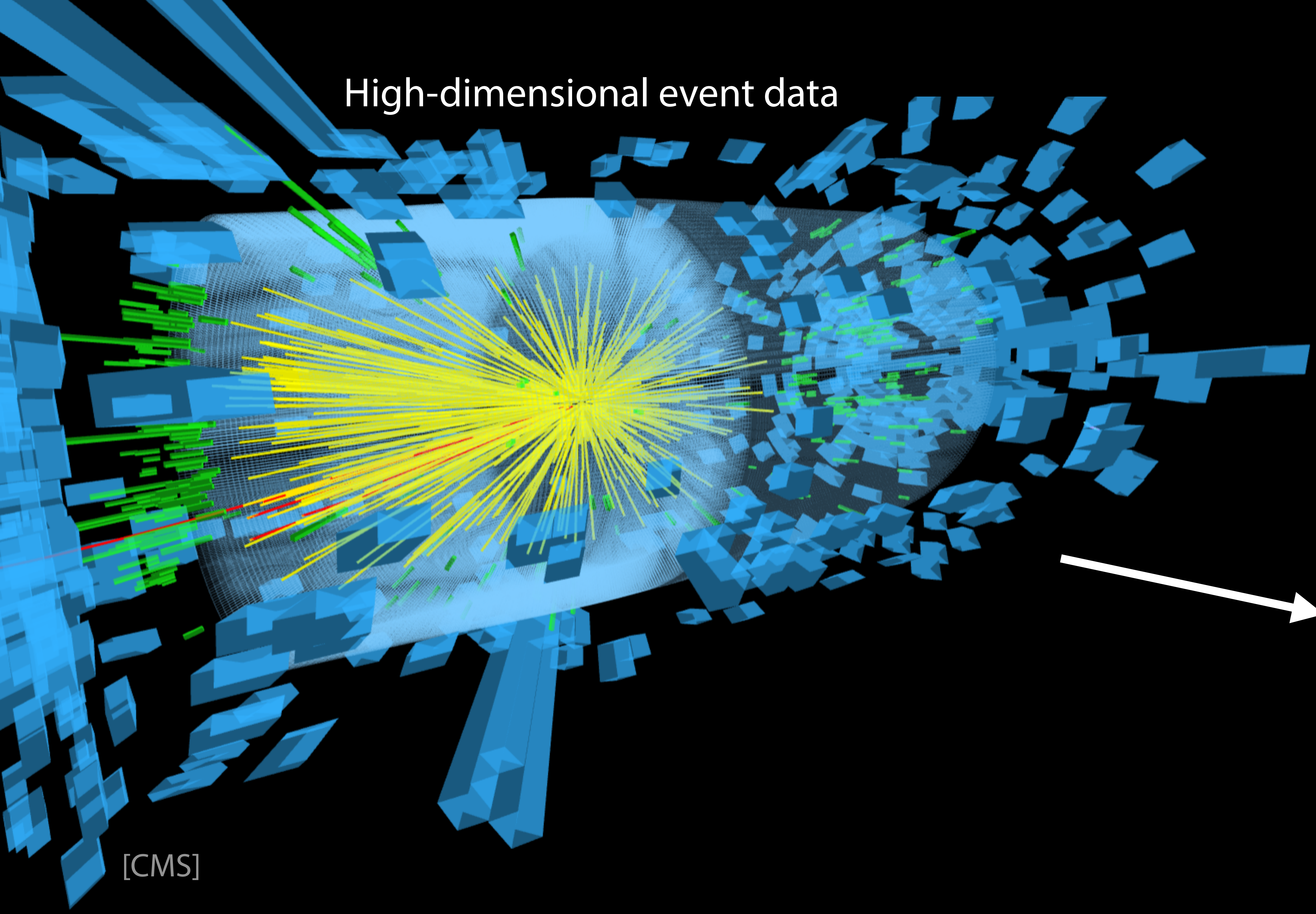
How machine learning can help us get the most out of high-precision particle physics models

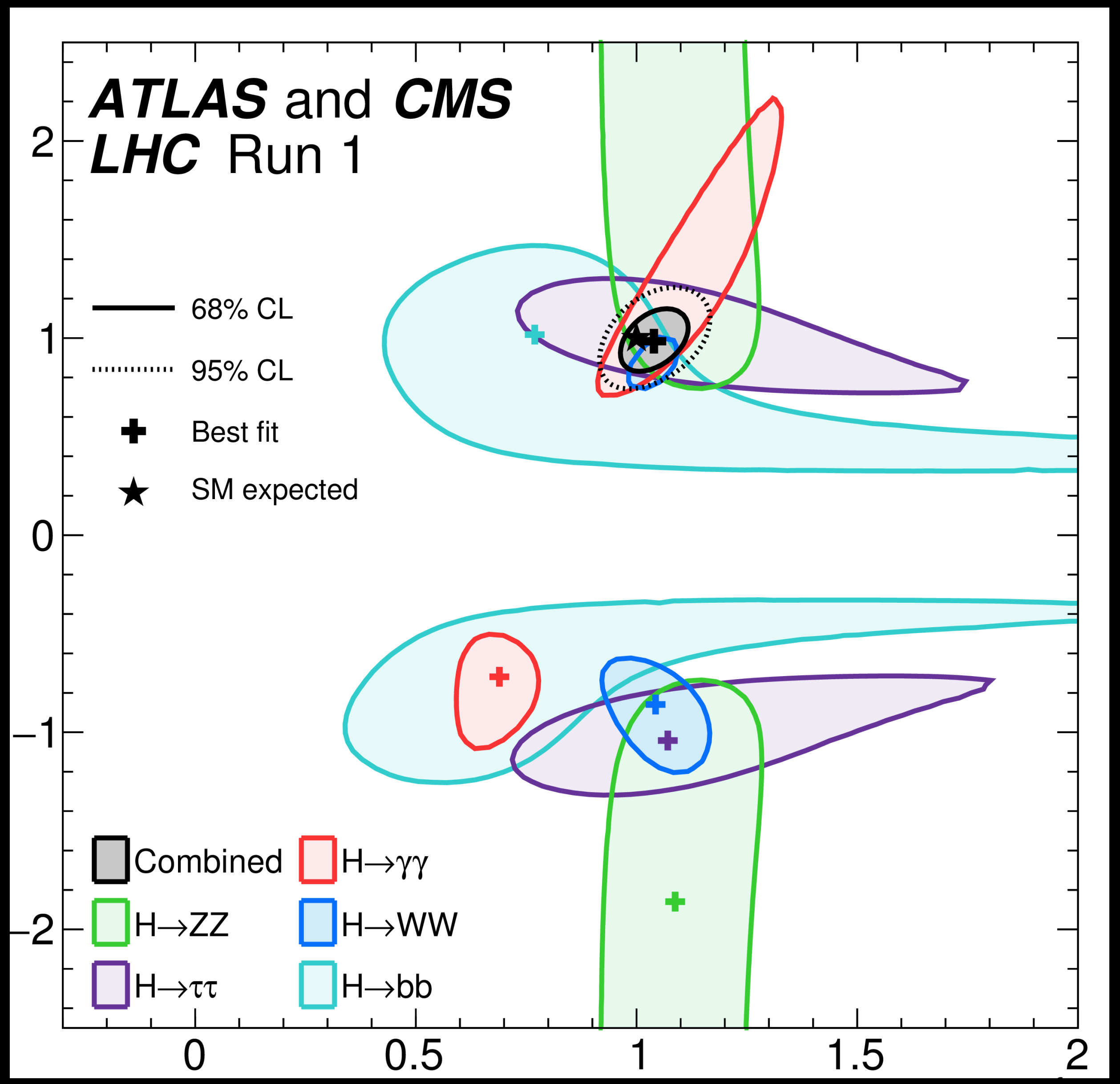
Johann Brehmer
New York University

DESY-HU theory seminar
November 12, 2020

High-dimensional event data



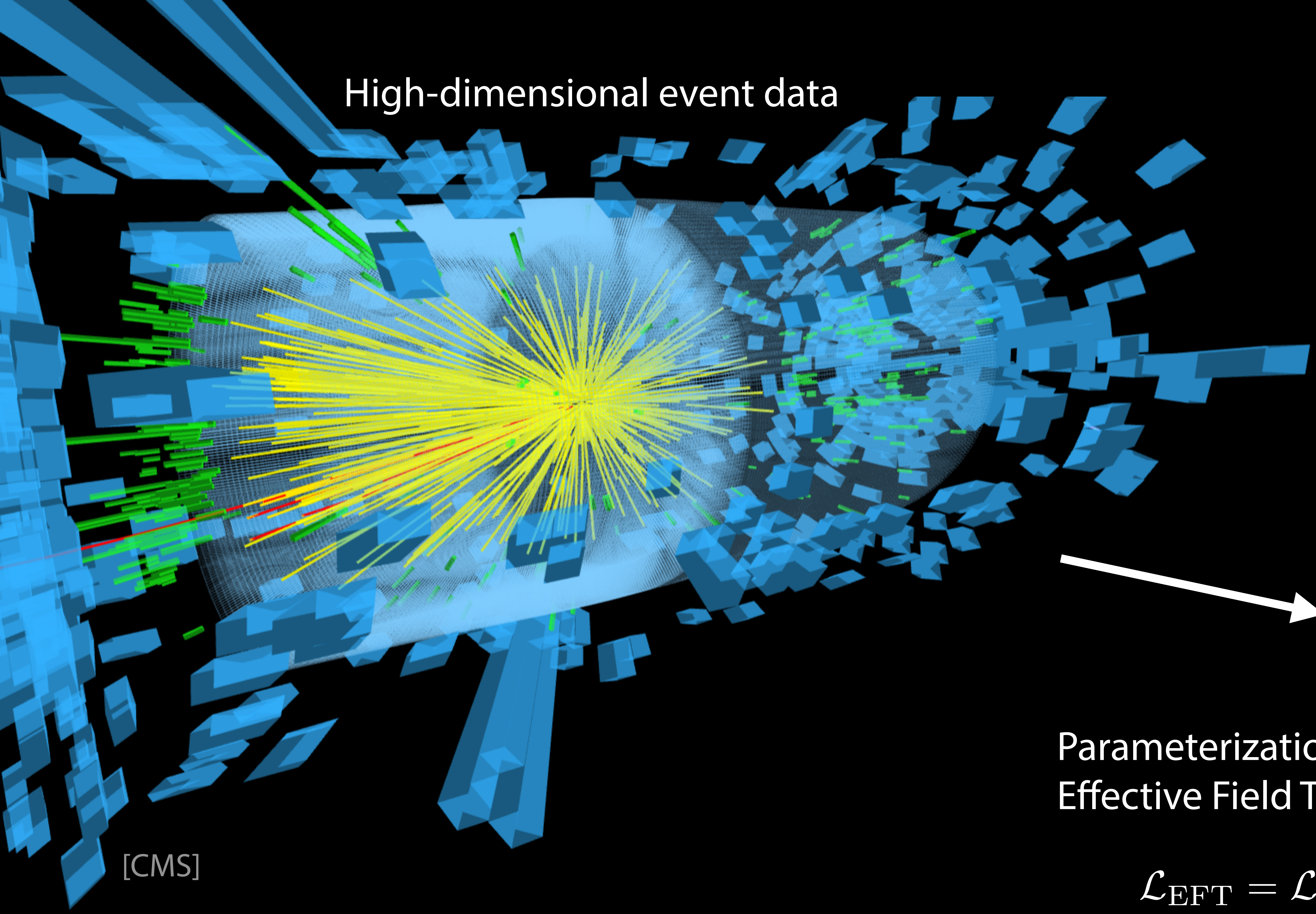
[CMS]



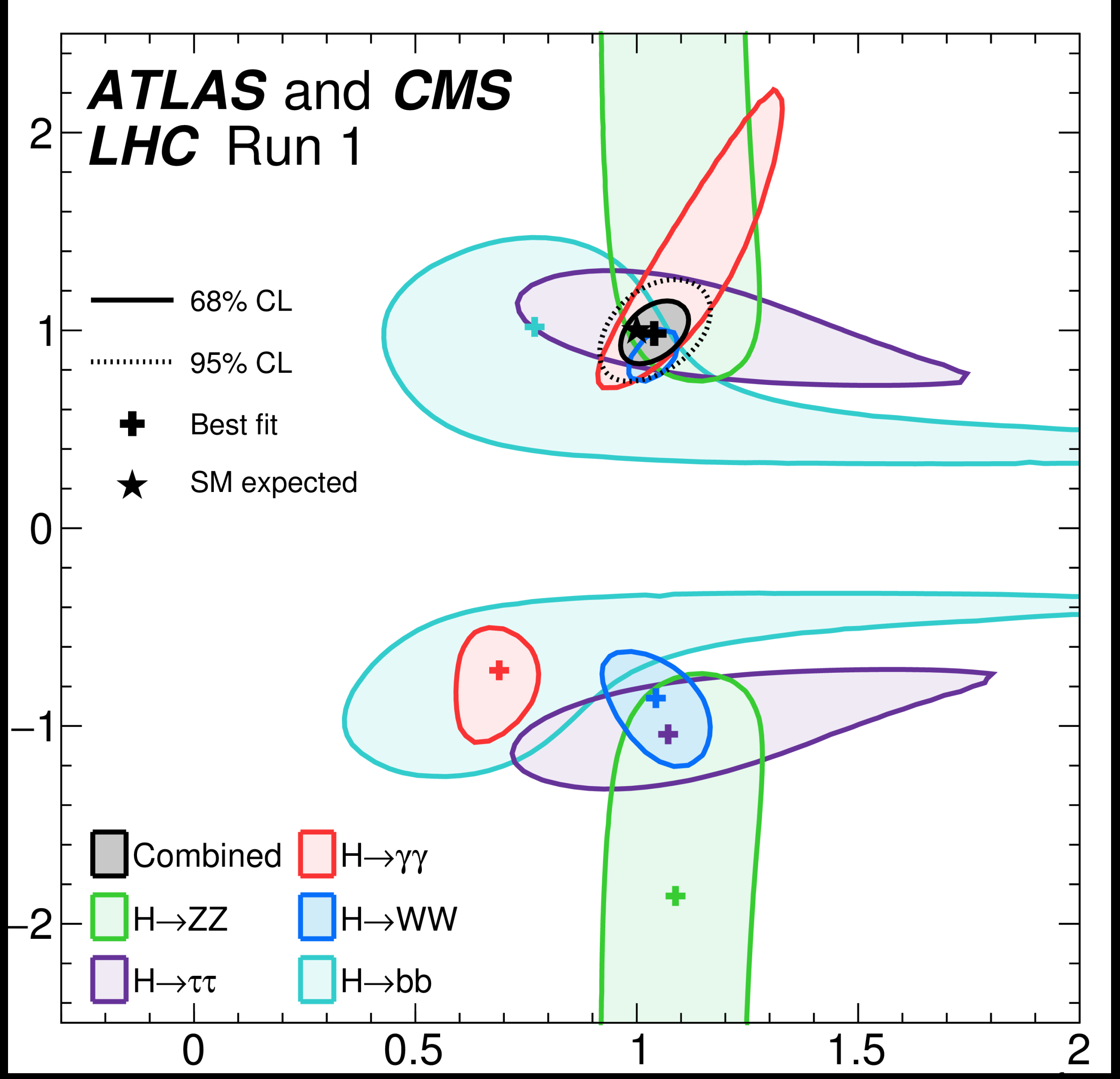
[ATLAS, CMS 1606.02266]

Precision constraints on new physics

High-dimensional event data



[CMS]



[ATLAS, CMS 1606.02266]

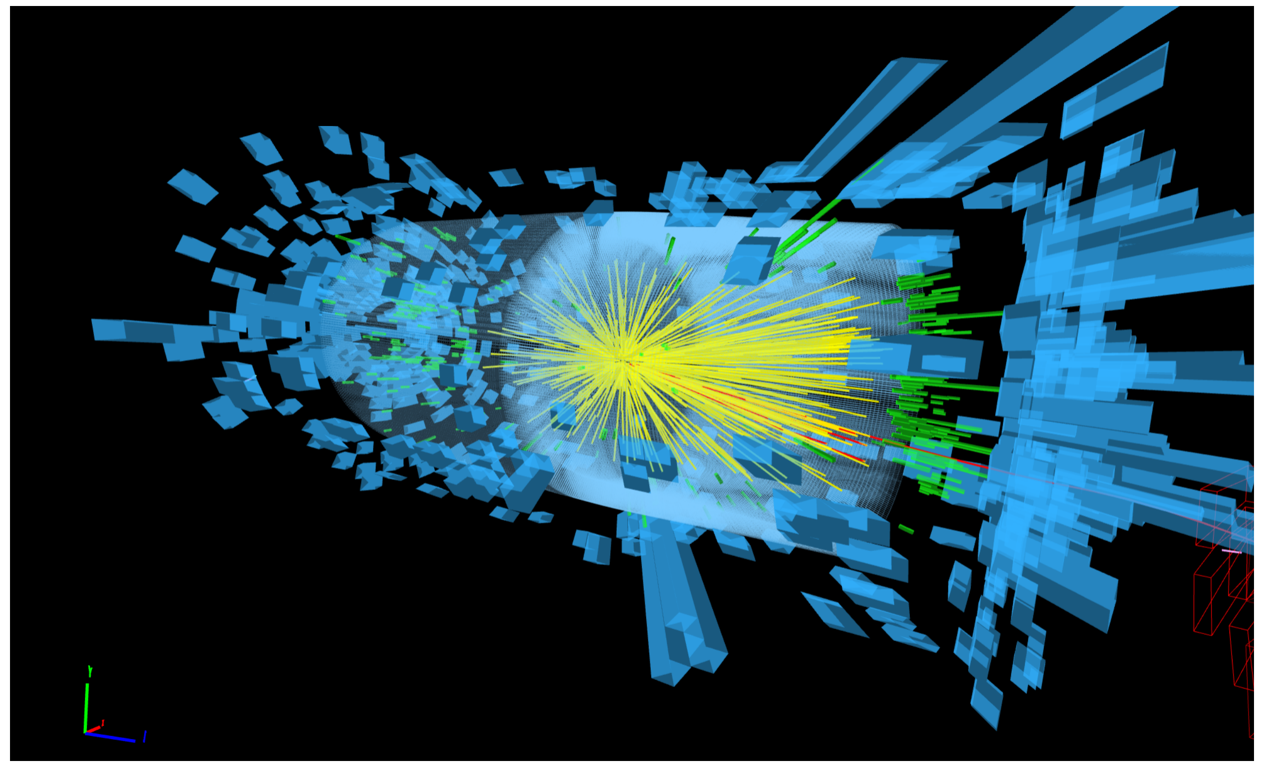
Precision constraints on new physics

Parameterization e.g. in Effective Field Theory:

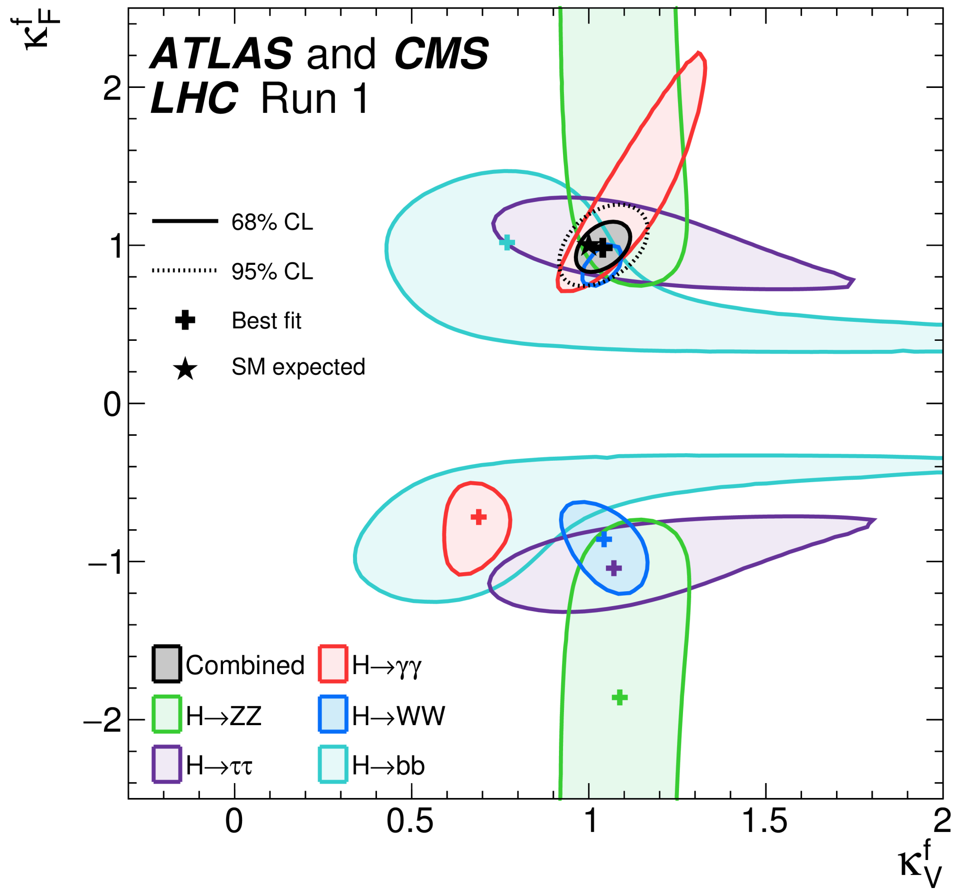
systematic expansion of new physics around Standard Model

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

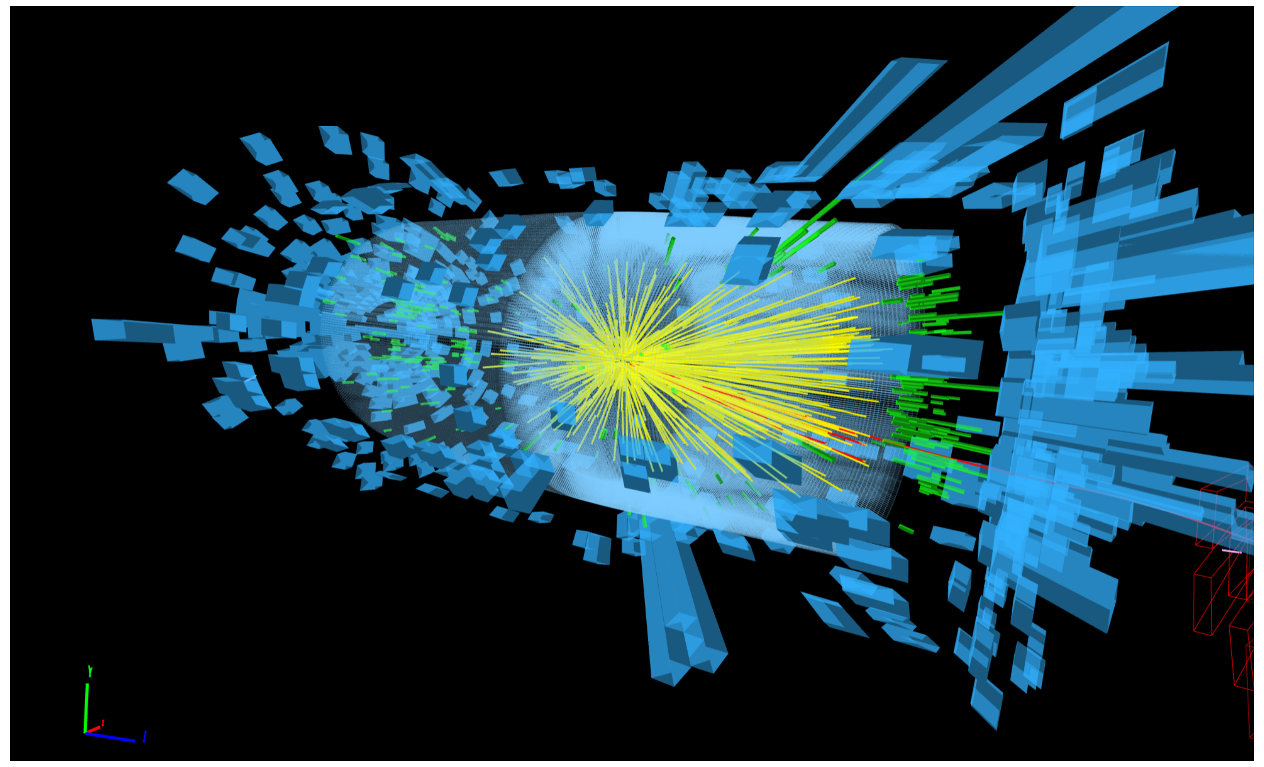
10s to 100s "universal" parameters to measure



