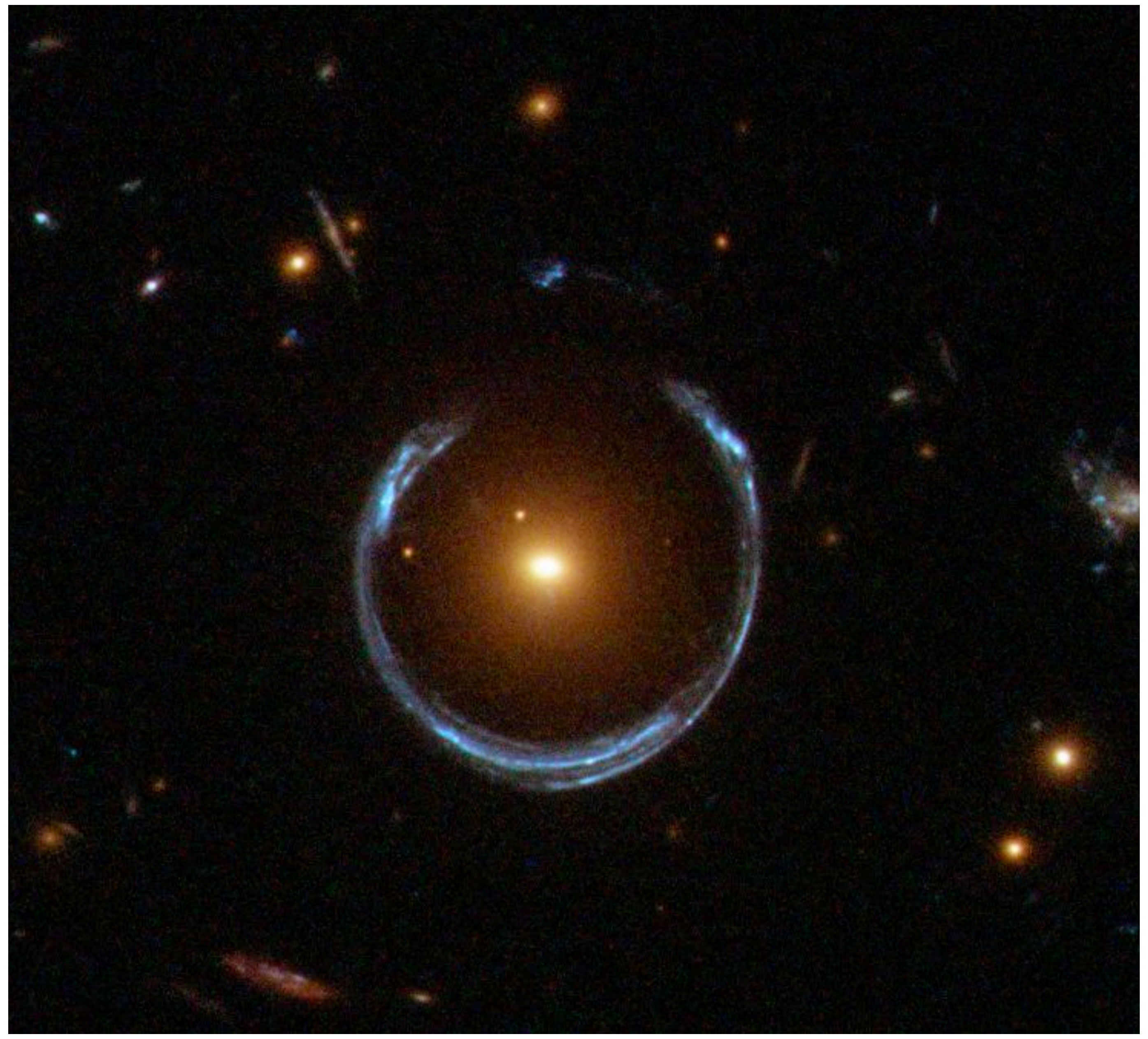
# All the things we didn't do

- More involved subhalo mass function
  - Warm DM with DM mass as parameter

- Realistic simulators
  - More diverse source and host galaxies (e.g. data-driven)
  - Realistic subhalo modelling (tidal disruption, redshift dependence…)
  - Line-of-sight substructure
  - Realistic observation model (variable exposure / PSF, multiple bands…)

- Use auxiliary information during inference

- Evaluation on real data



[ESA/Hubble/NASA]

⇒ Our method should scale to a realistic setting, but will require more simulations and careful sanity checks

# Bonus material: $\mathscr{M}$-flows

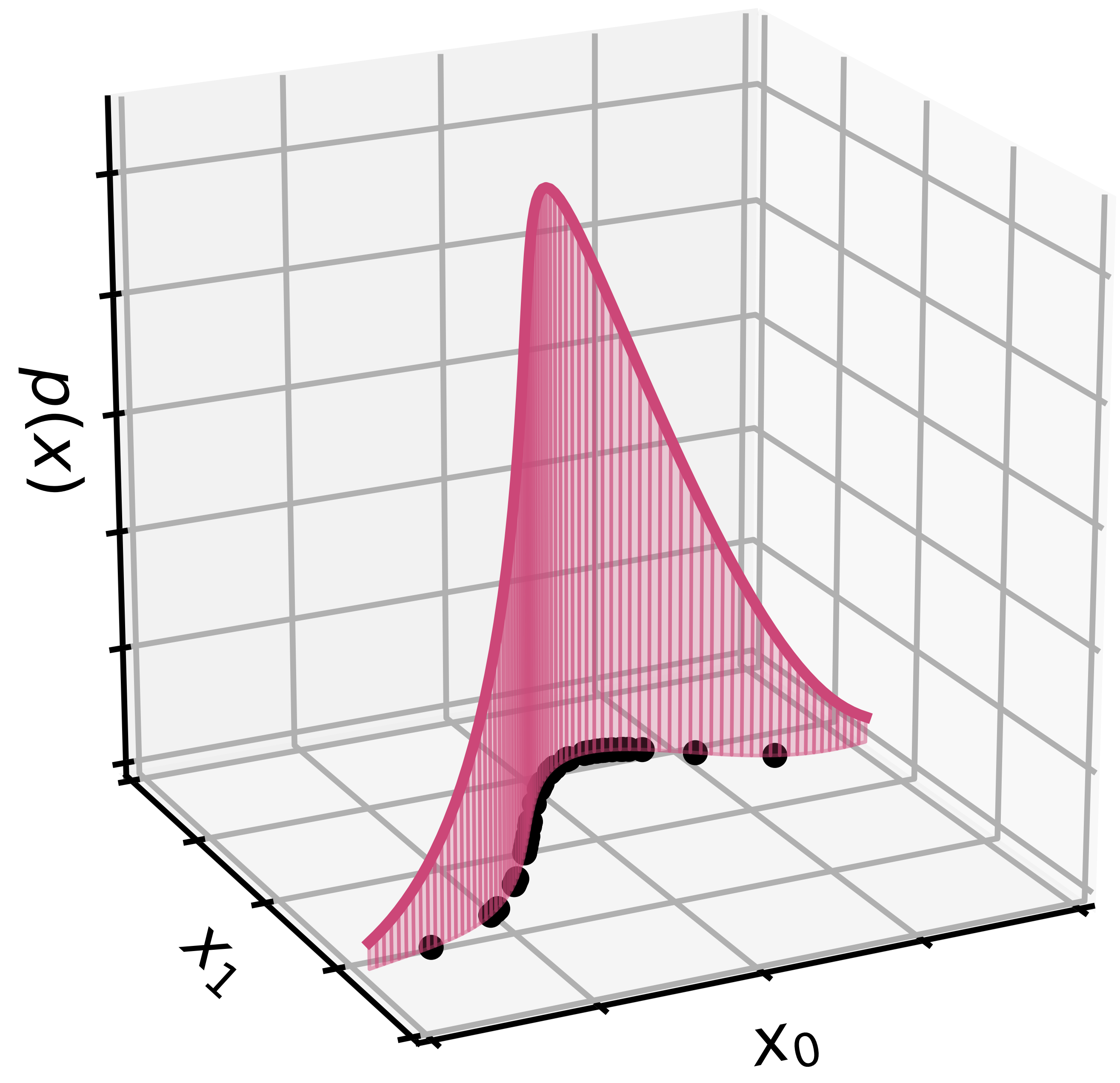
# $\mathcal{M}$-flows

[JB, K. Cranmer 2003.13913]

Often data is restricted to a lower-dimensional manifold embedded in the data space

$\mathcal{M}$-flows are a new probabilistic / generative model that

- describe data as a tractable probability density on a lower-dimensional manifold
- learn manifold and density from data



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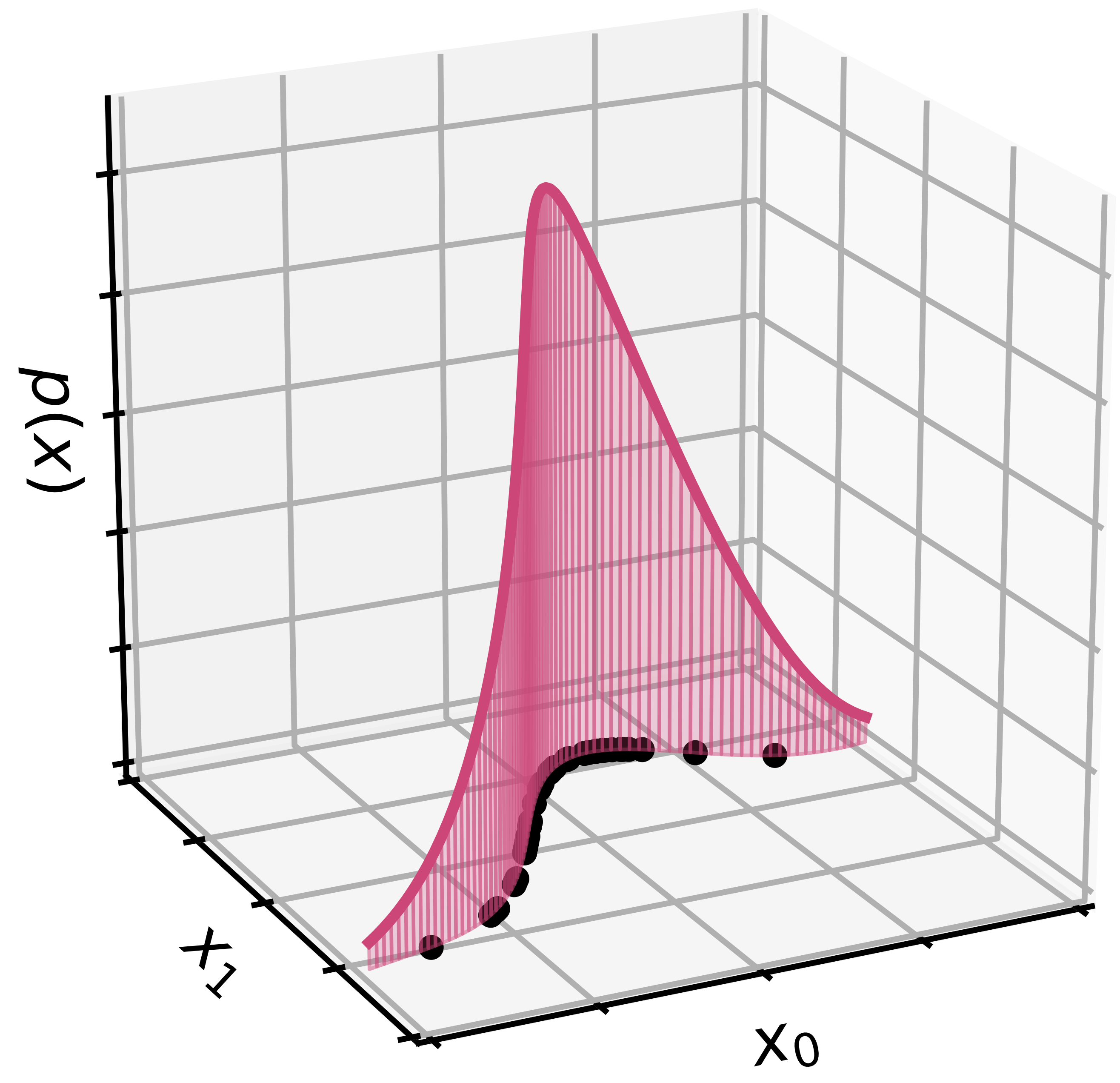