High-dimensional
event data x



Constraints on
parameters θ

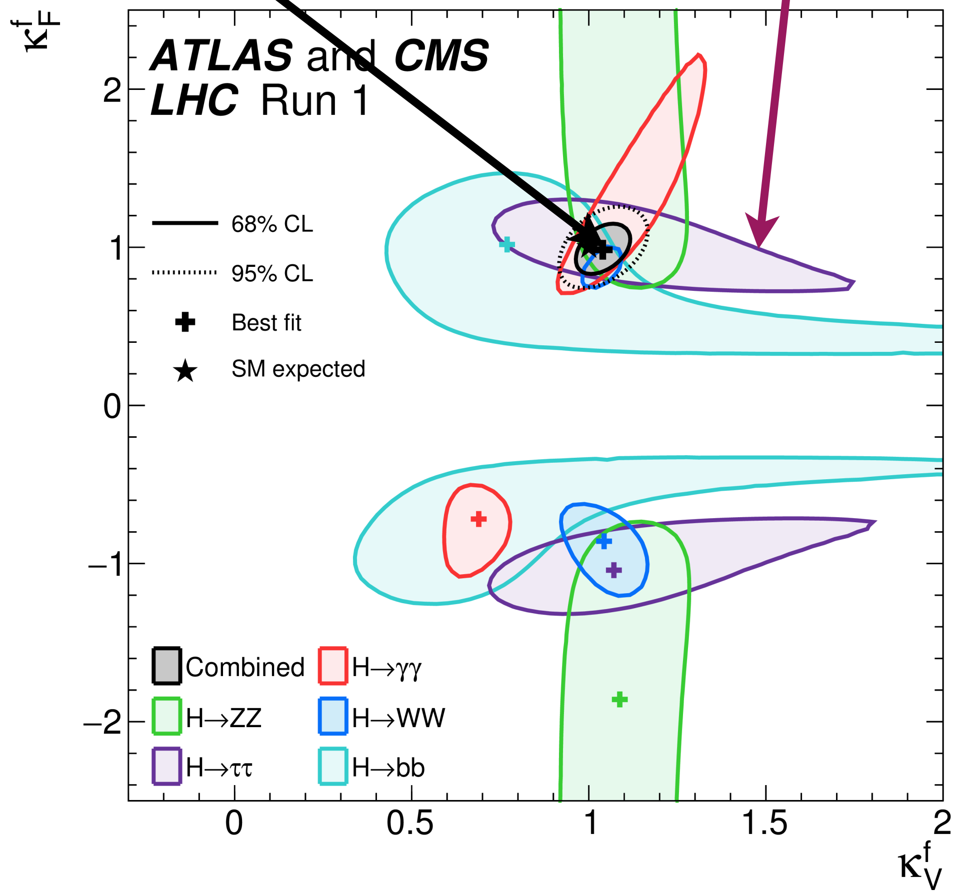


High-dimensional event data x

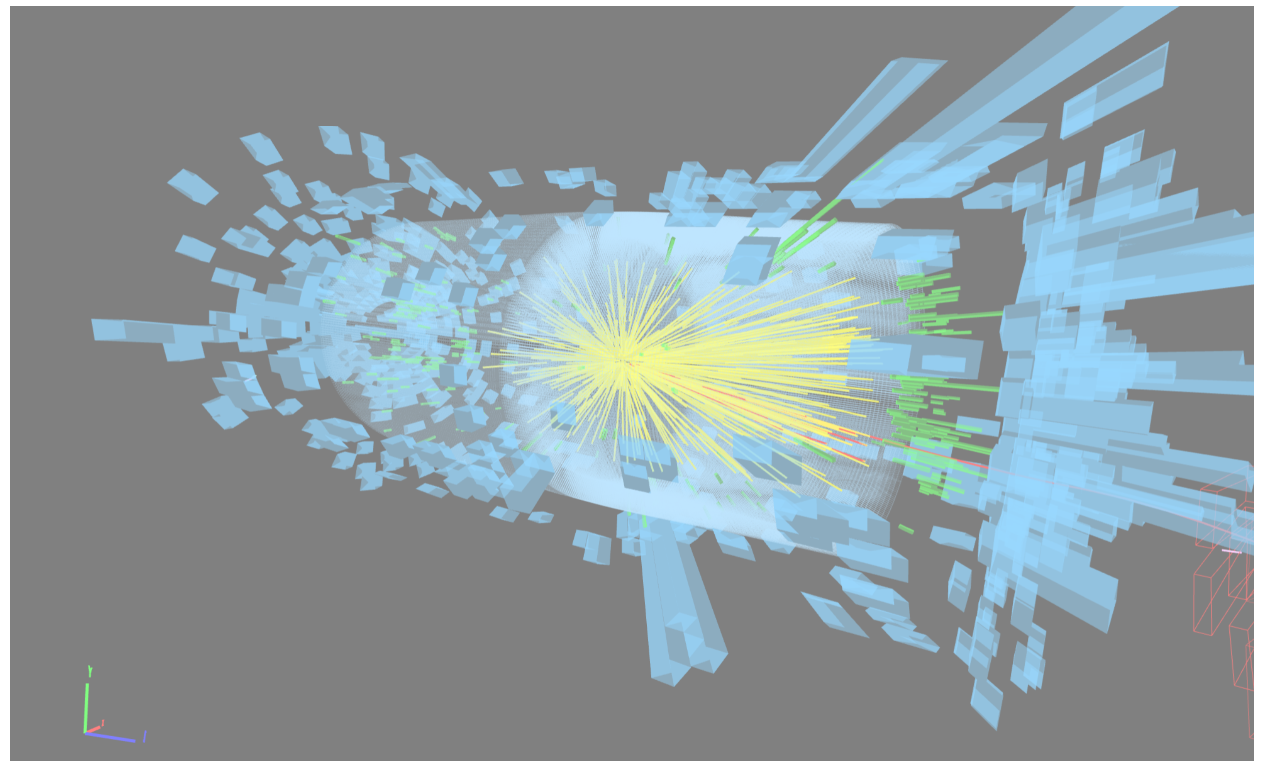
Likelihood function
$p(x|\theta)$

Maximum-likelihood estimator

Confidence limits based on likelihood ratio tests

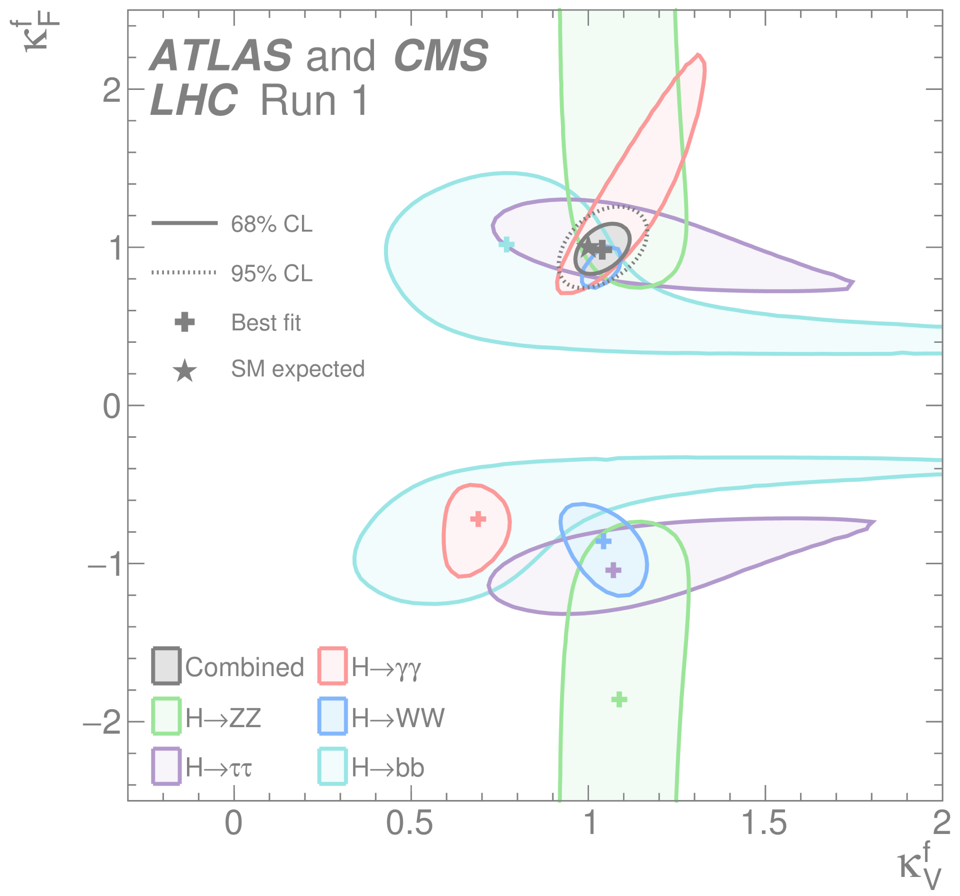


Constraints on parameters θ



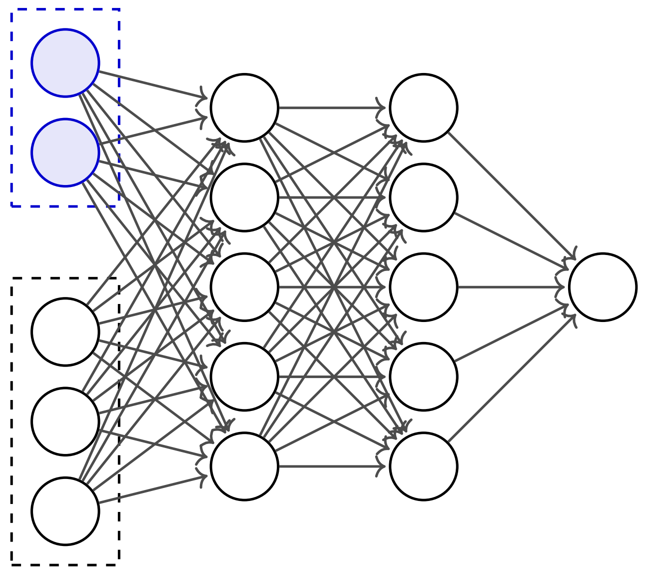
High-dimensional event data x

Likelihood function
$p(x|\theta)$

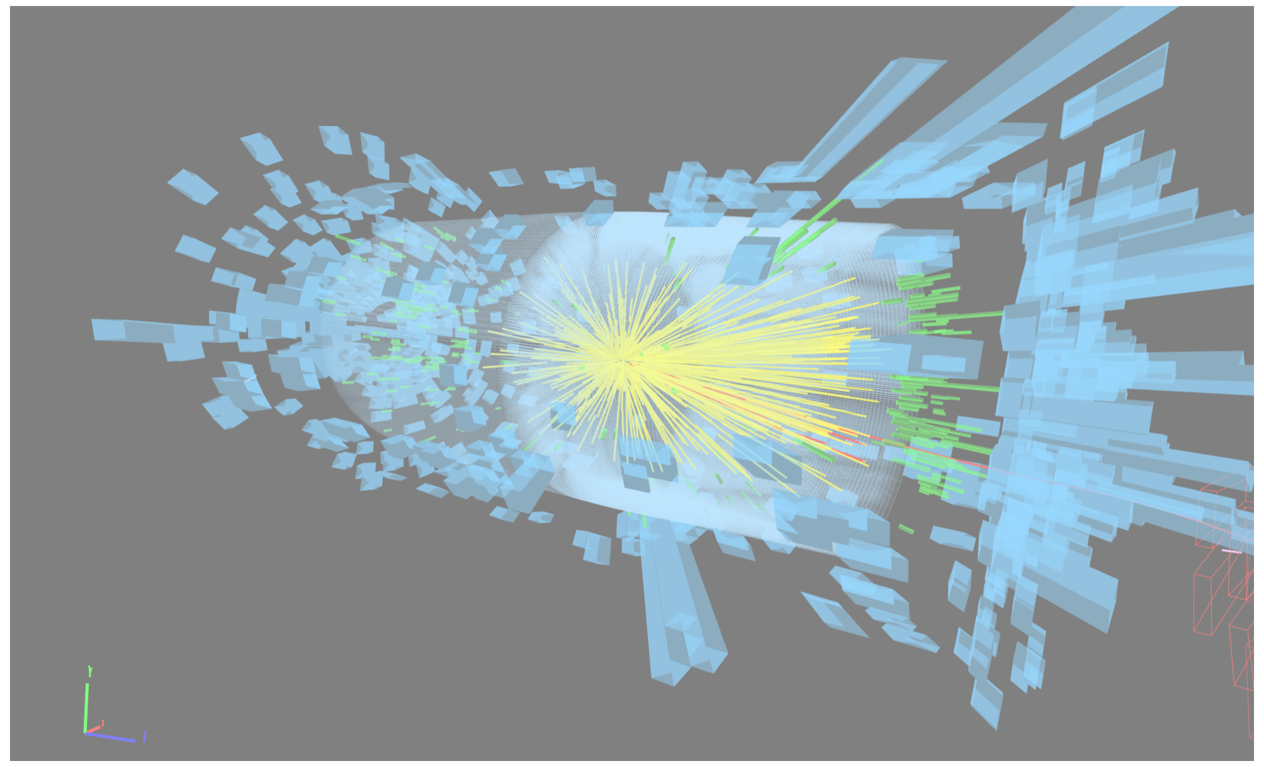


Constraints on parameters θ

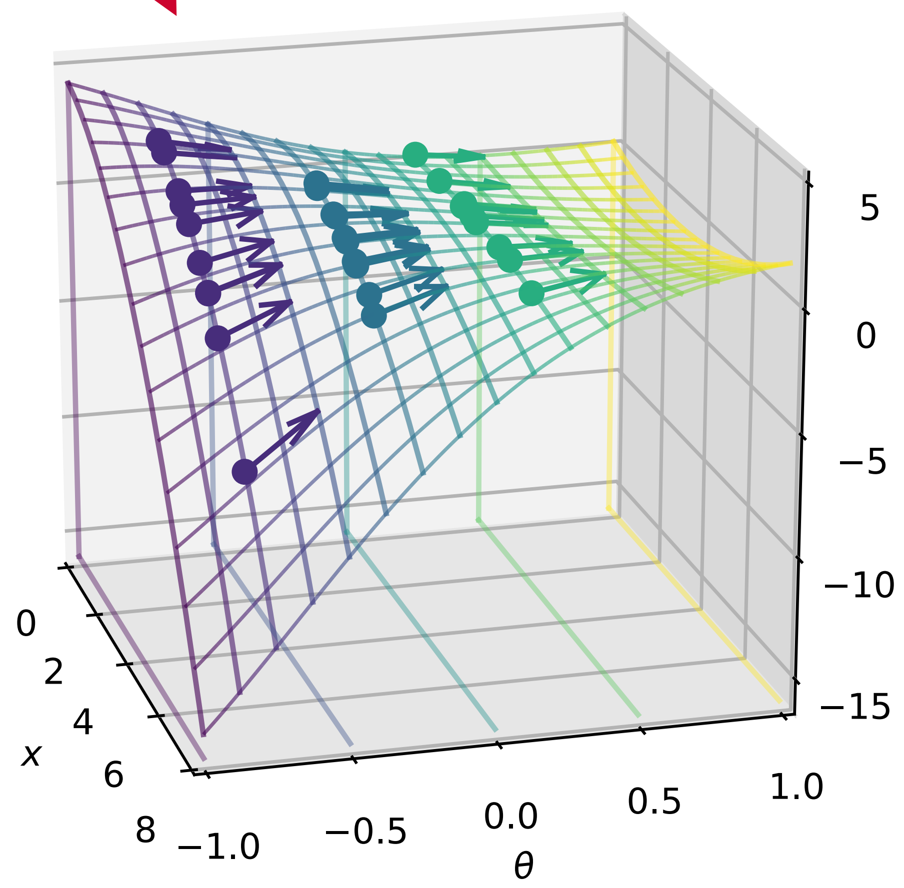
Surprisingly, when we want to use high-dimensional data and have to deal with the detector response, we do not have a good way to calculate the likelihood.



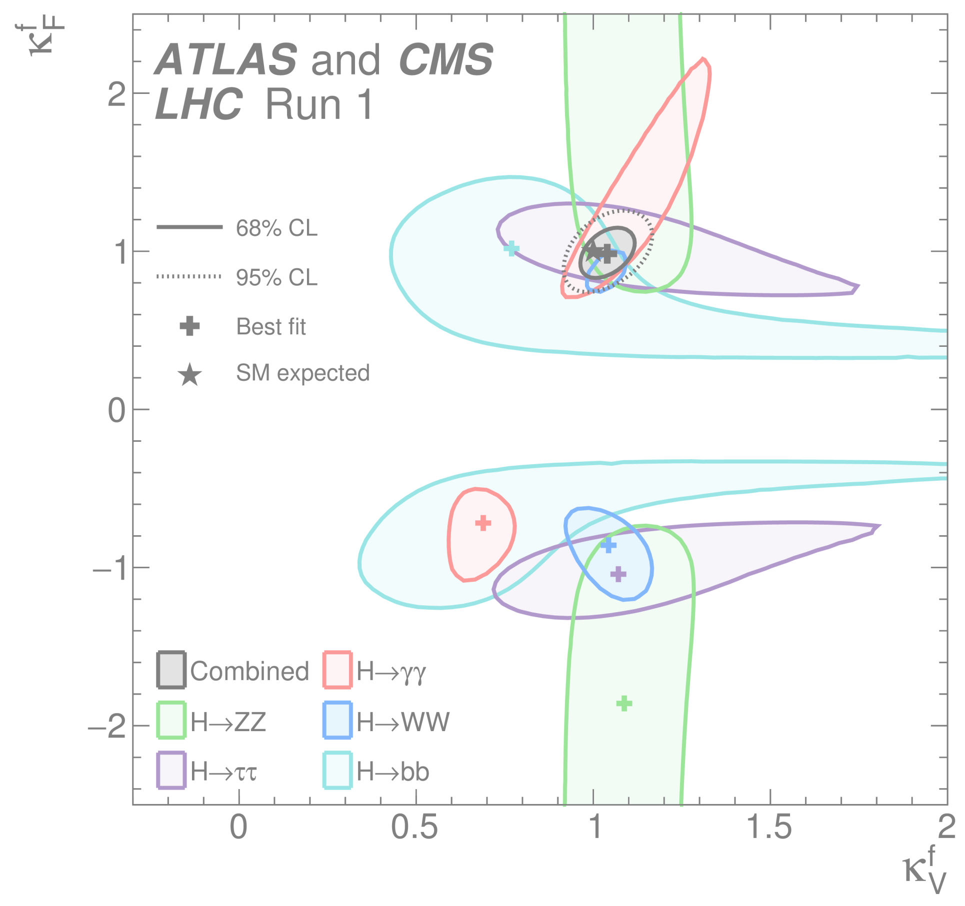
Machine learning



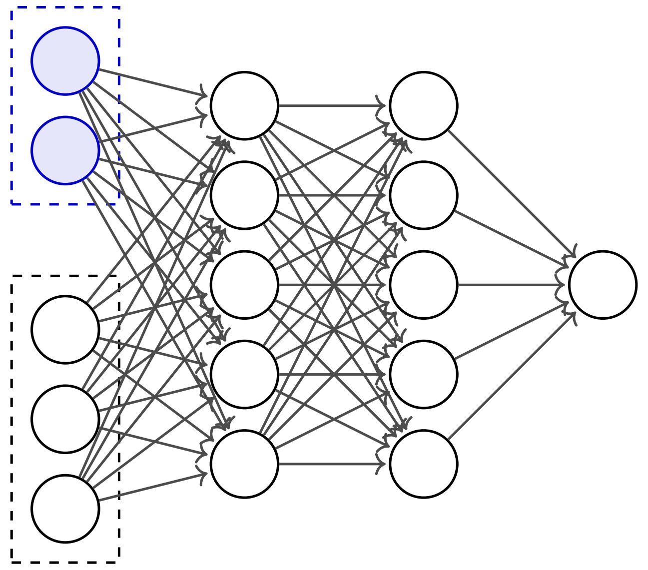
High-dimensional event data x



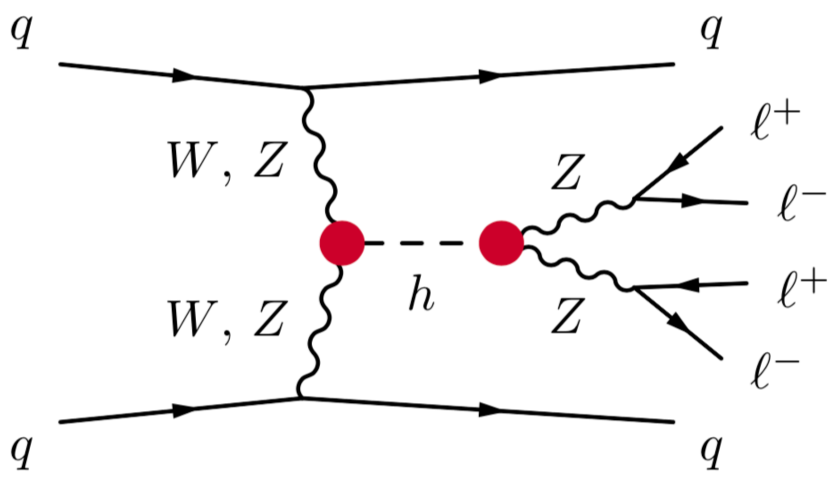
Estimator of the likelihood $p(x|\theta)$



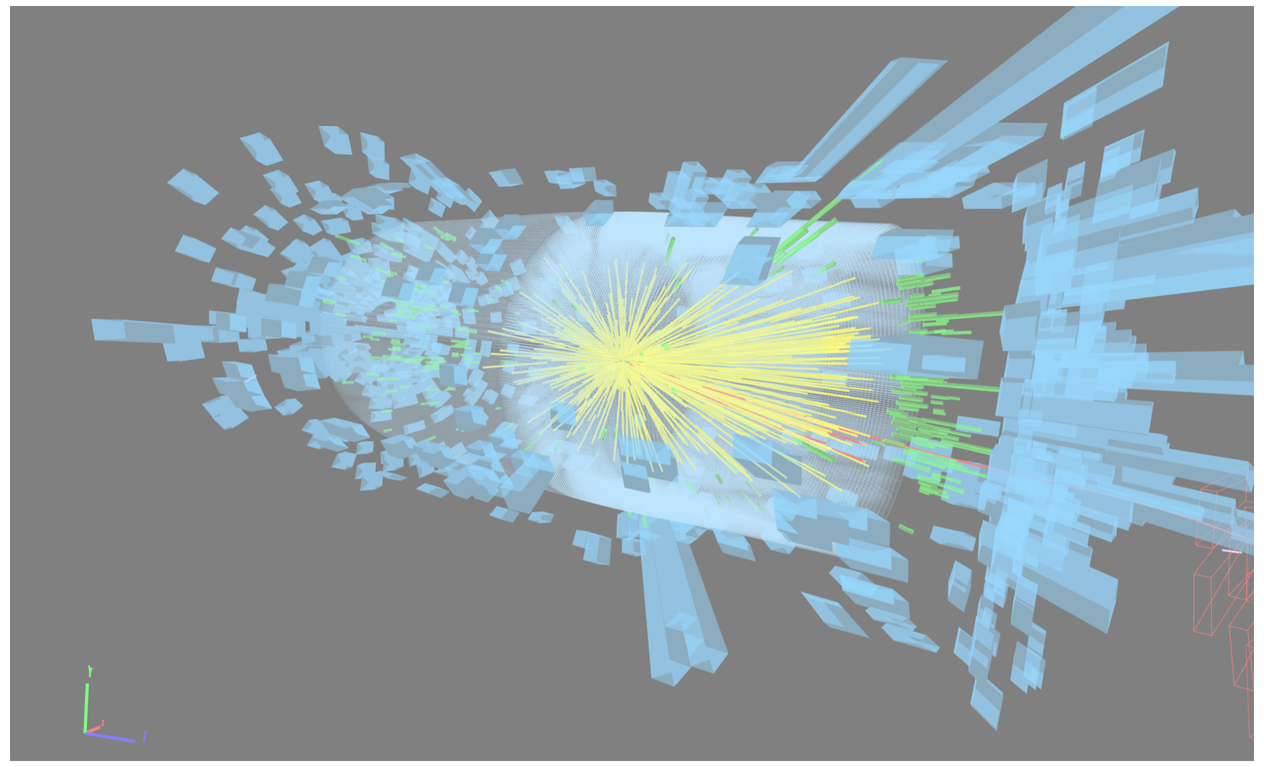
Constraints on parameters θ



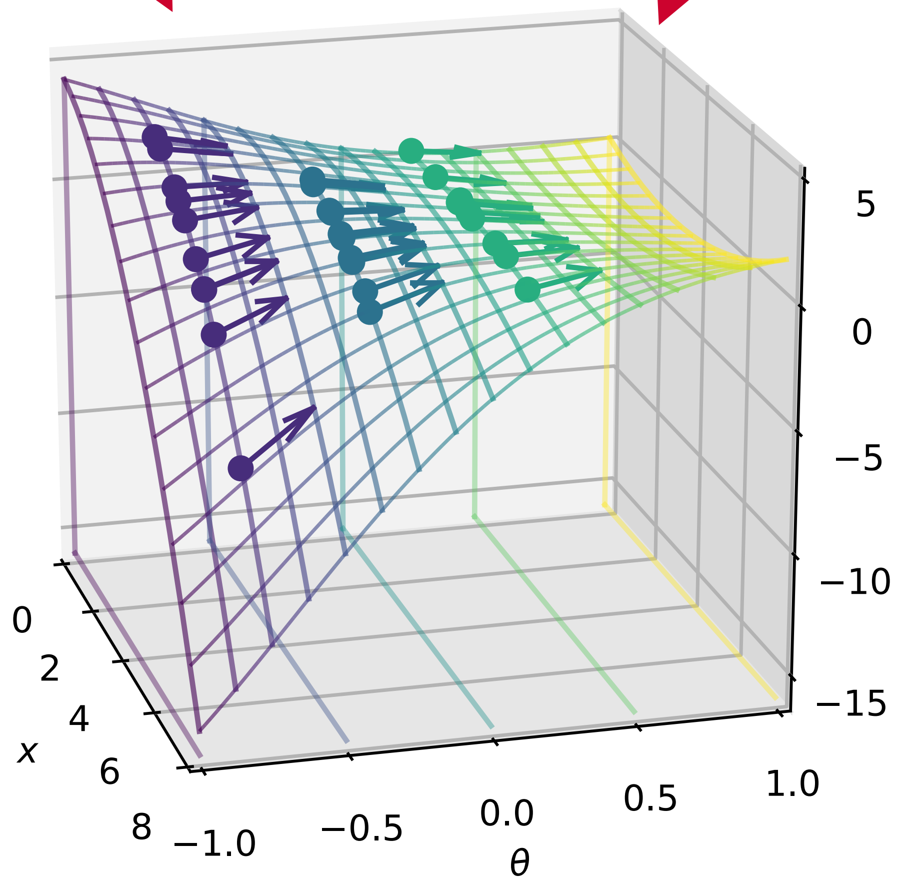
Machine learning



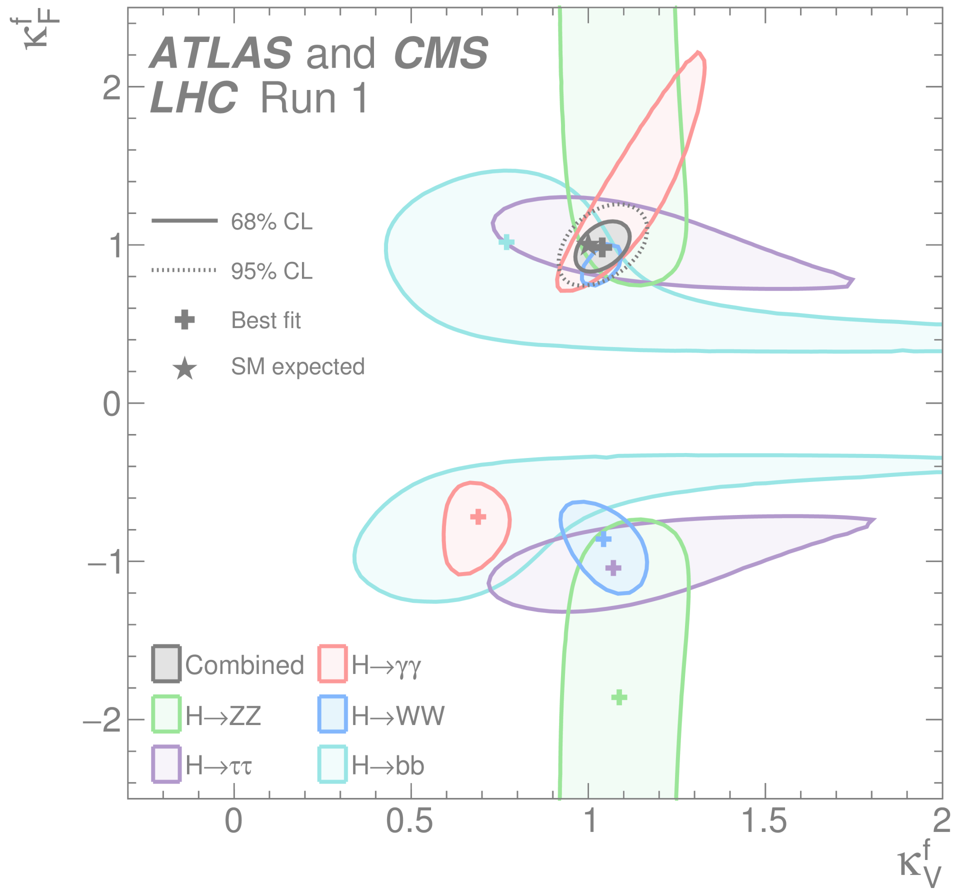
Physics insight:
matrix element information



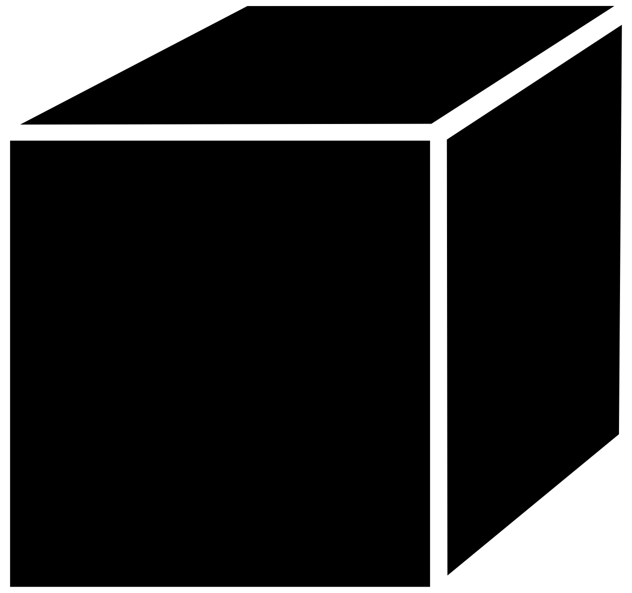
High-dimensional
event data x



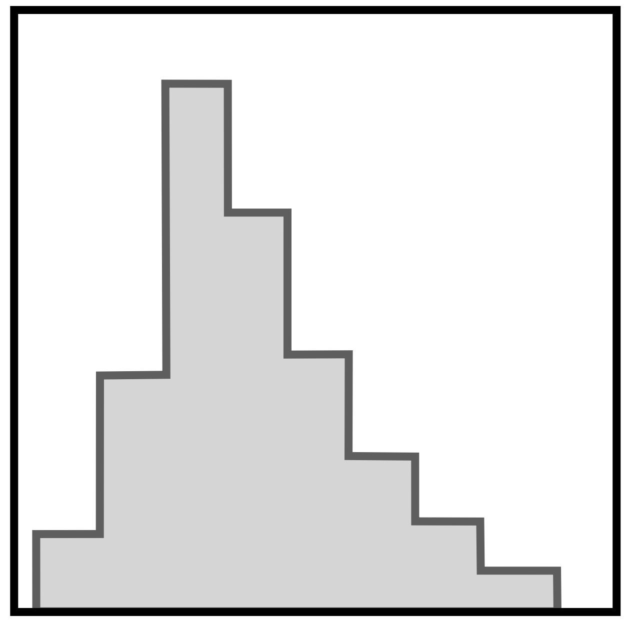
Estimator of the
likelihood $p(x|\theta)$



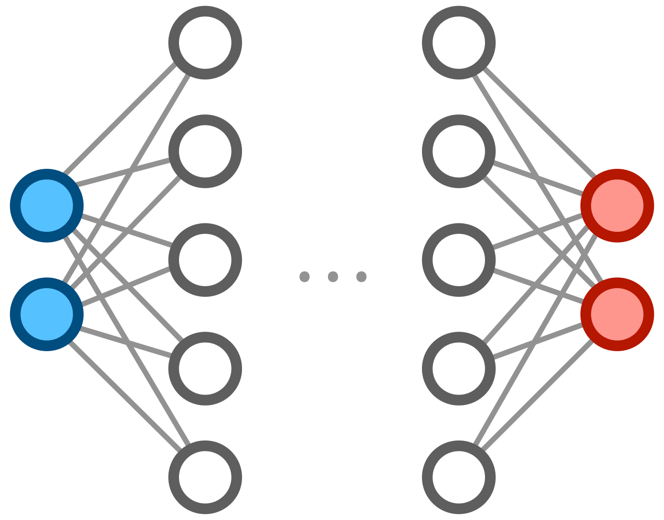
Constraints on
parameters θ



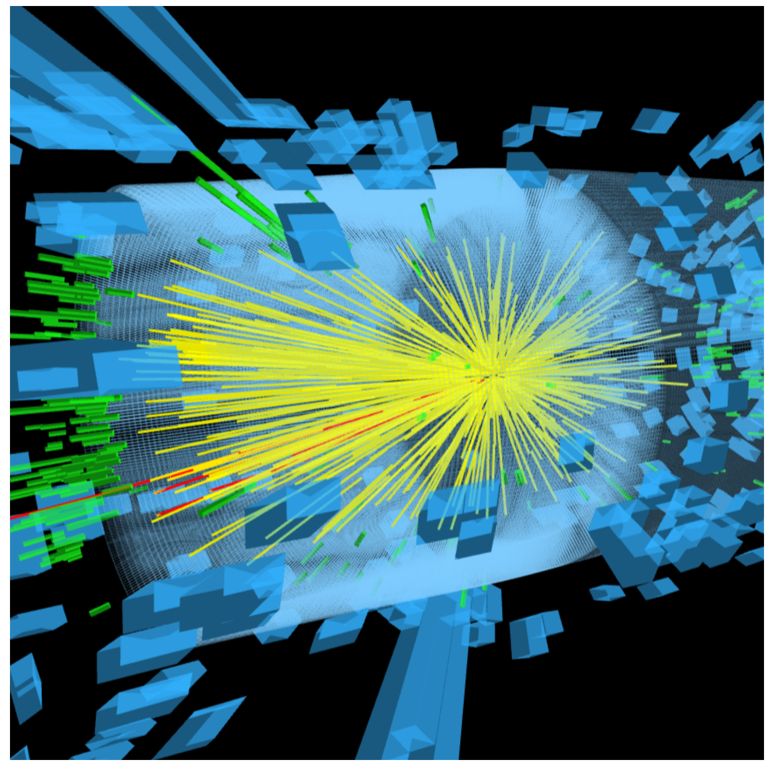
1. The simulation-based inference problem



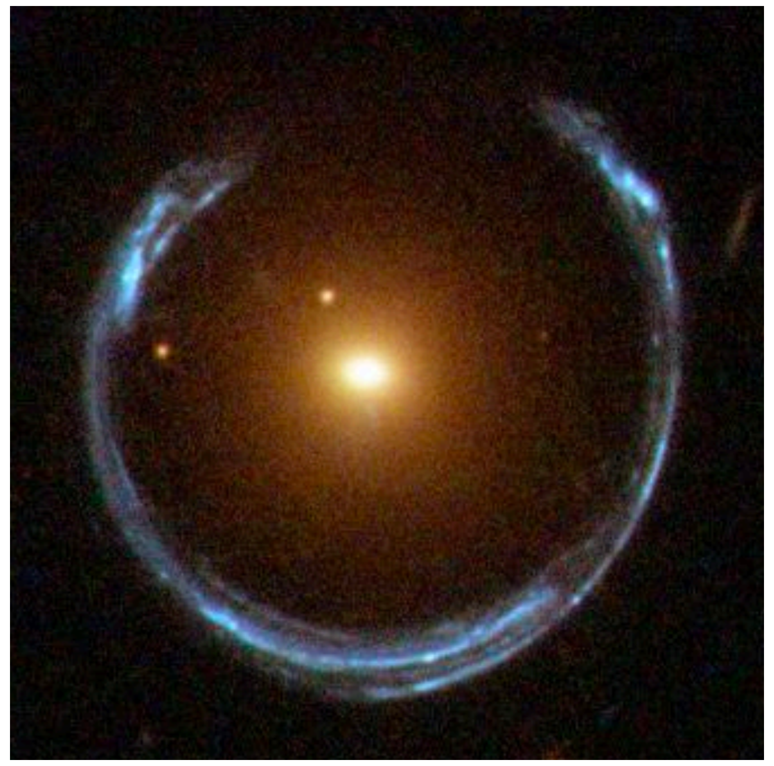
2. Why has that not stopped us before?