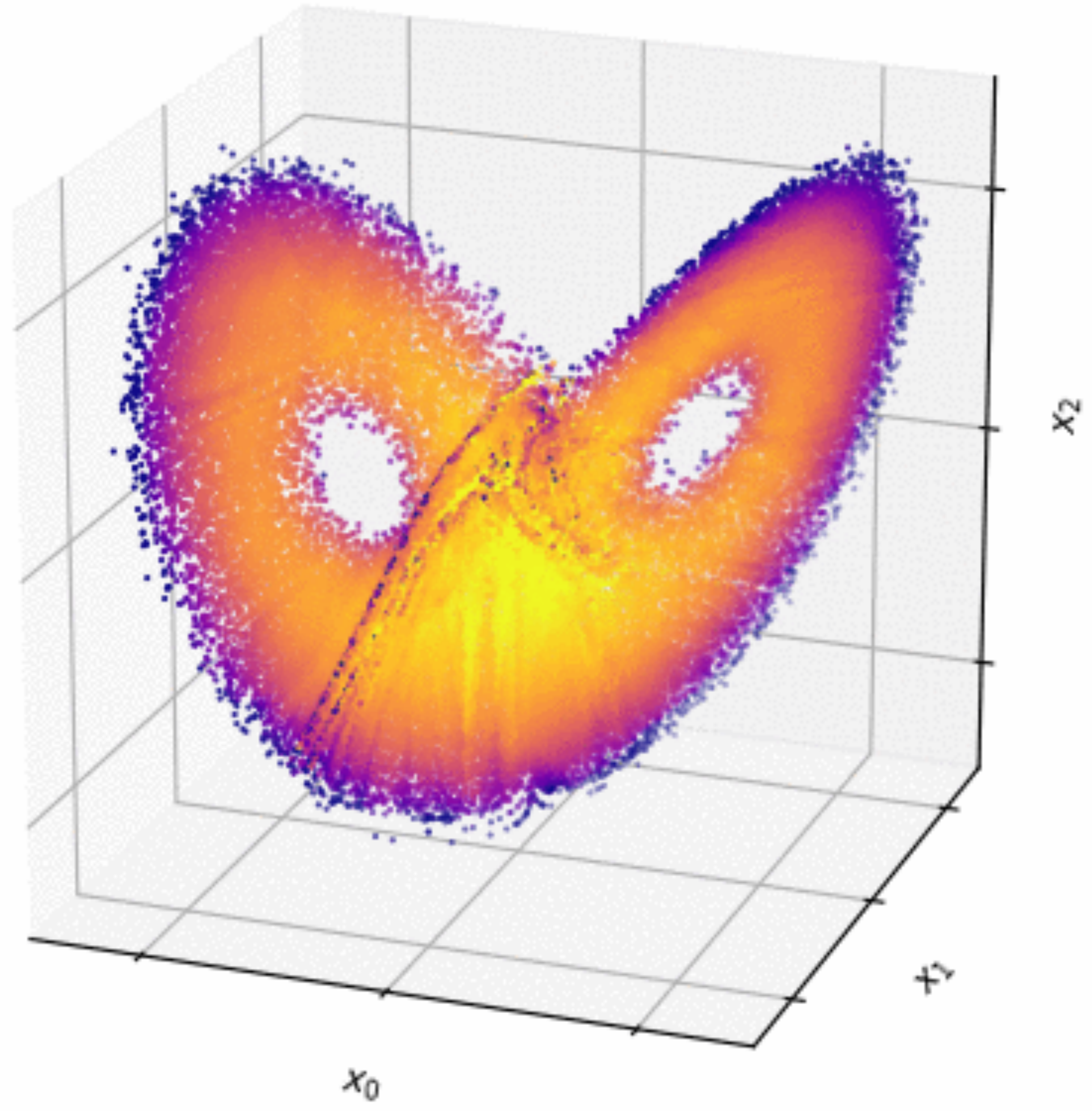

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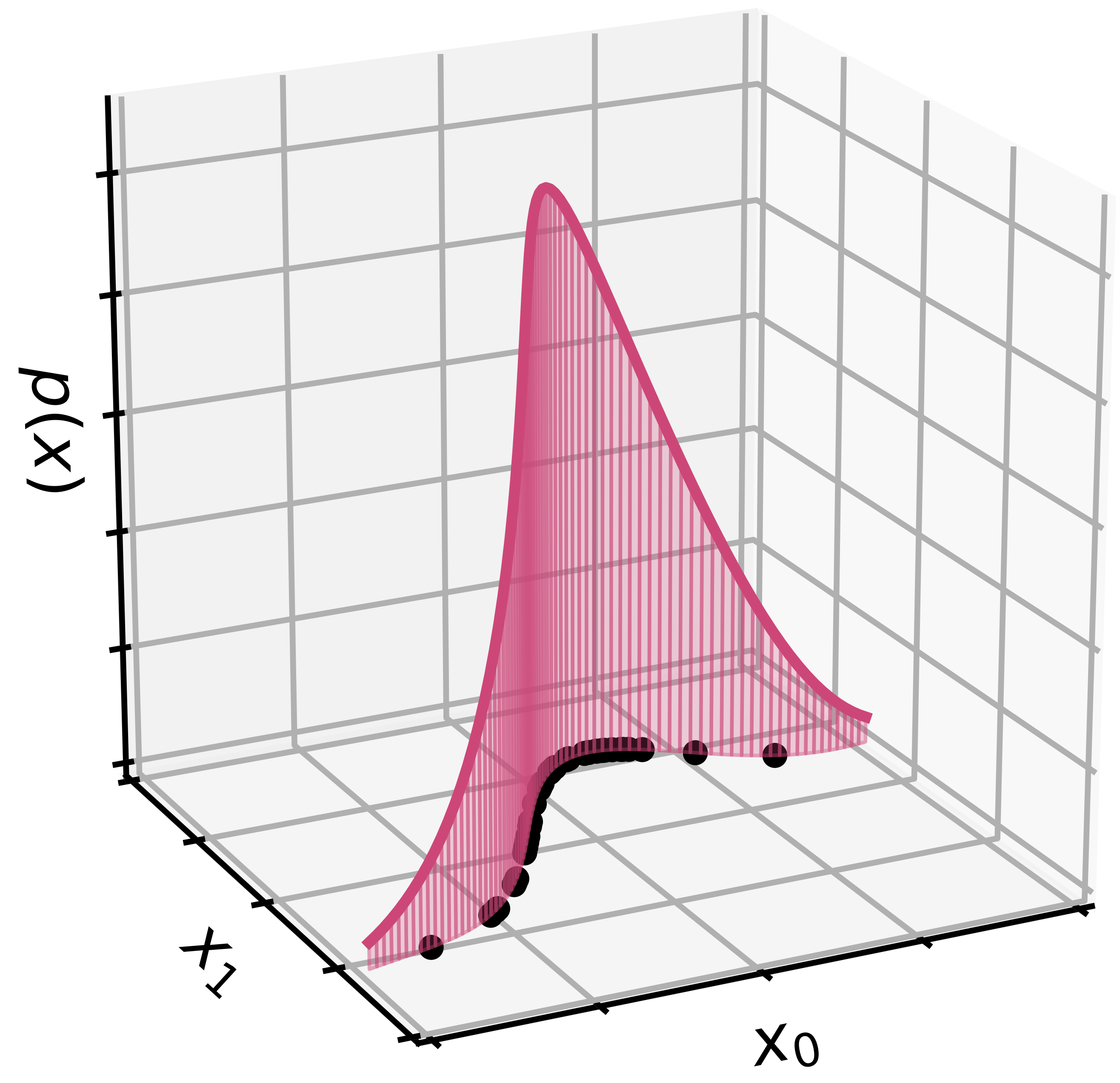
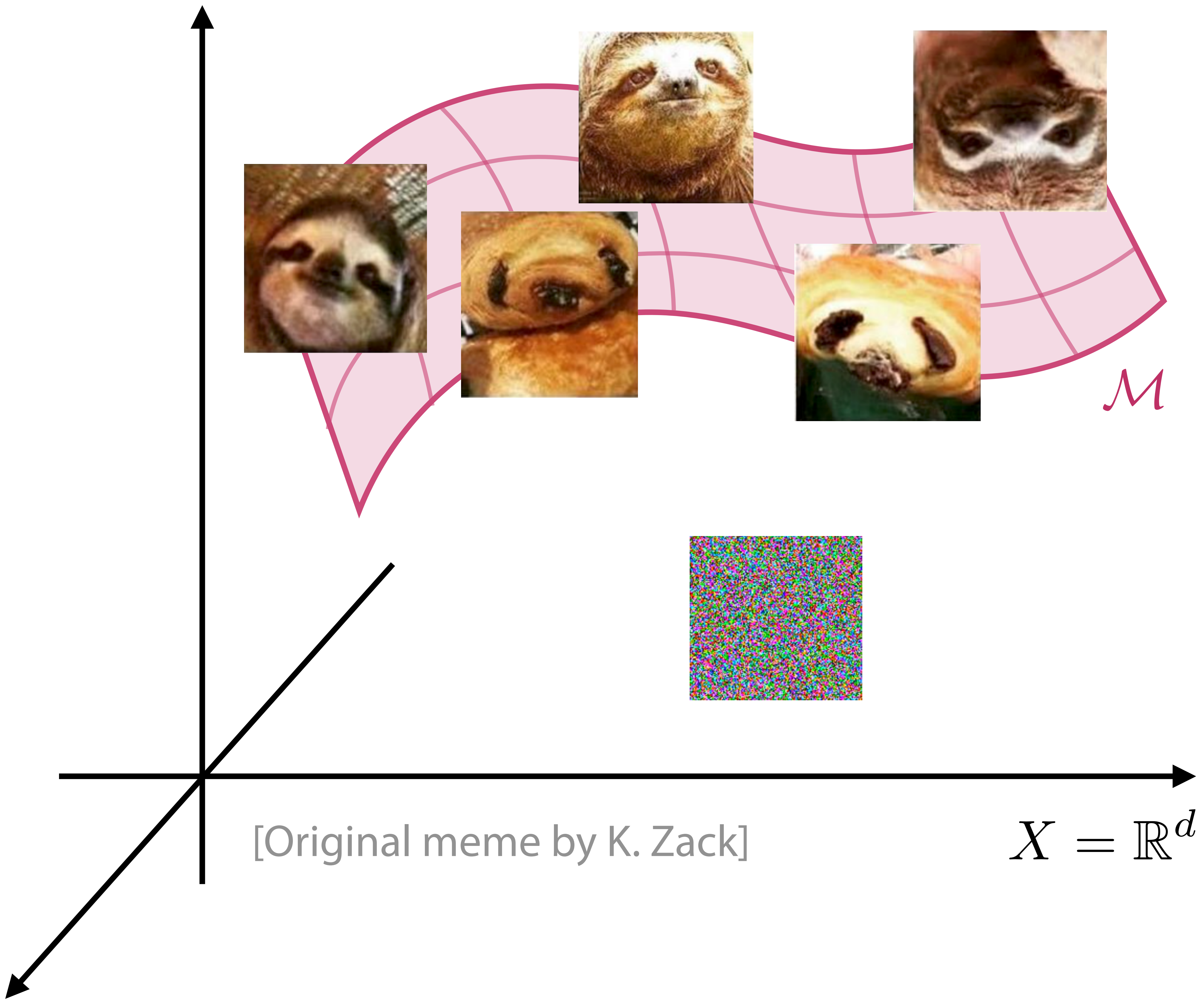



# The manifold hypothesis

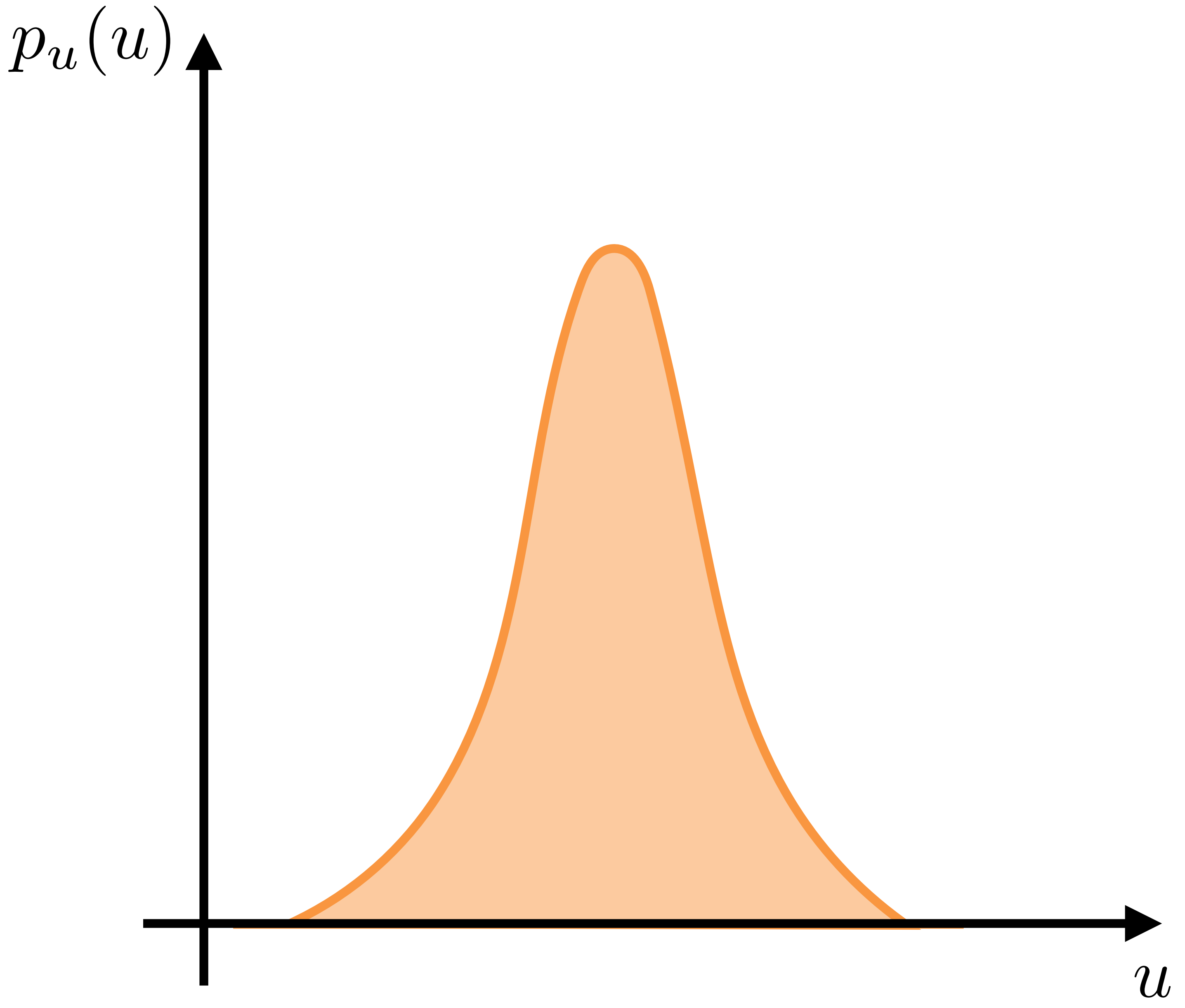
Data often live on a $n$-dimensional manifold embedded in the $d$-dimensional ambient space

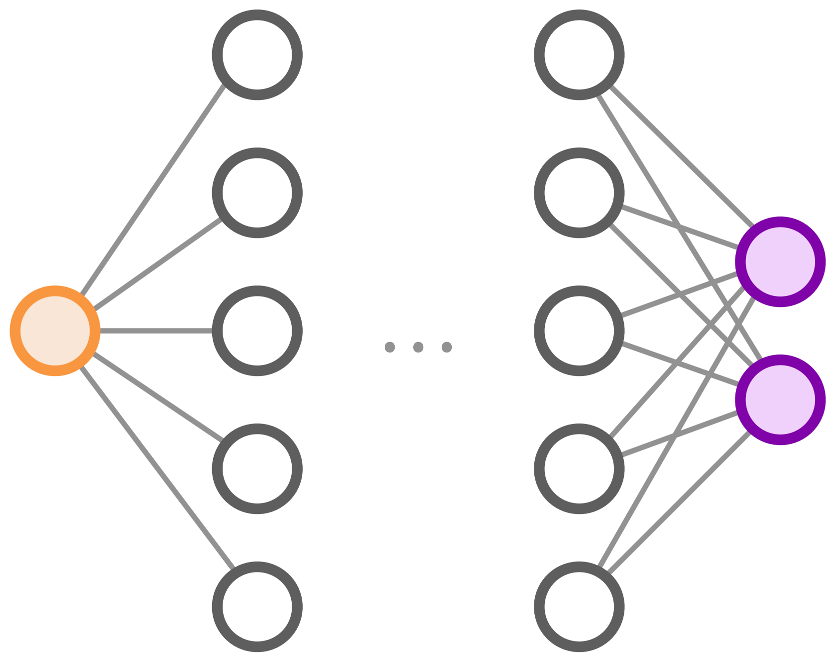


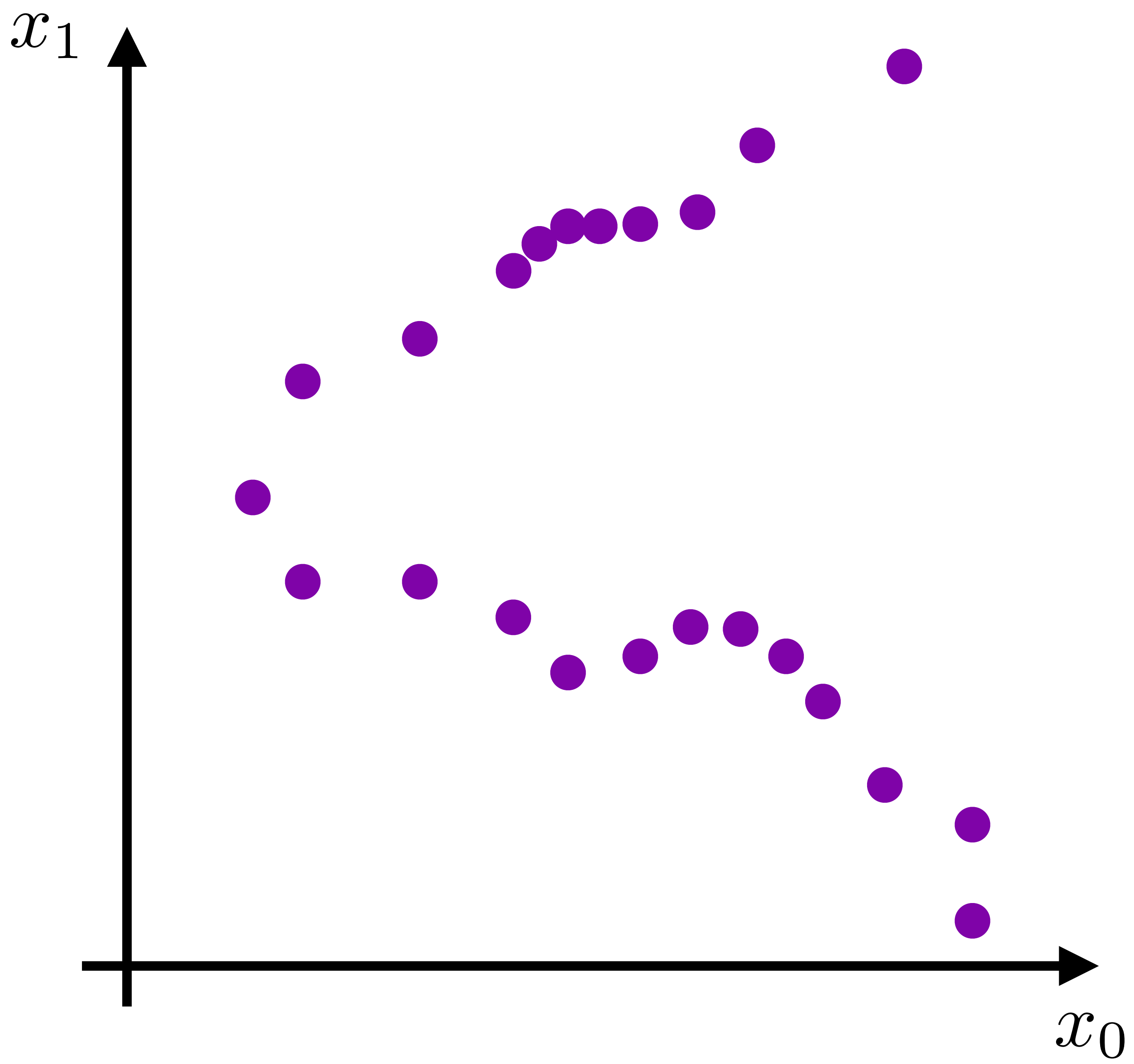

- Robot arms, molecules: limited degrees of freedom
- Particle physics: energy-momentum conservation, on-shell conditions, redundant observables
- Many other high-dimensional datasets (e.g. images): empirical evidence for (approximate) data manifold
  [L. Cayton 2005; …]

# Generative adversarial networks (GANs)

[I. Goodfellow et al 1406.2661]




$u \sim p_u(u)$

$g$

$x$

$n$-dim. latent variables

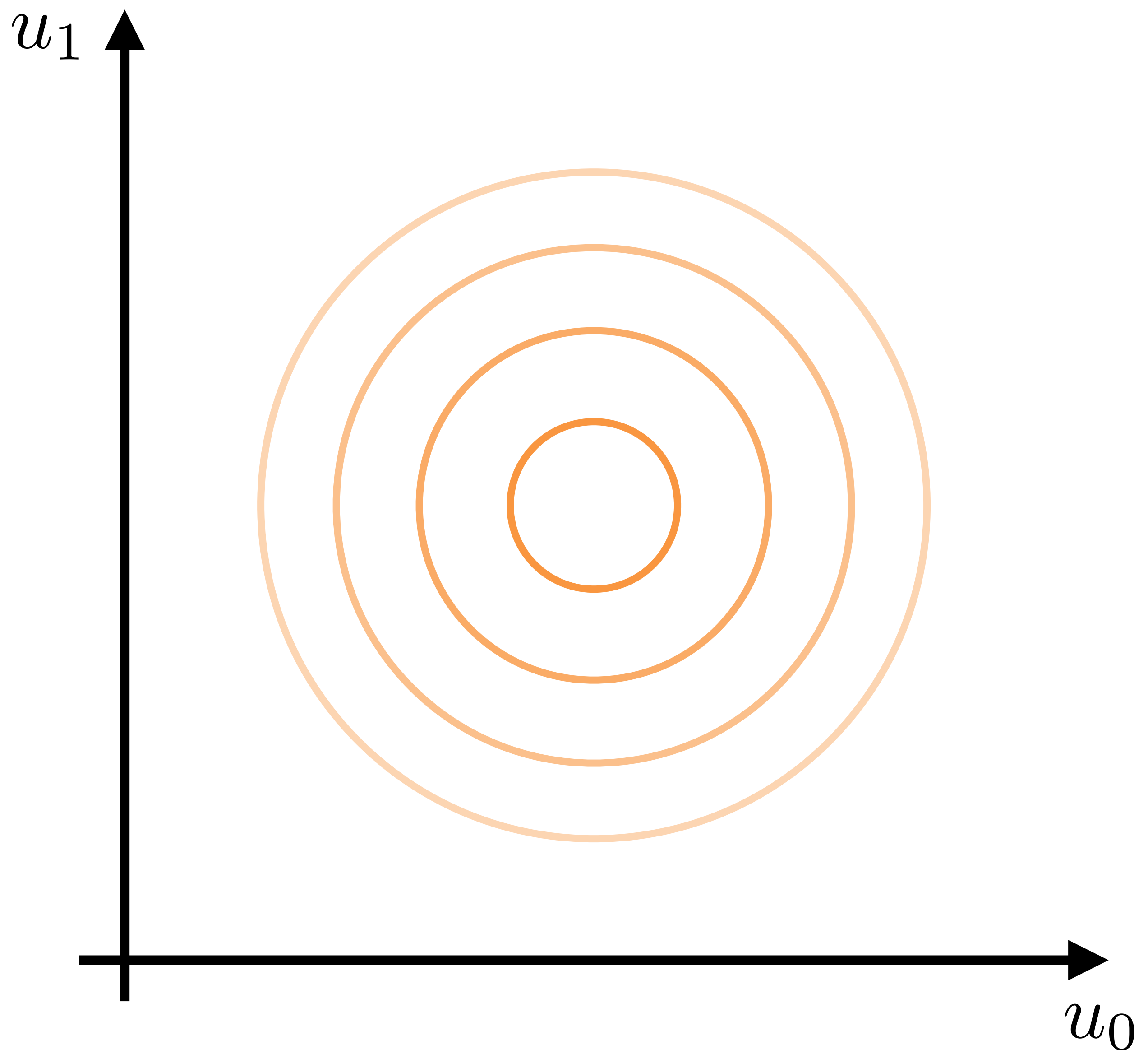
unconstrained NN

implicit density over $\mathcal{M}$

$p_{\mathcal{M}}(x)$ intractable

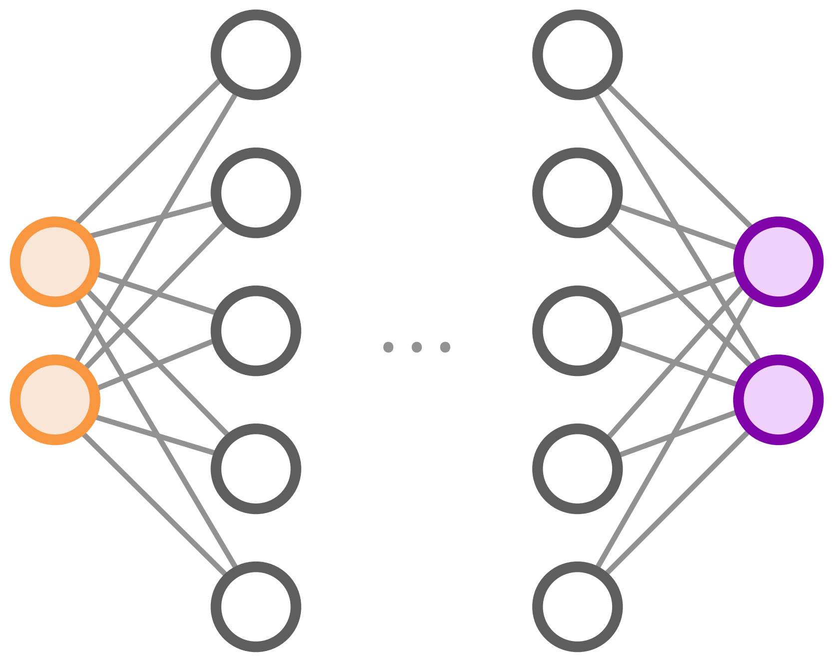
# Normalizing flows in the ambient data space

[G. Papamakarios et al 1912.02762]



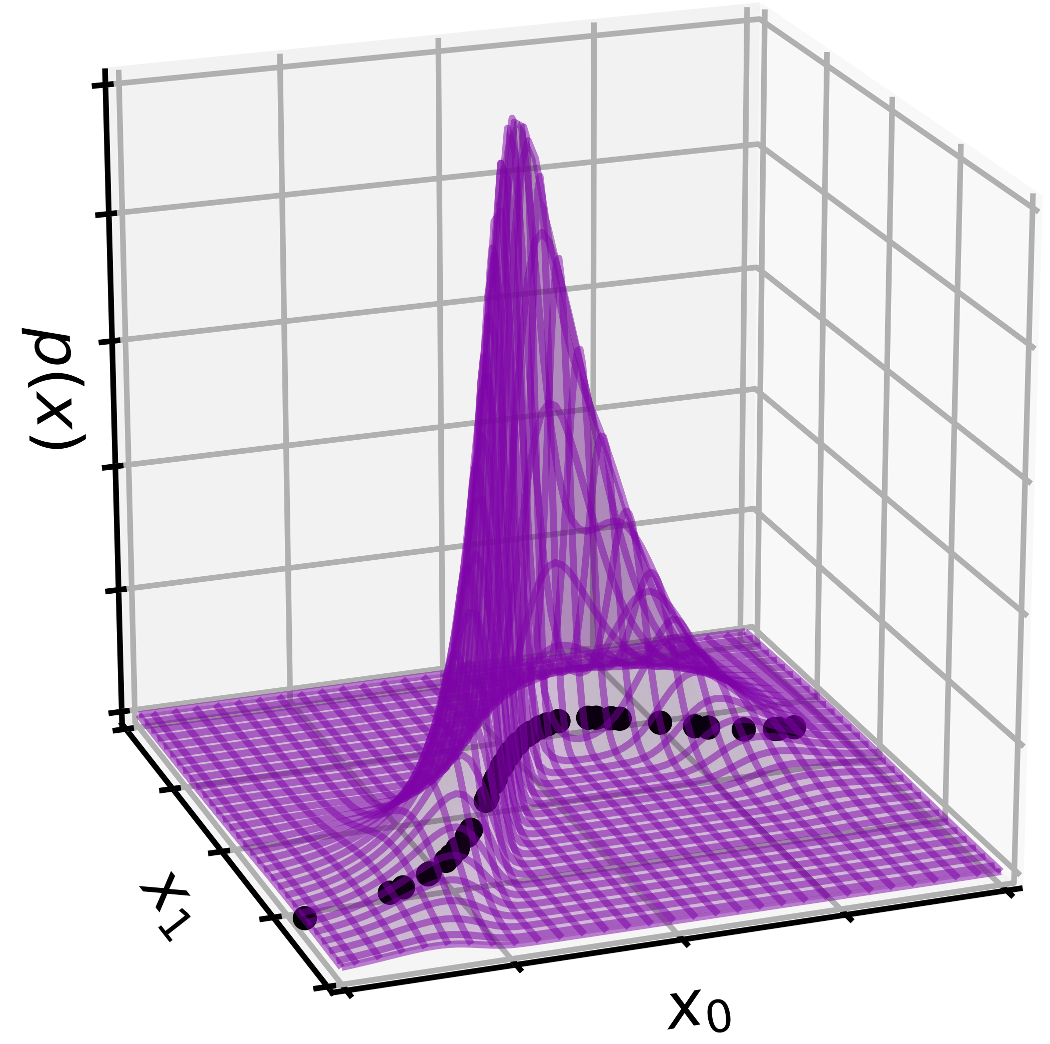

$u \sim p_u(u)$

*d*-dim. latent variables



$f$

invertible NN



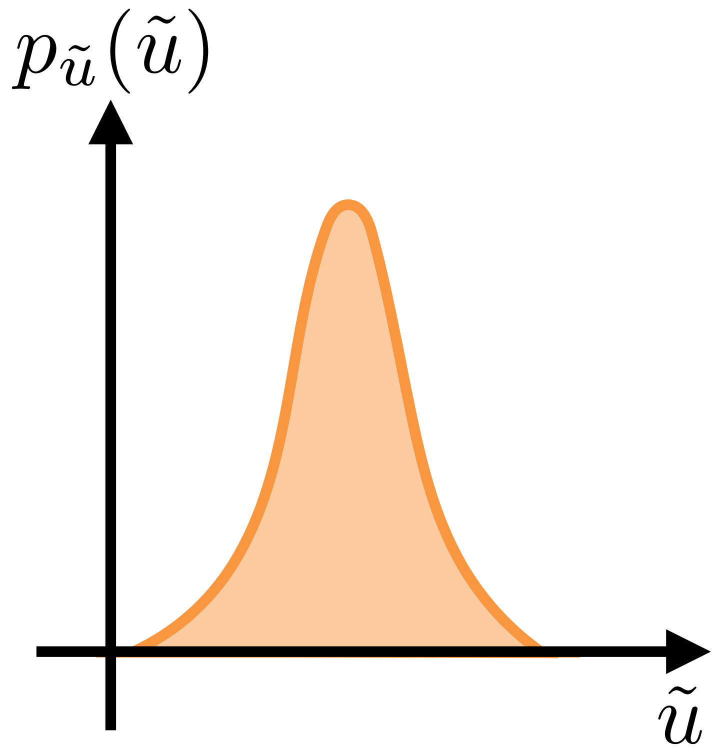

$x$

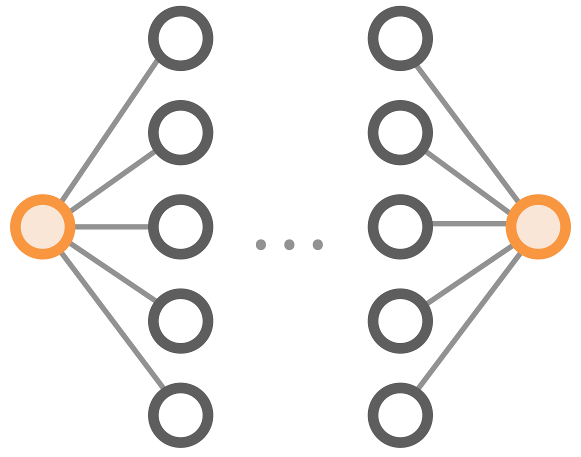
tractable density over ambient data space

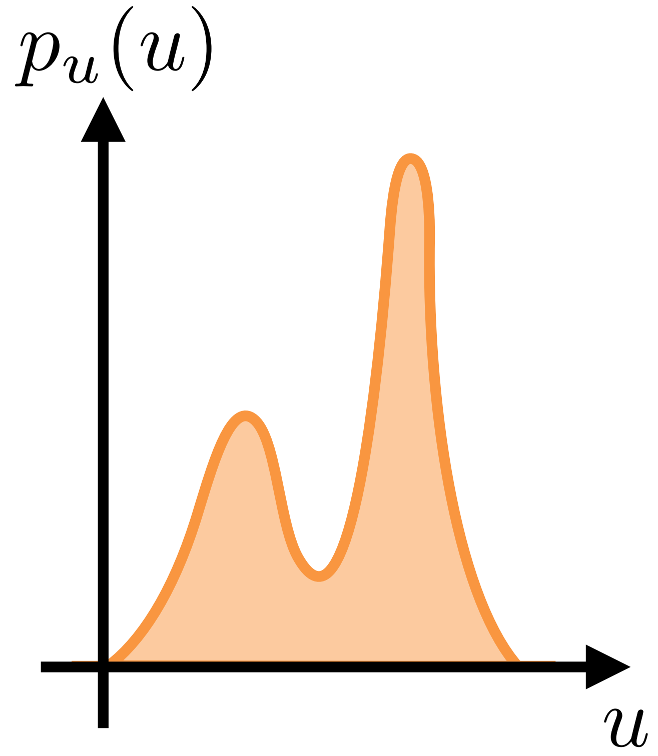
$$p_x(x) = p_u(f^{-1}(x))\,|\det J_f(f^{-1}(x))|^{-1}$$

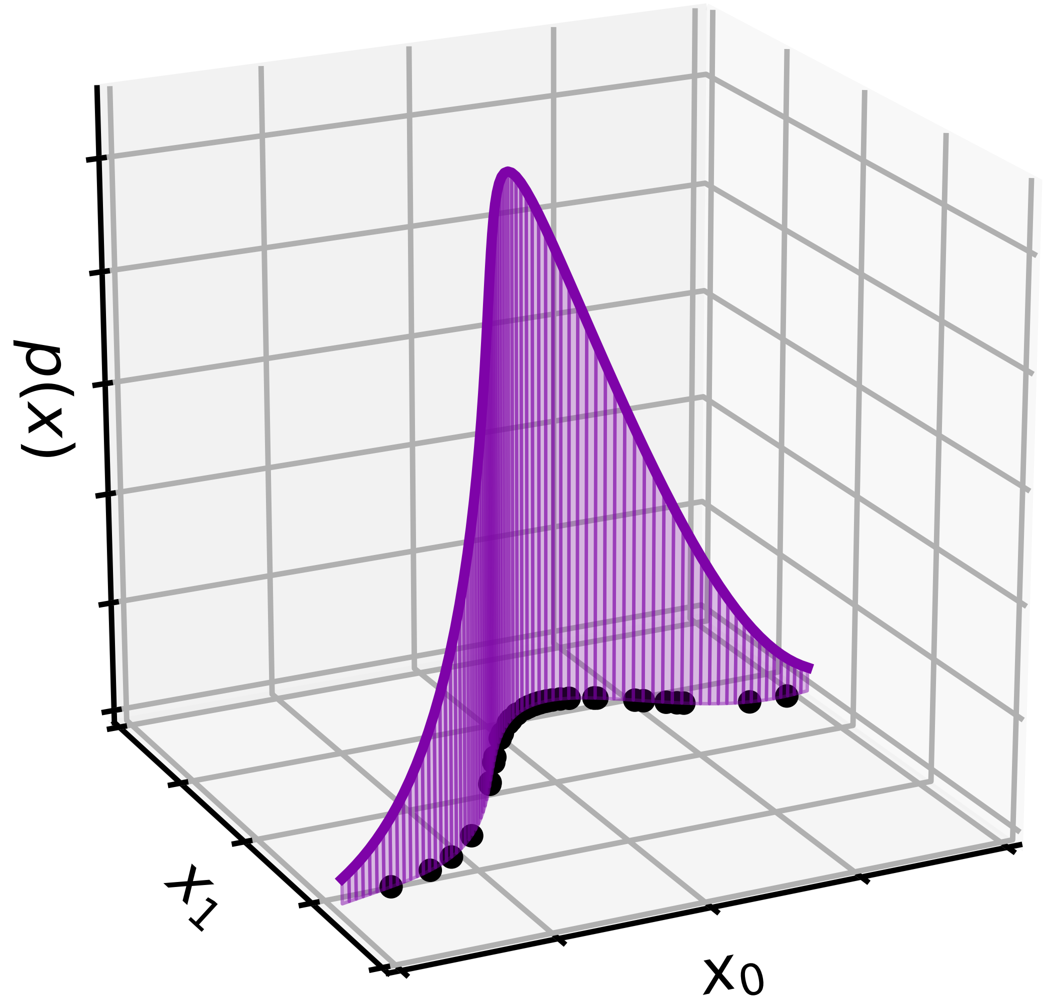
# Flows on a prescribed manifold

[M. Gemici et al 1611.02304; D. Rezende et al 2002.02428]





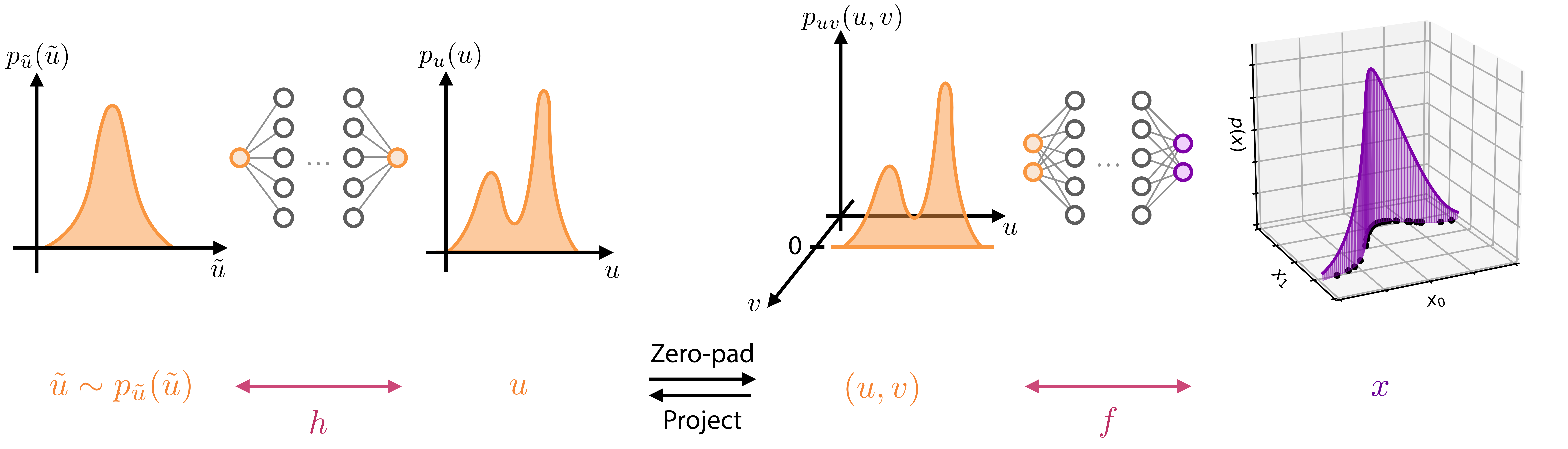

$\tilde u \sim p_{\tilde u}(\tilde u)$ $\xleftrightarrow{h}$ $u$ $\xleftrightarrow{g^*}$ $x$

$n$-dim. latents | invertible NN | $n$-dim. latents | prescribed chart | tractable density over $\mathcal{M}^*$

$$p_{\mathcal{M}^*}(x) = p_{\tilde u}(\tilde u)\ \left|\det J_h(\tilde u)\right|^{-1} \cdot \left|\det[J_{g^*}^T(u) J_{g^*}(u)]\right|^{-\frac{1}{2}}$$

# $\mathcal{M}$-flows

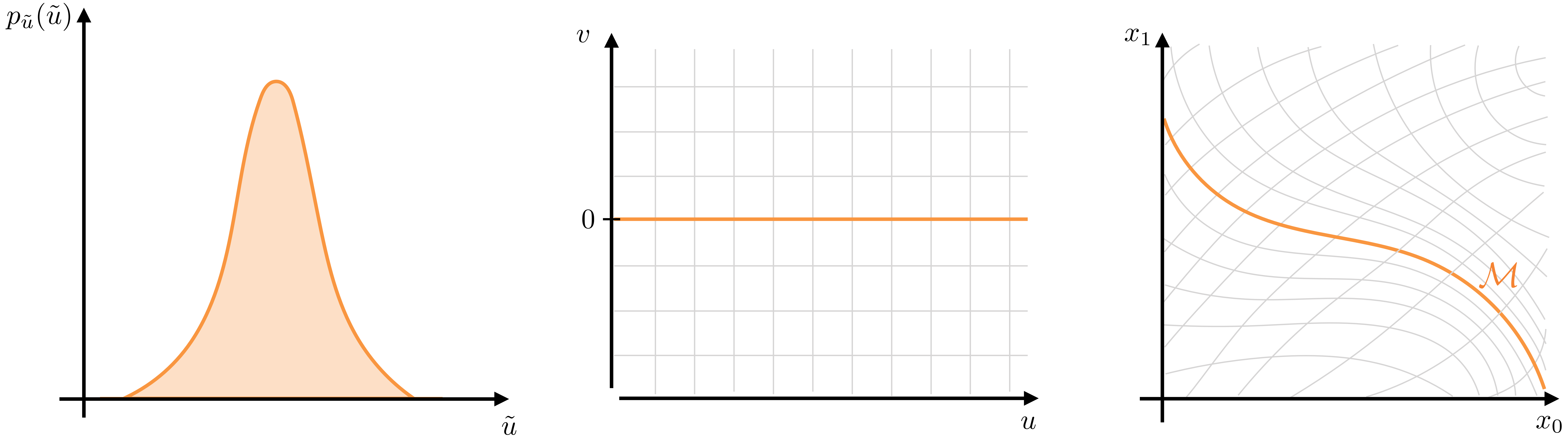
[JB, Kyle Cranmer 2003.13913]