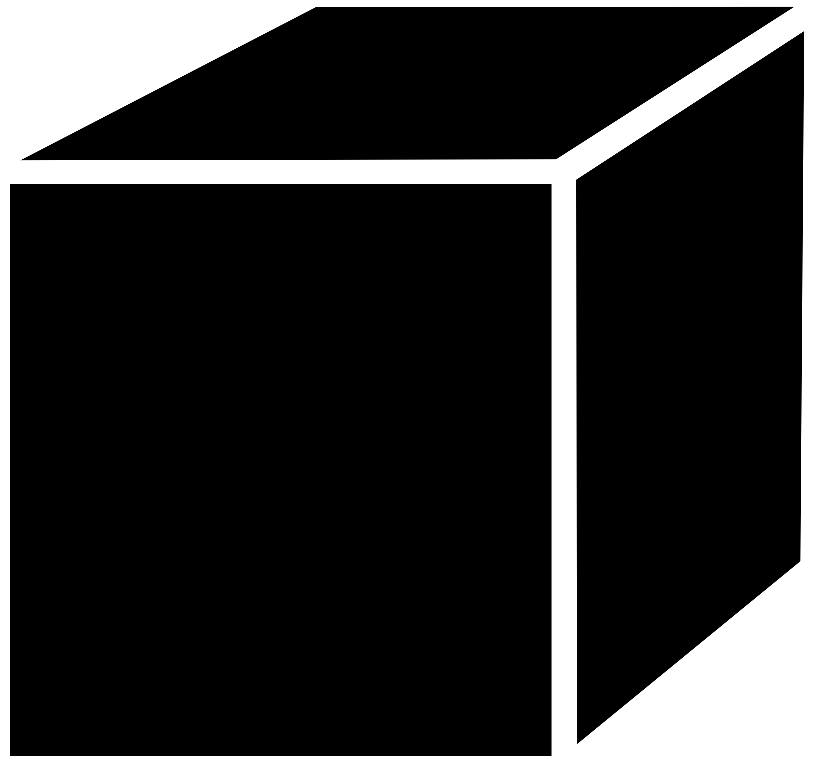
3. Machine learning methods



4. Examples



5. Beyond the LHC



1. Particle physics measurements as a simulation-based inference problem

Modelling particle physics processes

Theory
parameters
θ

Evolution

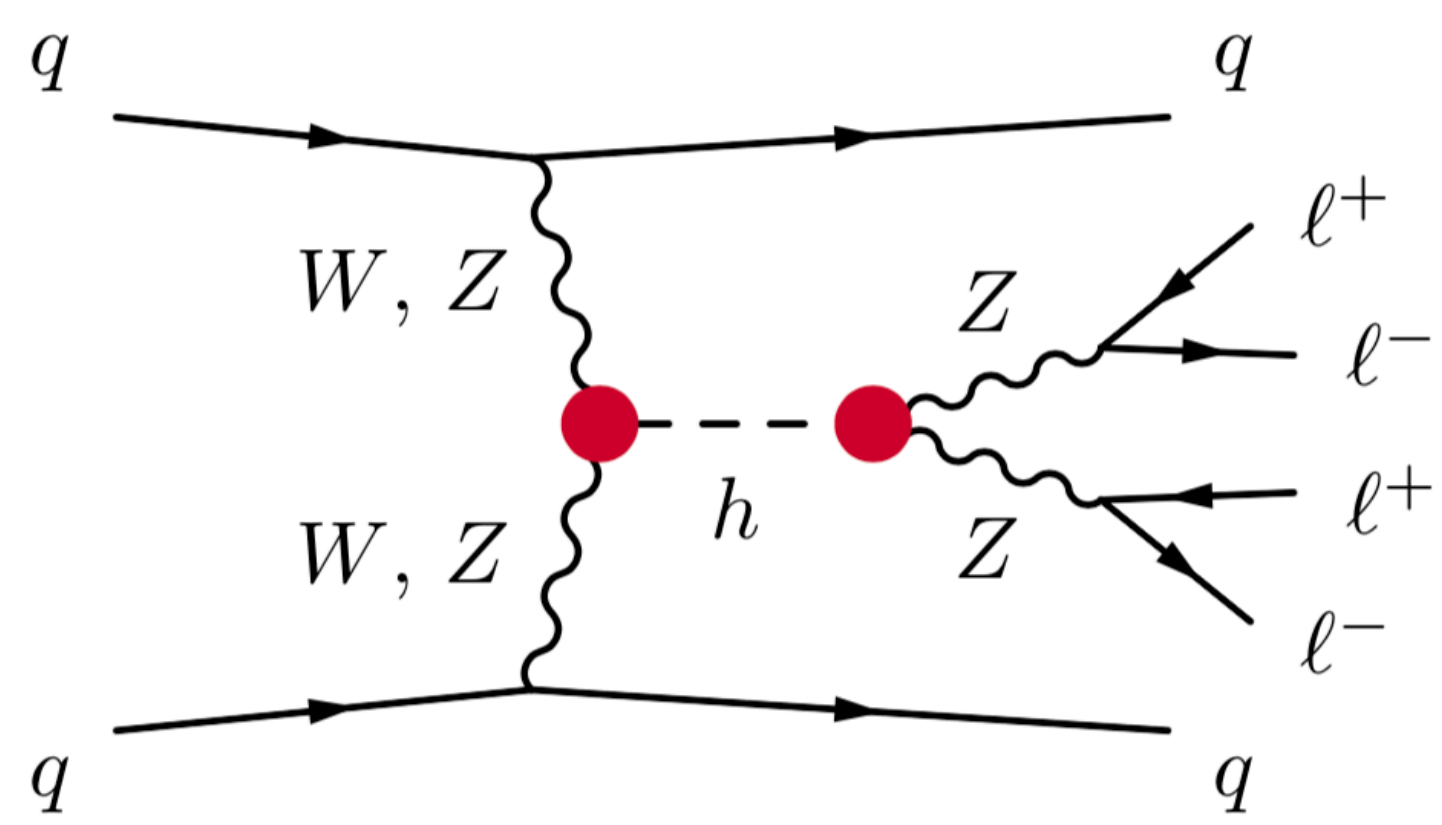
Modelling particle physics processes

Latent variables

Parton-level momenta

Theory parameters

$$z_p \longleftarrow \theta$$



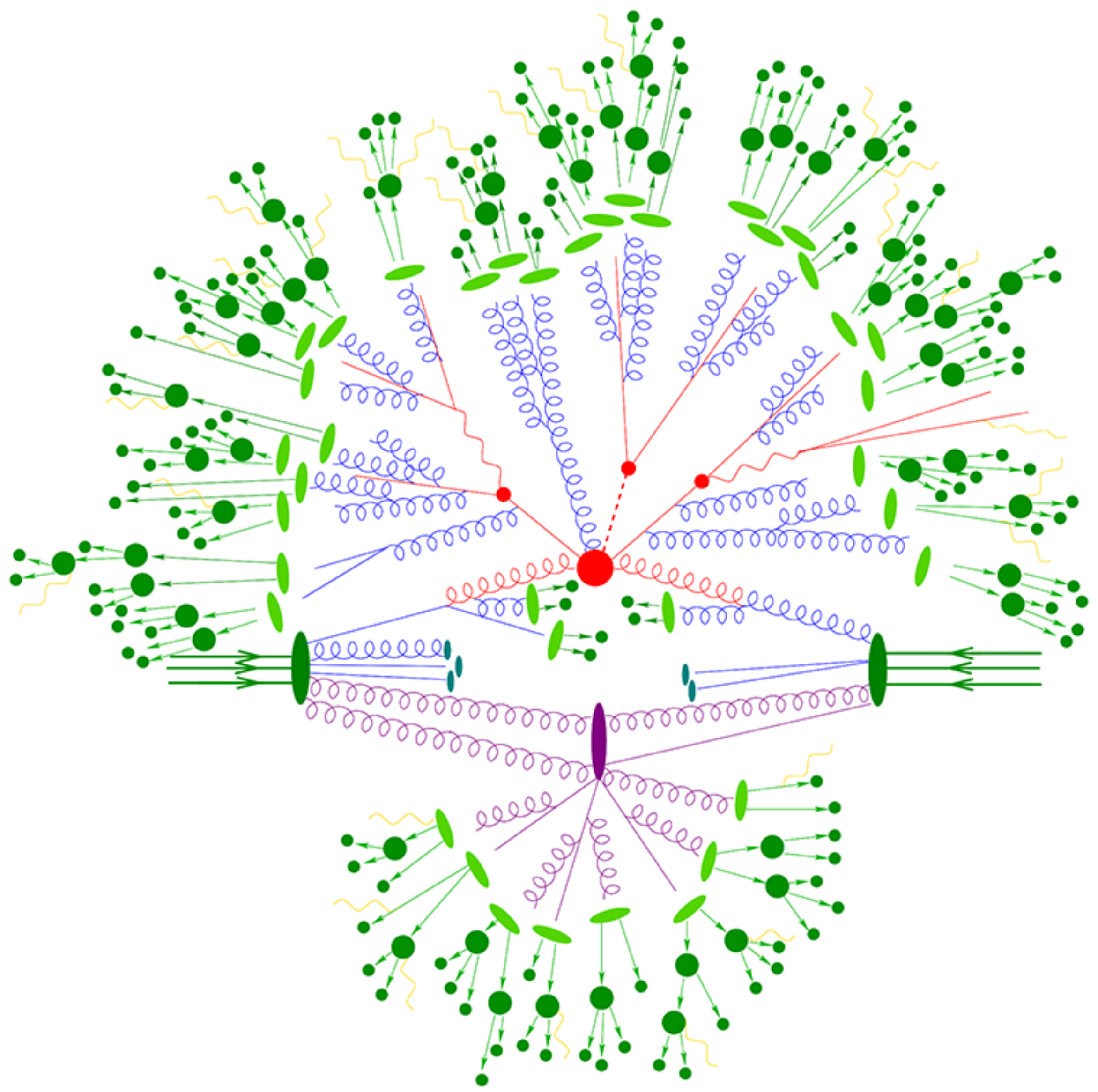
Evolution

Modelling particle physics processes

Latent variables

Shower splittings	Parton-level momenta	Theory parameters
z_s	z_p	θ

$$z_s \longleftarrow z_p \longleftarrow \theta$$



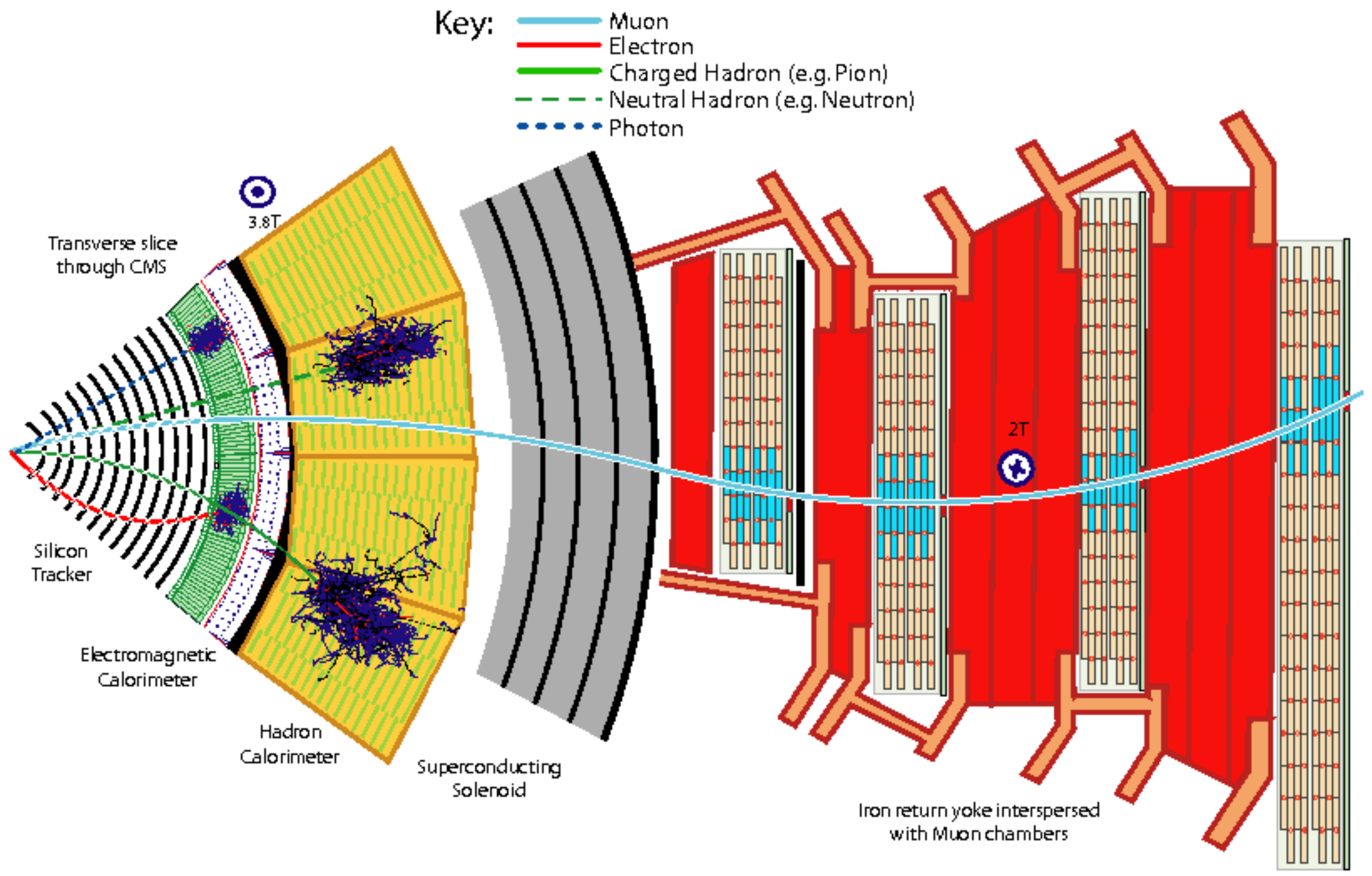
[F. Krauss]

Evolution

Modelling particle physics processes

Latent variables

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



[CMS]

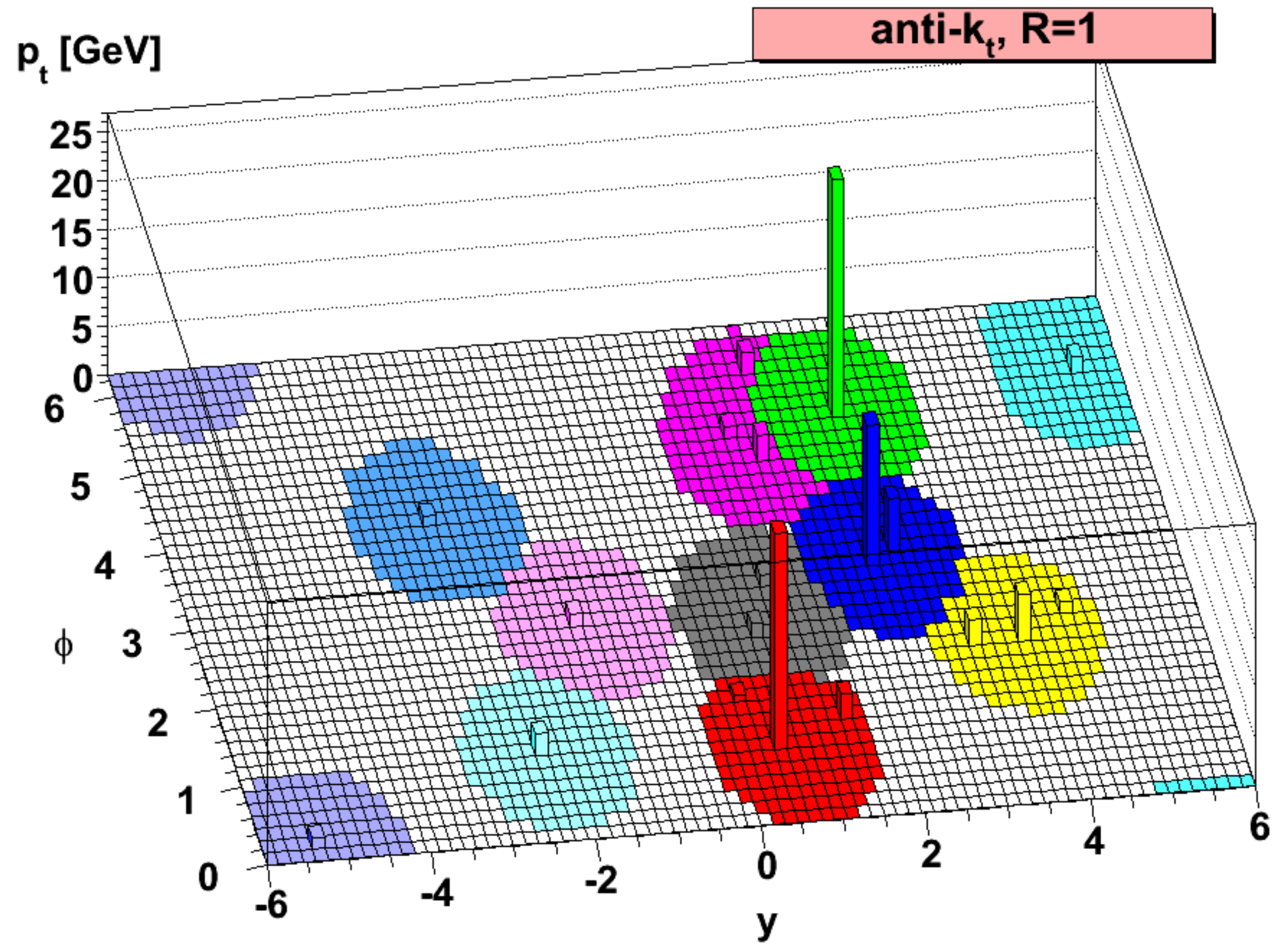
$\longleftarrow$

Evolution

Modelling particle physics processes

Latent variables

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



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

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

GEANT4 A SIMULATION TOOLKIT

MADGRAPH5_aMC@NLO

$\longleftarrow$ Prediction (simulation)

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	$\longleftarrow$	θ

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

$\longrightarrow$

Inference

Modelling particle physics processes

Latent variables

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

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

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

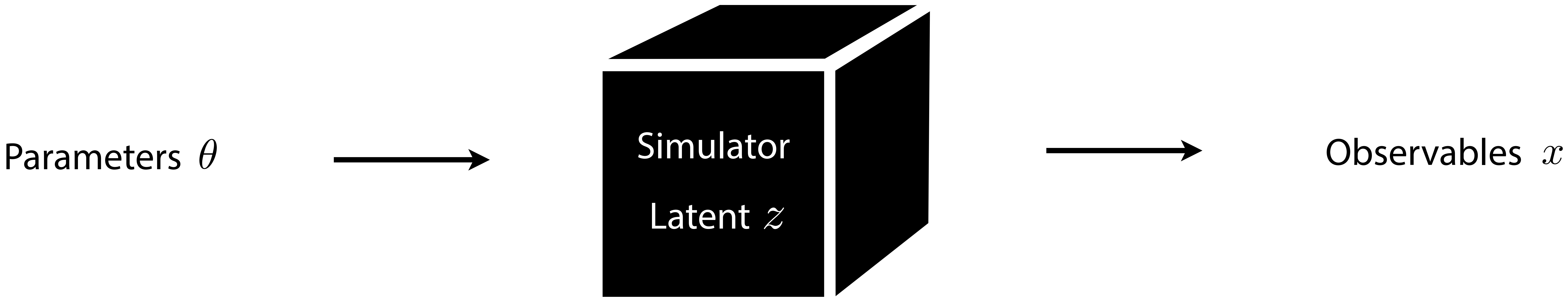
It's infeasible to calculate the integral over this enormous space!

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

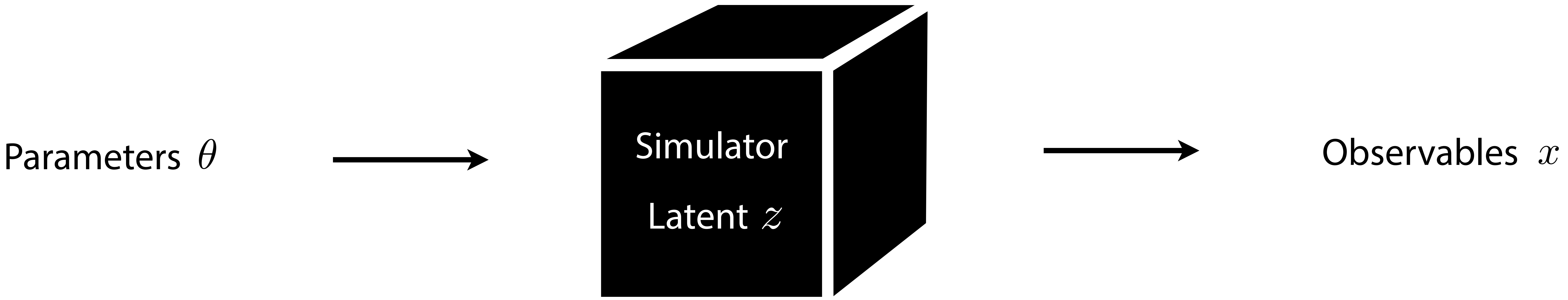
$\longrightarrow$

Inference

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

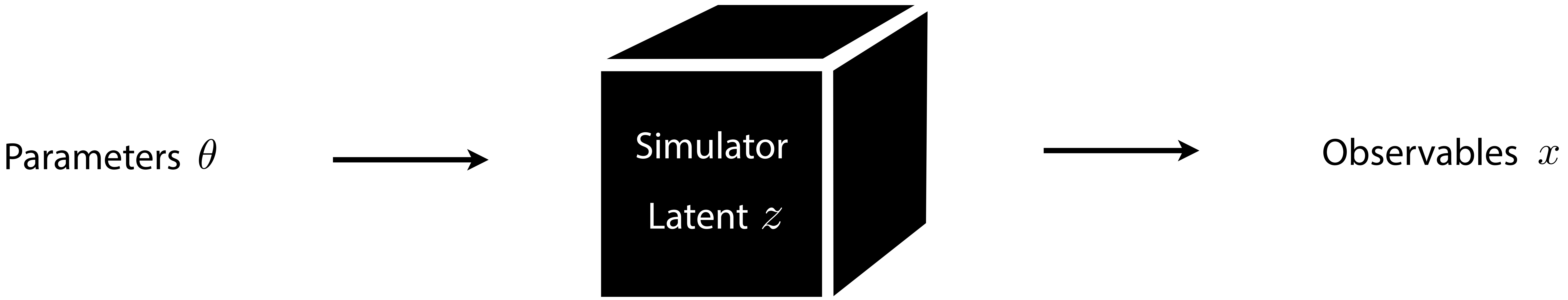


The problem of simulation-based ("likelihood-free") inference



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

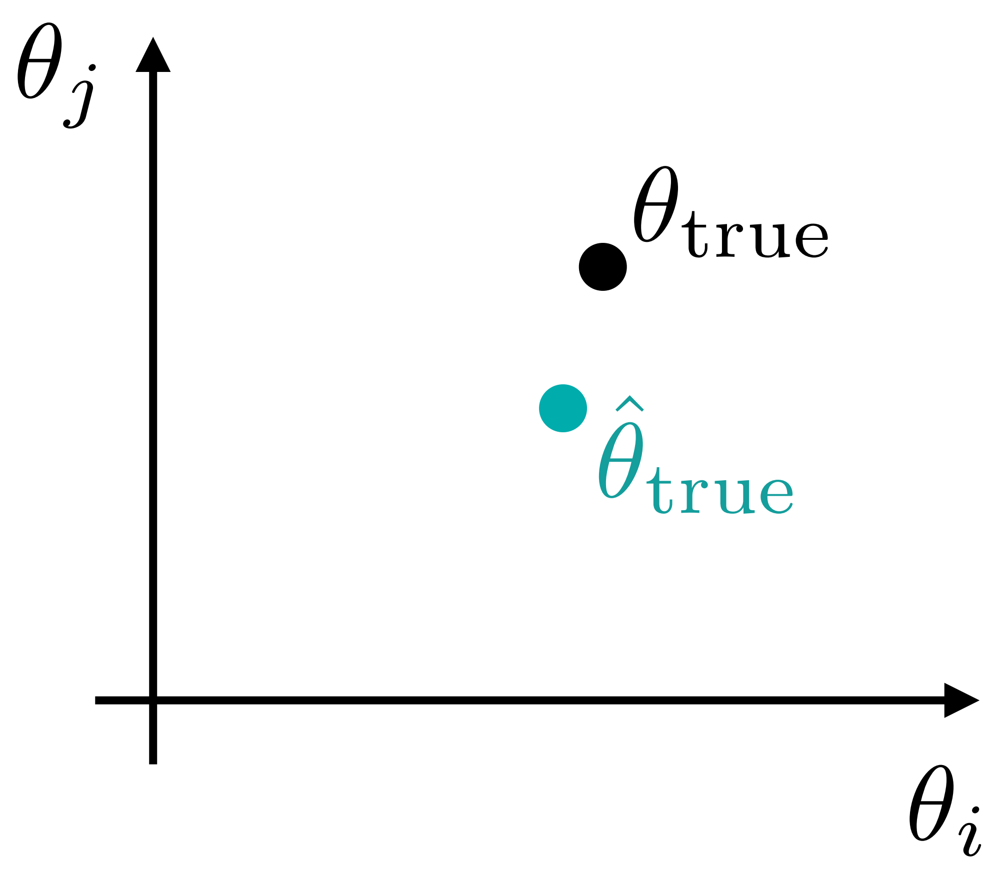
- a simulator that lets you generate N samples $x_i \sim p(x_i|\theta_i)$ (for parameters θ_i of our choice),
- observed data $x_{\mathrm{obs}} \sim p(x_{\mathrm{obs}}|\theta_{\mathrm{true}})$, and
- a prior $p(\theta)$,

Three problem statements

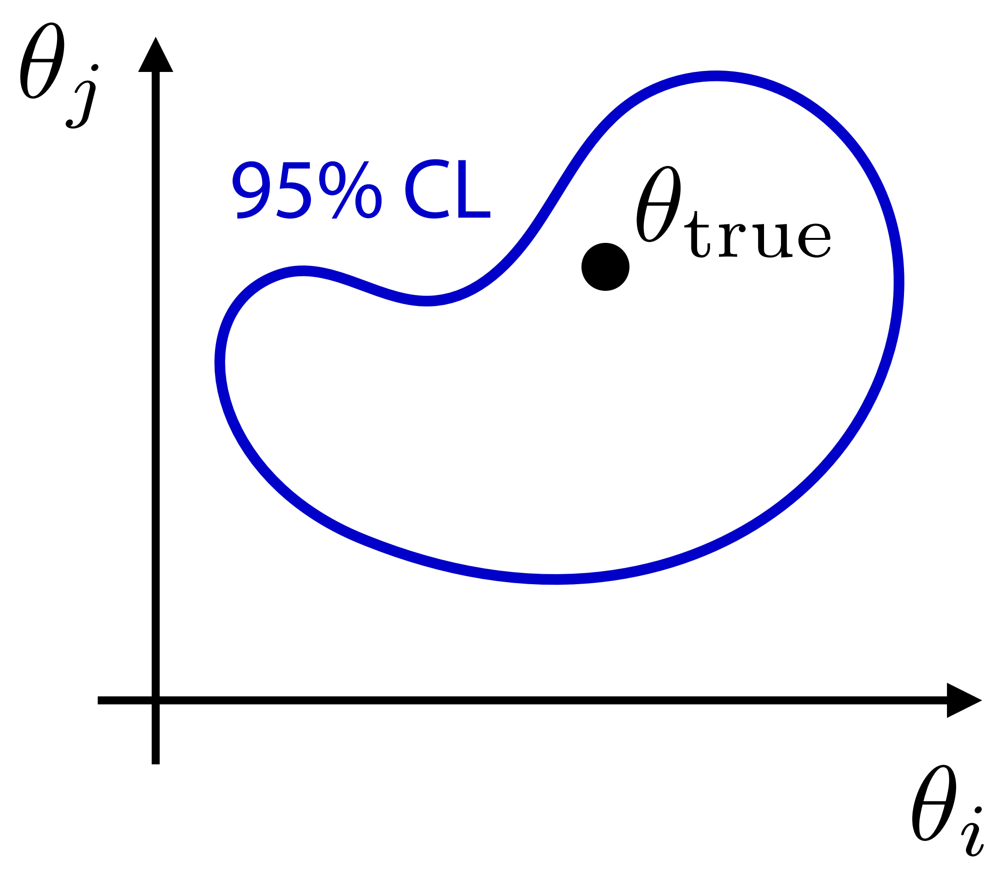
Given

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

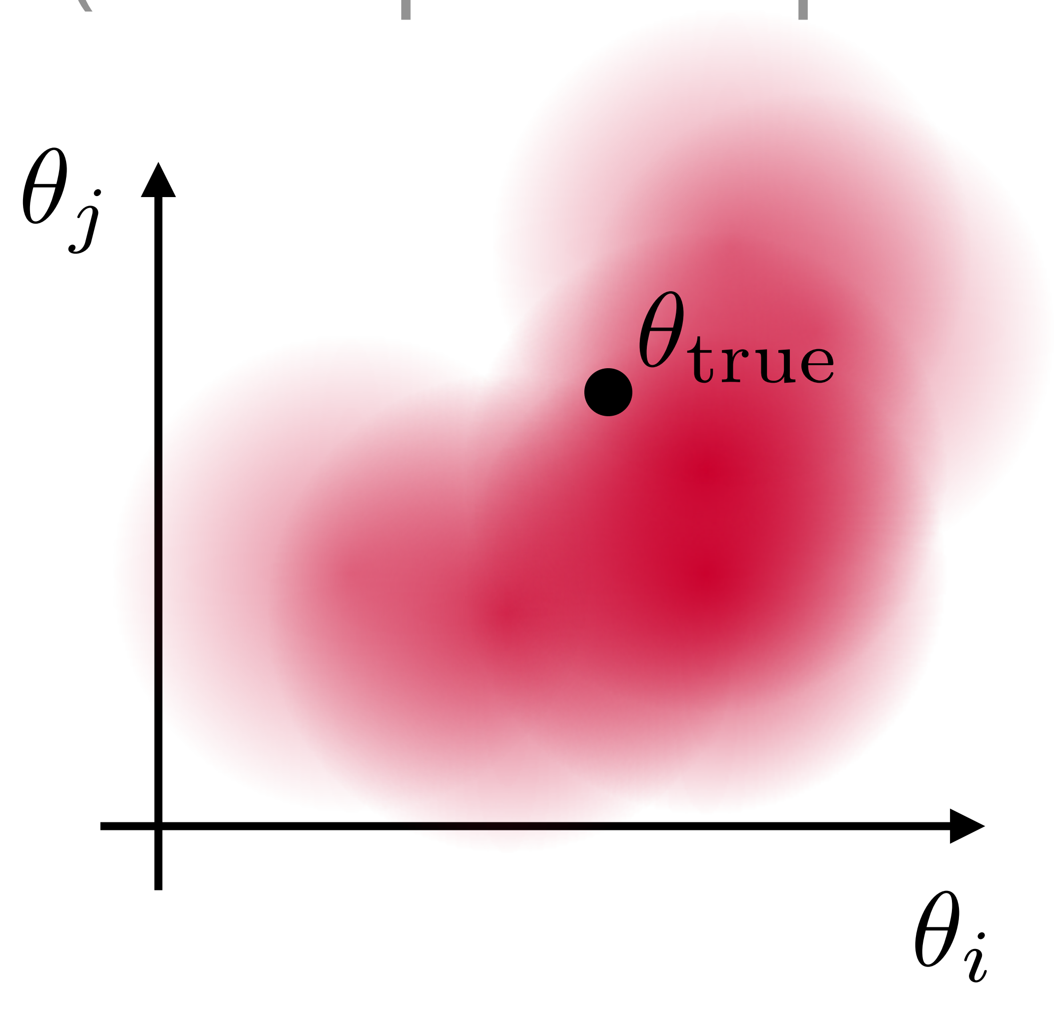
a) estimate $\hat{\theta}_{\text{true}}$
(e.g. MLE)

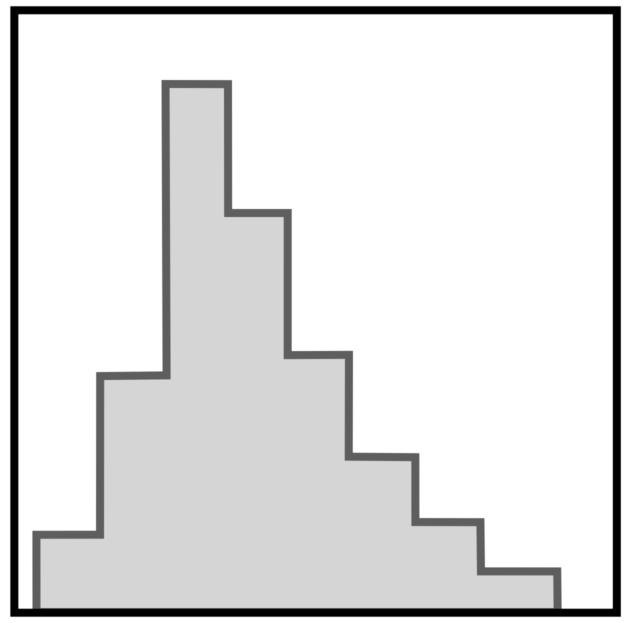


b) construct confidence sets
(e.g. likelihood ratio tests)



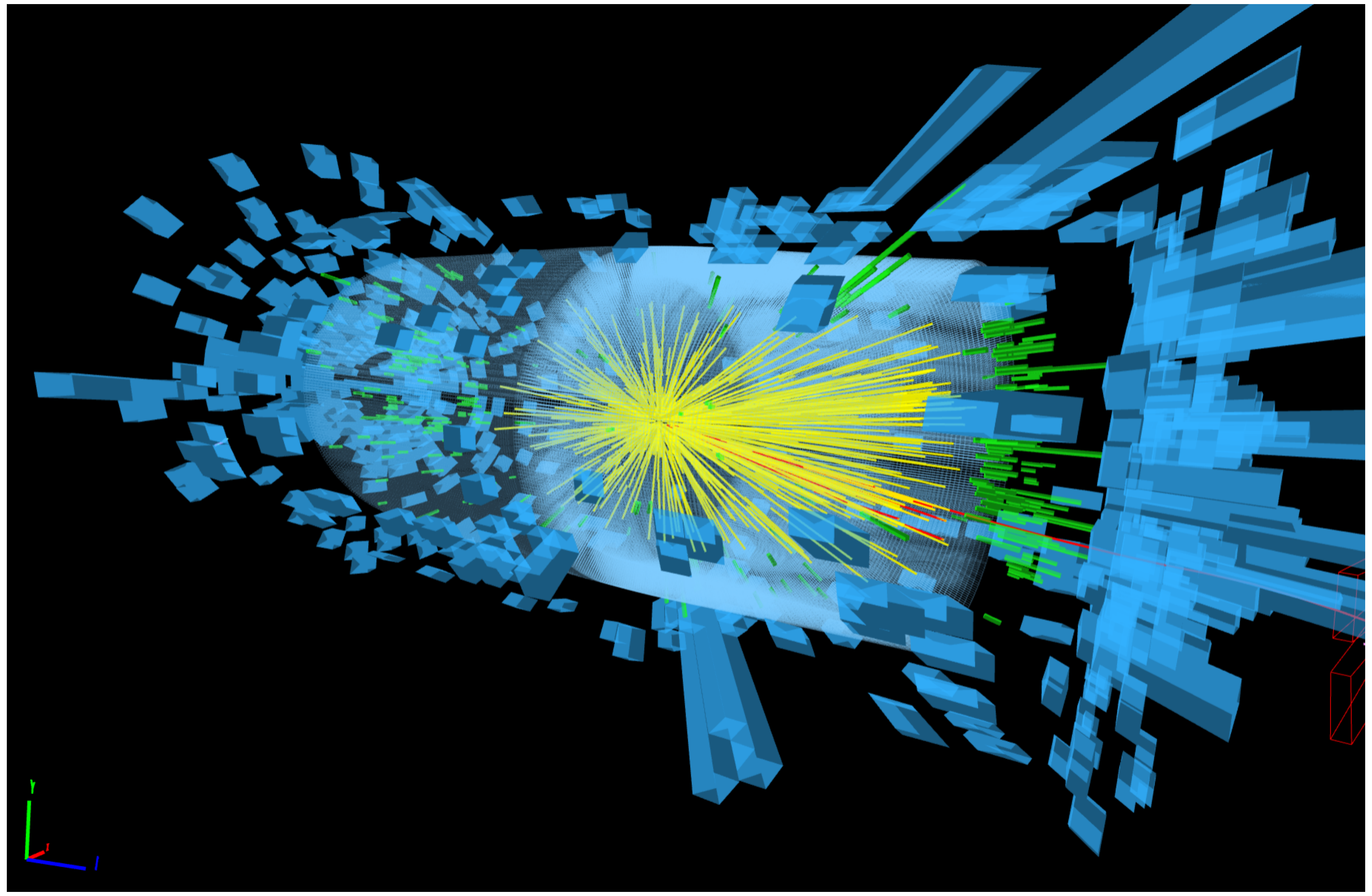
c) estimate the posterior
(or sample from posterior)