$n$-dim. latents | inv. NN | $n$-dim. latents | embed | $d$-dim. latents | inv. NN | tractable density over $\mathcal{M}$

$$p_{\mathcal{M}}(x) = p_{\tilde{u}}(\tilde{u}) \, |\det J_h(\tilde{u})|^{-1} \cdot \left|\det\left[\begin{pmatrix}\mathbb{1} & 0\end{pmatrix} J_f(u)^T J_f(u) \begin{pmatrix}\mathbb{1} \\ 0\end{pmatrix}\right]\right|^{-\frac{1}{2}}$$

# Evaluating data on or off the manifold



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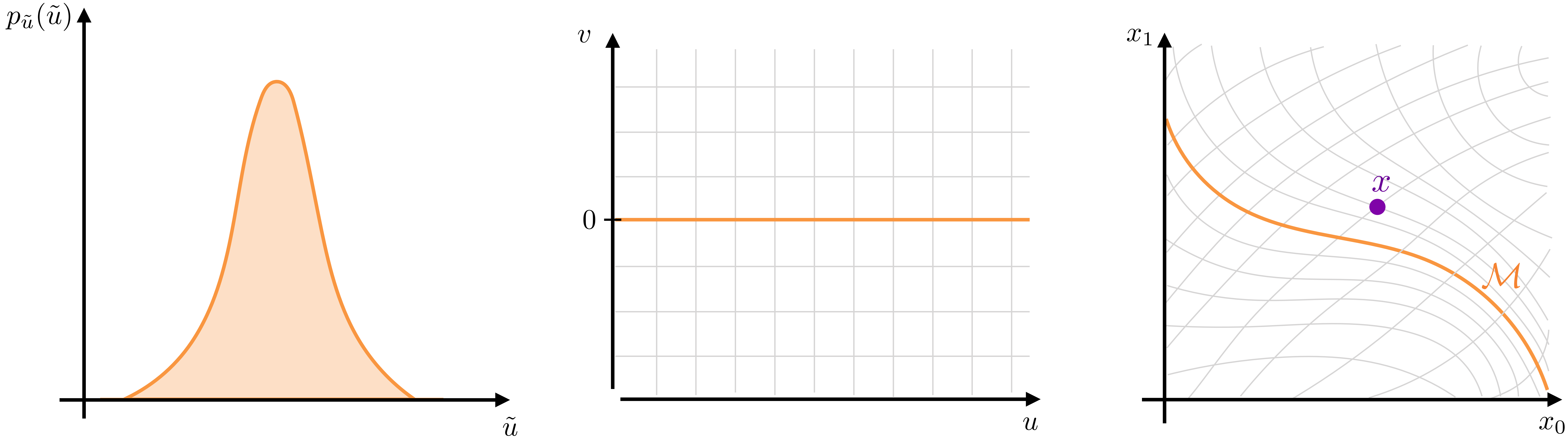

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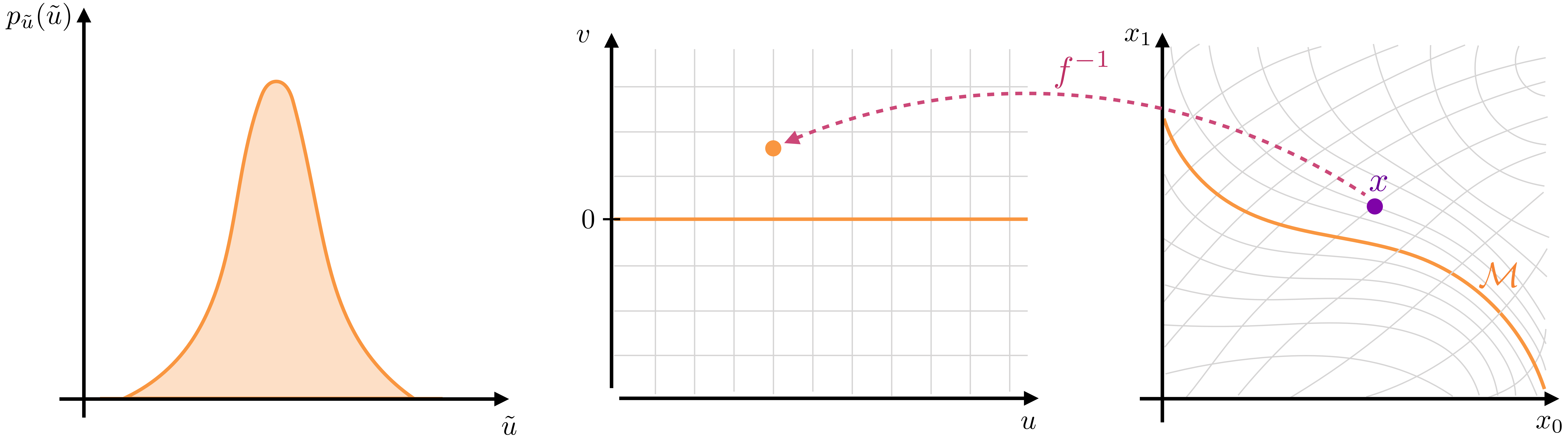

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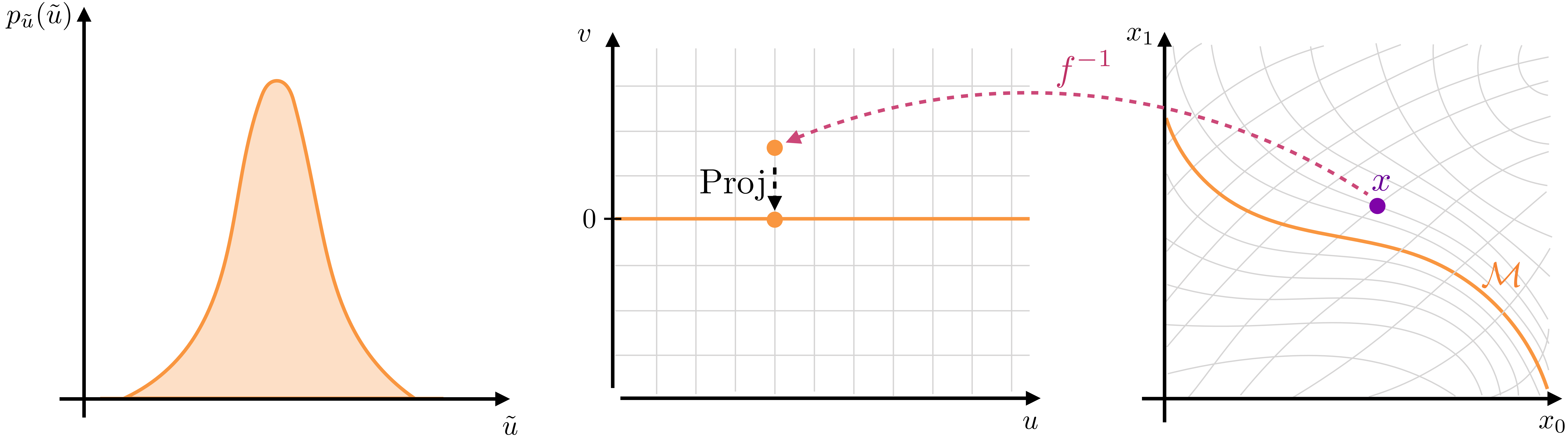

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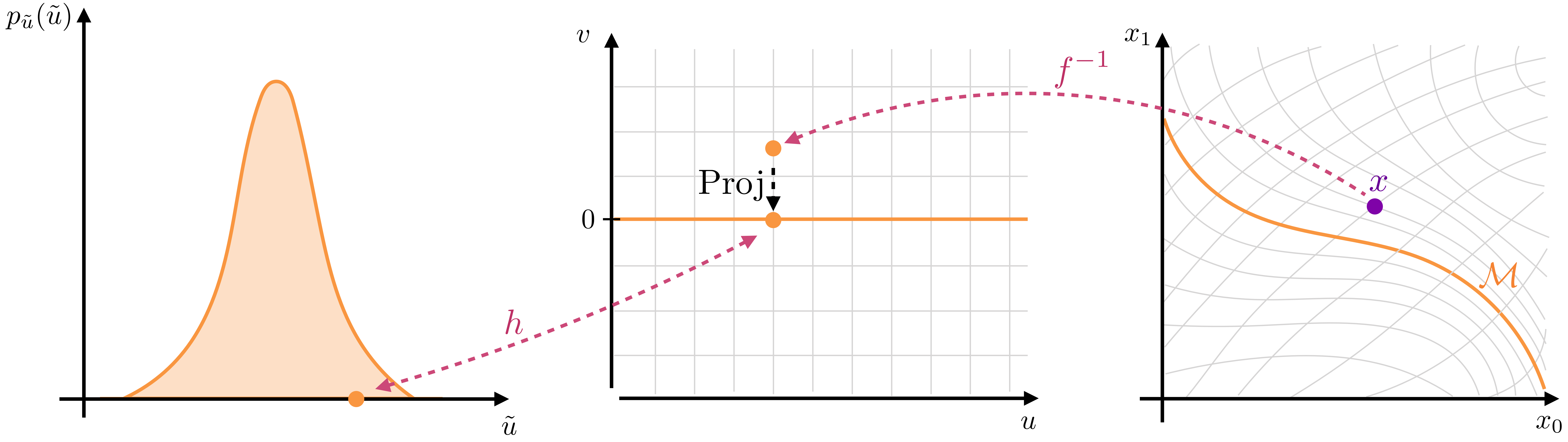

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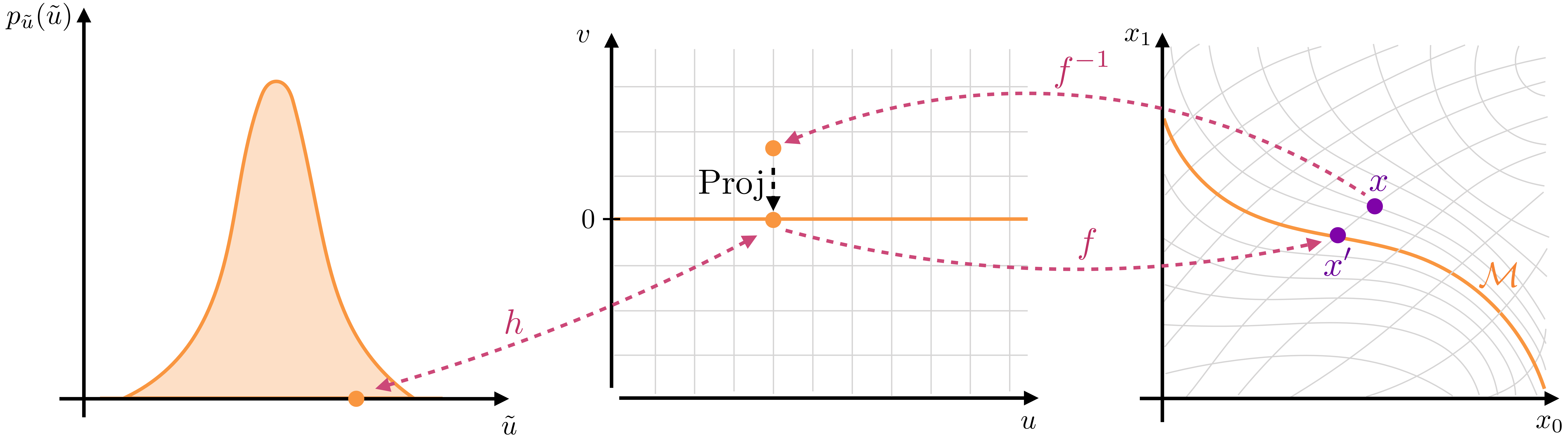

# Evaluating data on or off the manifold


Input $x$

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Input $x$ ⇝ Representation $\tilde{u}$ (dimensionality reduction)

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⇝ Reconstruction error $\|x - x'\|$ (training, OOD detection)

# Evaluating data on or off the manifold


Input $x$

- ⇝ Representation $\tilde{u}$ (dimensionality reduction)
- ⇝ Projection to manifold $x'$ (denoising)
- ⇝ Reconstruction error $\|x - x'\|$ (training, OOD detection)
- ⇝ Likelihood after projection $p_{\mathcal{M}}(x')$ (training, inference)

# Generative models vs. the data manifold

| Model | Manifold | Chart | Generative | Tractable density | Restr. to manifold |
|---|---|---|---|---|---|
| Ambient flow (AF) | no | no | ✓ | ✓ | no |
| Flow on prescr. manifold | prescribed | prescribed | ✓ | ✓ | ✓ |
| GAN | learned | no | ✓ | no | ✓ |
| VAE | learned | no | ✓ | only ELBO | (no) |
| $\mathcal{M}$-flow | learned | learned | ✓ | ✓ (potentially slow) | ✓ |

# Maximum likelihood is not enough

Likelihood defined after projection to $\mathcal{M}$,
which is defined through NN weights $\phi_f$

Family of likelihoods $p_{\phi_f}(x|\phi_h)$
rather than one likelihood $p(x|\phi_f, \phi_h)$

⇒ Learning $\phi_f$ by maximum

likelihood is unstable

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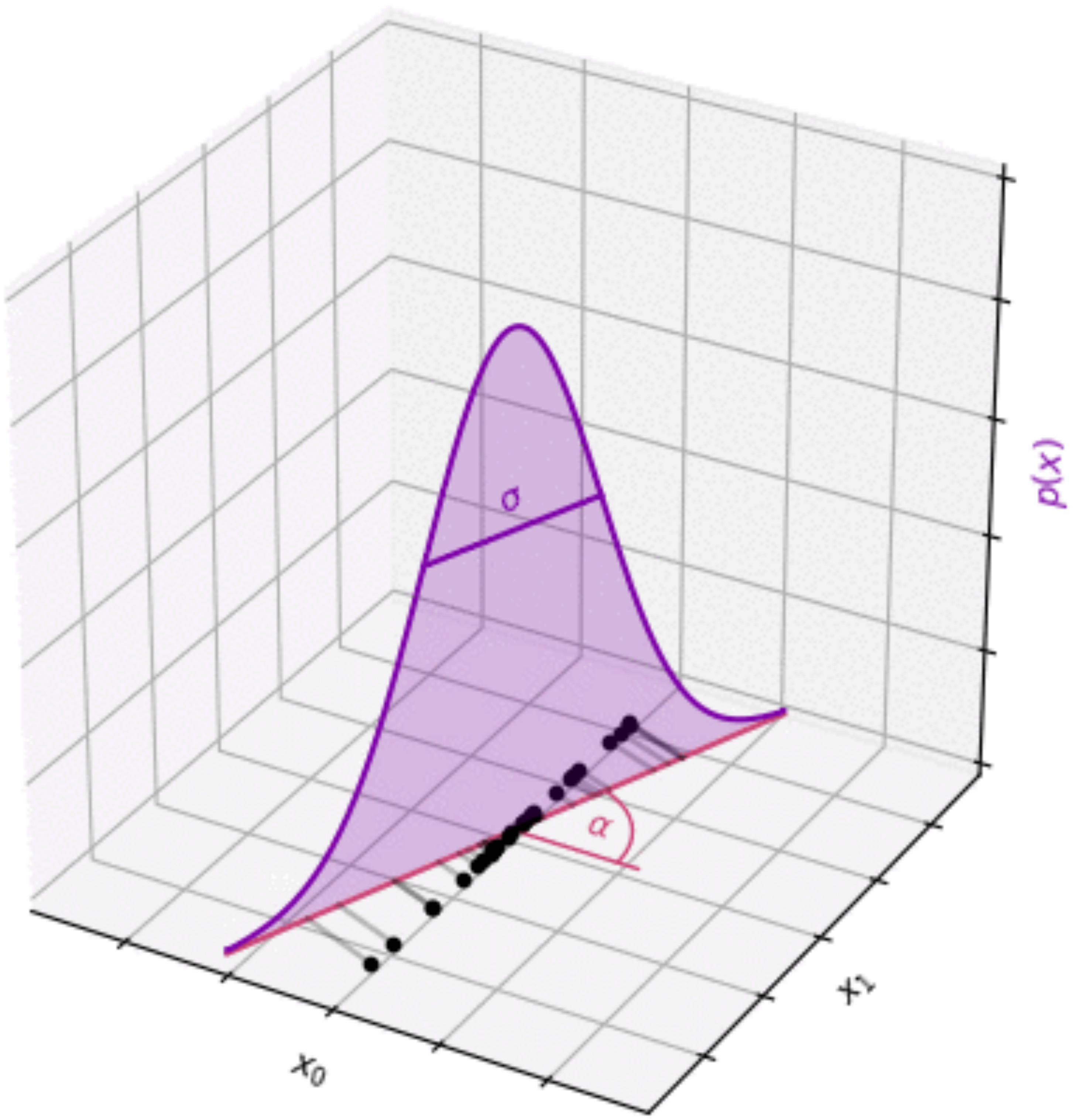

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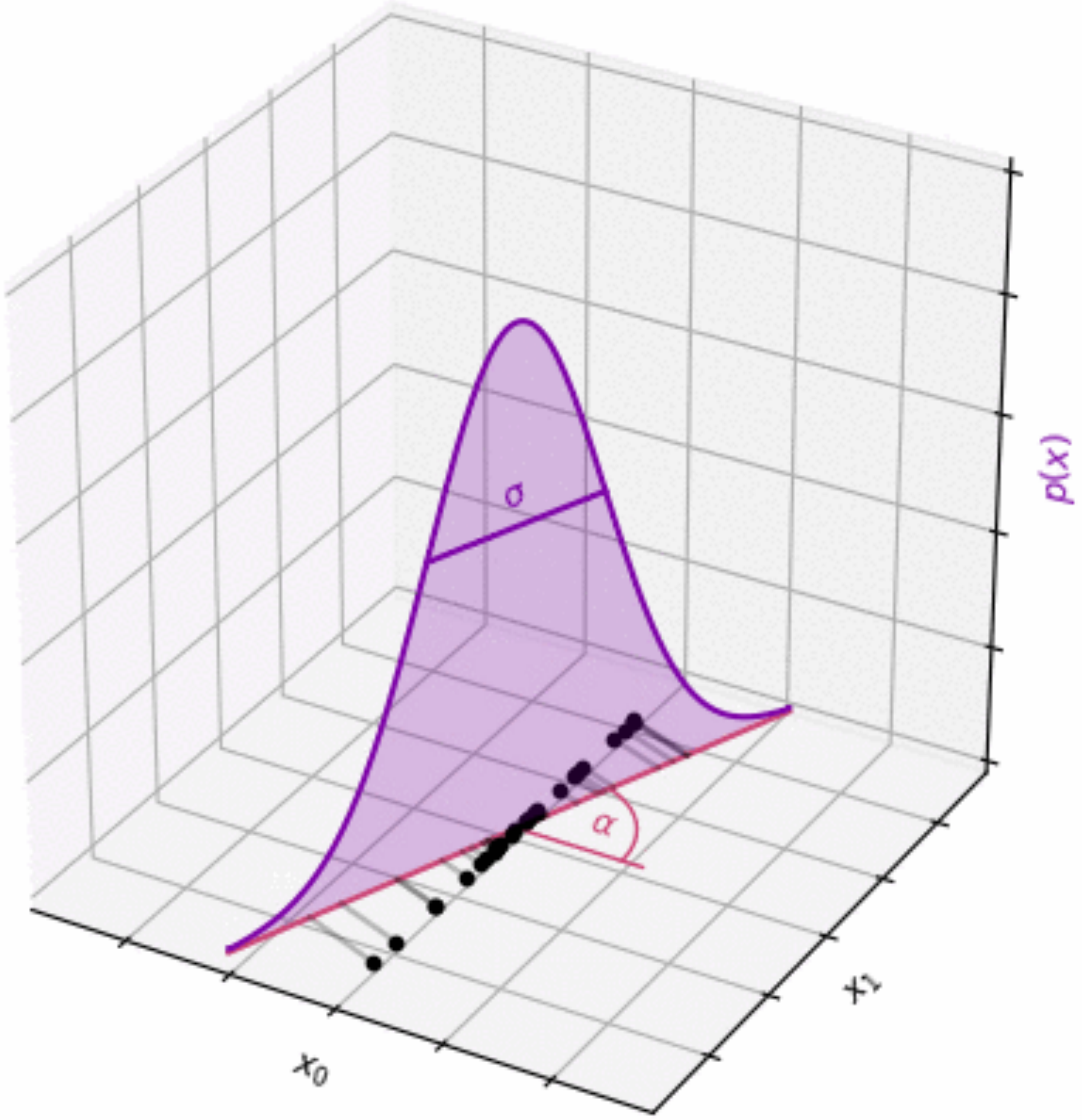
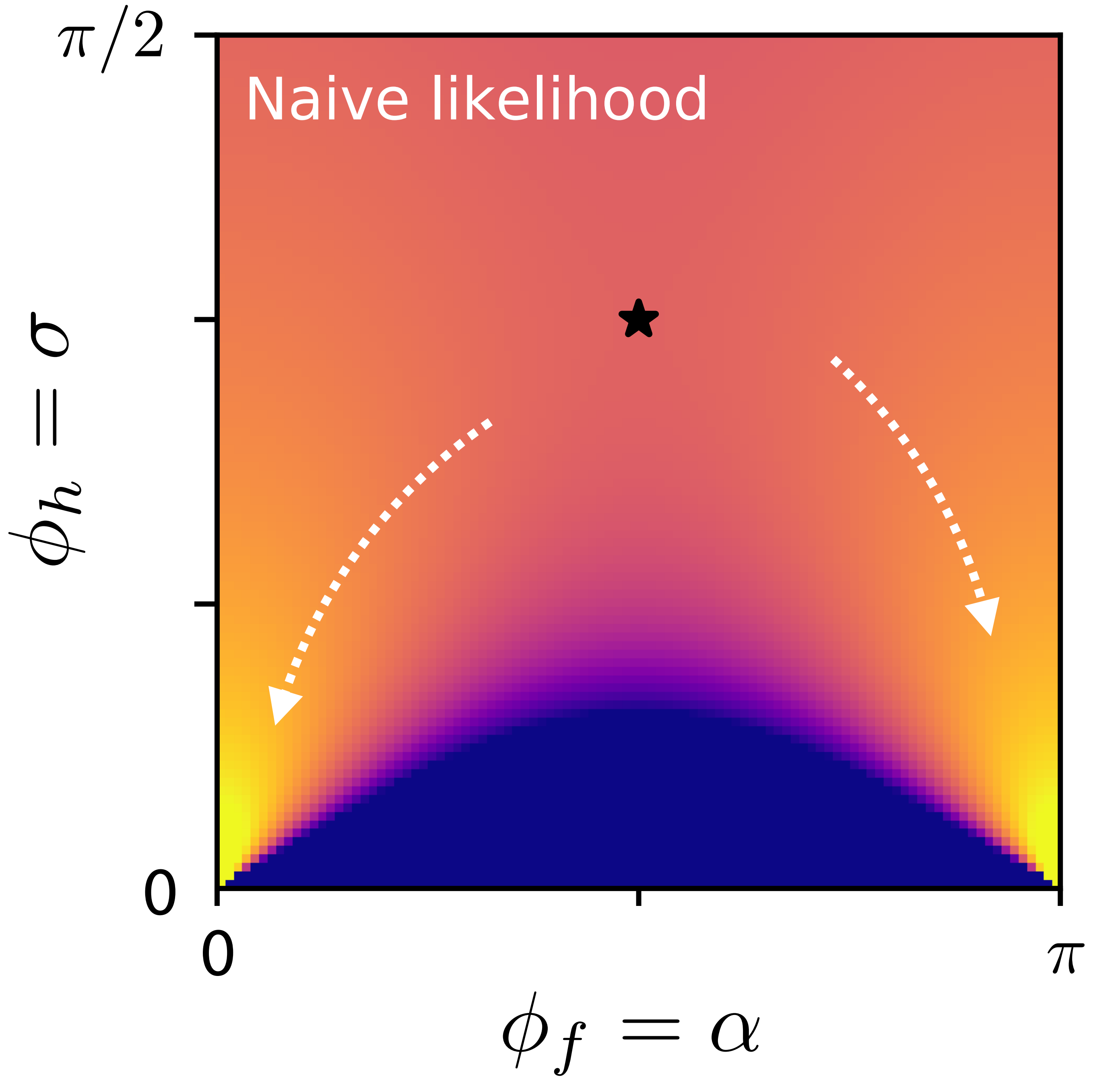
$\Rightarrow$ Learning $\phi_f$ by maximum likelihood is unstable

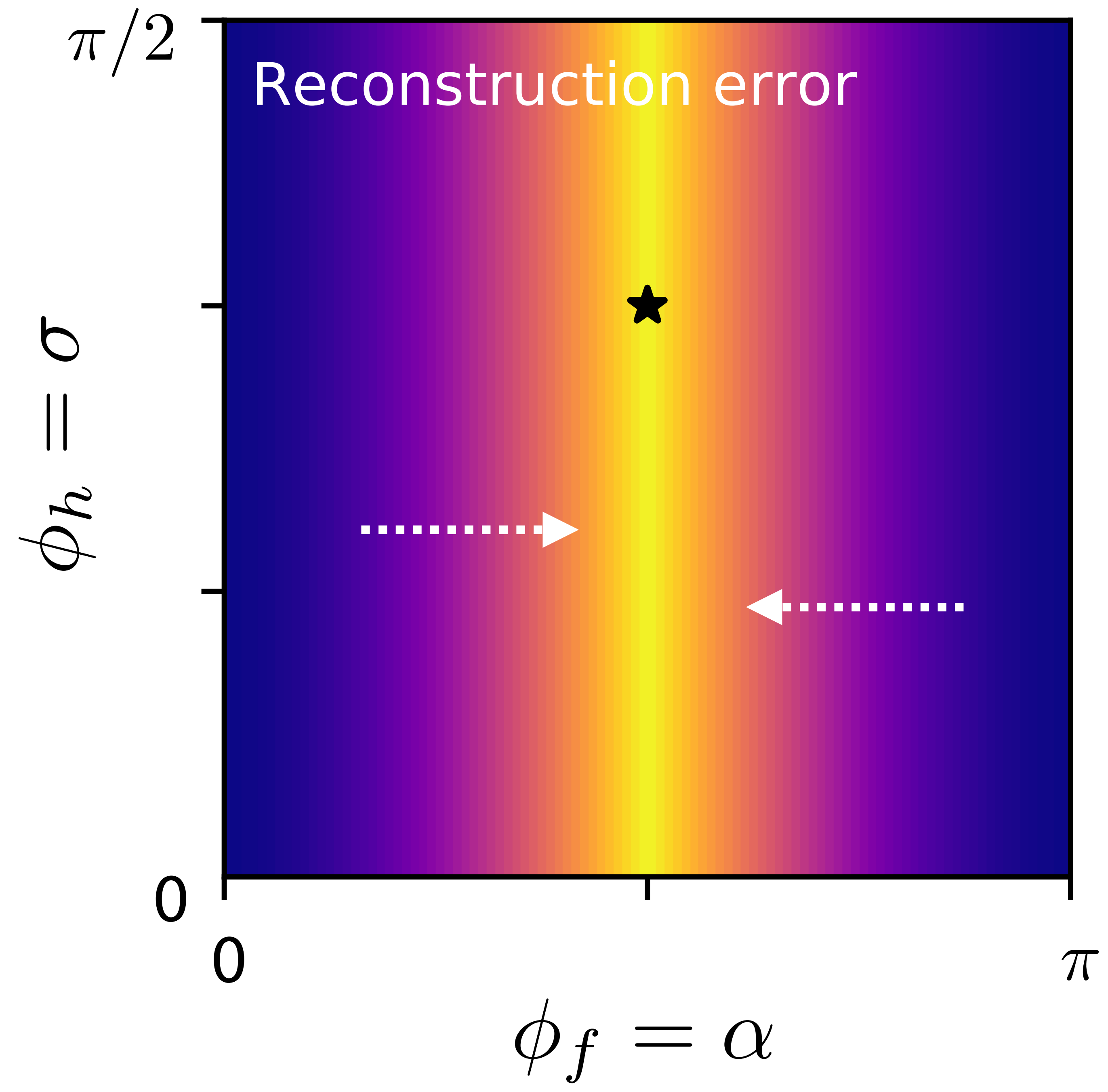


# M/D training

Solution: separate training in two phases!

- Manifold phase:
  update $\phi_f$ (and thus $\mathcal{M}$) by minimizing $\|x - x'\|$



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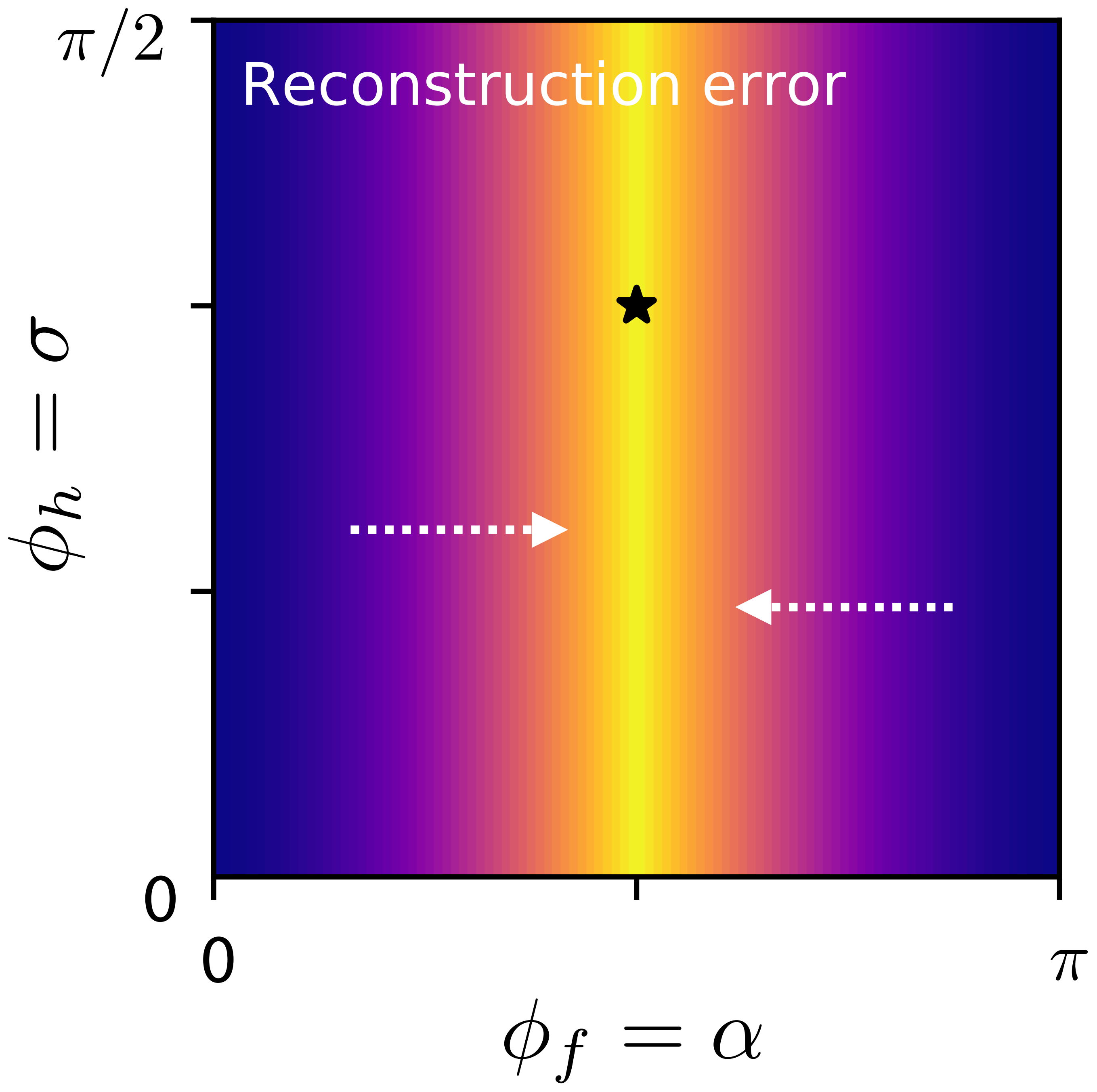
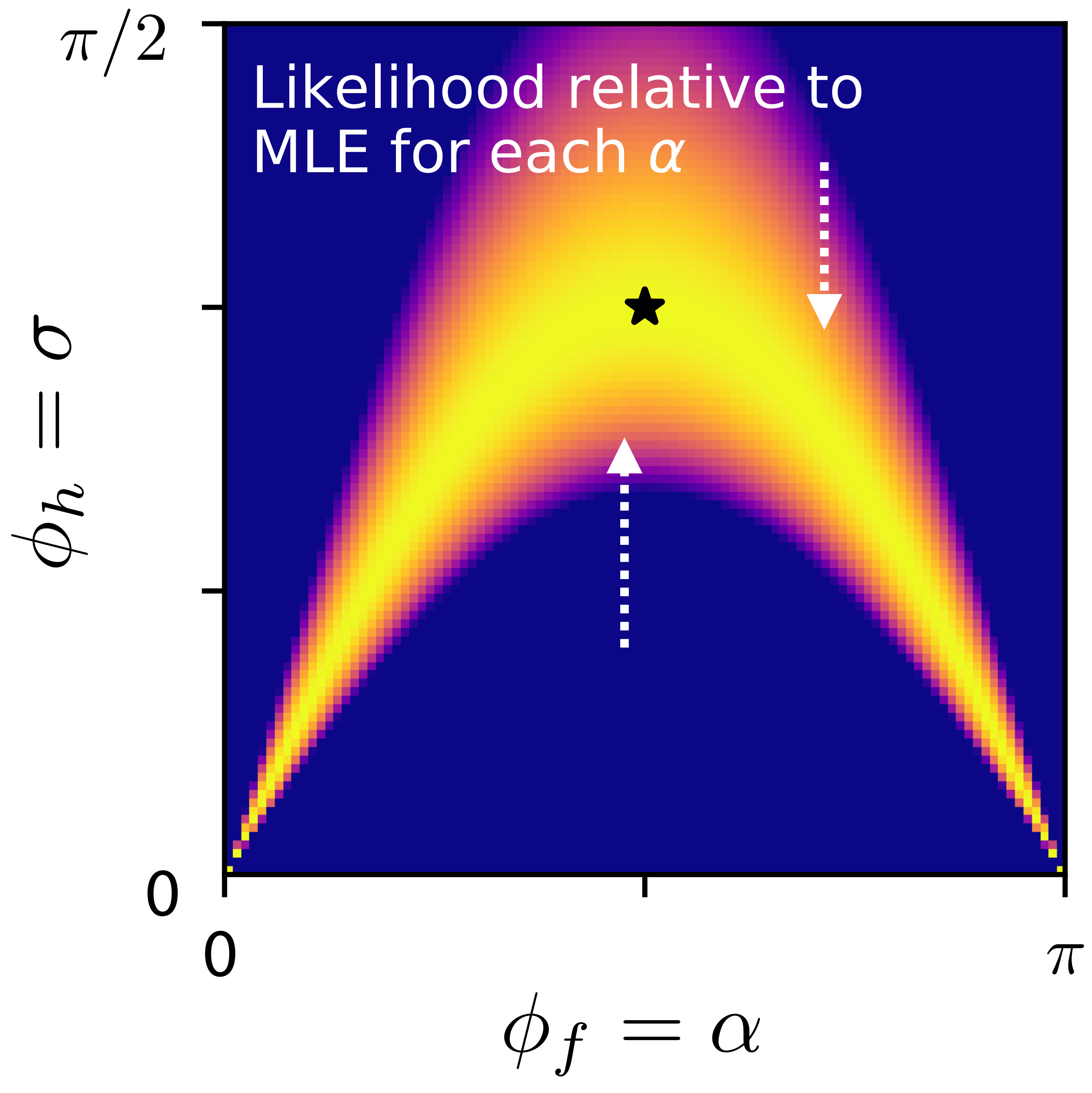



- Density phase:
  update $\phi_h$ (and thus $p_\mathcal{M}(x)$) by maximum likelihood (keeping $\mathcal{M}$ fixed)



# A second problem… and an accidental solution

The likelihood becomes expensive to evaluate for high-dimensional $x$:

$$\log p_{\mathcal{M}}(x) = \log p_{\tilde{u}}(h^{-1}(u)) - \log \det J_h(h^{-1}(u)) - \frac{1}{2} \log \det \left[ (\mathbb{1}\ 0)\, J_f^T(u)\, J_f(u) \begin{pmatrix} \mathbb{1} \\ 0 \end{pmatrix} \right]$$