2. Why has that not stopped us before?

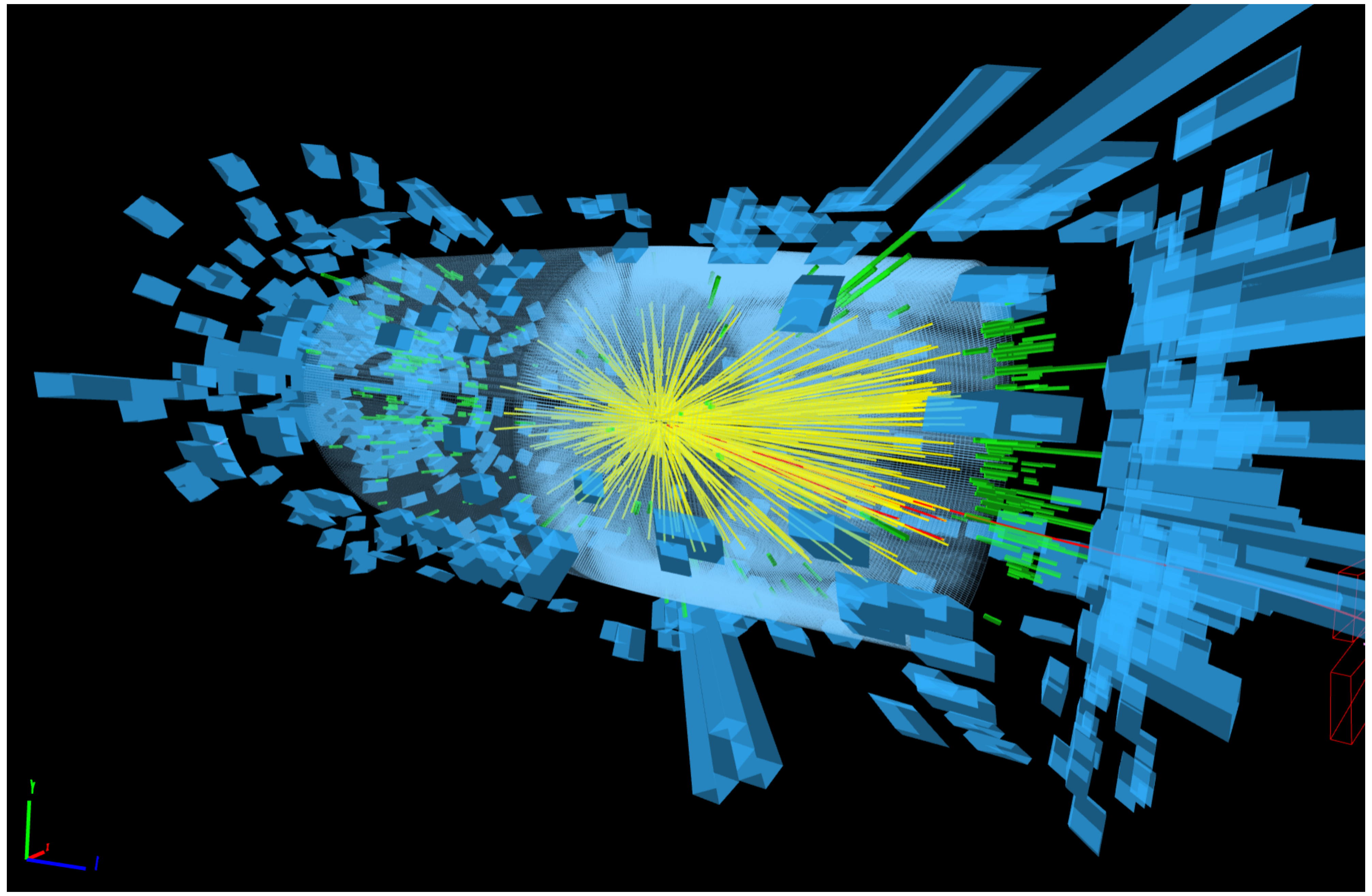
Solve it with summary statistics

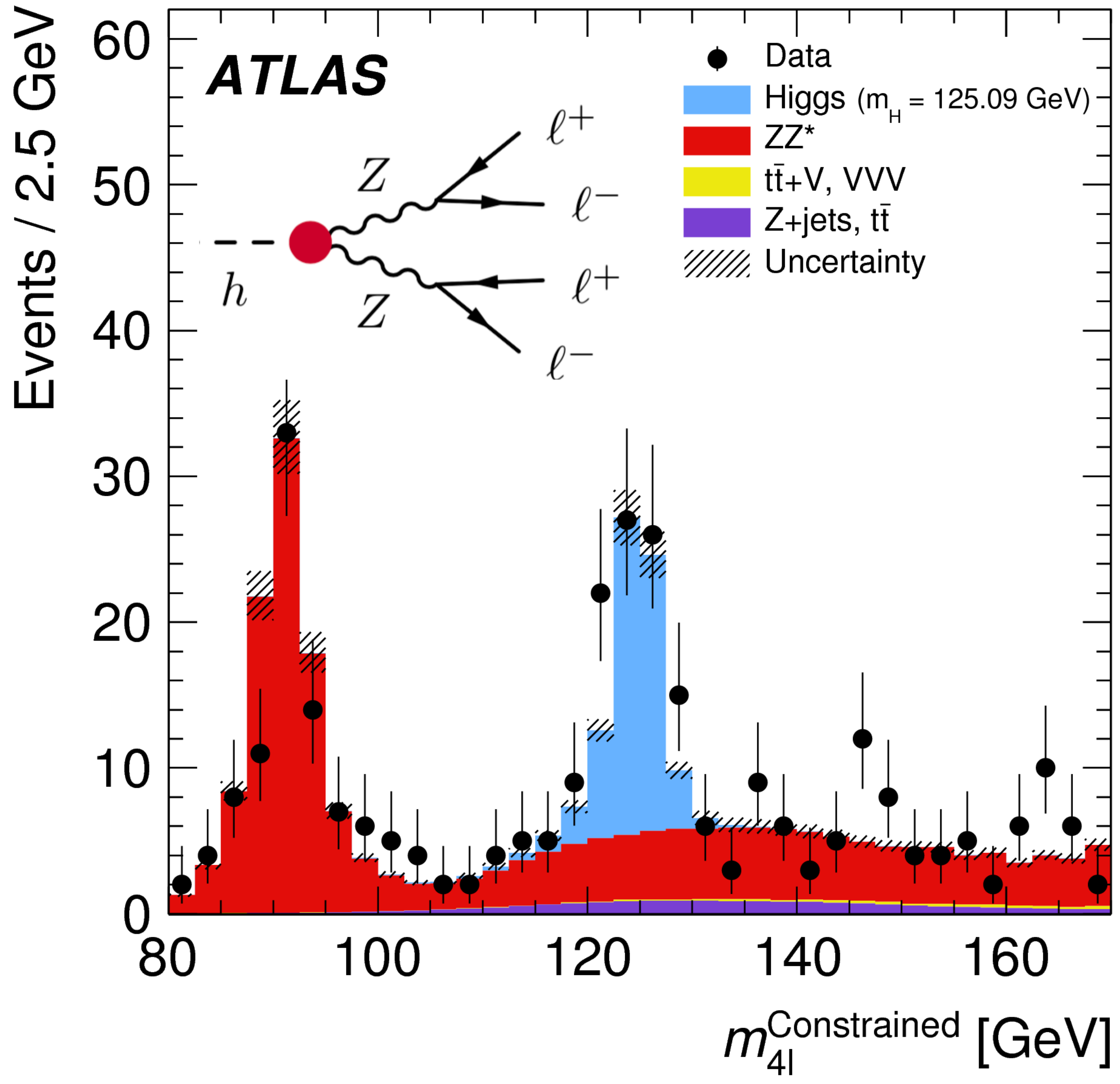


High-dimensional event data x

$p(x|\theta)$ 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, …

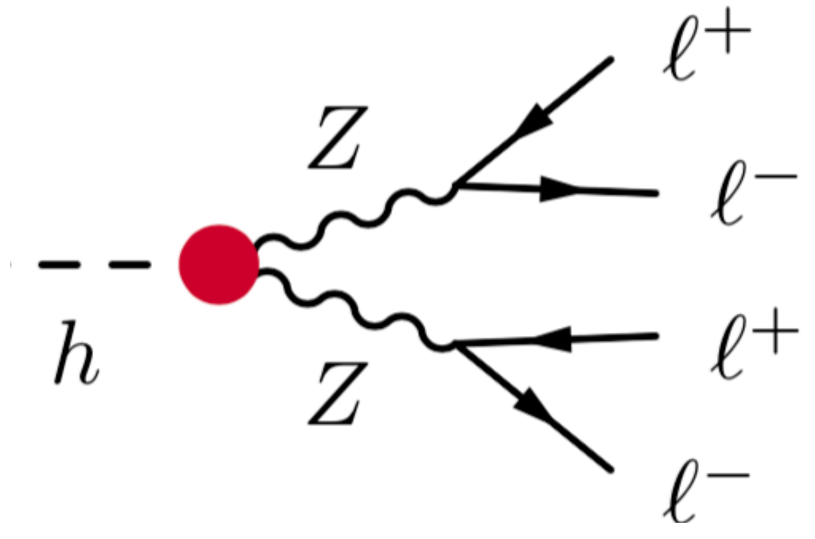
Summary statistics for LHC measurements?

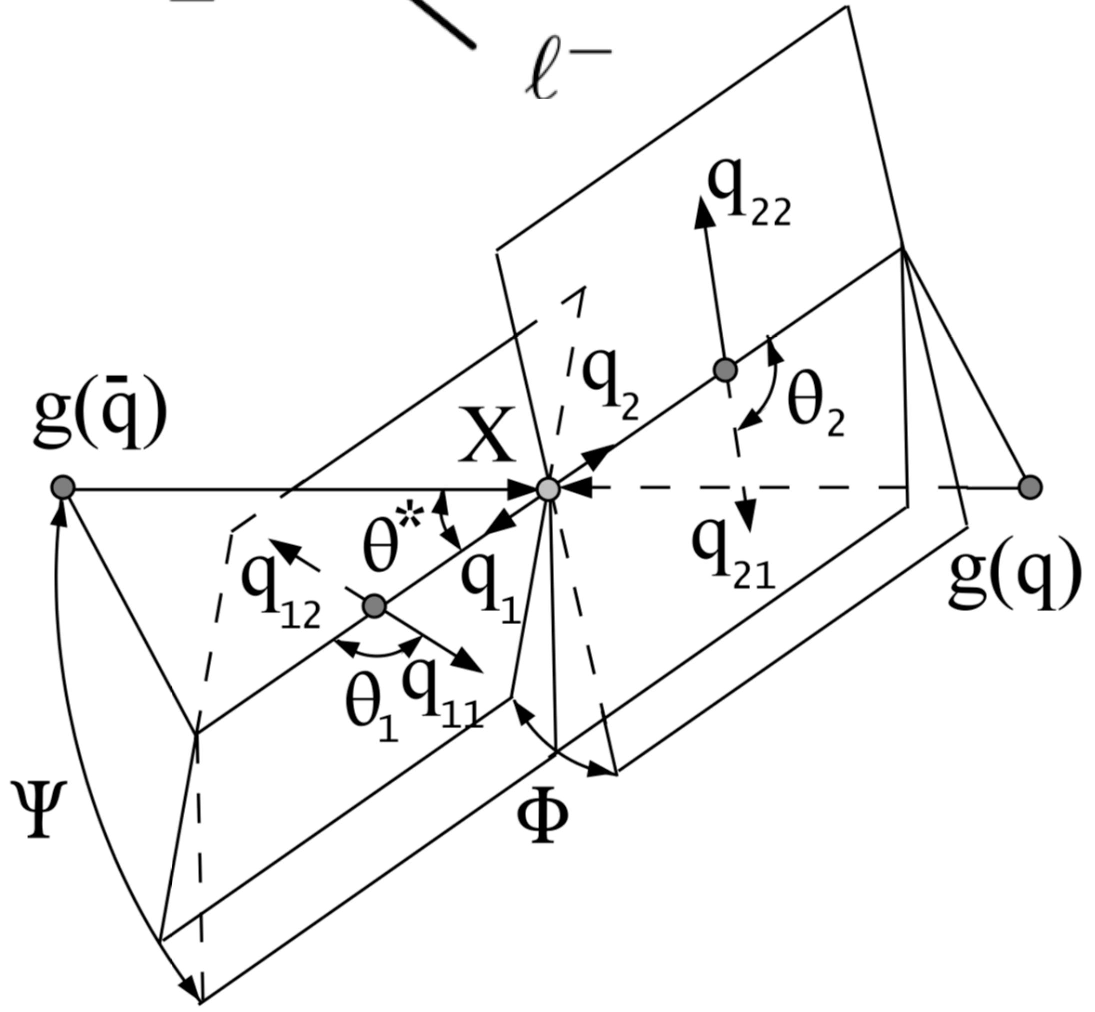
- In many LHC problems there is no single good summary statistics: compressing to any x' loses information!
  [JB, K. Cranmer, F. Kling, T. Plehn 1612.05261; JB, F. Kling, T. Plehn, T. Tait 1712.02350]

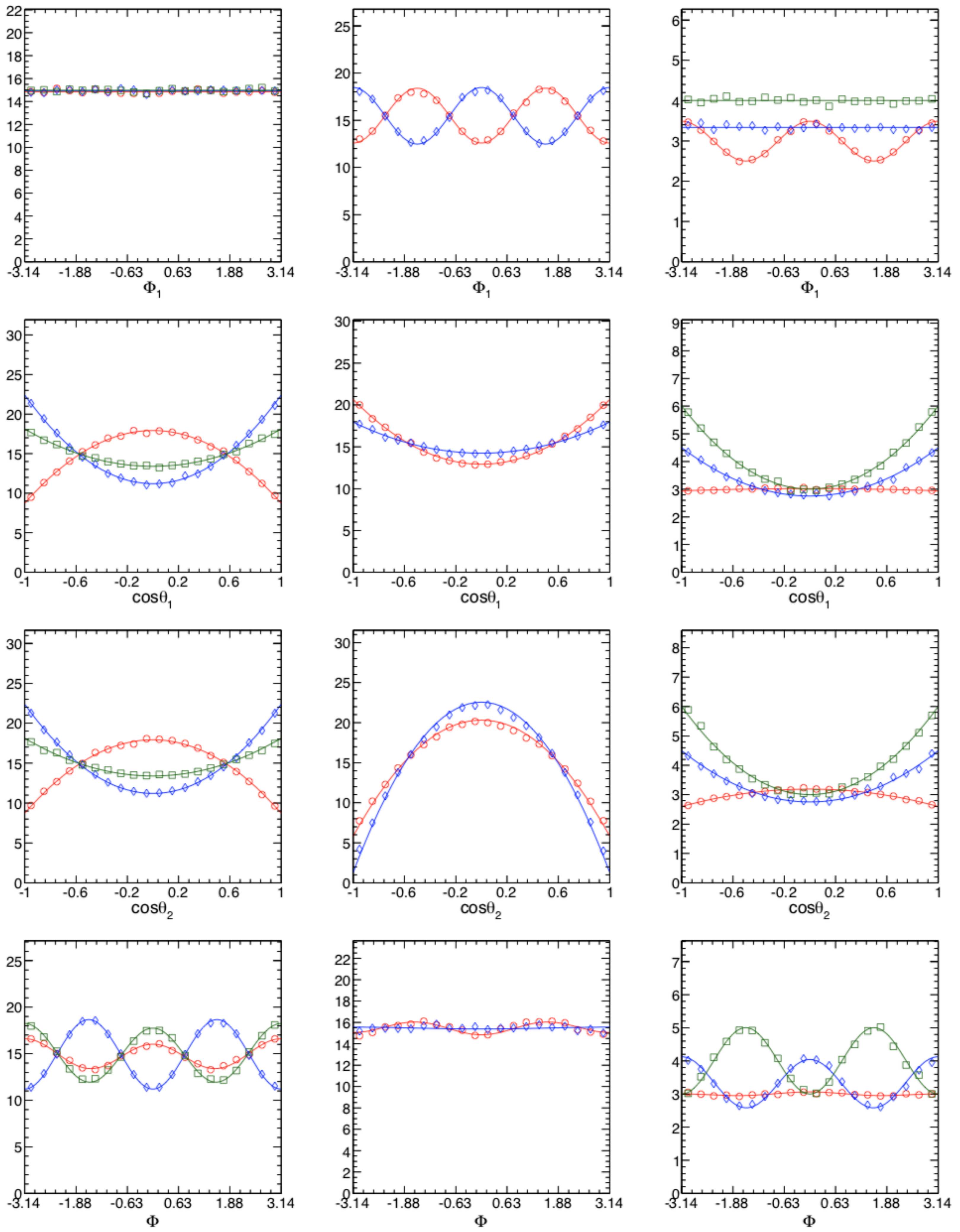
- Ideally: analyze all trustworthy high-level features (reconstructed four-momenta…), or some form of low-level features, including correlations
  (“fully differential cross section”)

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]







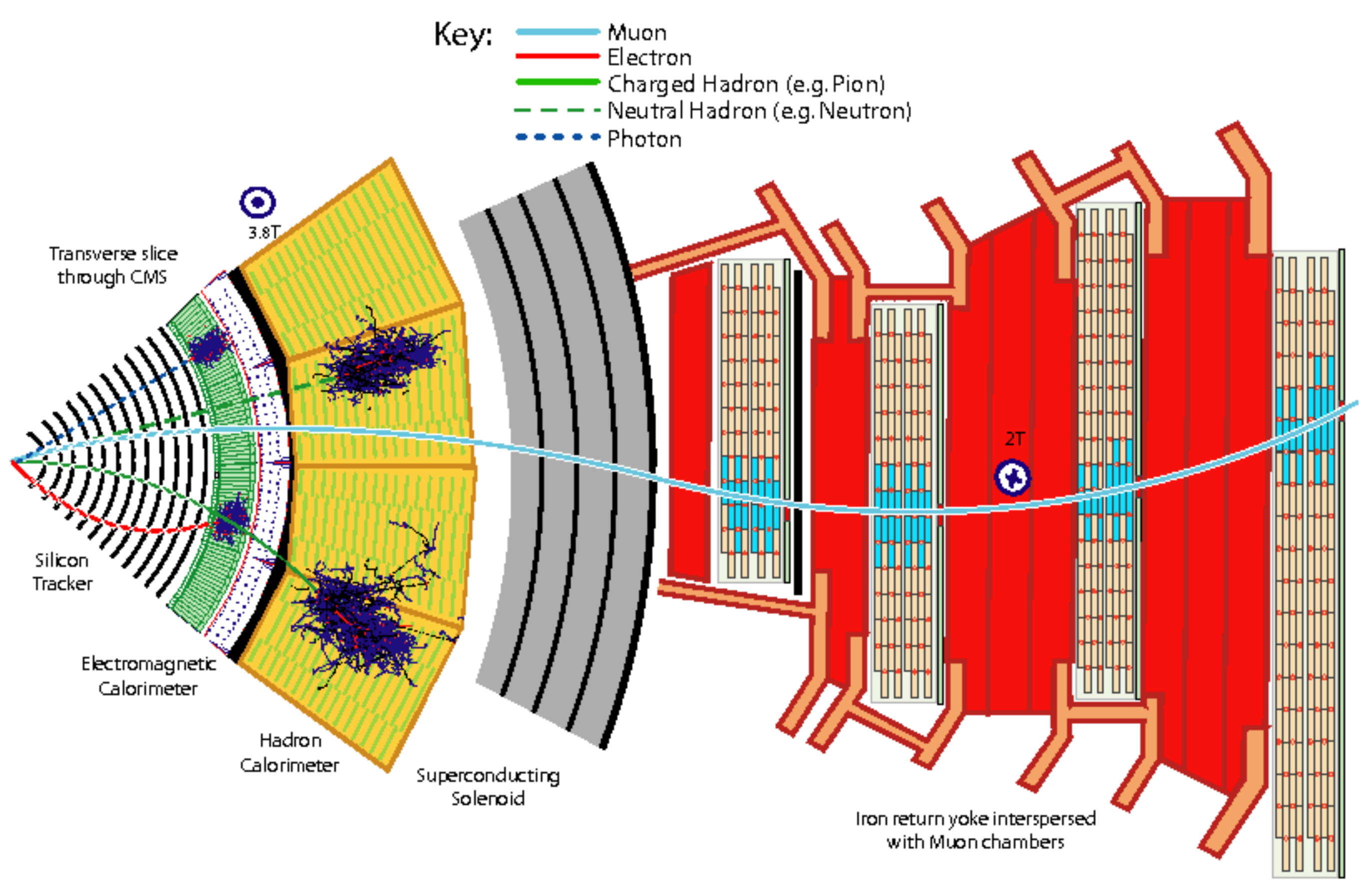
[Bolognesi et al. 1208.4018]

- 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

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

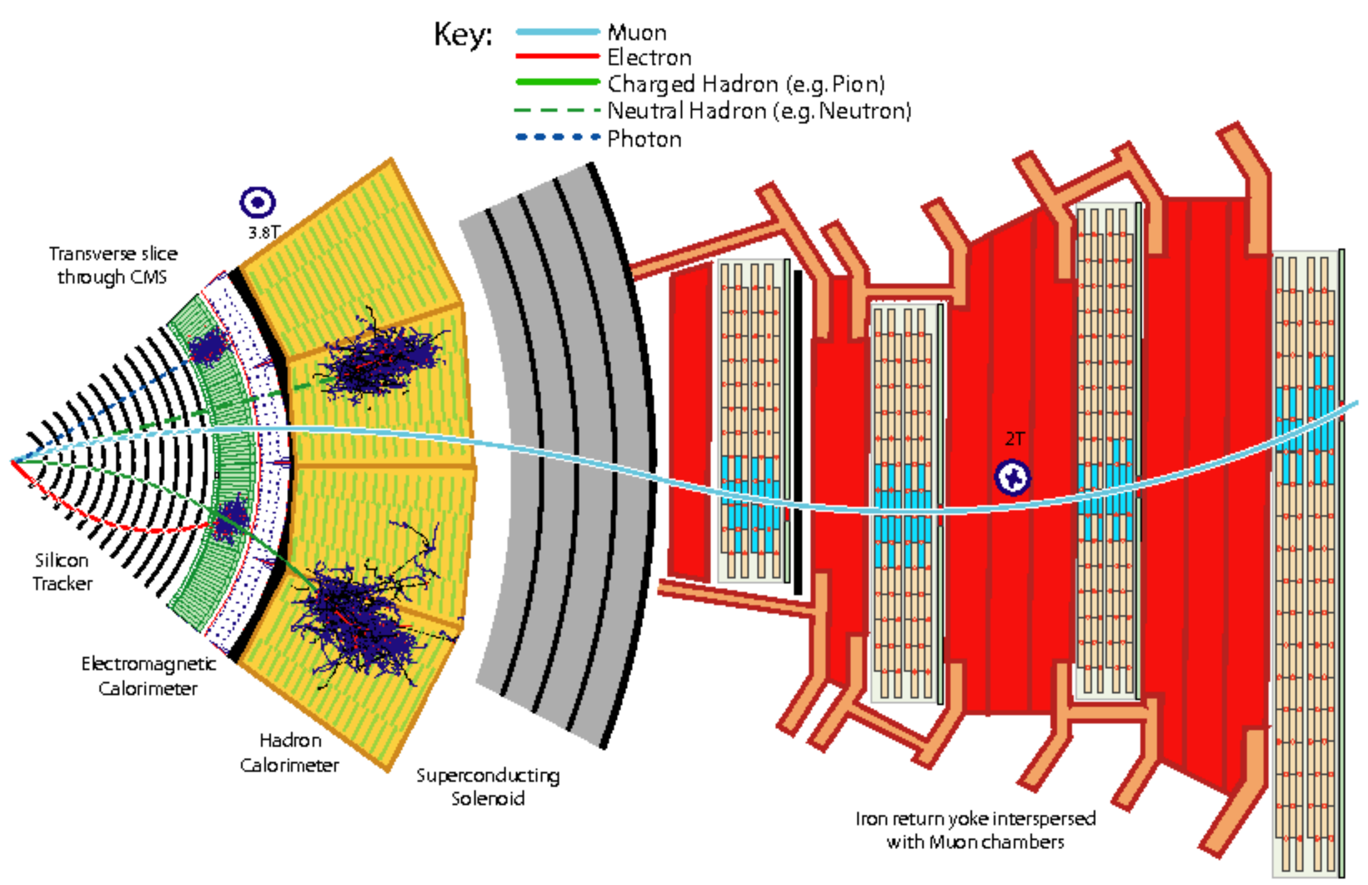


[CMS]

Solve it by approximating the integral

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

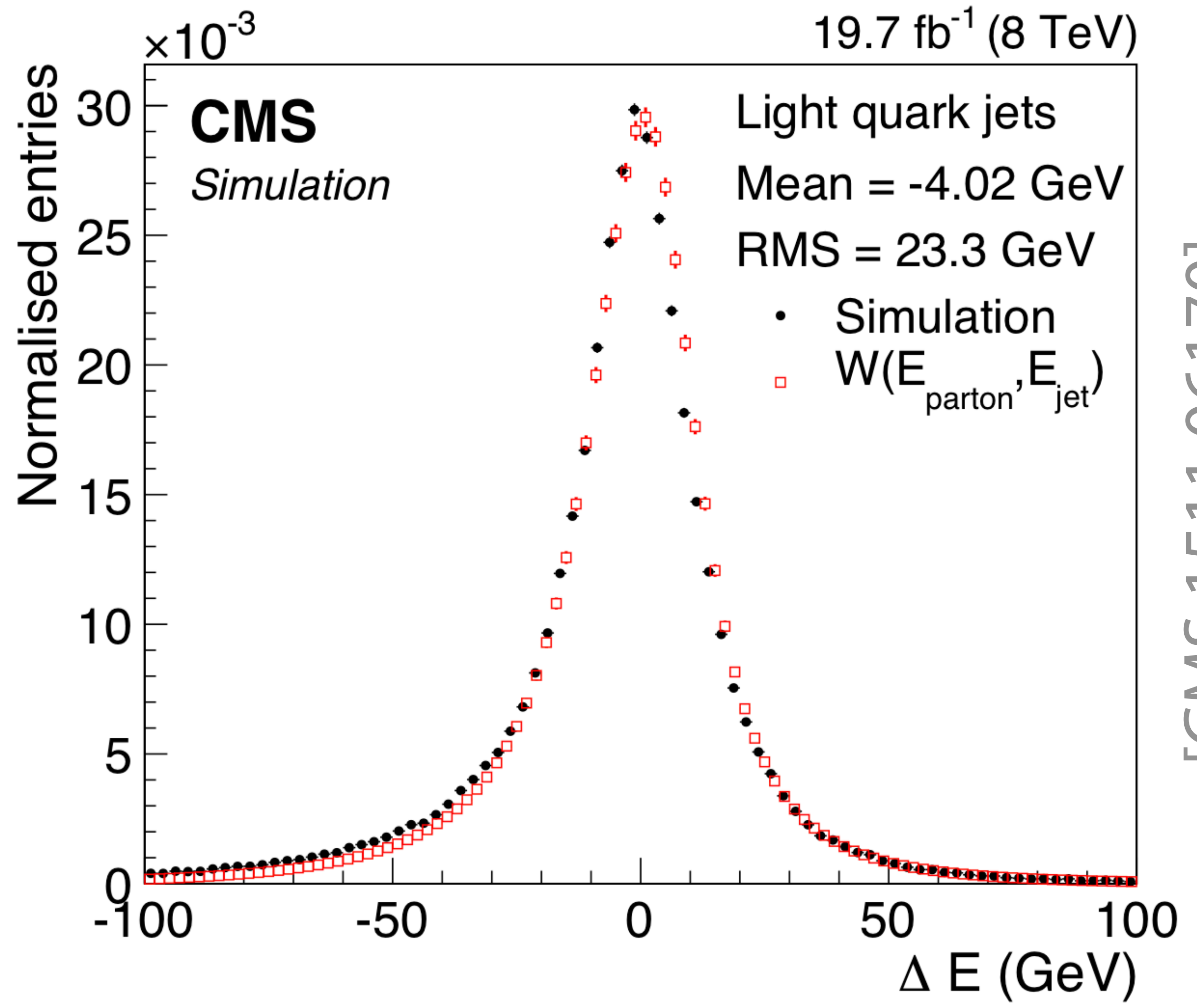
$$p(x|\theta) = \int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p \; p(x|z_d)\, p(z_d|z_s)\, p(z_s|z_p)\, p(z_p|\theta)$$



[CMS]

- 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

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

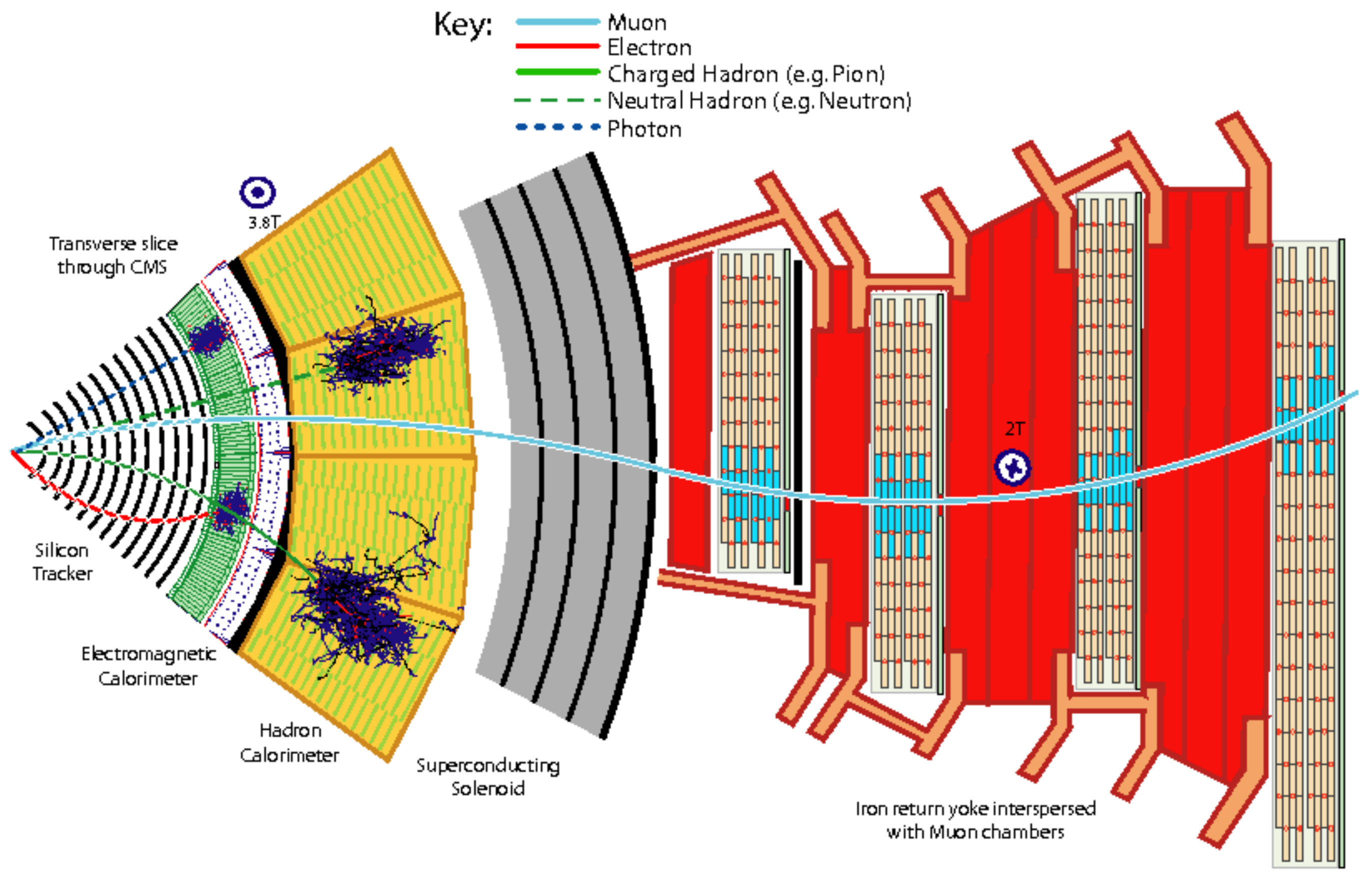


[CMS 1511.06170]

Solve it by approximating the integral

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

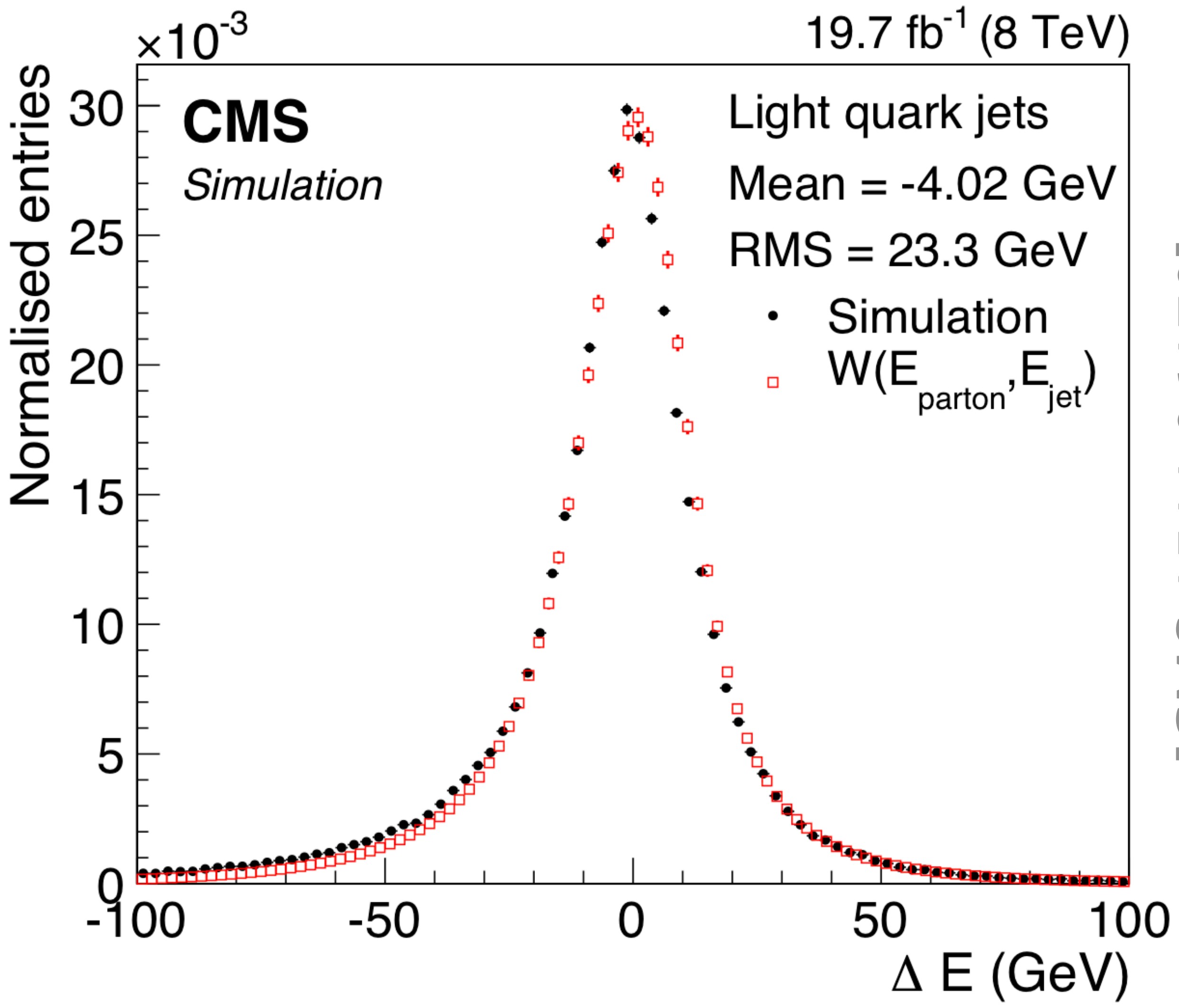
$$p(x|\theta) = \int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p \; p(x|z_d)\, p(z_d|z_s)\, p(z_s|z_p)\, p(z_p|\theta)$$



[CMS]

- 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

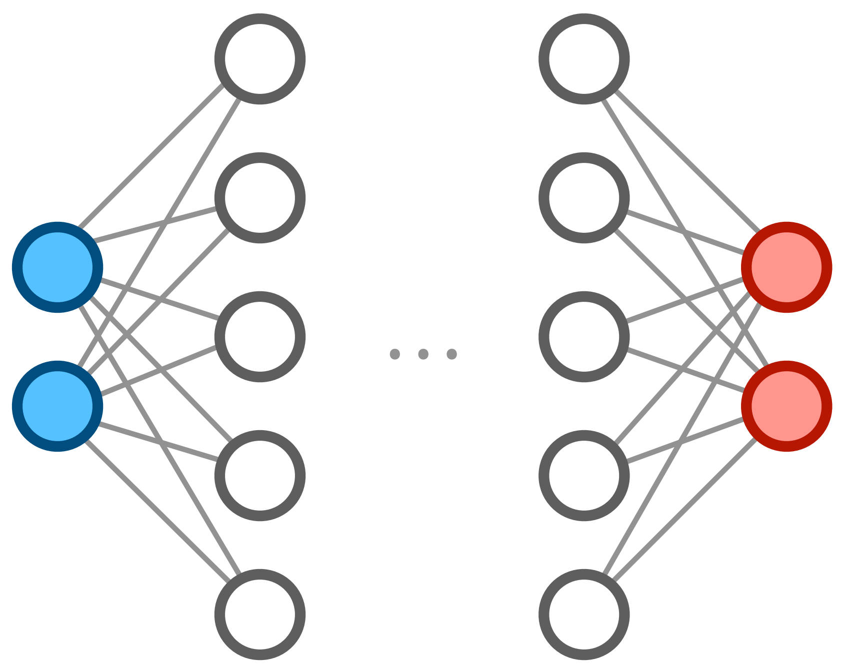
$$\hat{p}(x|\theta) = \int \mathrm{d}z_p \; \hat{p}(x|z_p)\, p(z_p|\theta)$$



[CMS 1511.06170]

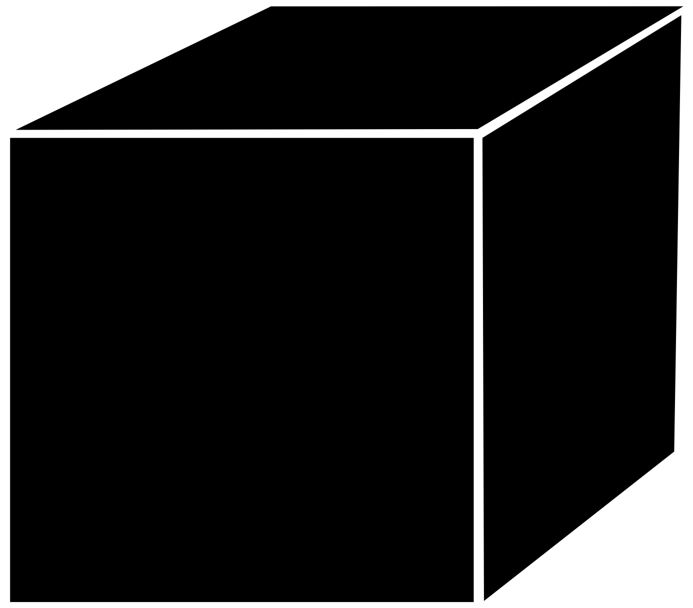
⇒ Uses matrix-element information, no summary statistics necessary, but:

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



3. Machine learning solutions

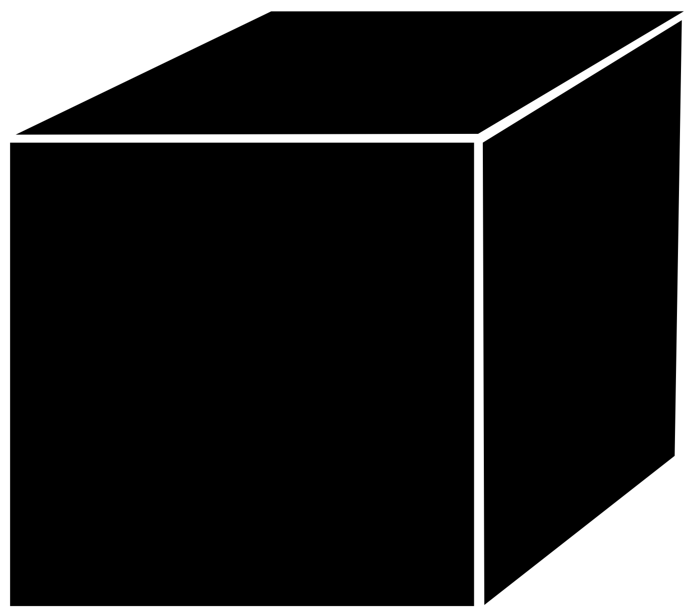
Get the best of two worlds

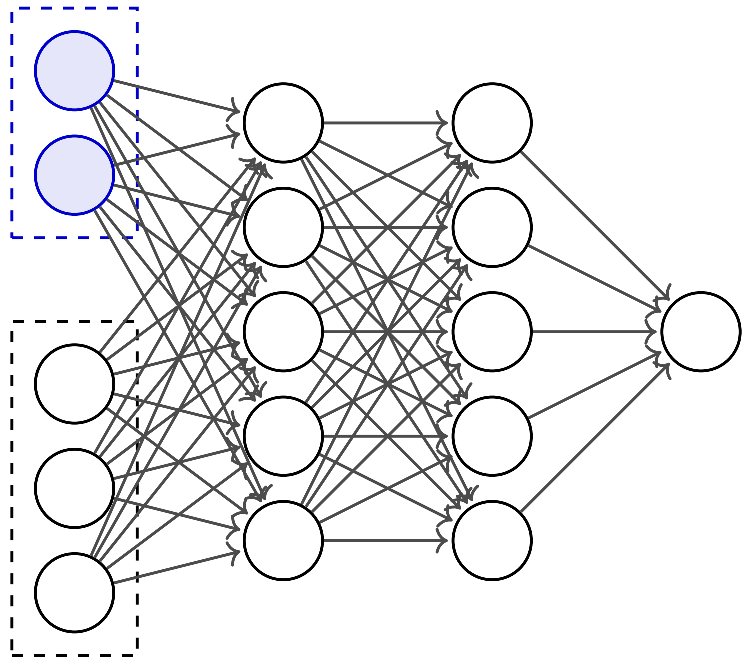


Simulators: focus on understanding

- based on mechanistic, causal model
- interpretable parameters

Get the best of two worlds





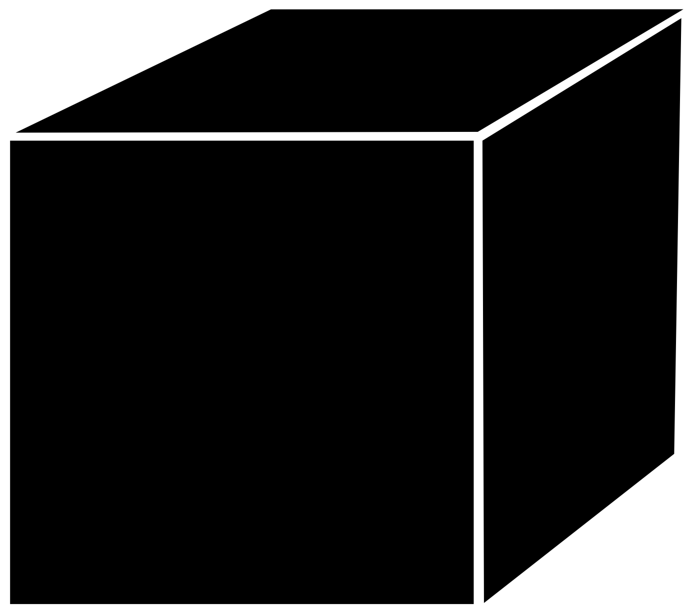
Simulators: focus on understanding

- based on mechanistic, causal model
- interpretable parameters

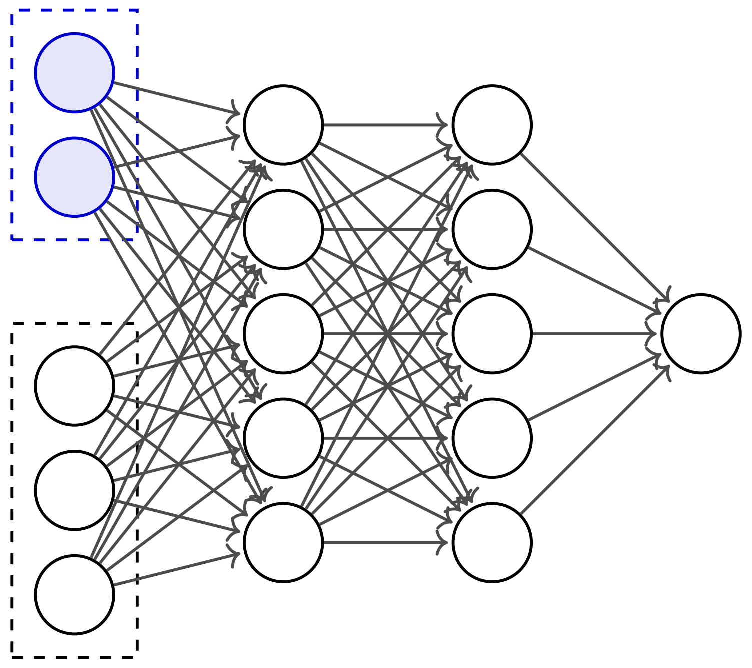
Machine learning models: focus on performance

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

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?

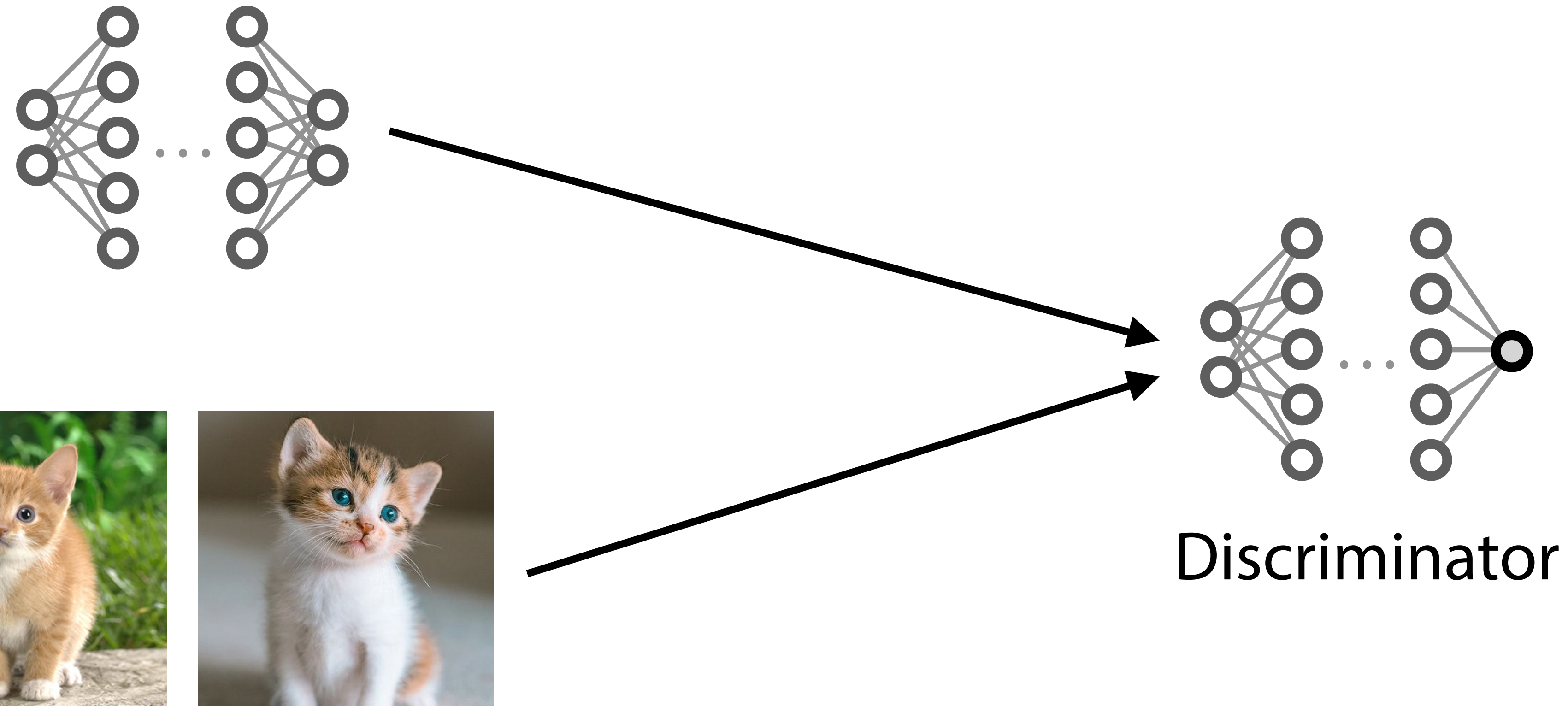
Idea 1: the likelihood ratio trick

- Generative Adversarial Networks (GANs):

[I. Goodfellow et al. 1406.2661]

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

Examples
(intractable likelihood $p_{\text{true}}(x)$)



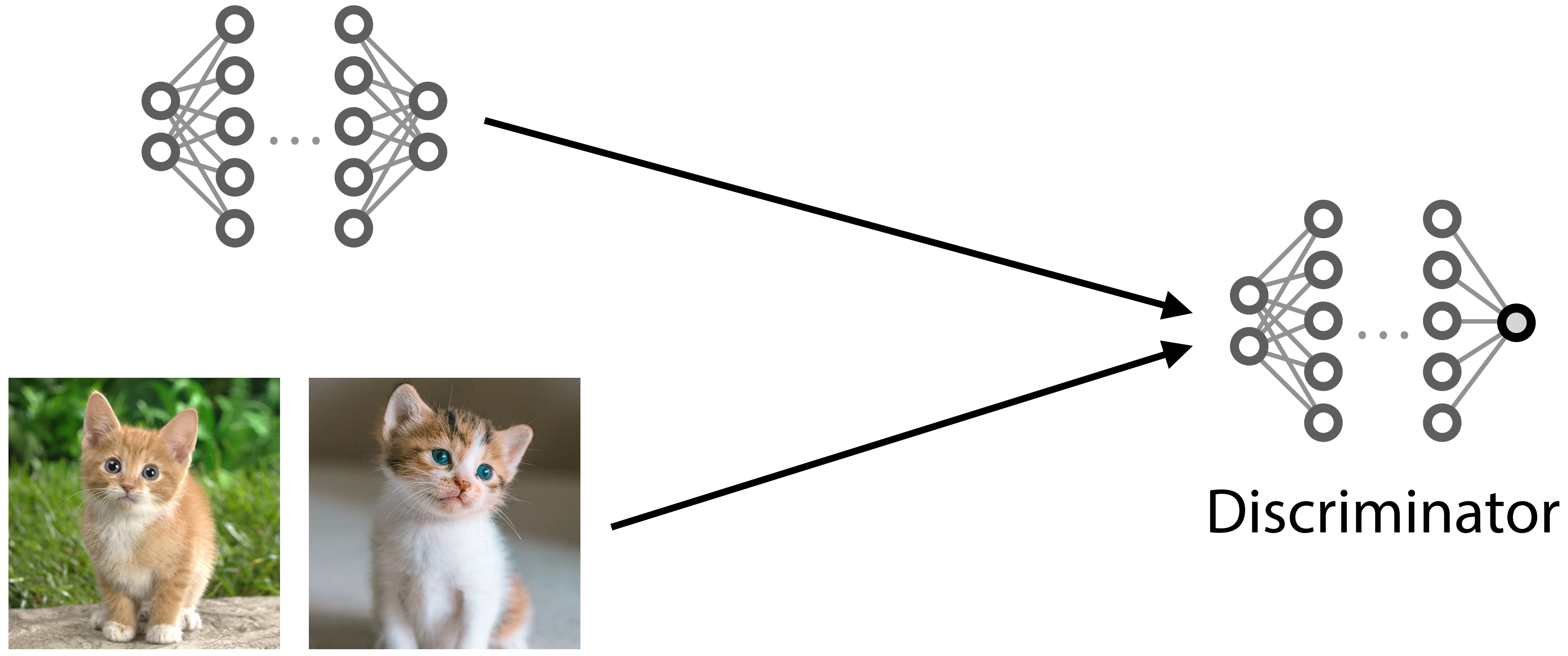
Idea 1: the likelihood ratio trick

- Generative Adversarial Networks (GANs):

[I. Goodfellow et al. 1406.2661]

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

Examples
(intractable likelihood $p_{\text{true}}(x)$)



Discriminator learns decision function

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

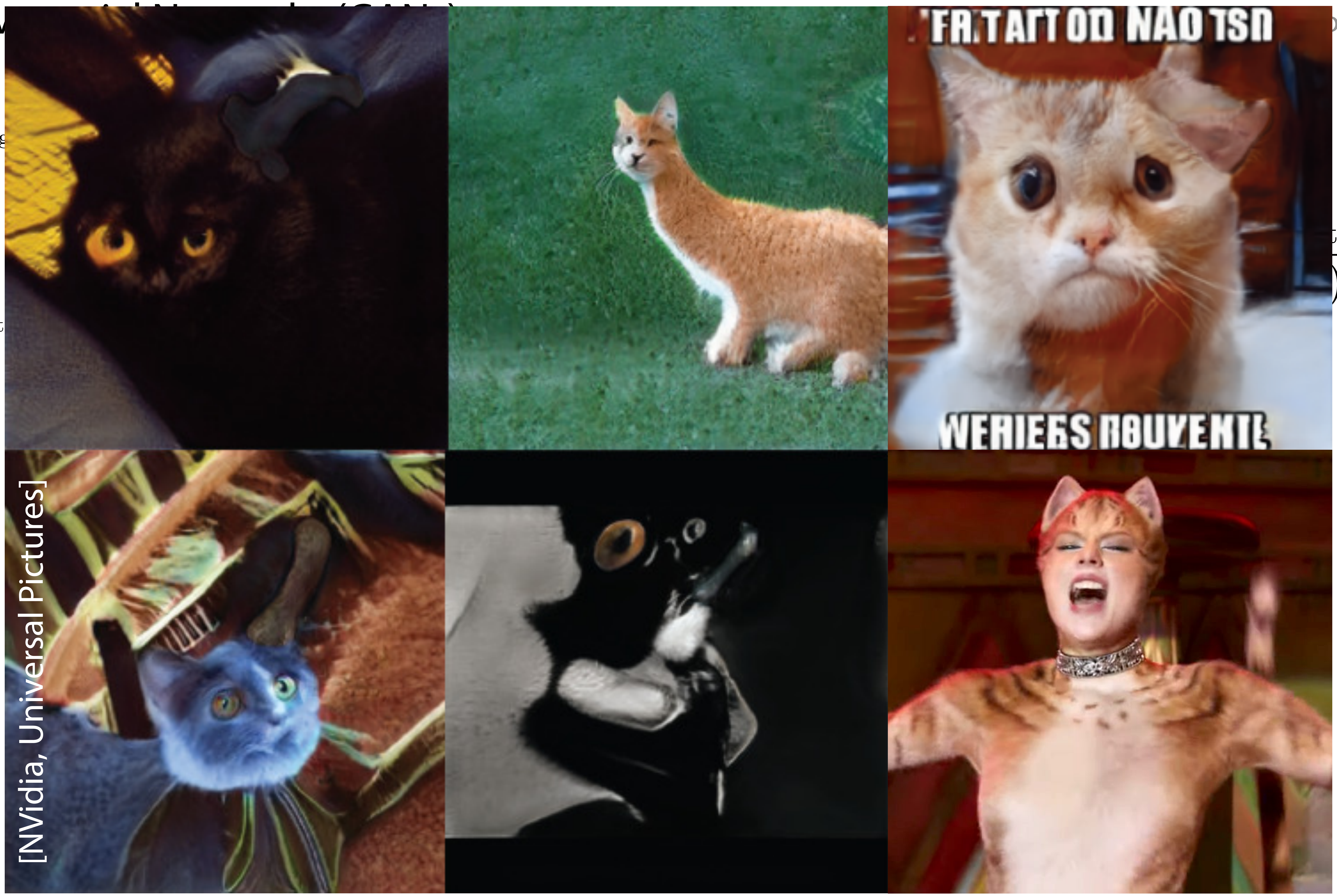
Idea 1: the likelihood ratio trick

- Generative Adv

odfellow et al. 1406.2661]

Generator
(intractable likelihood p_g

Examples
(intractable likelihood p_t



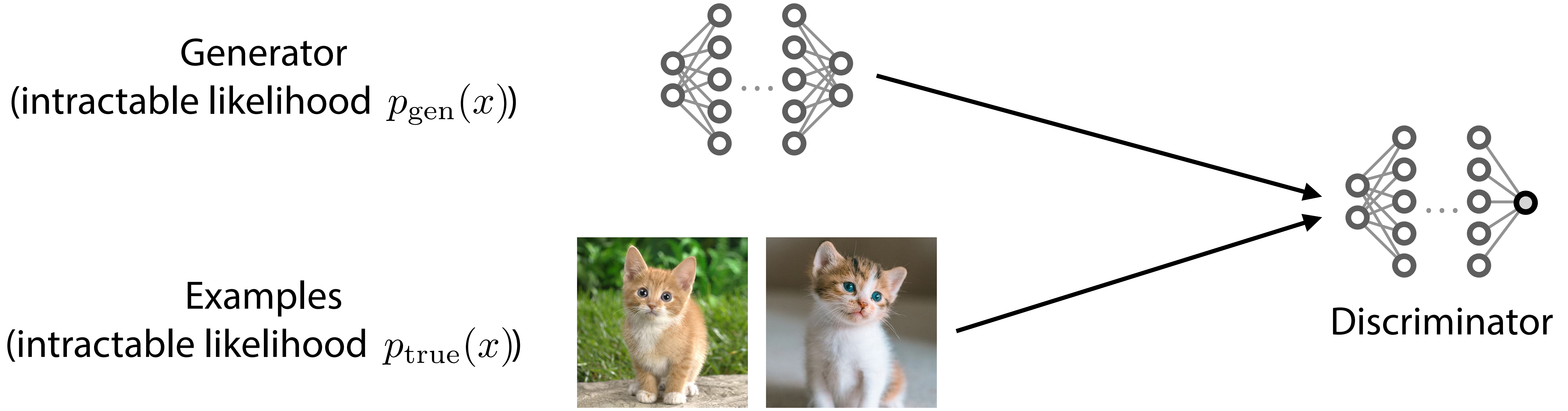
[NVidia, Universal Pictures]

decision function

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

Idea 1: the likelihood ratio trick

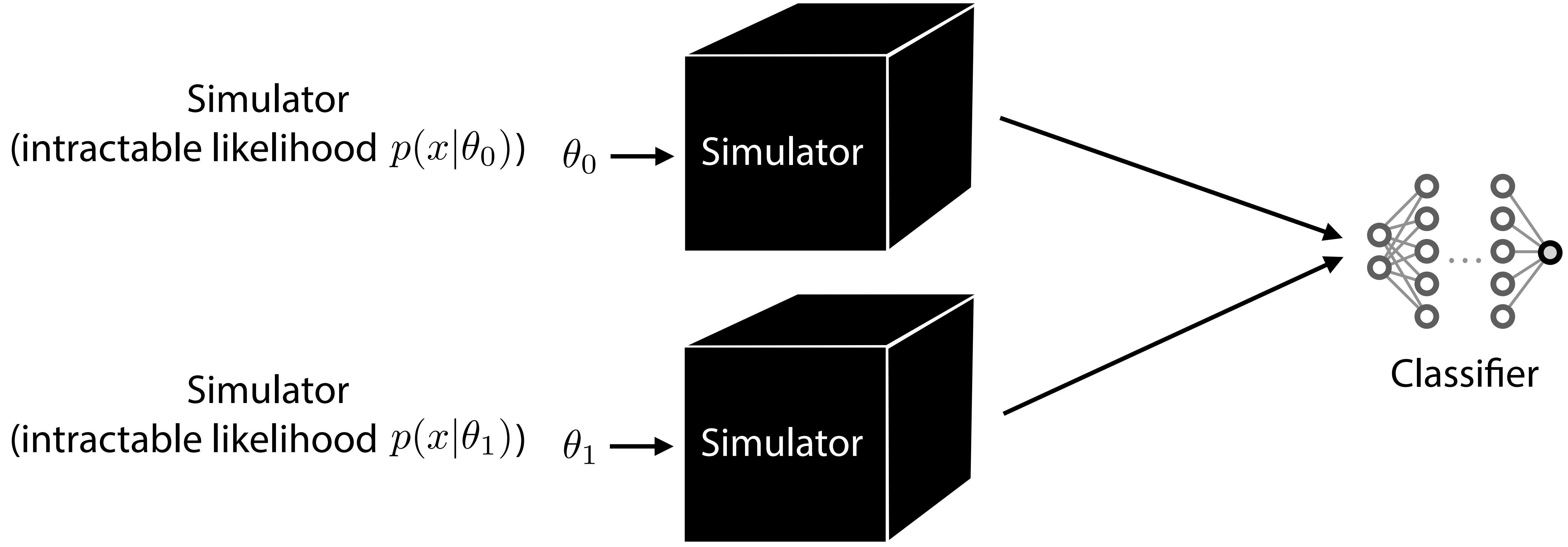
- Generative Adversarial Networks (GANs): [I. Goodfellow et al. 1406.2661]



Discriminator learns decision function

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

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

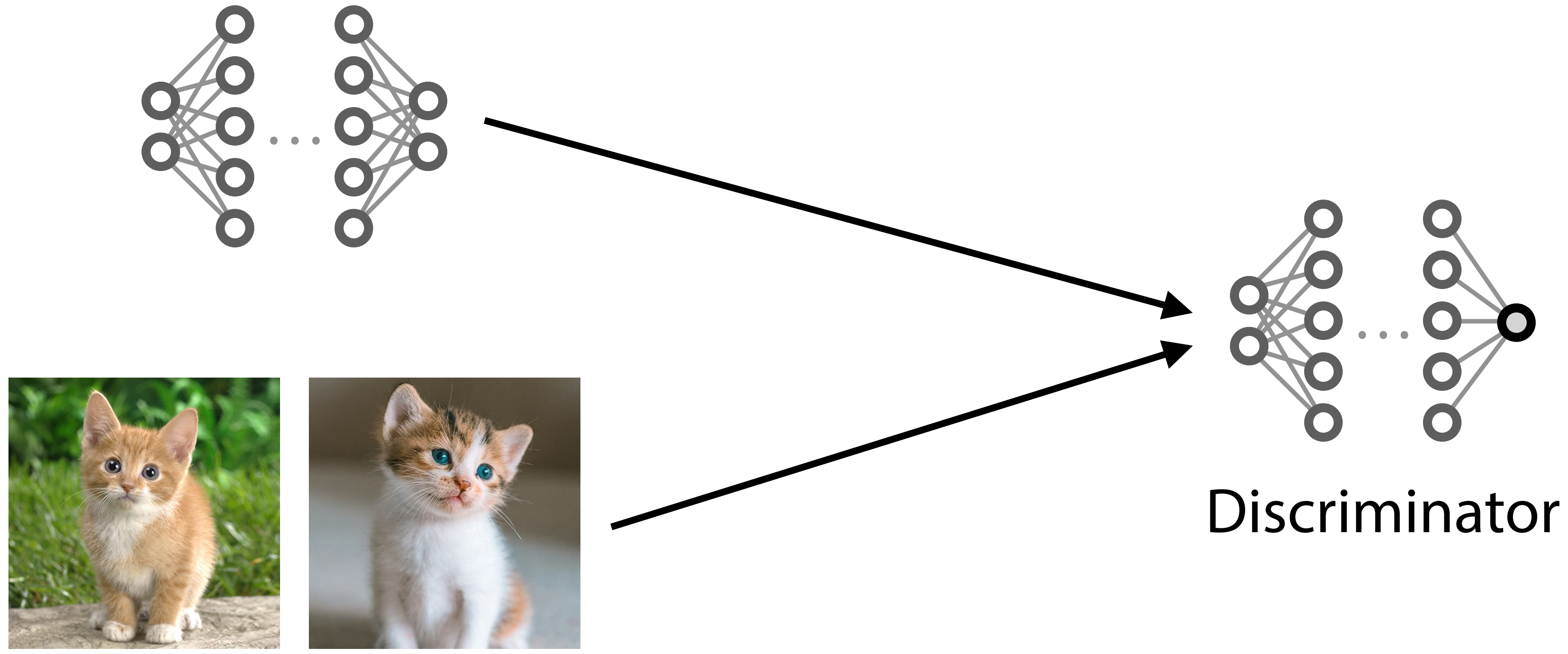


Idea 1: the likelihood ratio trick

- Generative Adversarial Networks (GANs): [I. Goodfellow et al. 1406.2661]