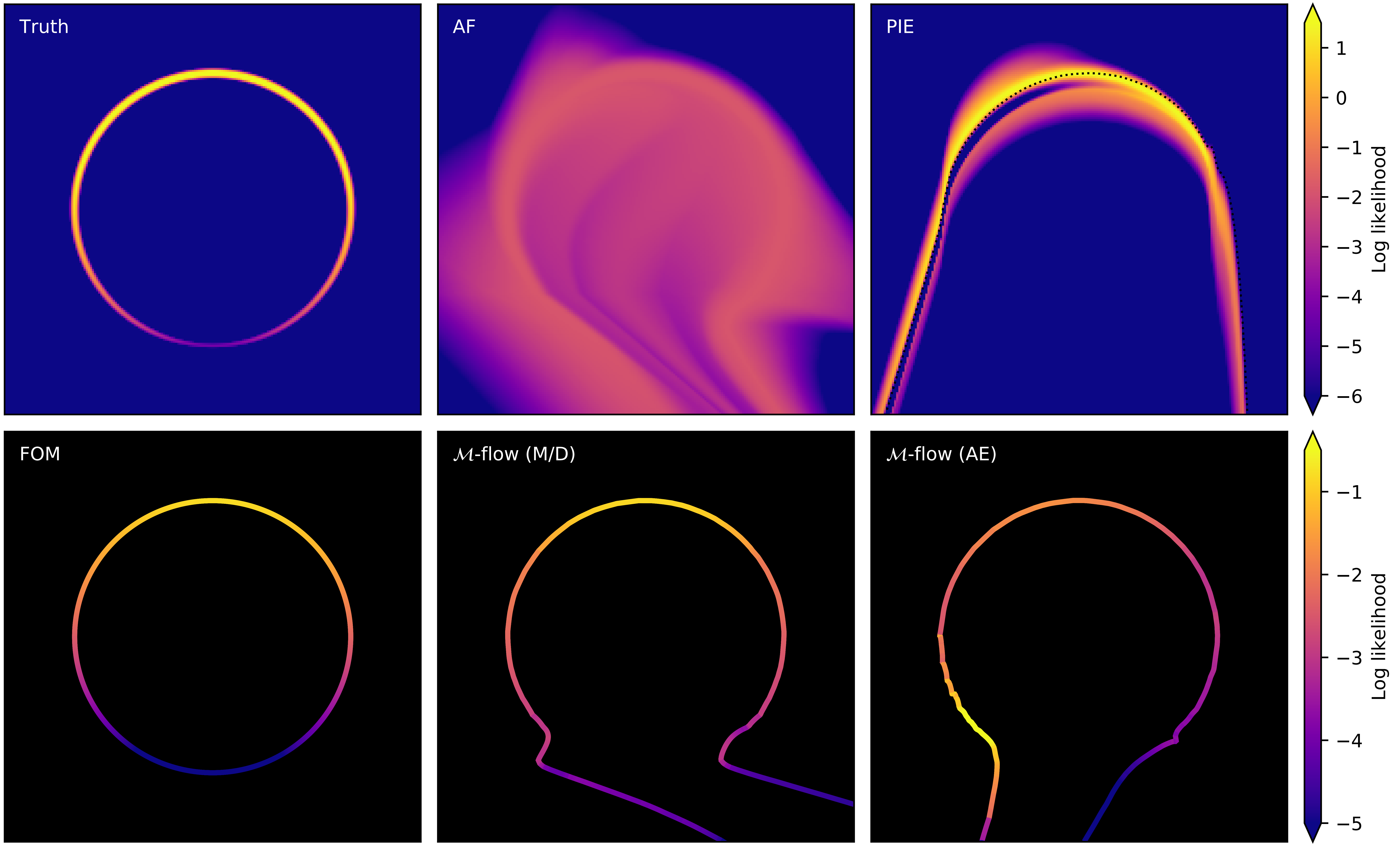
Cannot separate determinant of product of non-square matrices

M/D training sidesteps this problem: density phase only requires gradient

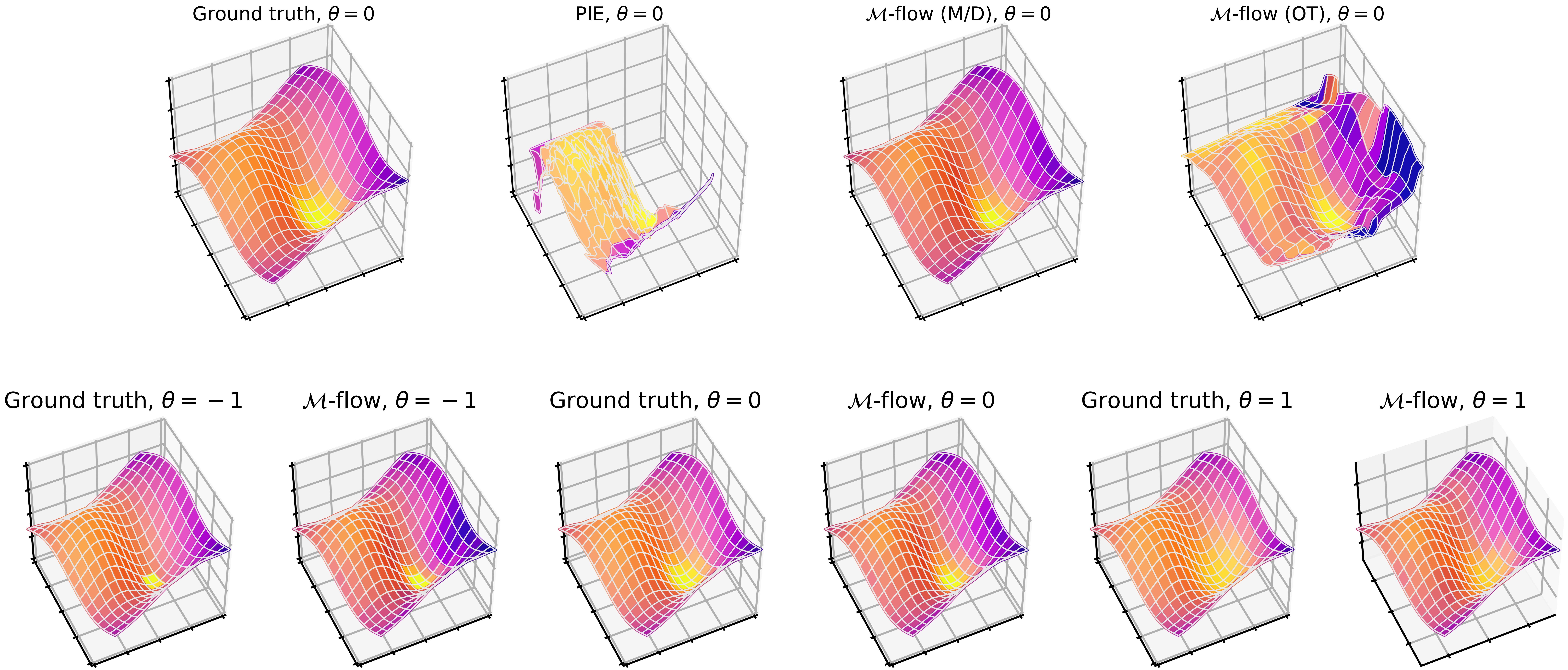
$$\nabla_{\phi_h} (\log p_{\mathcal{M}}(x)) = \nabla_{\phi_h} \left(\log p_{\tilde{u}}(h^{-1}(u))\right) - \nabla_{\phi_h} \left(\log \det J_h(h^{-1}(u))\right) - \underbrace{\nabla_{\phi_h} \frac{1}{2} \log \det \left[ (\mathbb{1}\ 0)\, J_f^T(u)\, J_f(u) \begin{pmatrix} \mathbb{1} \\ 0 \end{pmatrix} \right]}_{=0},$$

which can be computed efficiently!

# Gaussian on a circle

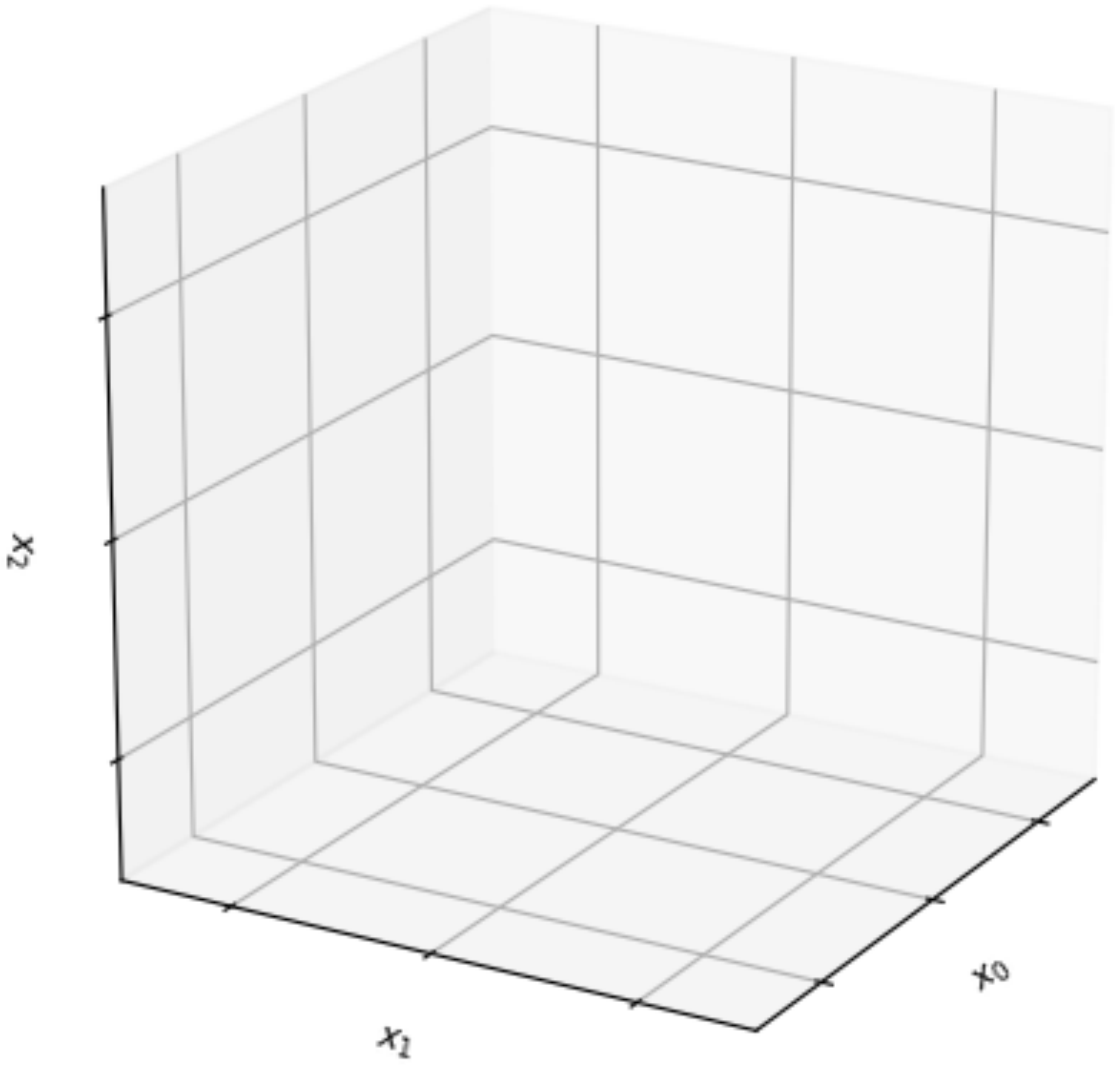


# Mixture model on a polynomial surface



# Lorenz attractor

[E. Lorenz 1963]




$$\frac{\mathrm{d}x_0}{\mathrm{d}t} = \sigma(x_1 - x_0)\,, \quad \frac{\mathrm{d}x_1}{\mathrm{d}t} = x_0(\rho - x_2) - x_1\,, \quad \frac{\mathrm{d}x_2}{\mathrm{d}t} = x_0 x_1 - \beta x_2\,.$$

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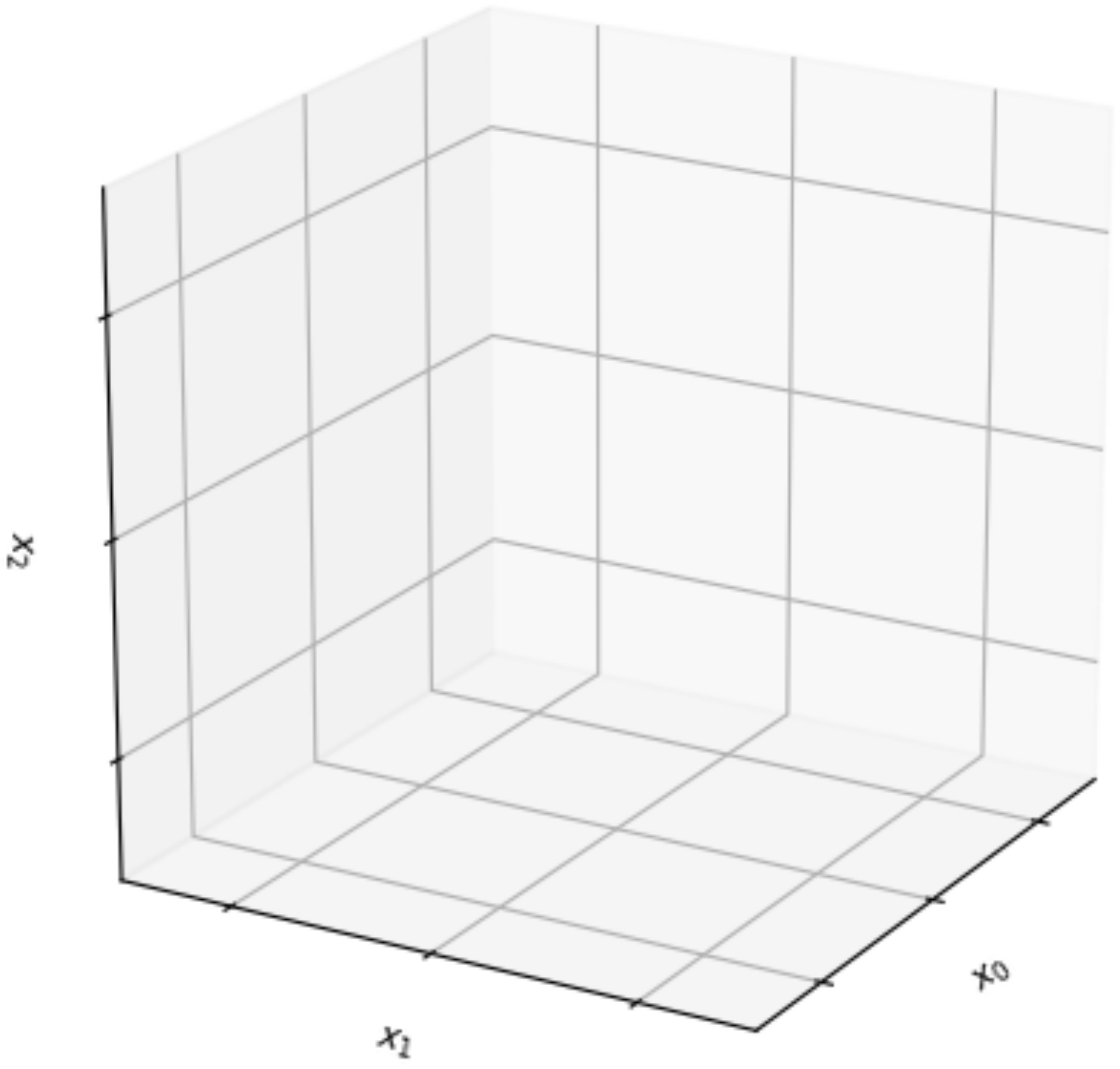
[E. Lorenz 1963]

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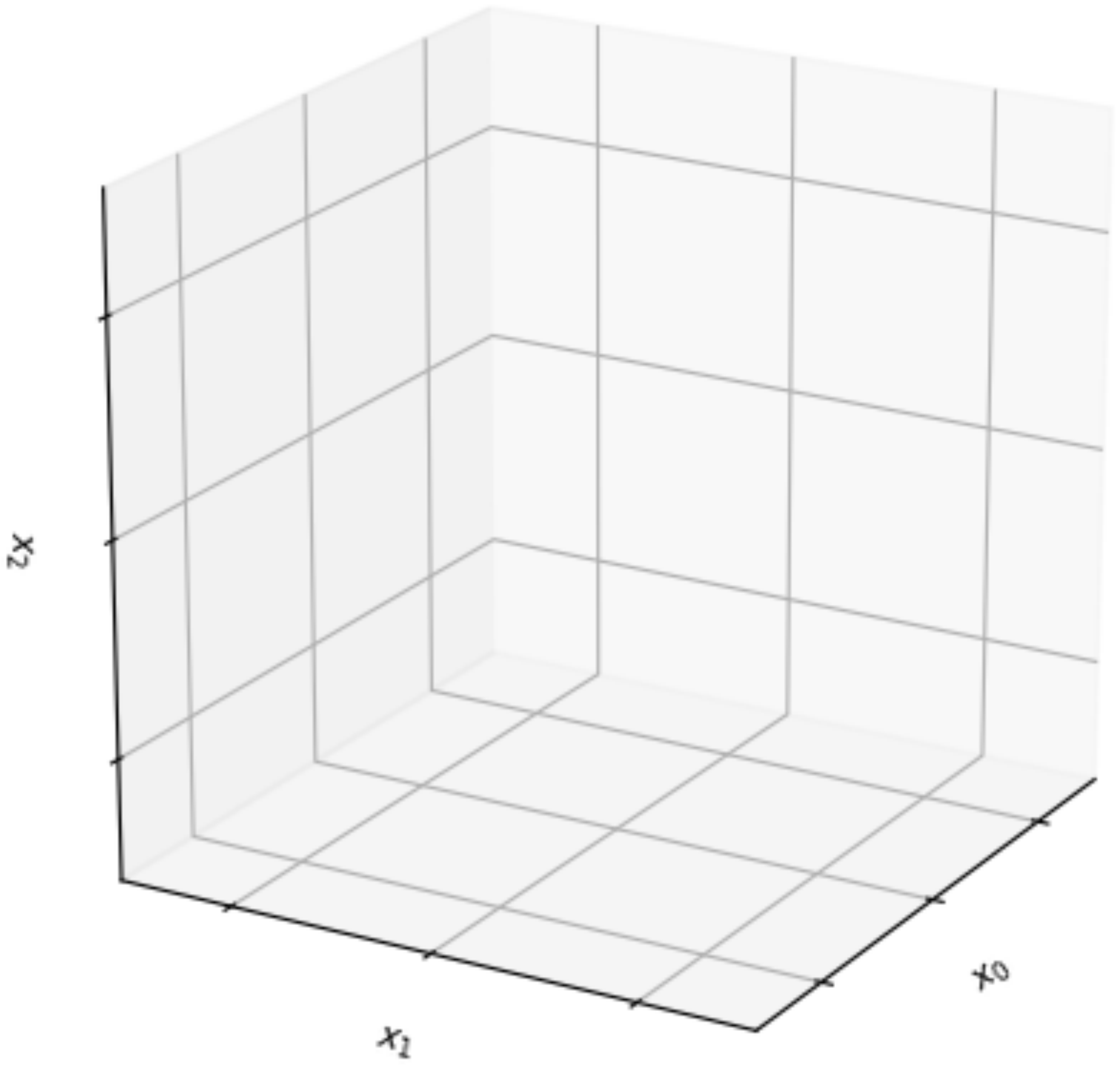