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

Examples
(intractable likelihood $p_{\mathrm{true}}(x)$)



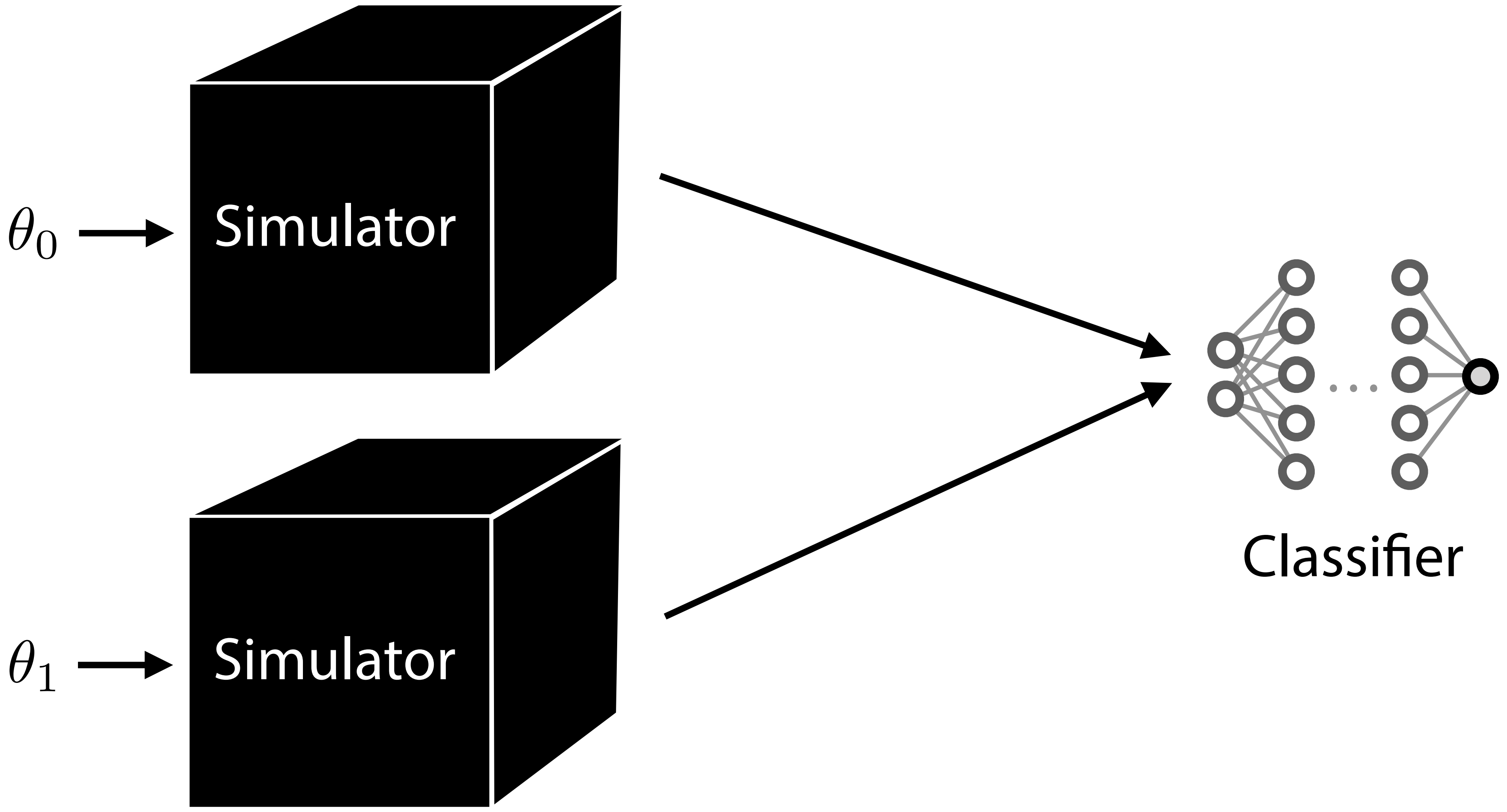
Discriminator learns decision function

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

- 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 $p(x|\theta_1)$)



Classifier learns decision function

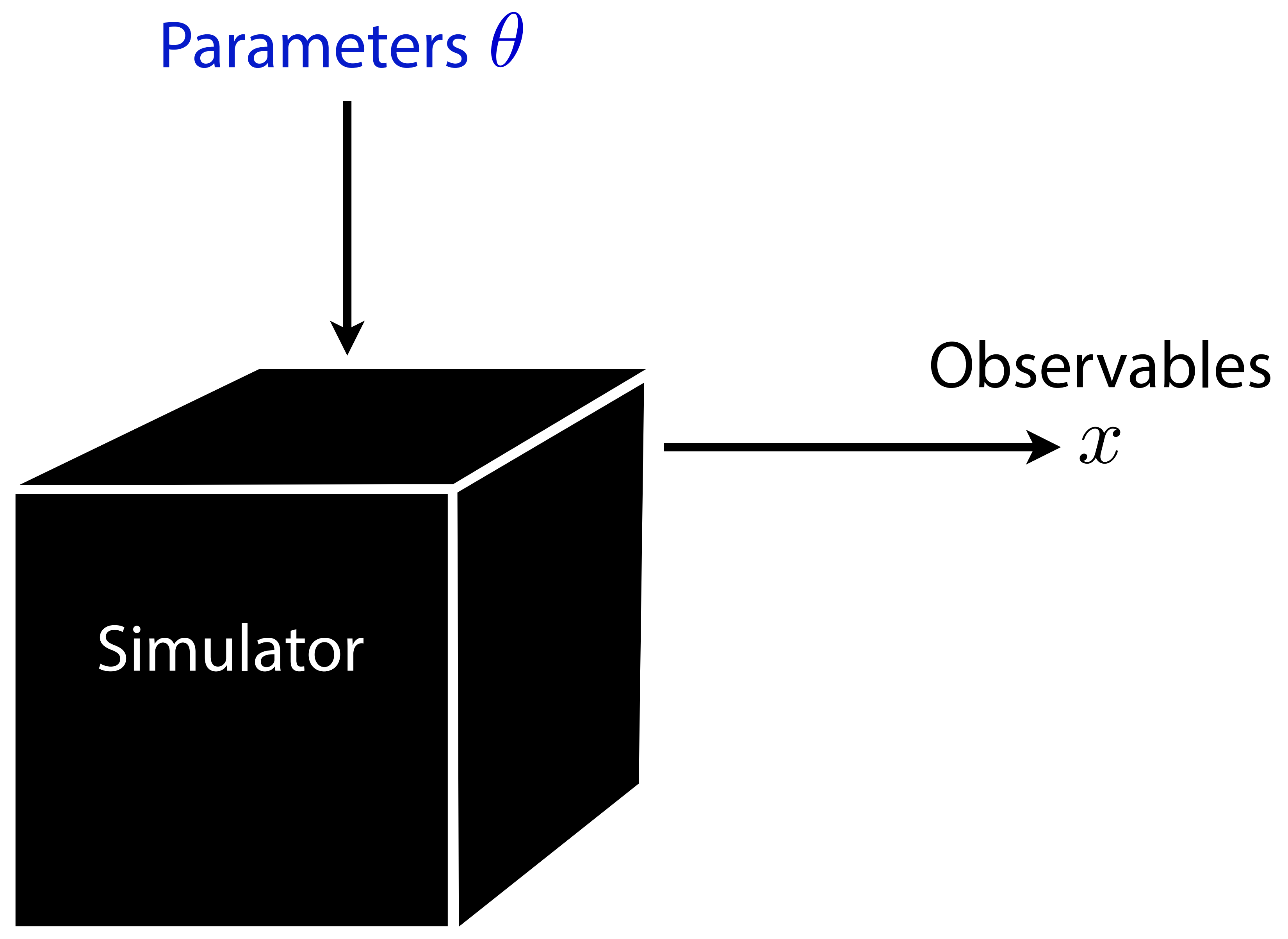
$$s(x) \to \frac{p(x|\theta_1)}{p(x|\theta_0) + p(x|\theta_1)}$$

⇒ 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]

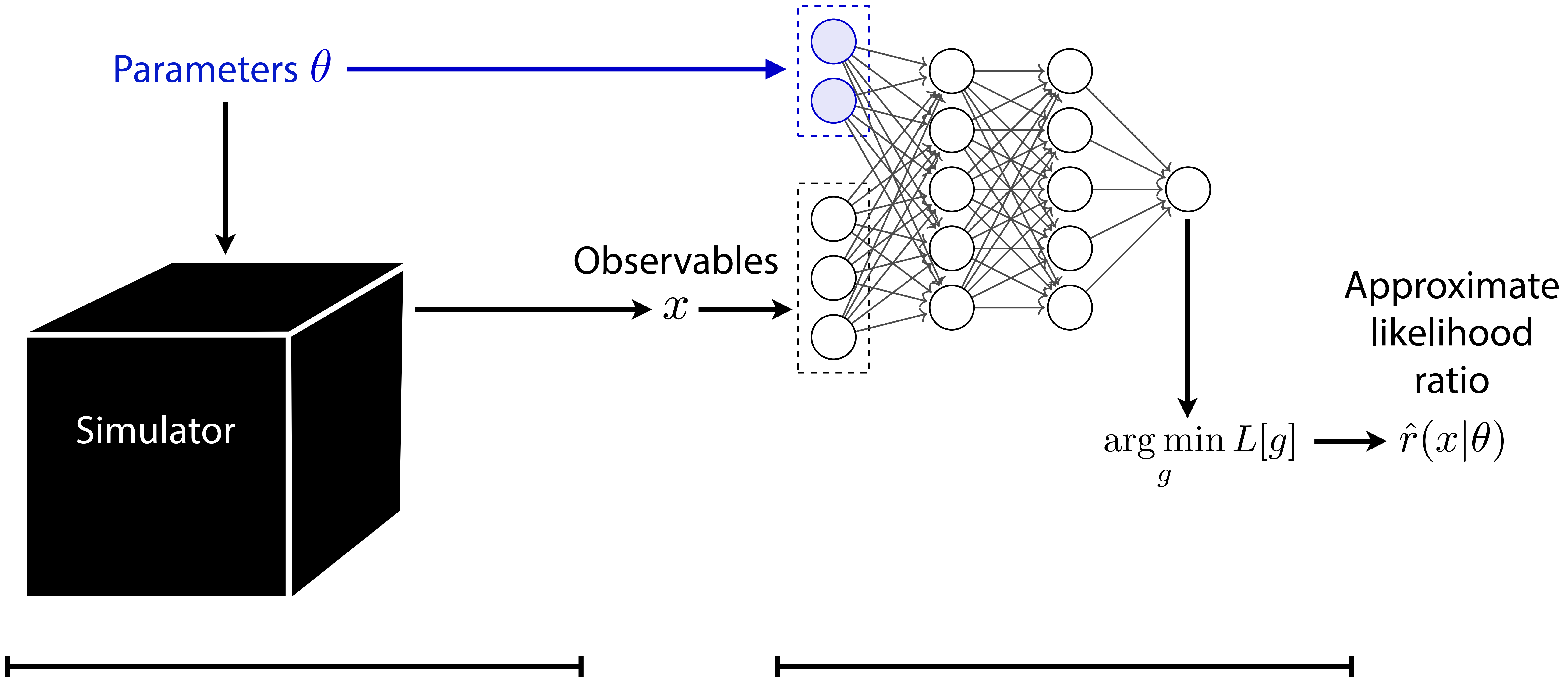


1. Simulation

Run simulator and save data

Inference by likelihood ratio trick

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



1. Simulation

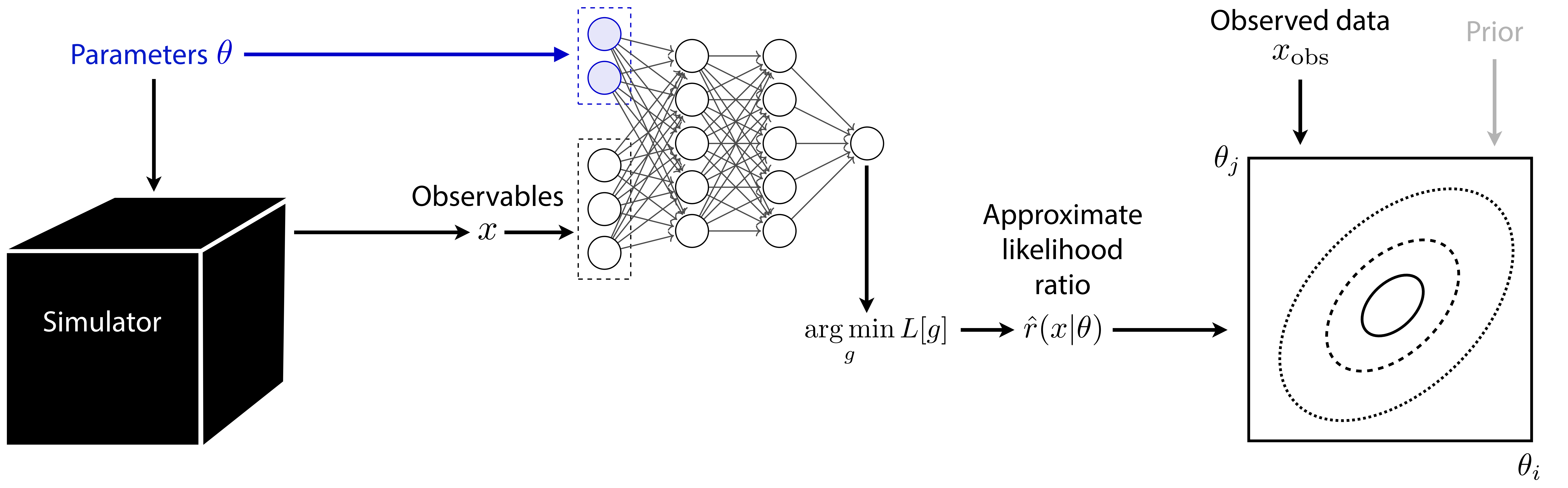
Run simulator and save data

2. Machine Learning

Train NN classifier, interpret as likelihood ratio estimator

Inference by likelihood ratio trick

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



1. Simulation

2. Machine Learning

3. Inference

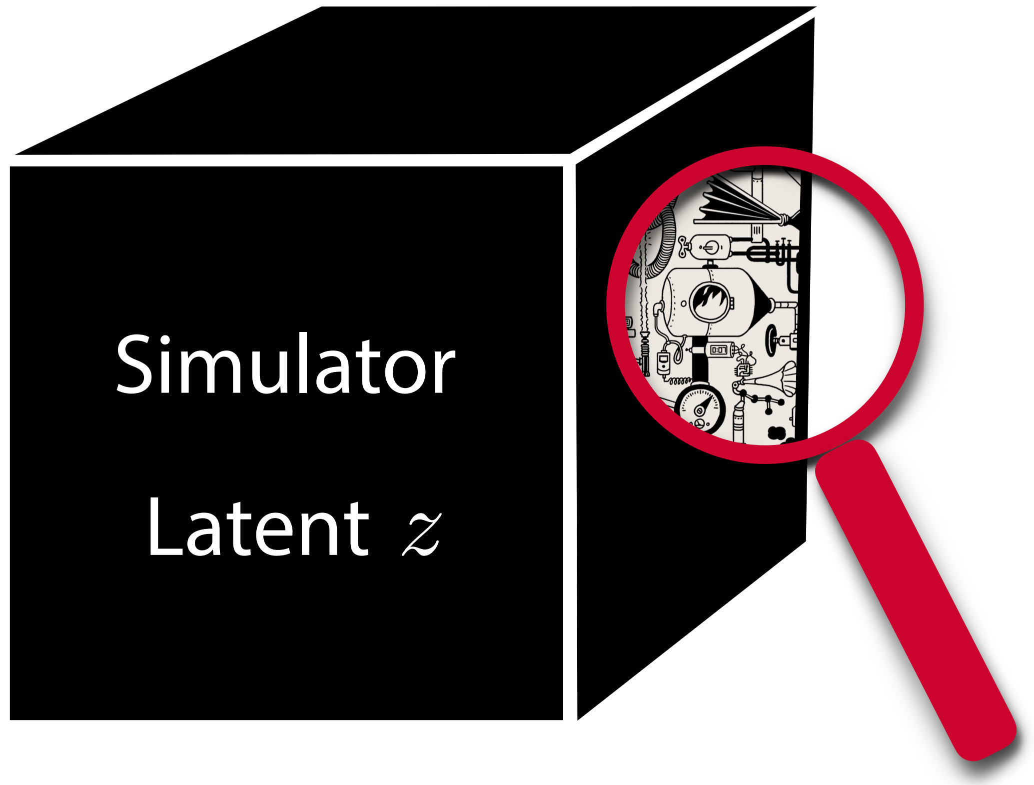
Run simulator and save data

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 $p(x|\theta) = \int \mathrm{d}z\, p(x, z|\theta)$,

but for each simulated event we can compute

- the joint likelihood ratio

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

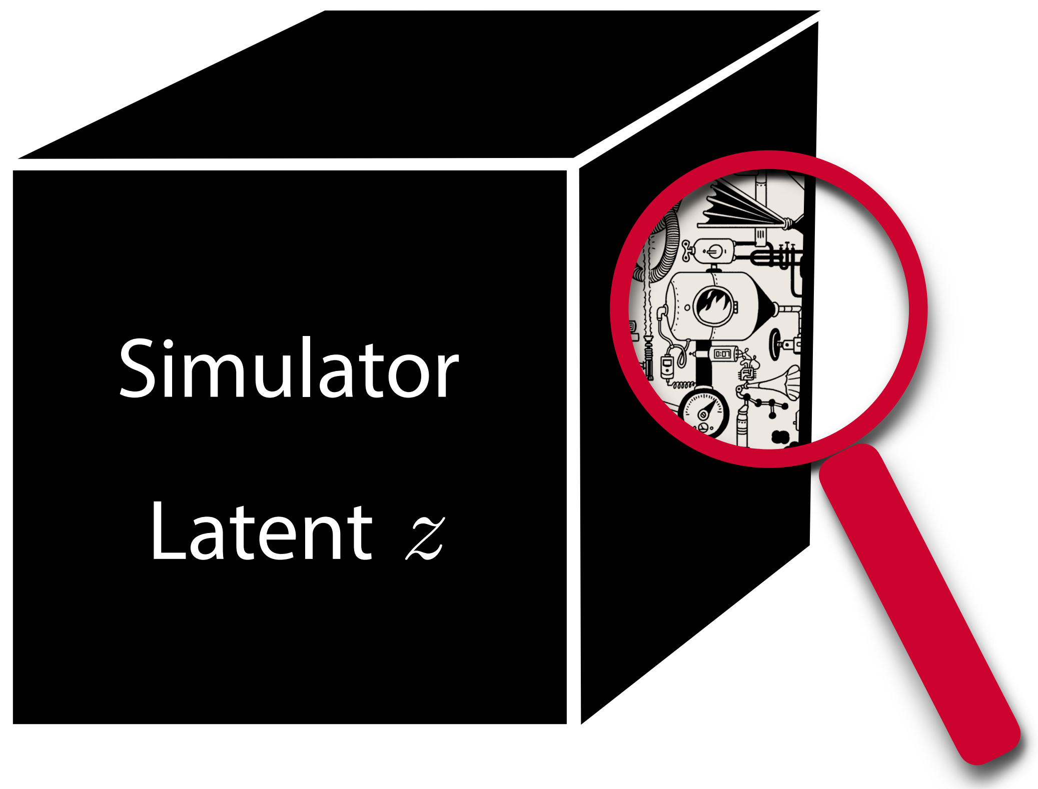
- the joint score

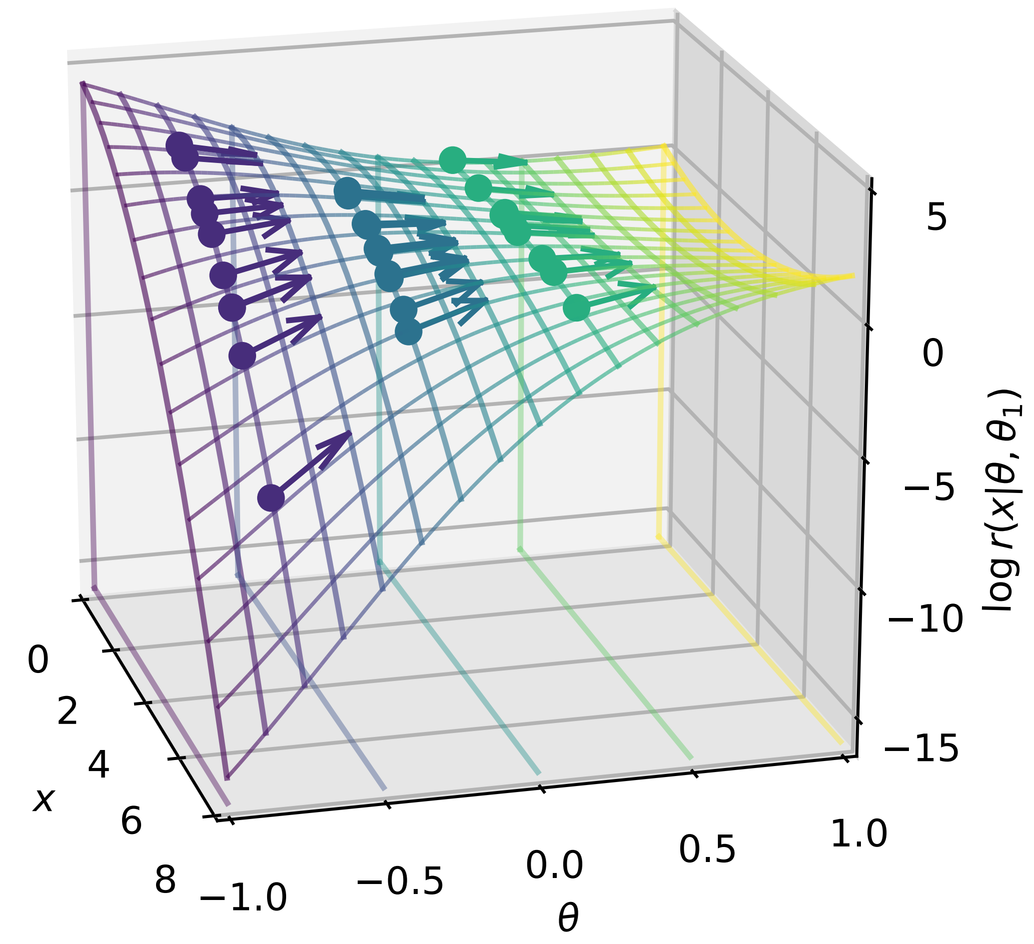
$$t(x, z|\theta) = \nabla_\theta \log p(x, z|\theta) \sim \frac{\nabla_\theta |\mathcal{M}|^2(z|\theta)}{|\mathcal{M}|^2(z|\theta)}$$

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

Idea 2: “mining gold”

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





We cannot compute $p(x|\theta) = \int \mathrm{d}z\, p(x, z|\theta)$,

but for each simulated event we can compute

- the joint likelihood ratio

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

- 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)

Why are they useful? One can show that

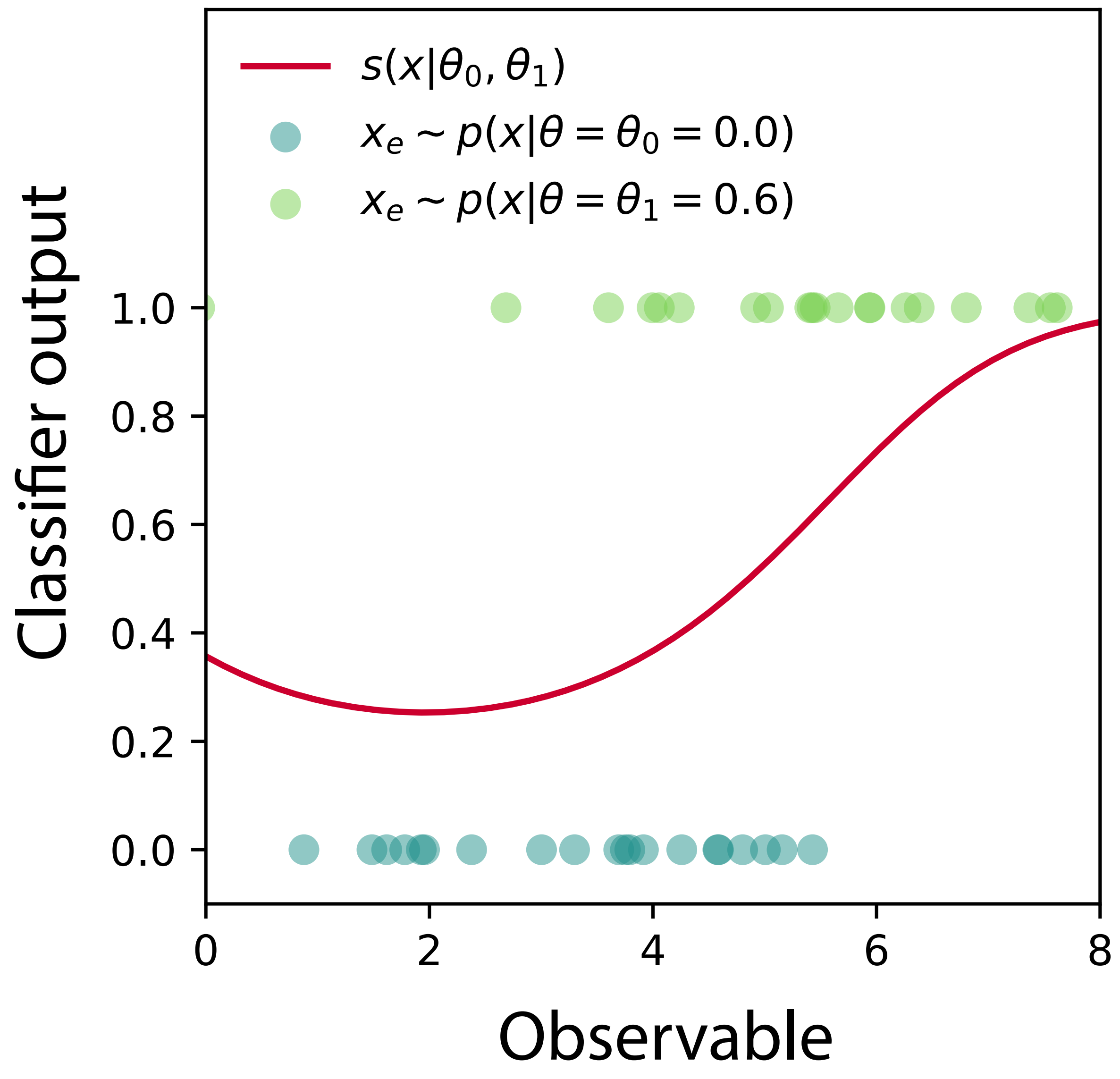
- the joint likelihood ratio is an unbiased estimator of the likelihood ratio
- the joint score provides unbiased gradient information

⇒ 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]