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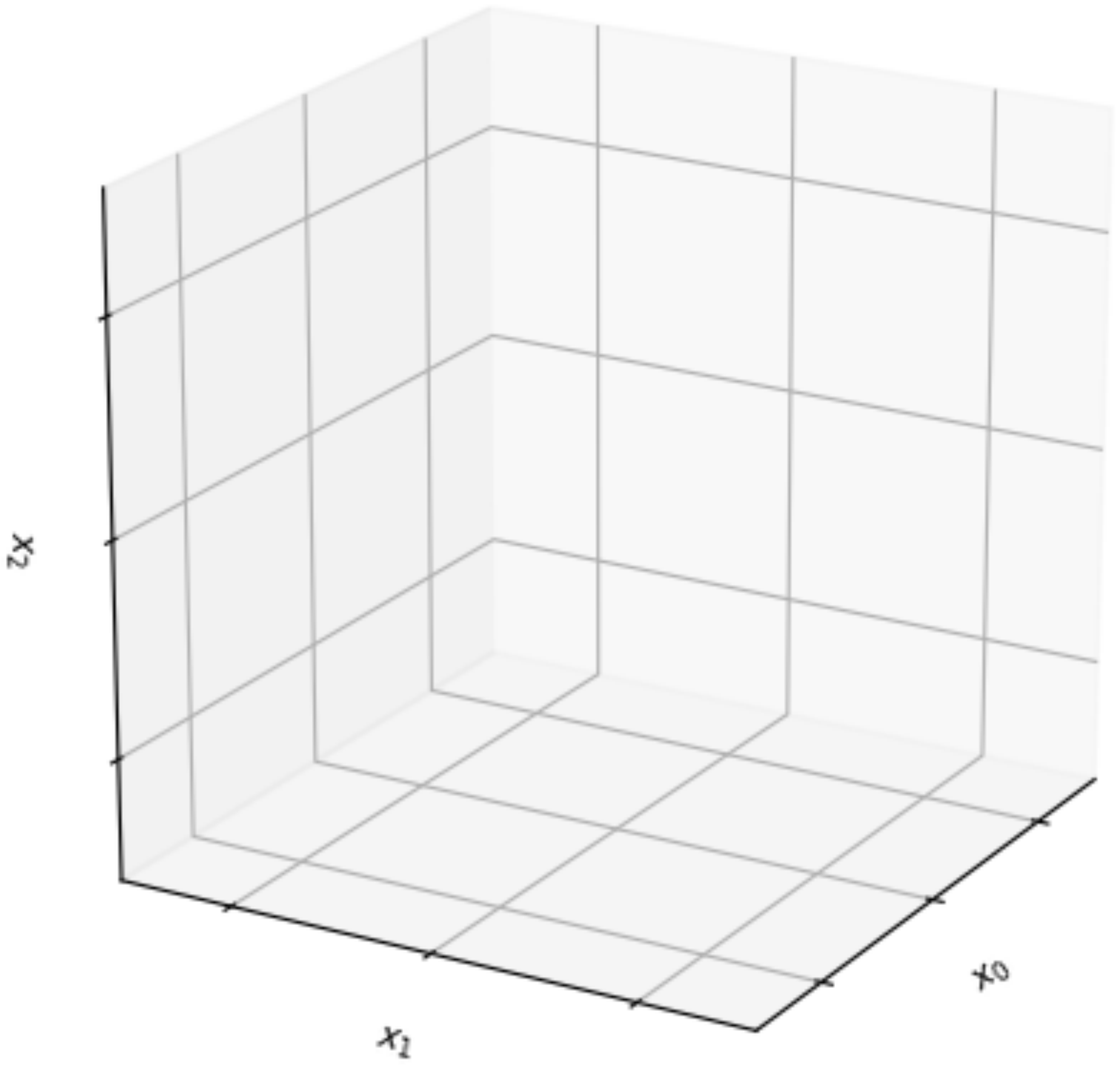


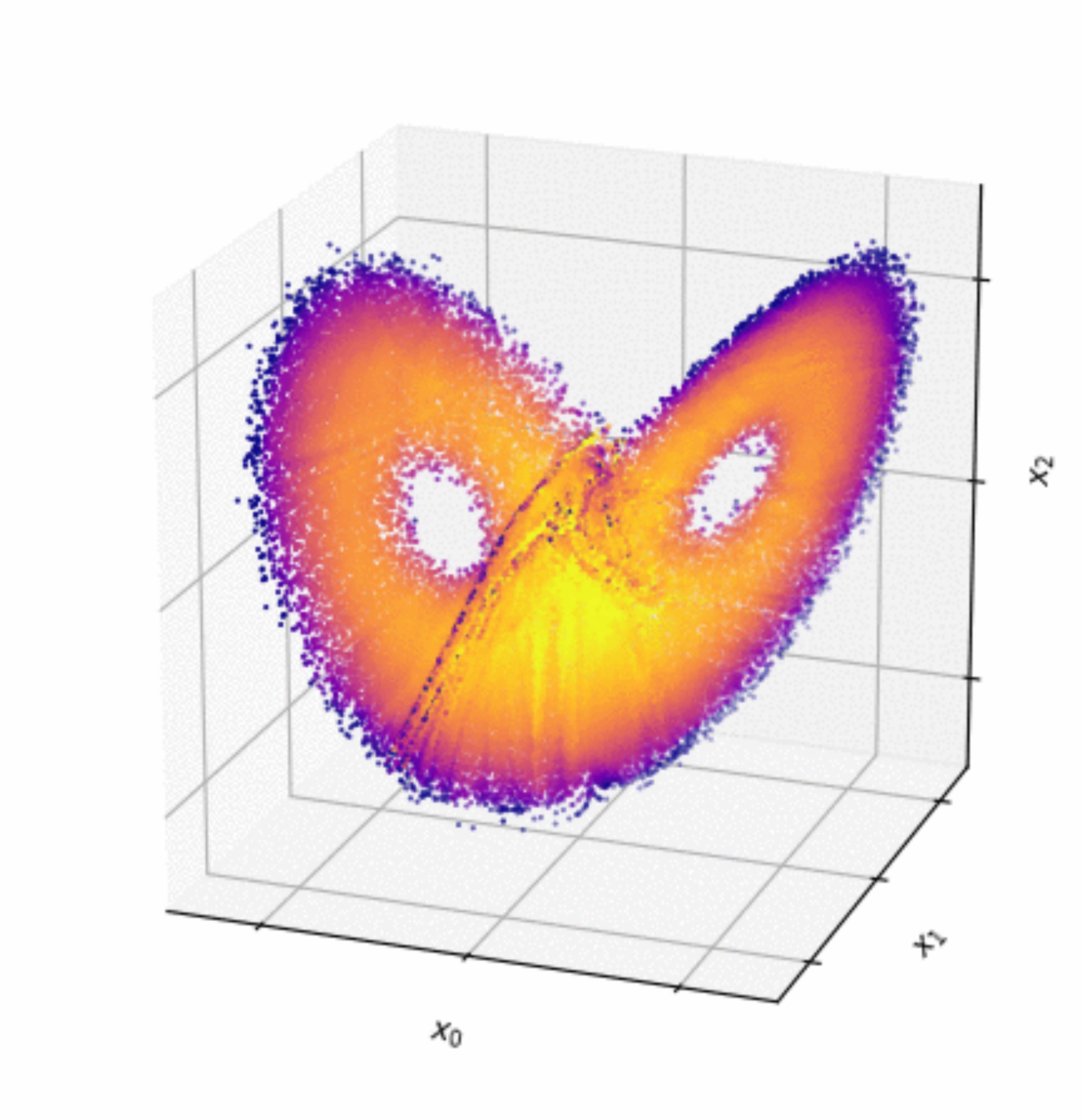


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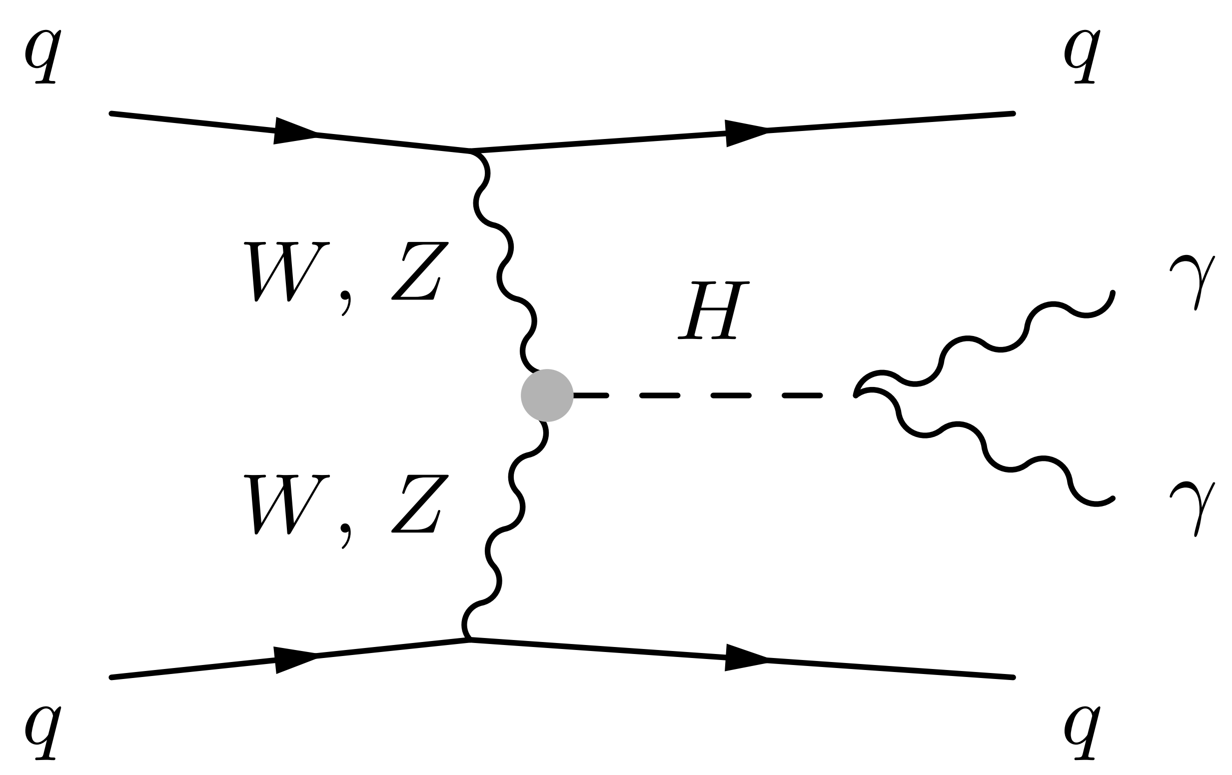
# Particle physics: structure

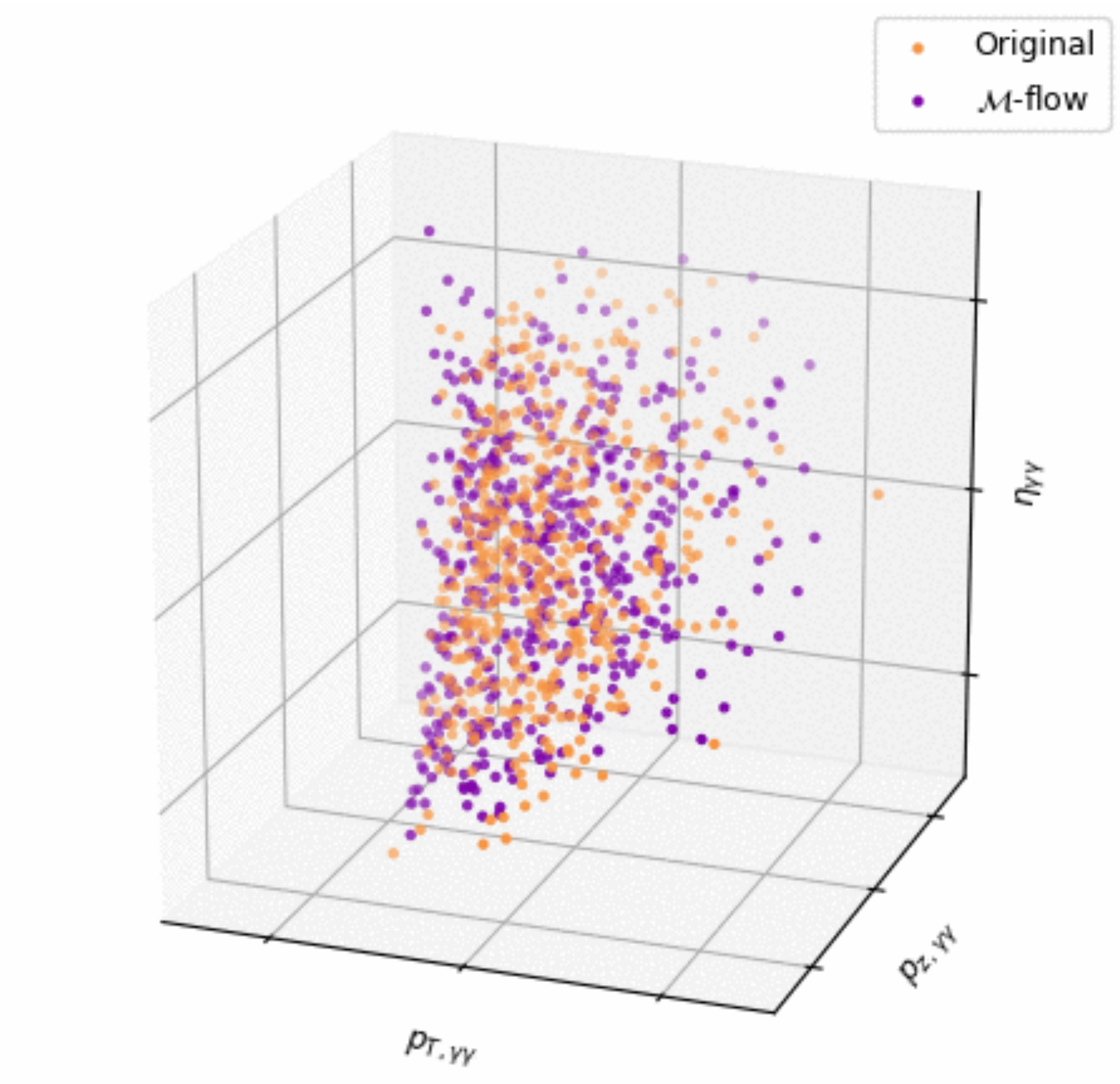



particle masses
("on-shell condition")

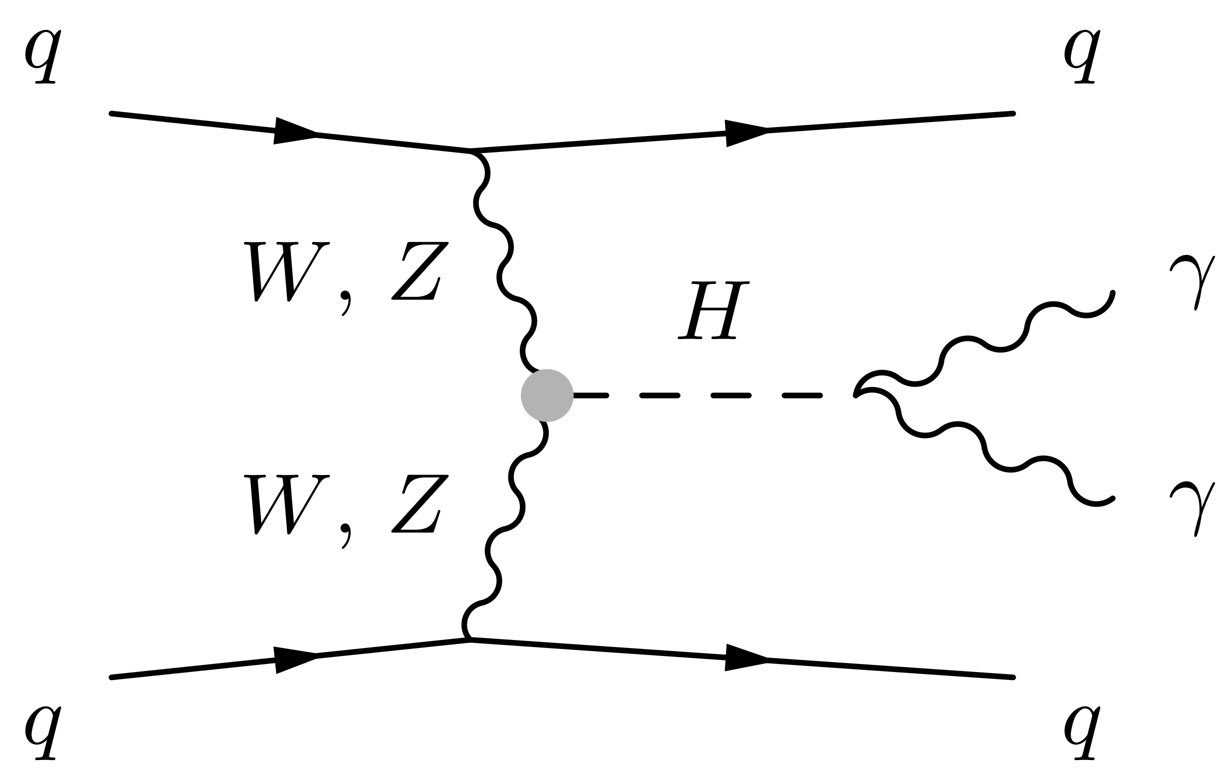
redundant
observables

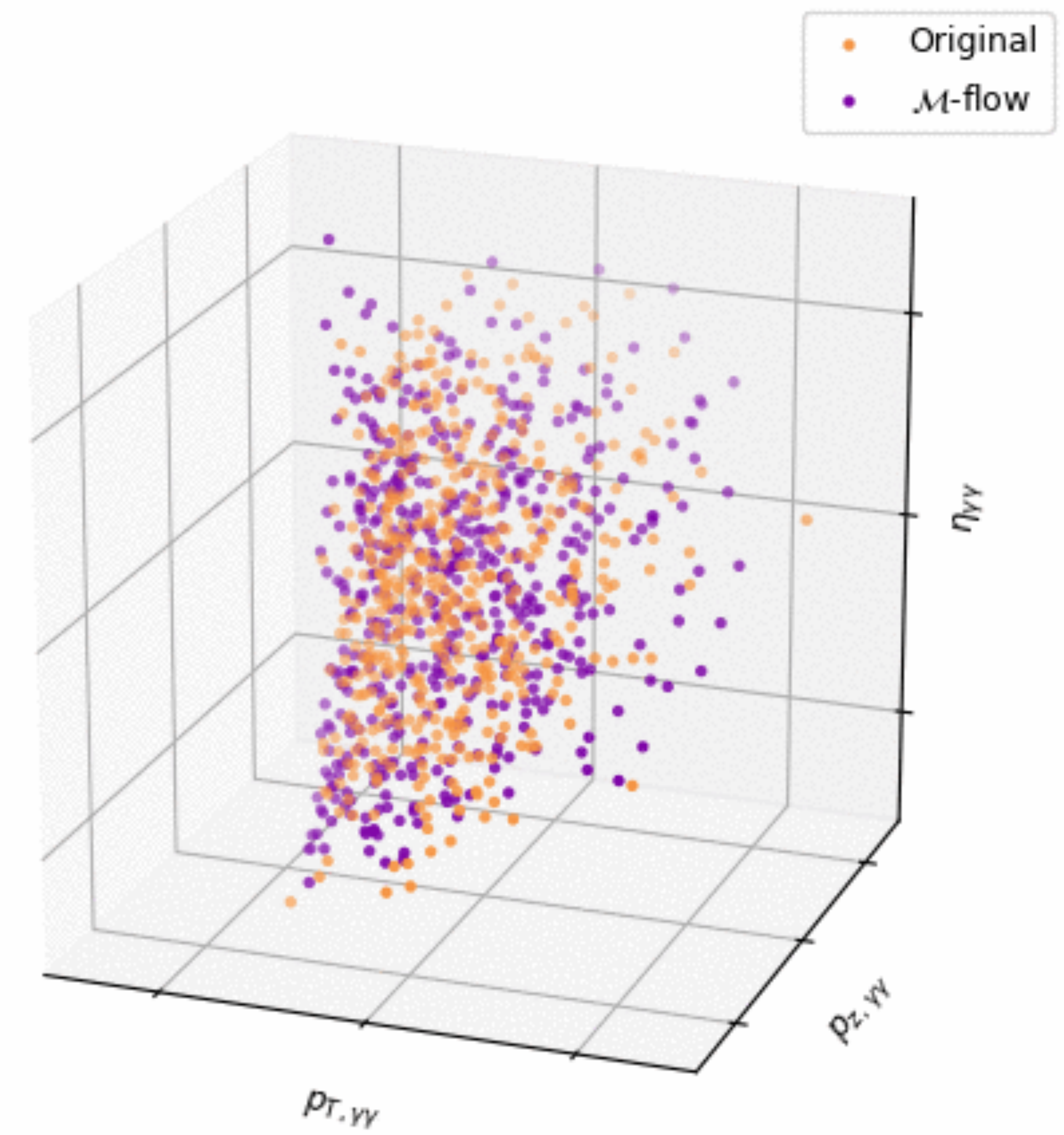
energy-momentum
conservation

14-dimensional manifold
embedded in 40-dimensional
data space



# Particle physics: structure



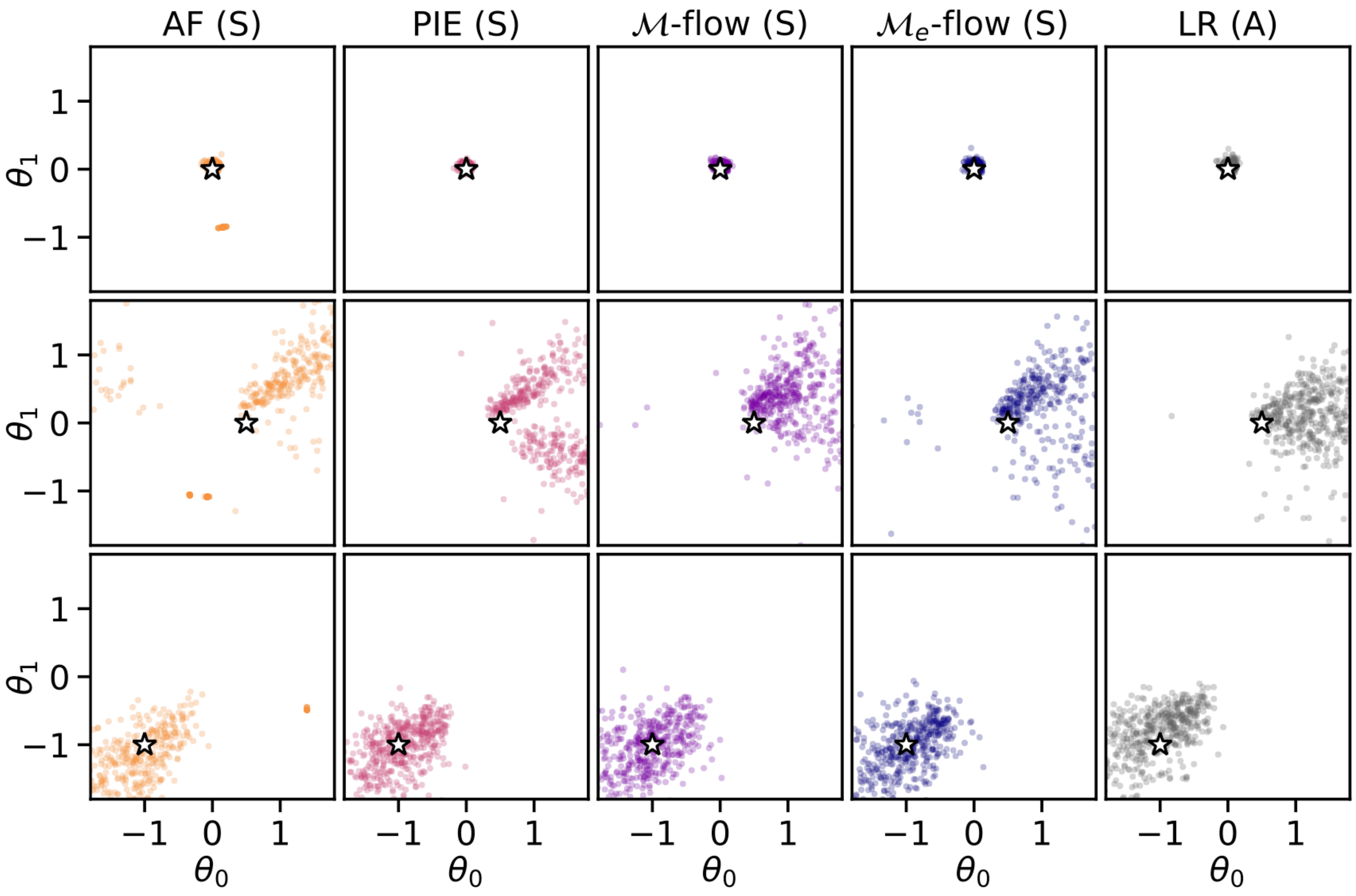

redundant observables

particle masses
("on-shell condition")

energy-momentum conservation

14-dimensional manifold
embedded in 40-dimensional
data space

# Particle physics: results

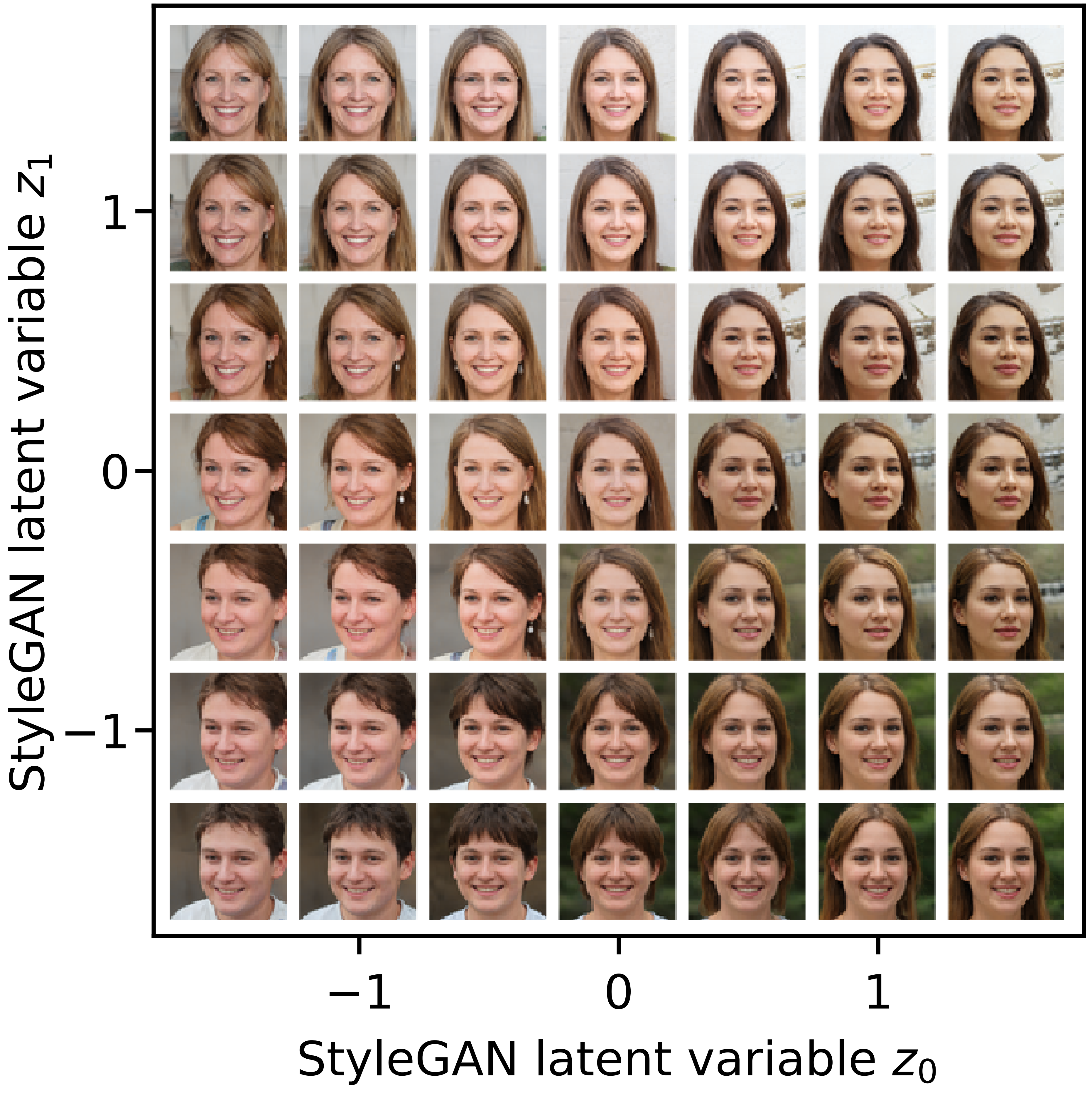


# Image manifolds

Q: How to make image datasets where we **know** that data lives on an $n$ -dimensional manifold?

A: take a pretrained GAN model, sample $n$ of its latent variables, and keep all others fixed

$n = 2$



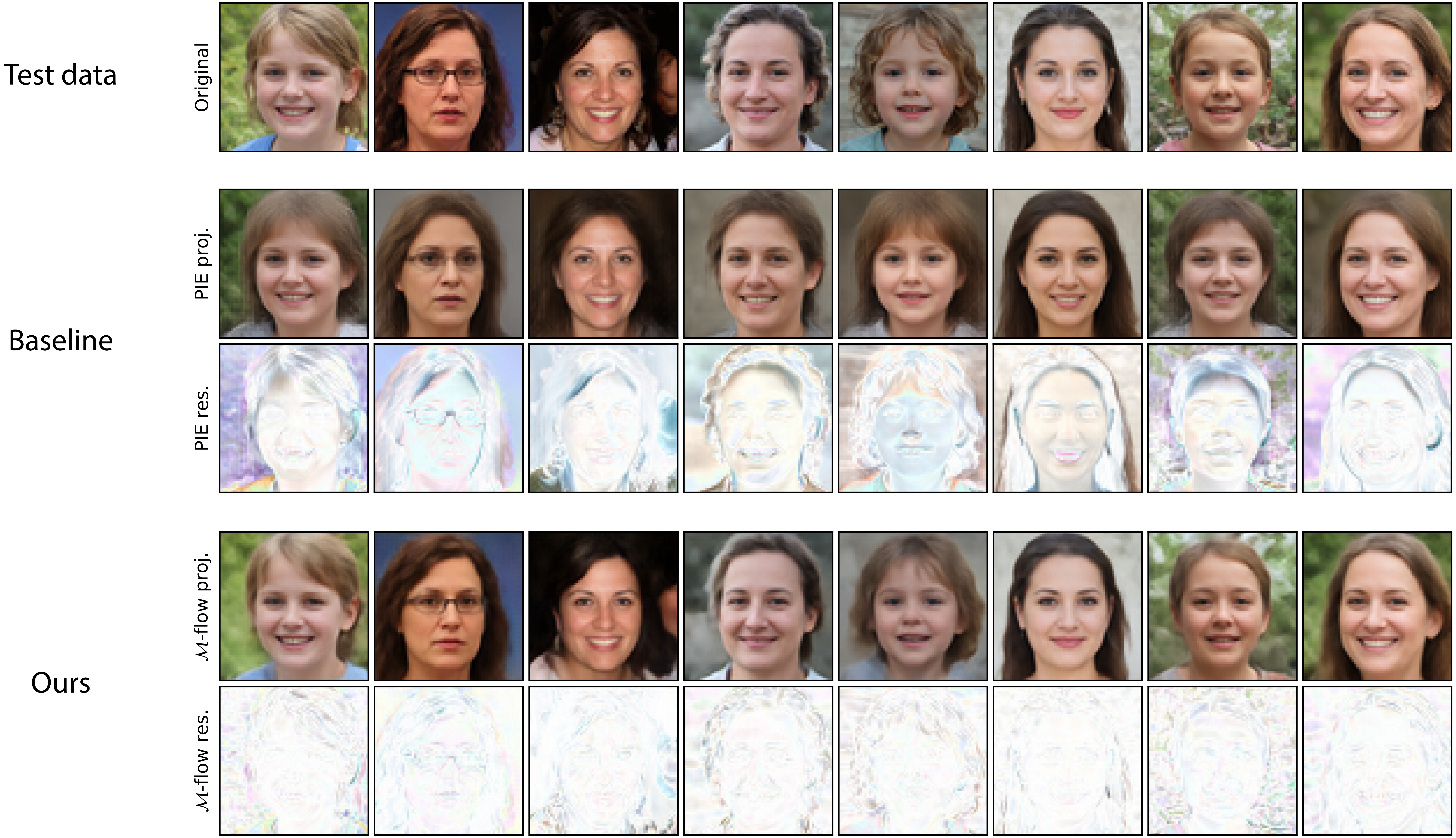
# Samples

Test data

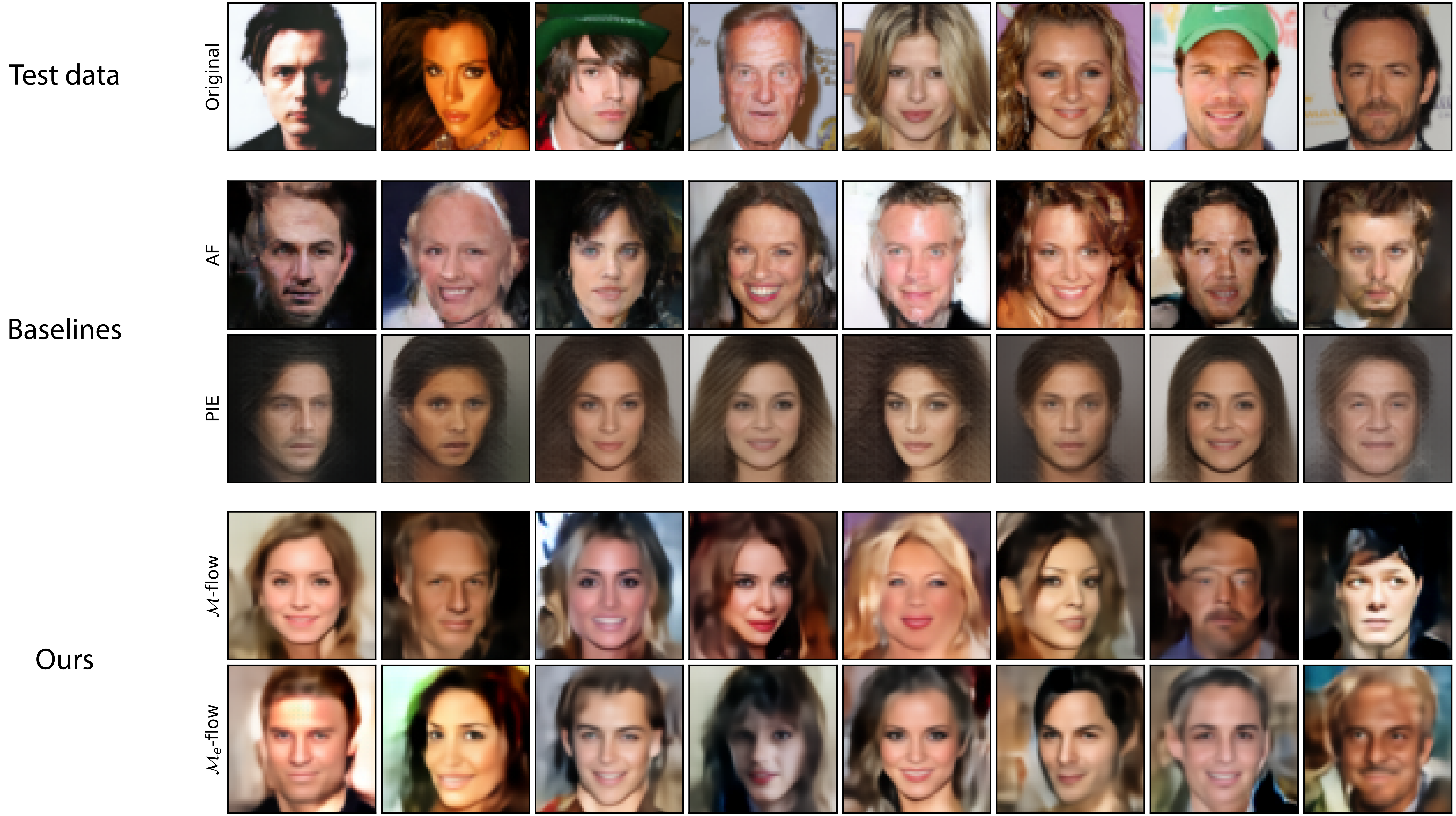
Baselines

Ours

# Projections to learned manifolds



# Real-world images: CelebA samples



# CelebA projections