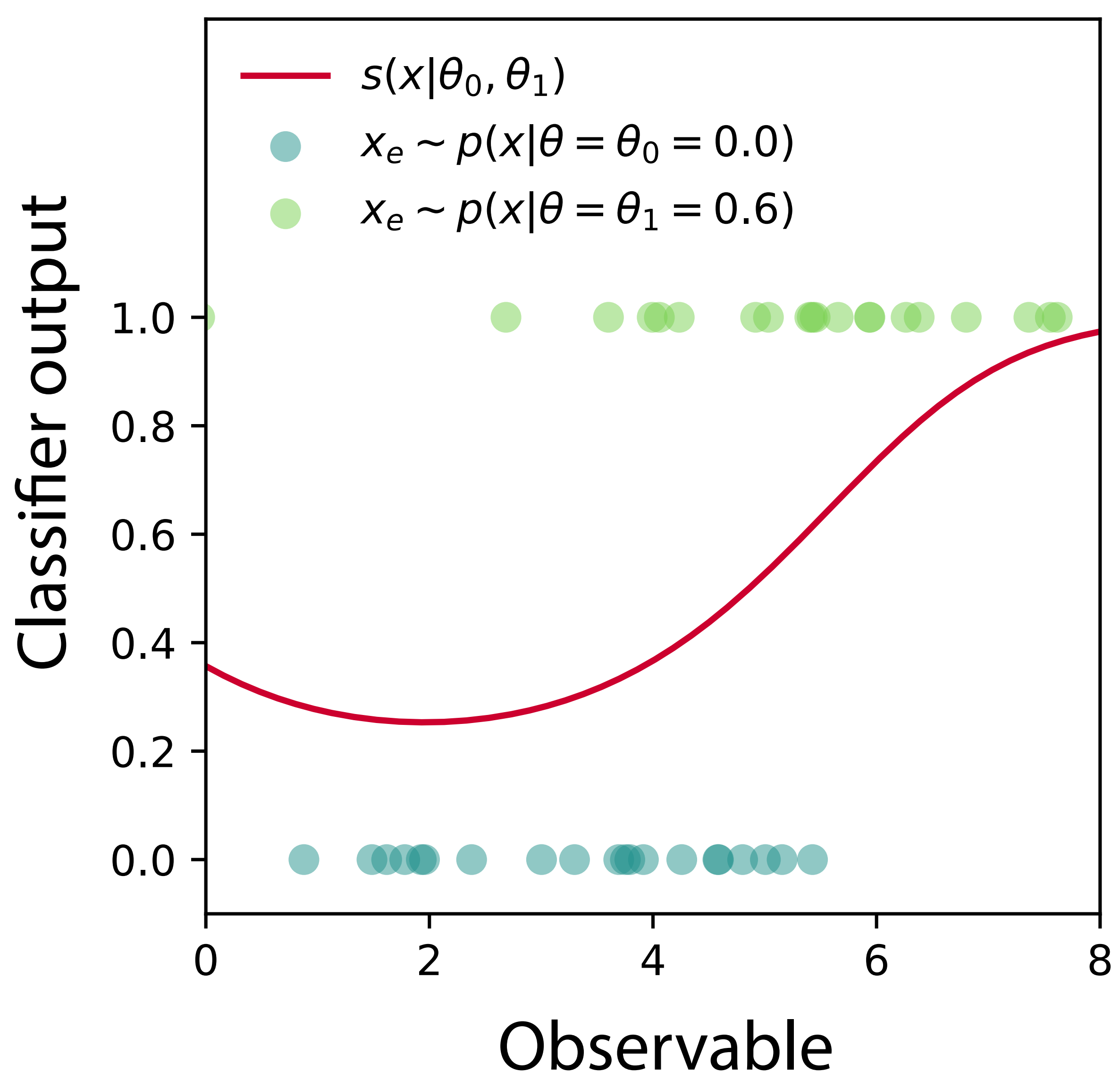
Likelihood ratio trick



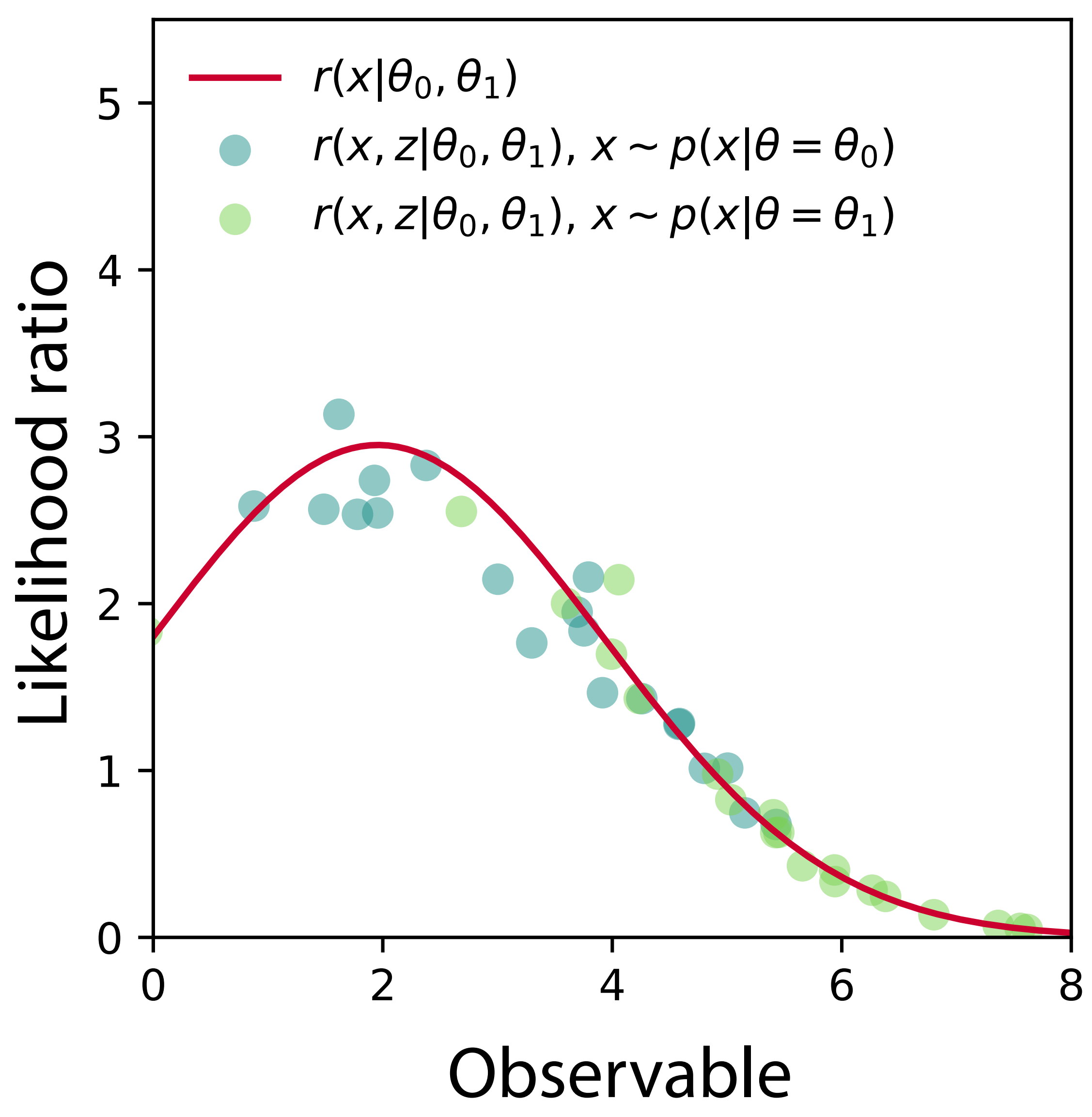
Mining gold adds information

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

Likelihood ratio trick

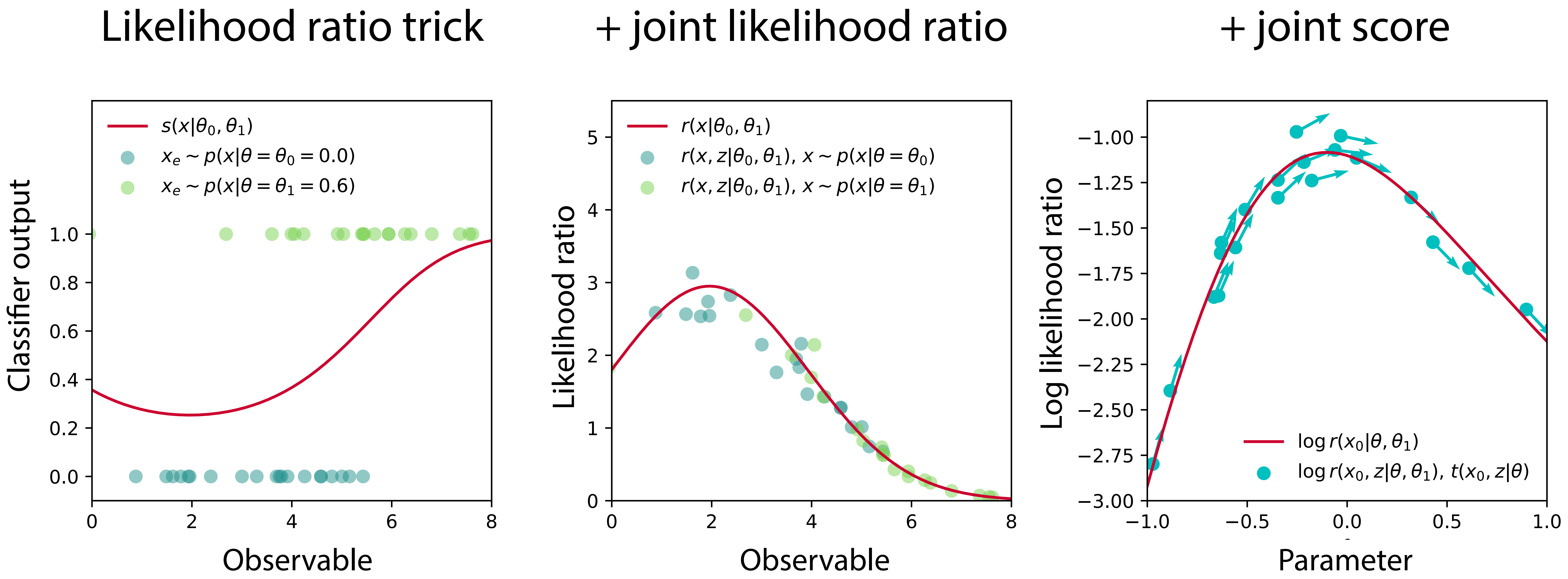


+ joint likelihood ratio



Mining gold adds information

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



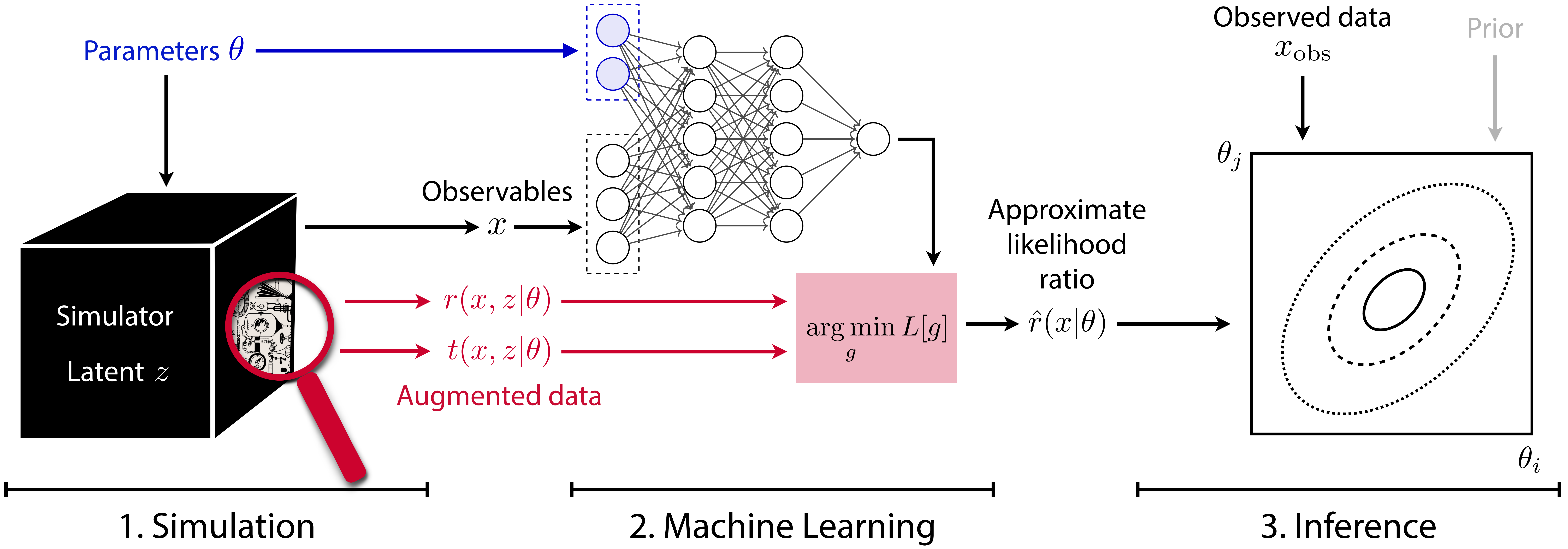
Mining gold adds information

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

Using more information = more sample-efficient inference

RASCAL

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



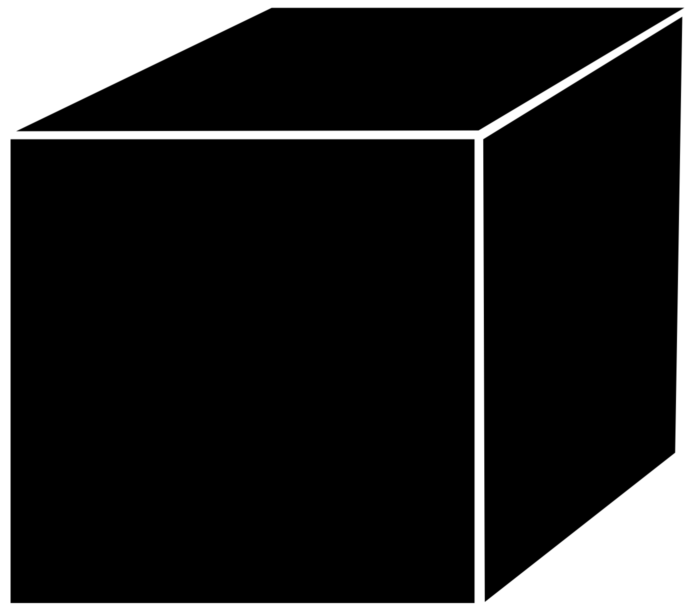
Extract joint likelihood ratio
and joint score from simulator

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

Simulation-based inference method zoo

Method	Approximations	Upfront cost	Evaluation
Summary statistics:			
Likelihood for summary stats ("histograms")	Reduction to summary stats	Fast	Fast
Approximate Bayesian Computation	Reduction to summary stats	Depends	Depends
Matrix elements:			
Matrix Element Method	Transfer fns	Fast	Slow
Optimal Observables	Transfer fns, optimal only locally	Fast	Slow
Neural networks:			
Neural likelihood	NN	Needs many samples	Fast
Neural posterior	NN	Needs many samples	Fast
Neural likelihood ratio	NN	Needs many samples	Fast
Neural networks + matrix elements:			
Neural likelihood (ratio) + gold mining (RASCAL)	NN	Needs less samples	Fast
Neural optimal observables (SALLY)	NN, optimal only locally	Needs less samples	Fast

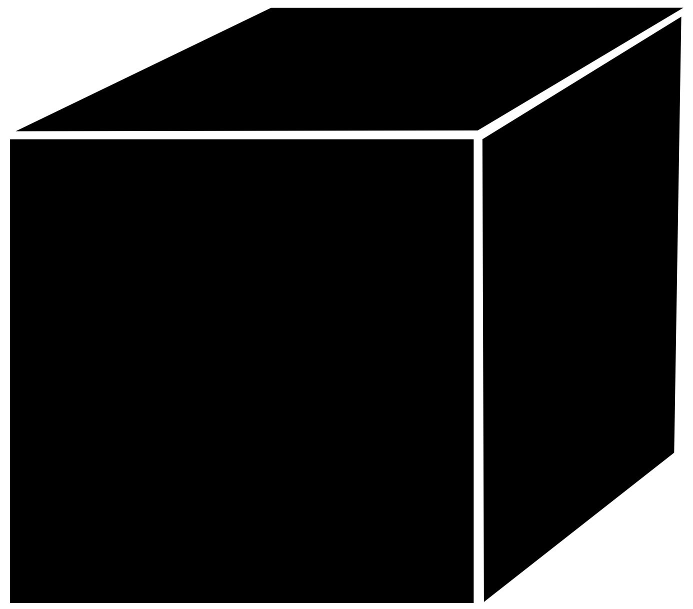
Systematics

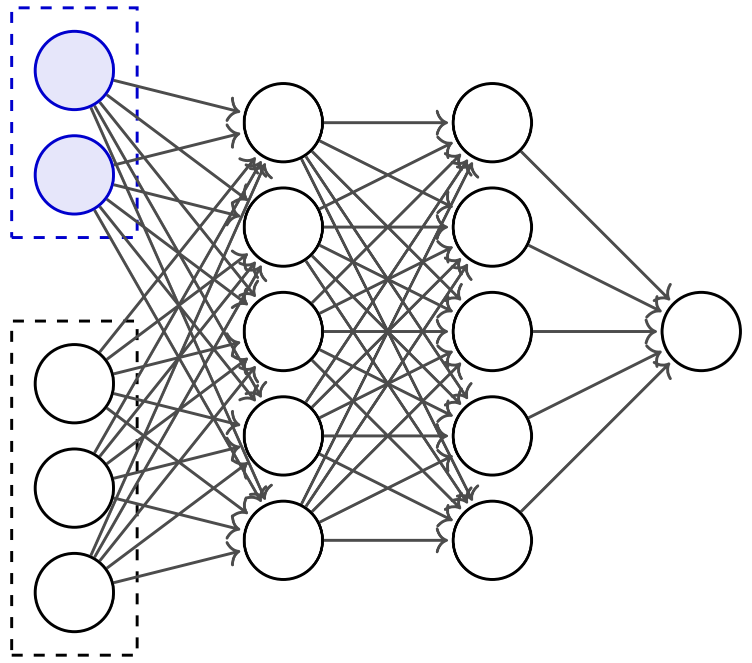


Can you trust the simulator?

- 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



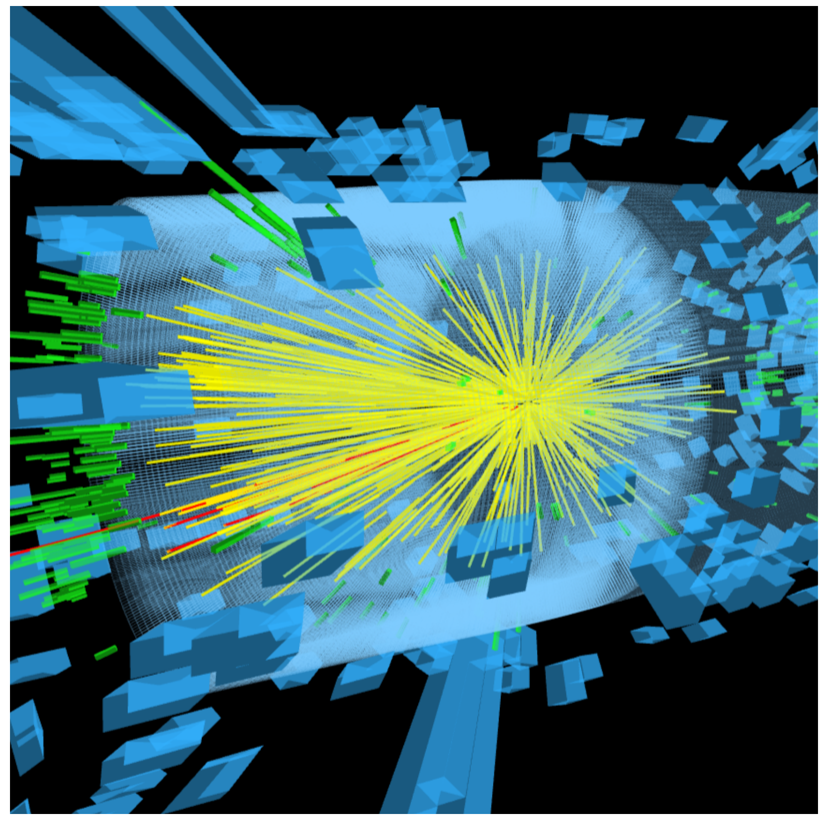


Can you trust the simulator?

- 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]

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]

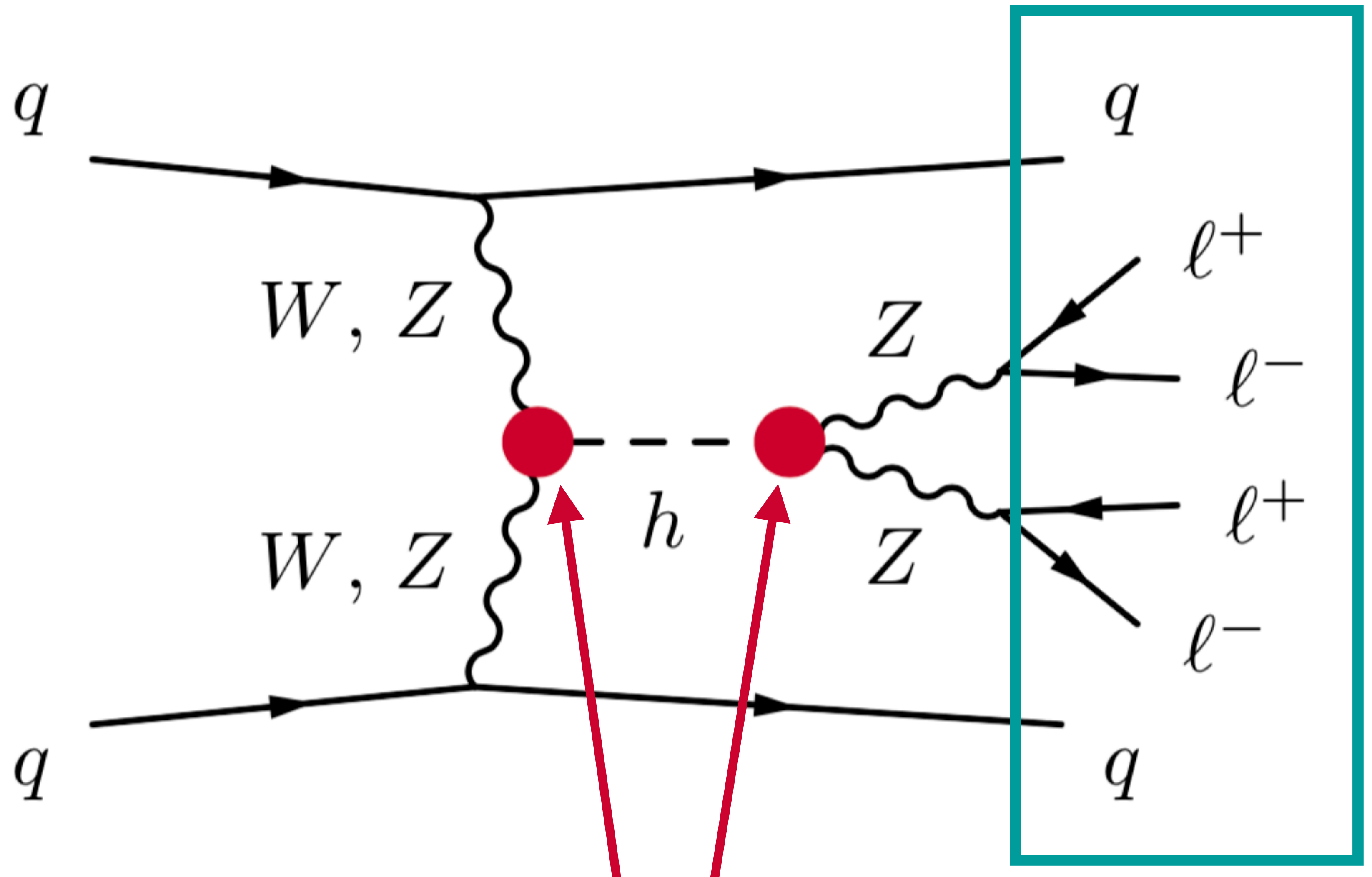


4. Examples

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



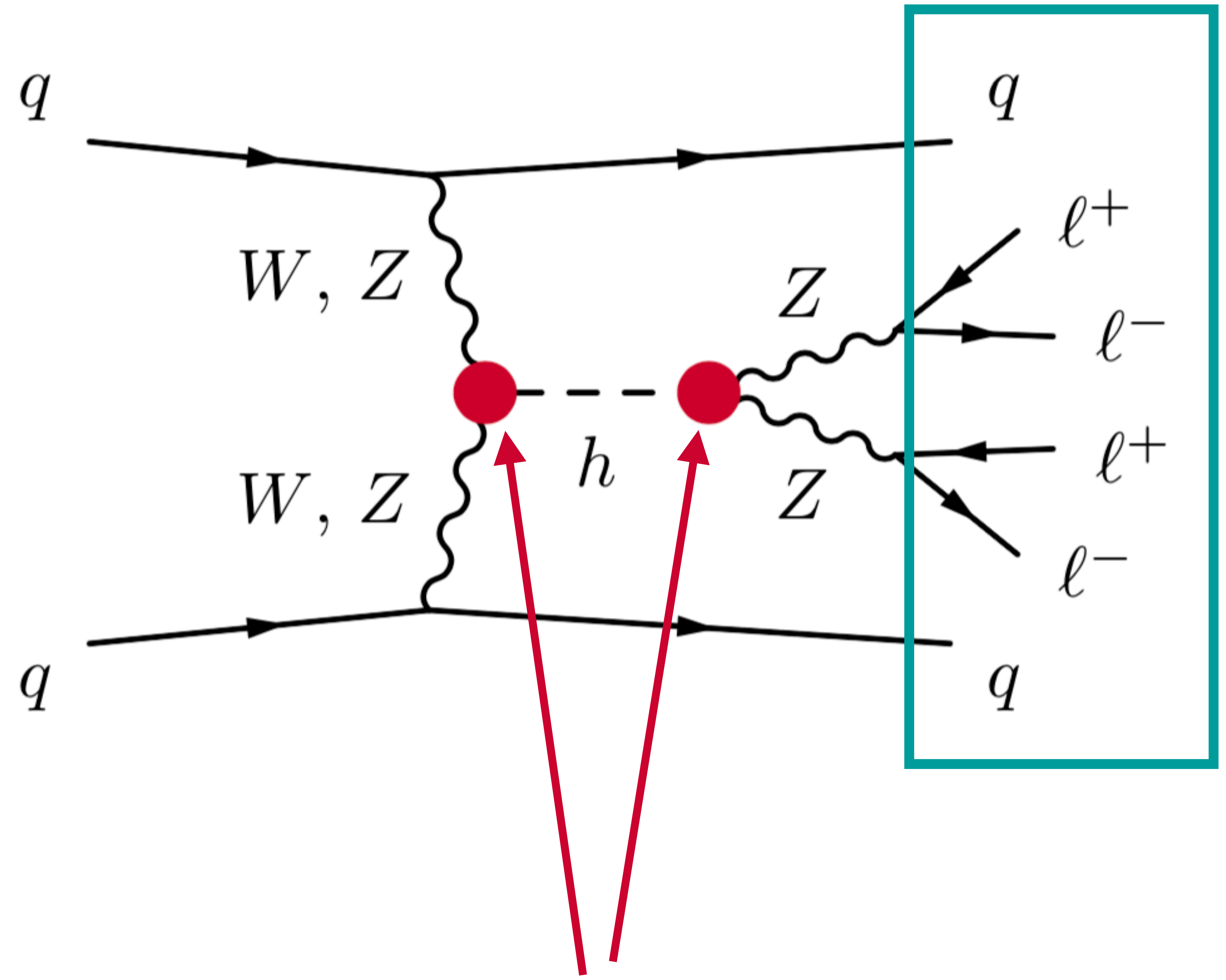
Exciting new physics might hide here!
We parameterize it with two EFT coefficients:

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

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:

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

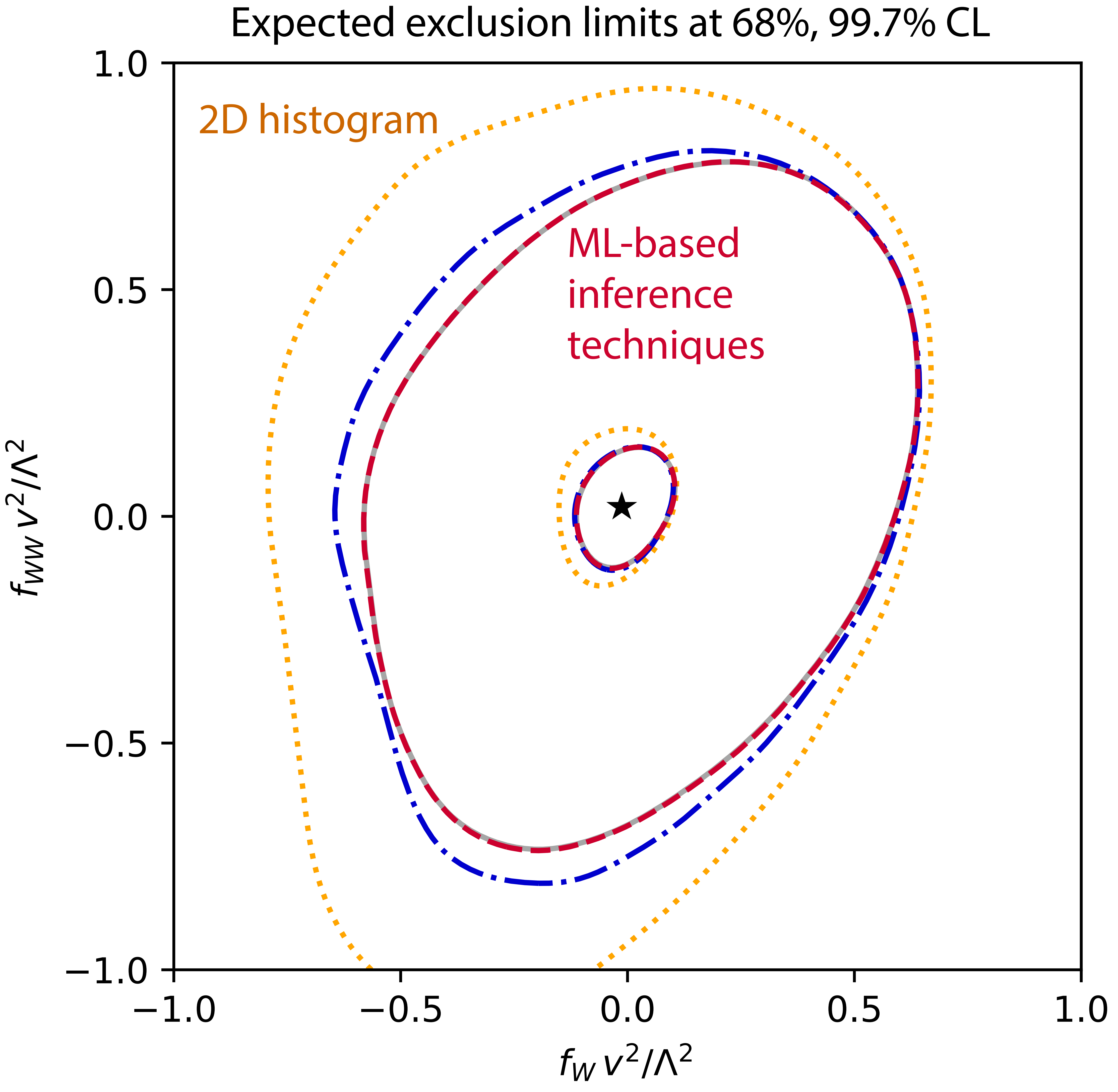
Goal: constrain the two EFT parameters

- 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

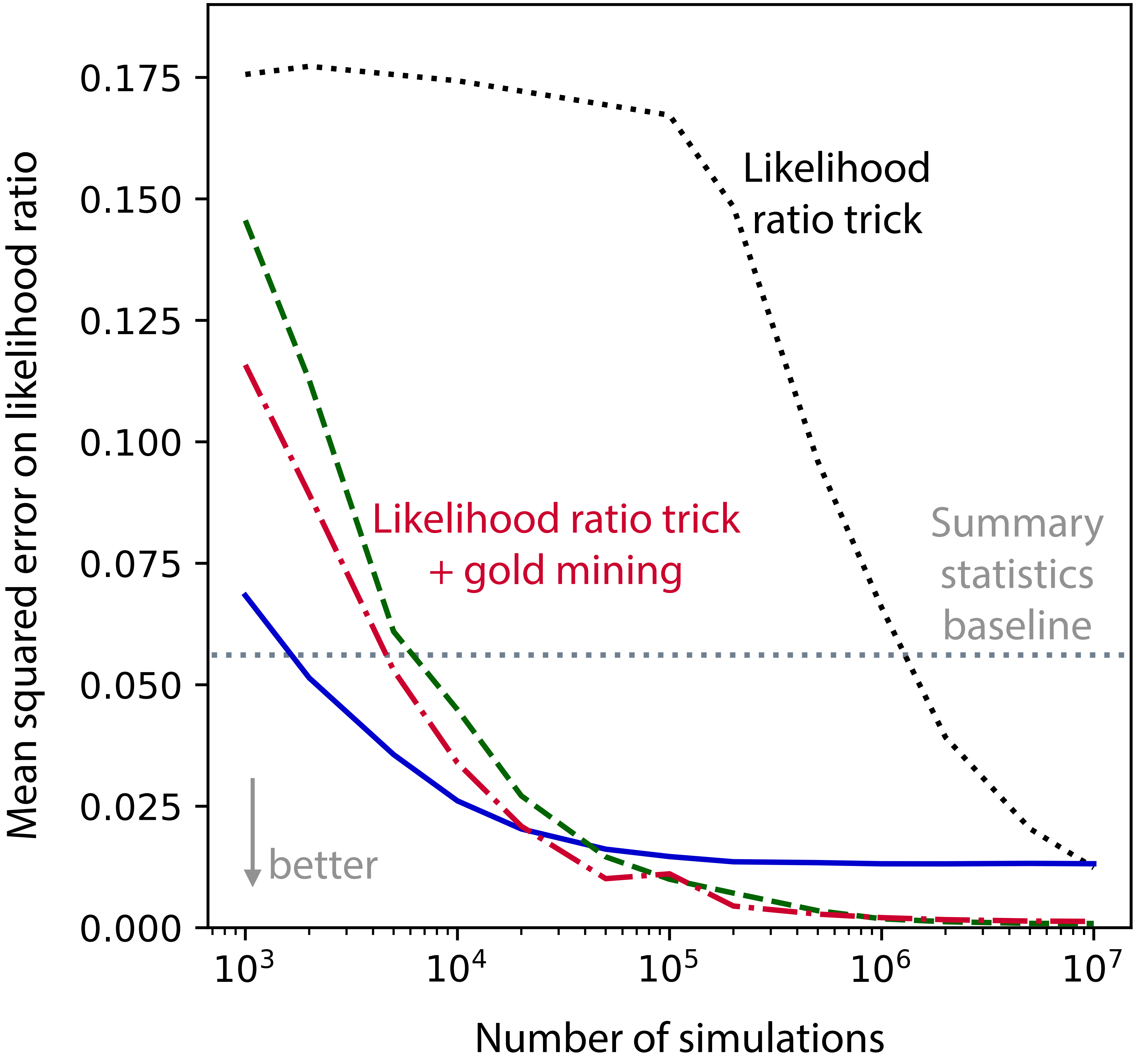
Stronger limits…



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:

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

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

Constraining operators in ttH effectively

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

- Pheno-level analysis of

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

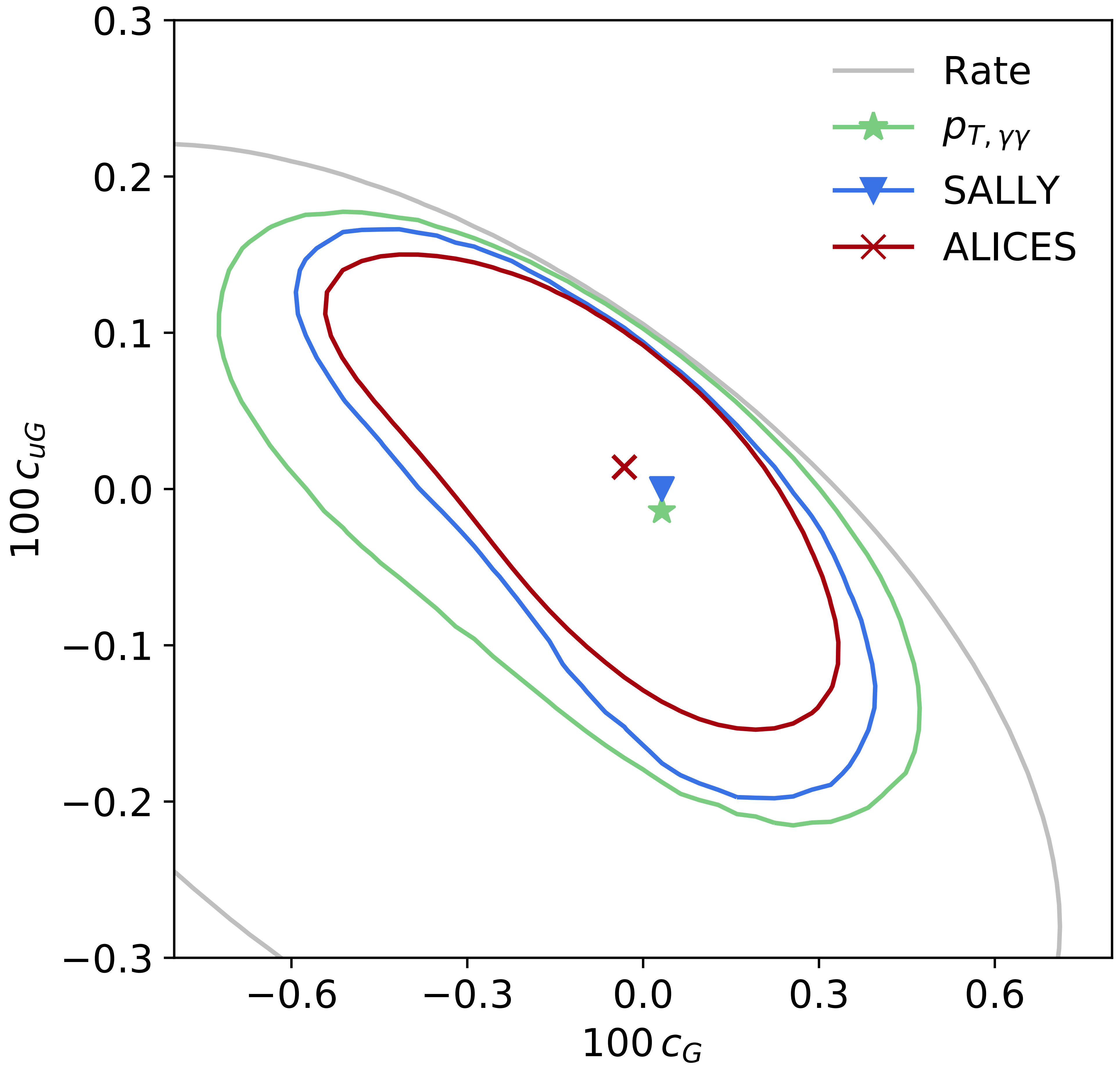
  with MadGraph + Pythia + Delphes

- Inference on three EFT operators:

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

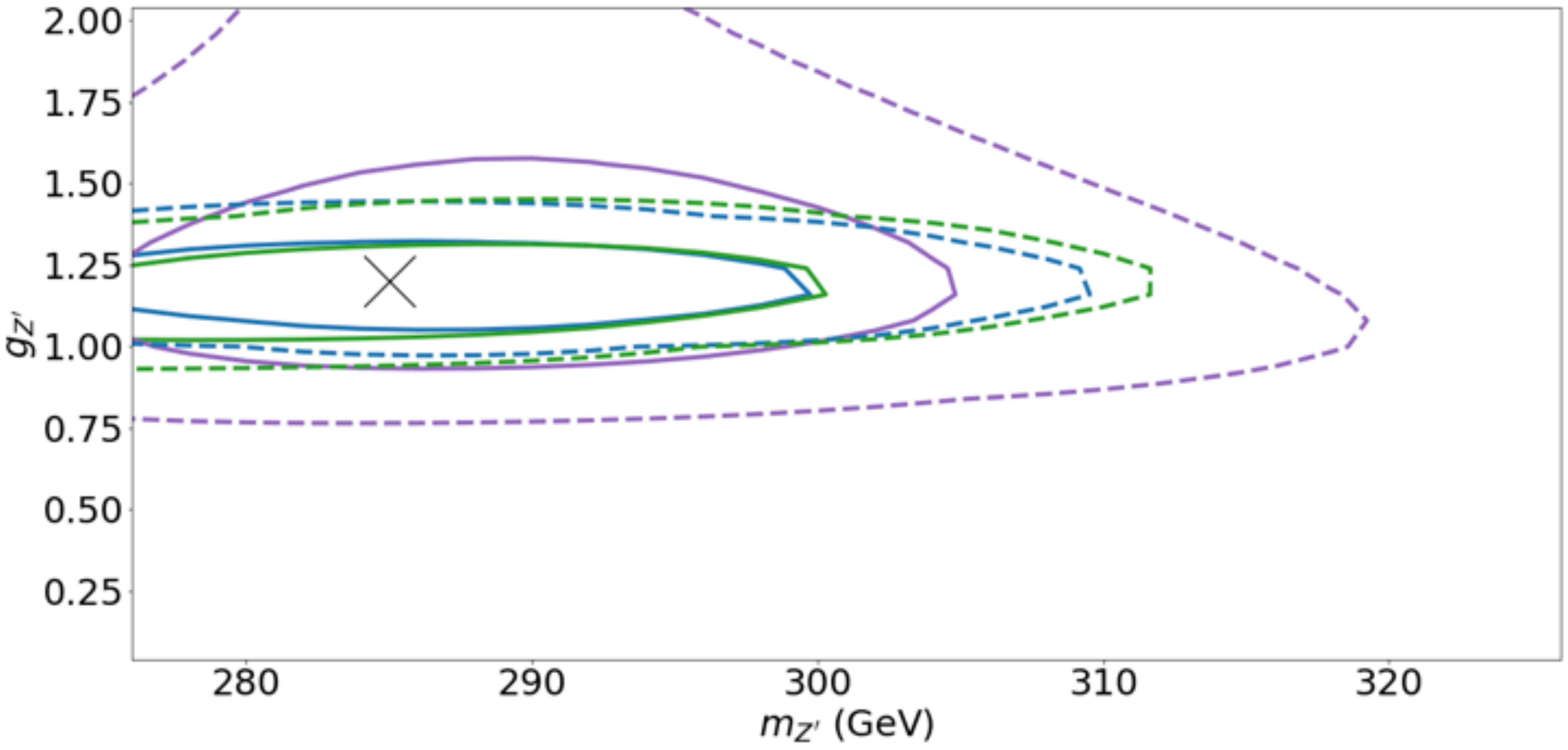
$$\mathcal{O}_{uG} = -\frac{4g_s}{m_W^2}y_u(H^\dagger \bar{Q}_L)\gamma^{\mu\nu}T_a u_R G^a_{\mu\nu}$$

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



Hunting $Z' \to jj$

[J. Hollingworth, D. Whiteson 2002.04699]

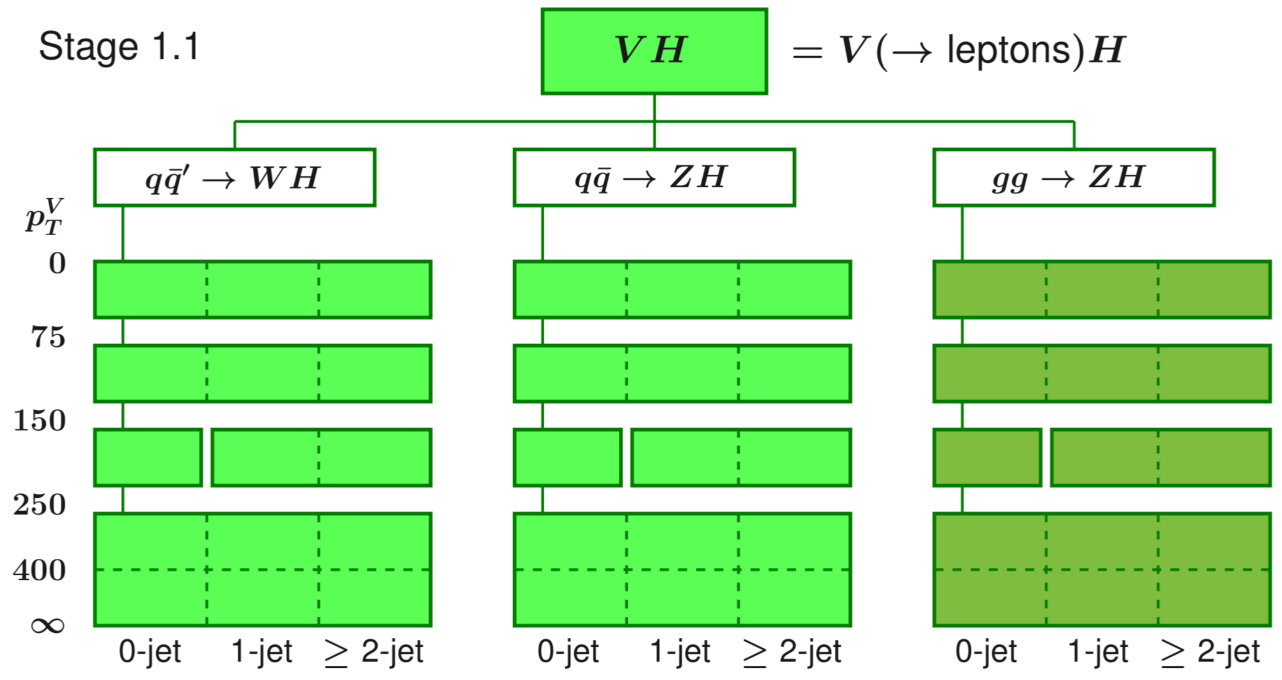


Multivariate analysis with new ML-based inference techniques leads to better expected limits than m_{jj} analysis

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

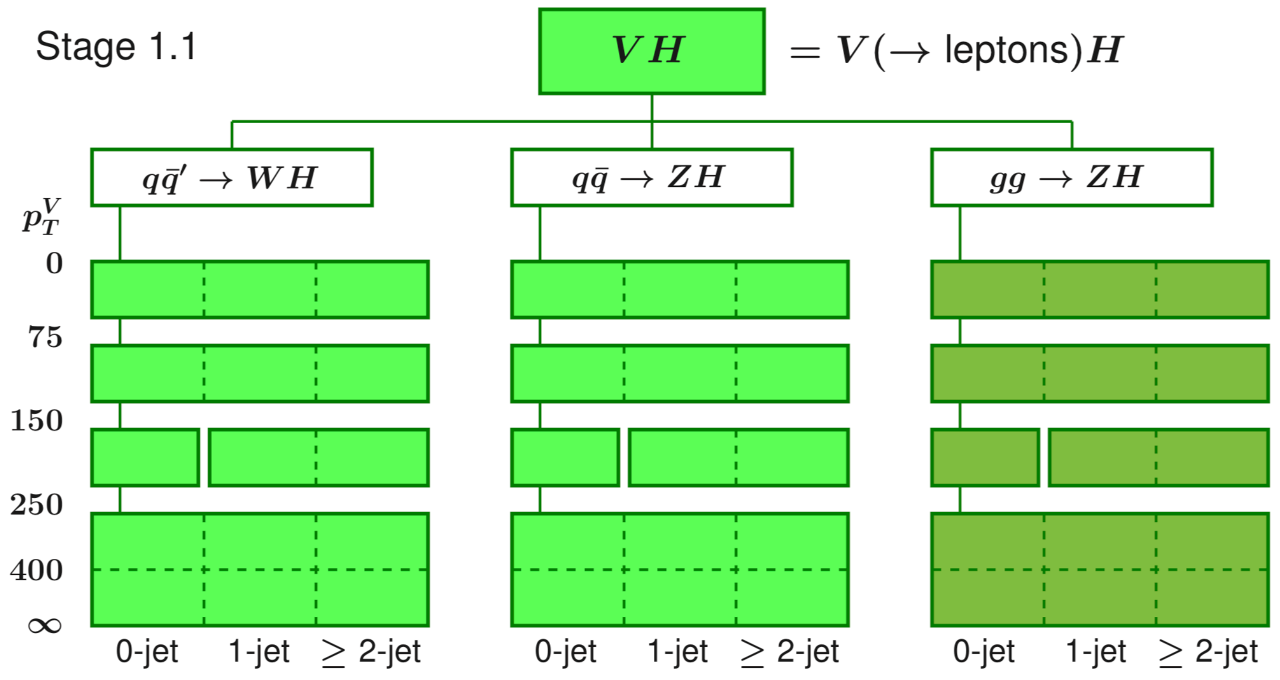
$$\tilde{\mathcal{O}}_{HD} = \mathcal{O}_{H\Box} - \frac{\mathcal{O}_{HD}}{4} = (\phi^\dagger\phi)\Box(\phi^\dagger\phi) - \frac{1}{4}(\phi^\dagger D^\mu\phi)^*(\phi^\dagger D_\mu\phi)$$
$$\mathcal{O}_{HW} = \phi^\dagger\phi W^a_{\mu\nu}W^{\mu\nu a}$$
$$\mathcal{O}^{(3)}_{Hq} = (\phi^\dagger i \overleftrightarrow{D}^a_\mu \phi)(\overline{Q}_L\sigma^a\gamma^\mu Q_L)\,,$$

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

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

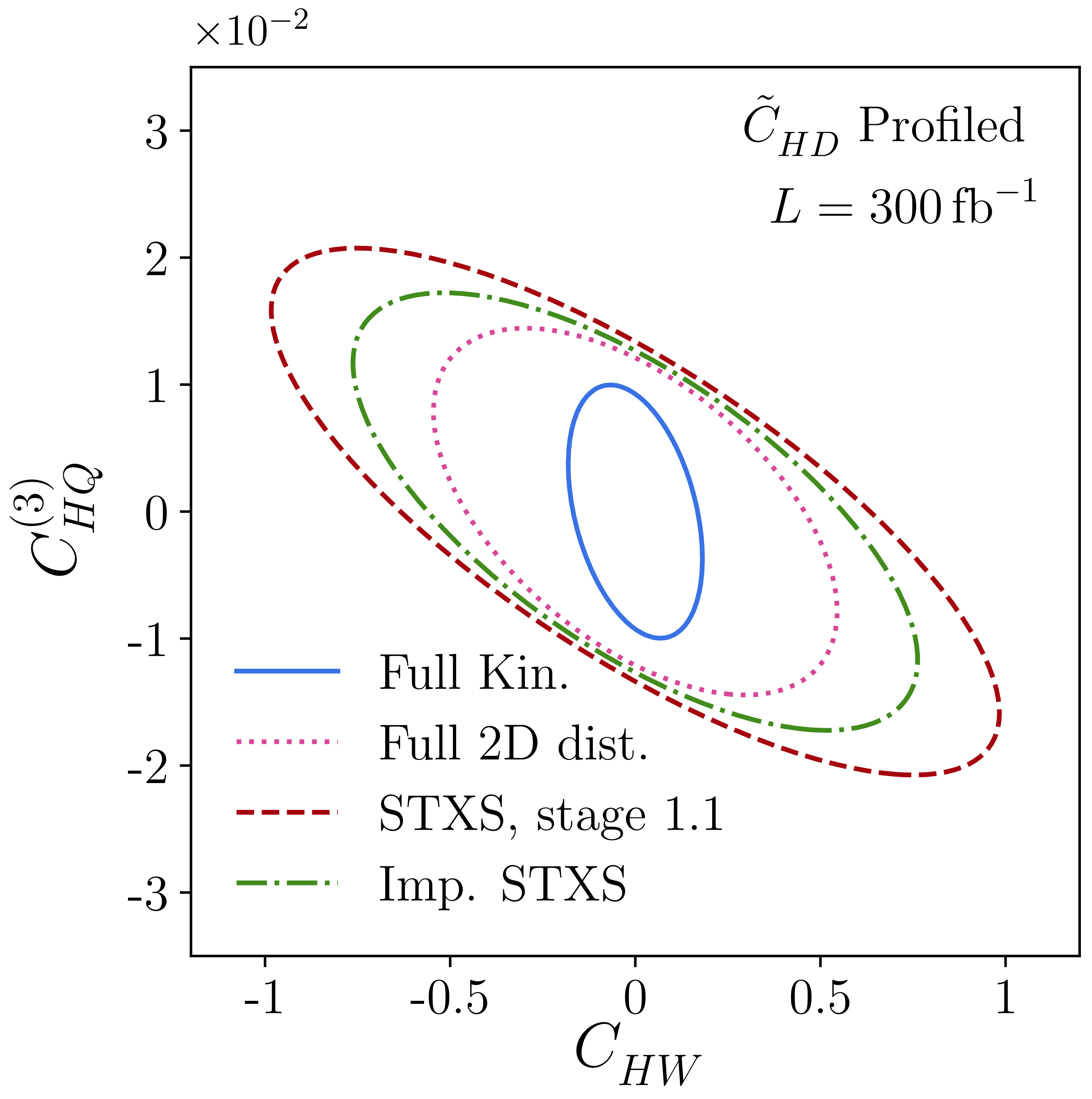
$$\tilde{\mathcal{O}}_{HD} = \mathcal{O}_{H\Box} - \frac{\mathcal{O}_{HD}}{4} = (\phi^\dagger\phi)\Box(\phi^\dagger\phi) - \frac{1}{4}(\phi^\dagger D^\mu\phi)^*(\phi^\dagger D_\mu\phi)$$

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

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

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

- 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

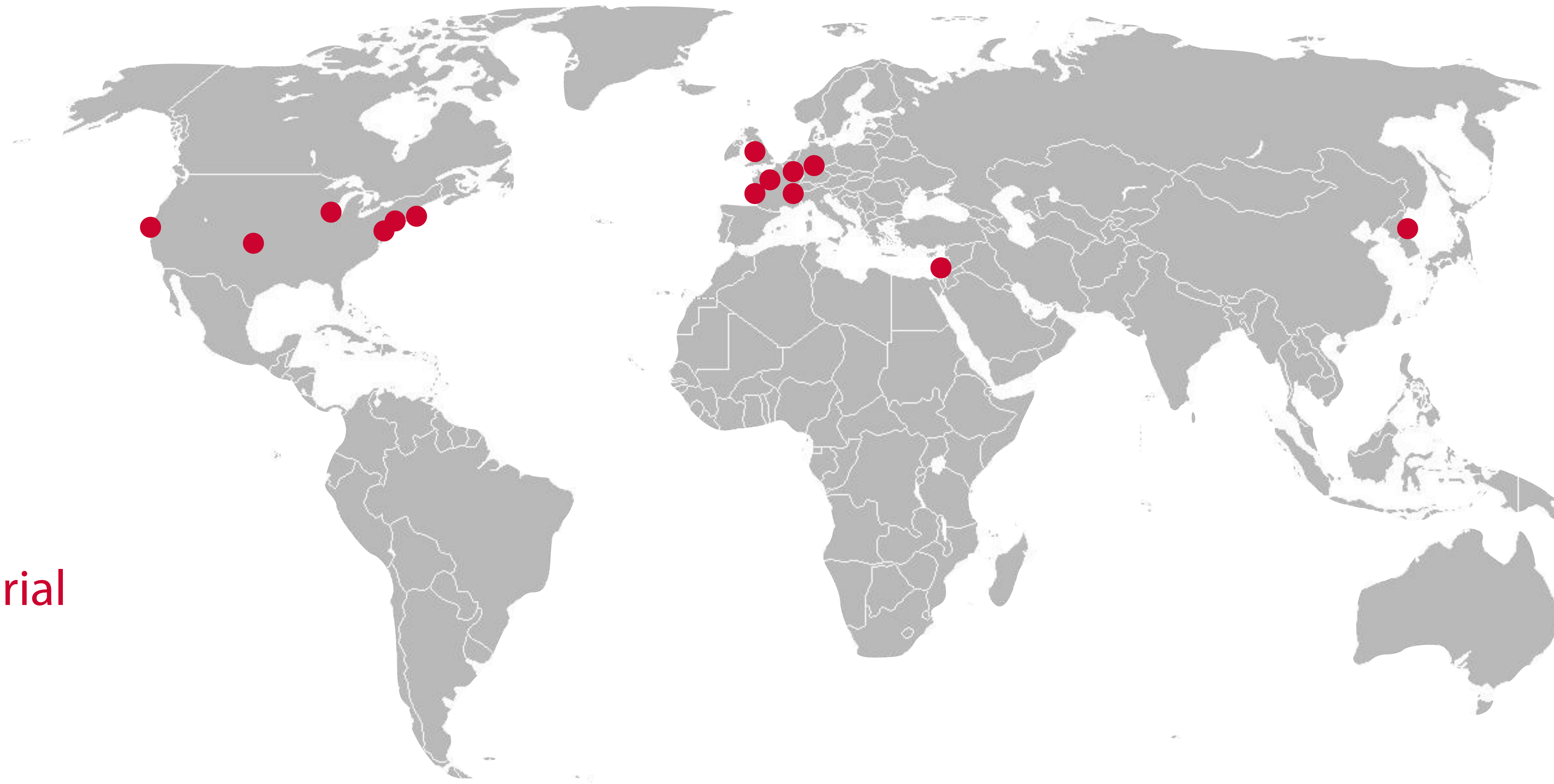
github.com/diana-hep/madminer

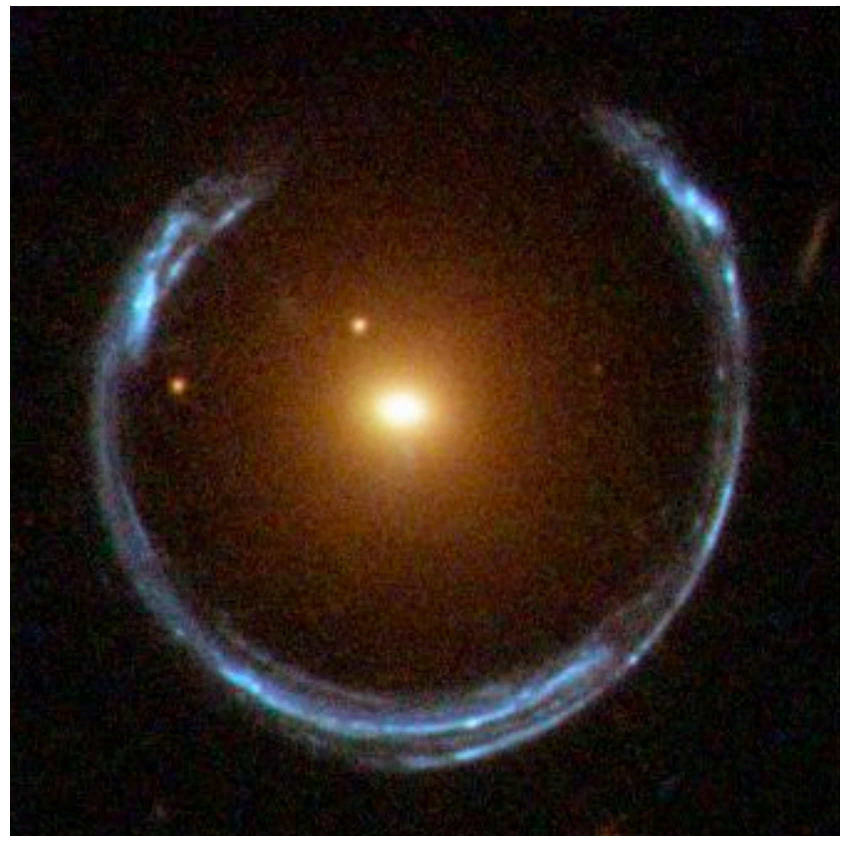
`pip install madminer`

hub.docker.com/u/madminertool

cranmer.github.io/madminer-tutorial

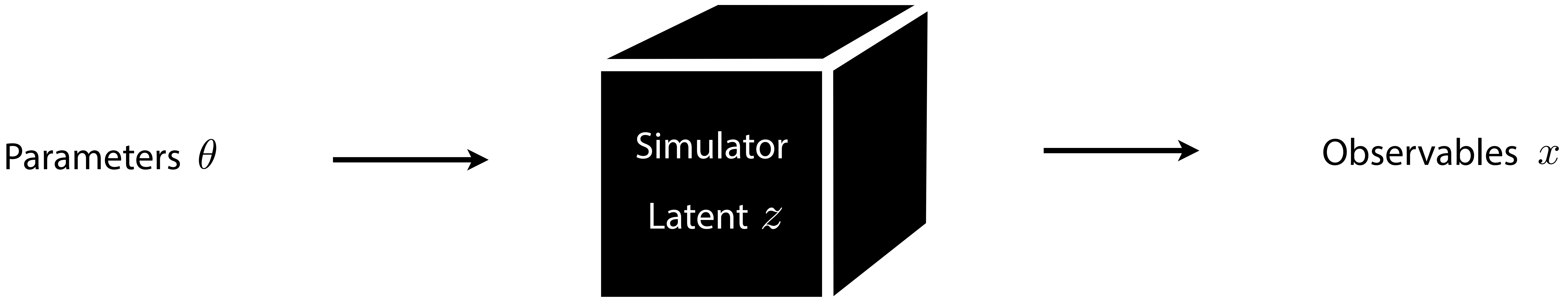
madminer.readthedocs.io





5. Beyond the LHC

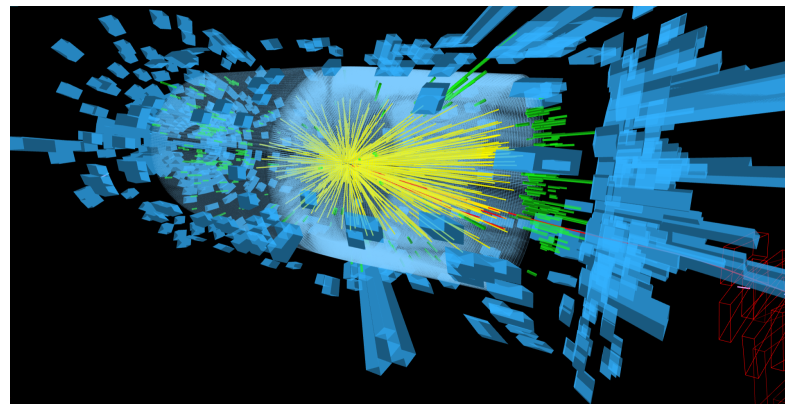
Simulation-based ("likelihood-free") inference problems…



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

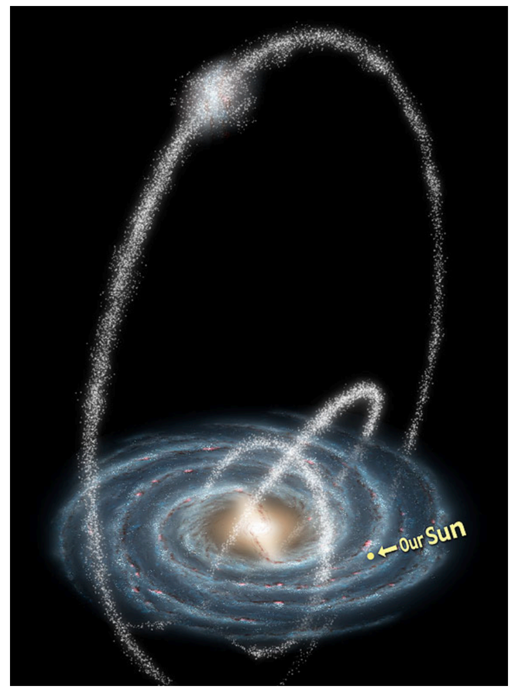
… appear in many fields of science



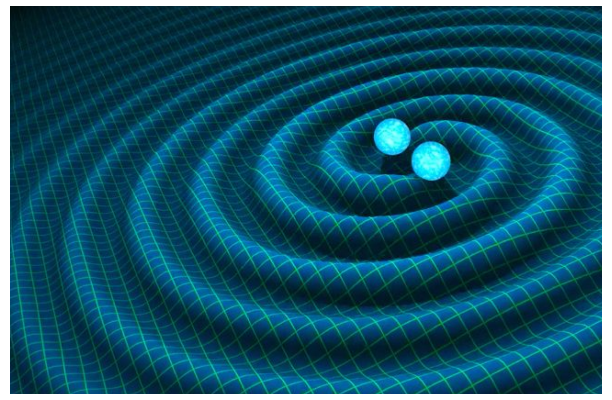
Collider experiments

[Ask me for image sources]

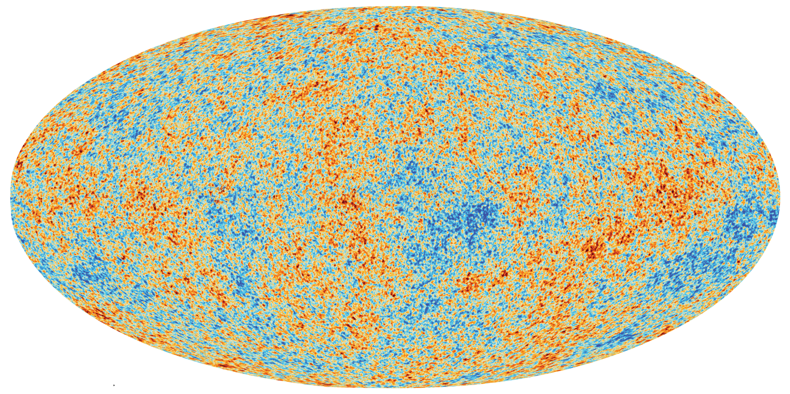
… appear in many fields of science



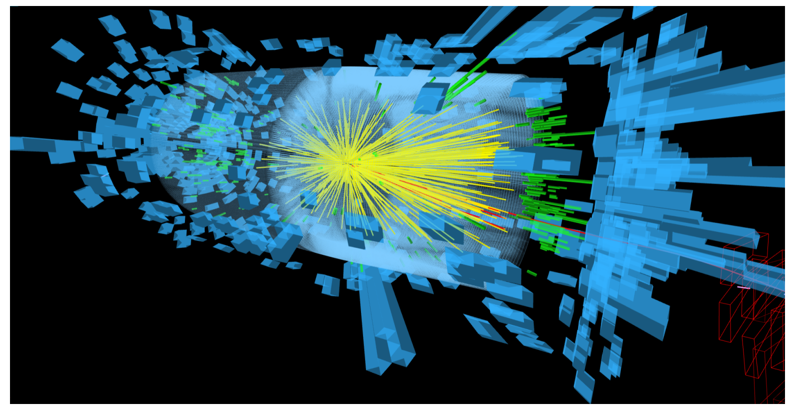
Stellar streams



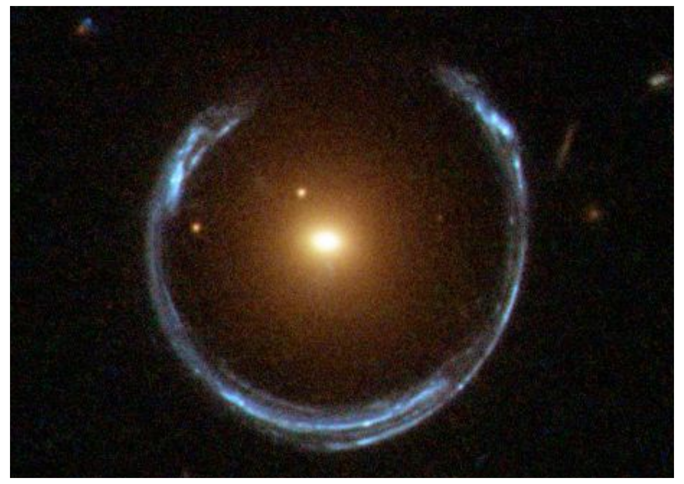
Gravitational waves



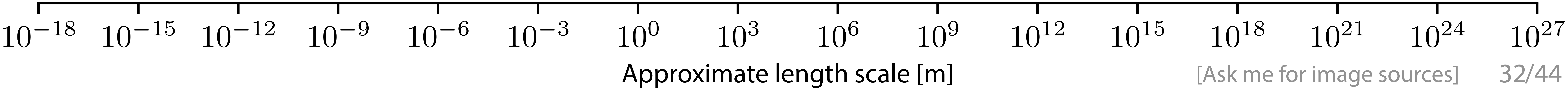
Evolution of the Universe



Collider experiments



Gravitational lensing

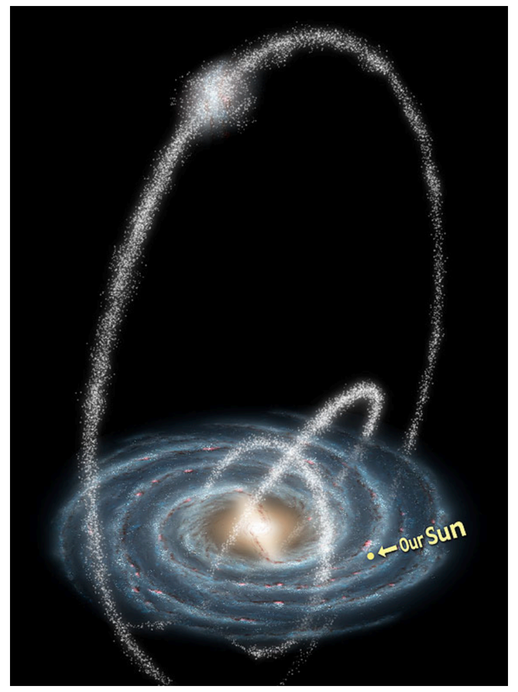


[Ask me for image sources]

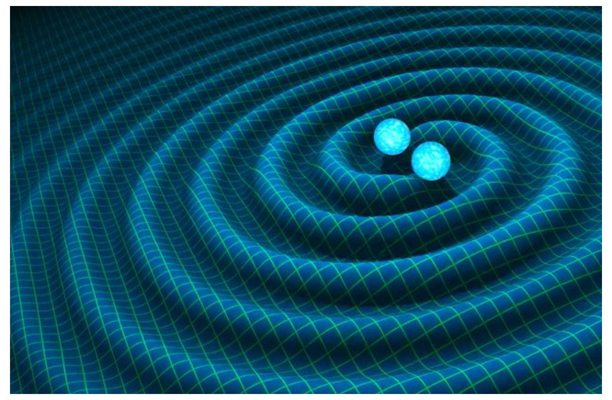
… appear in many fields of science

Chemical reactions

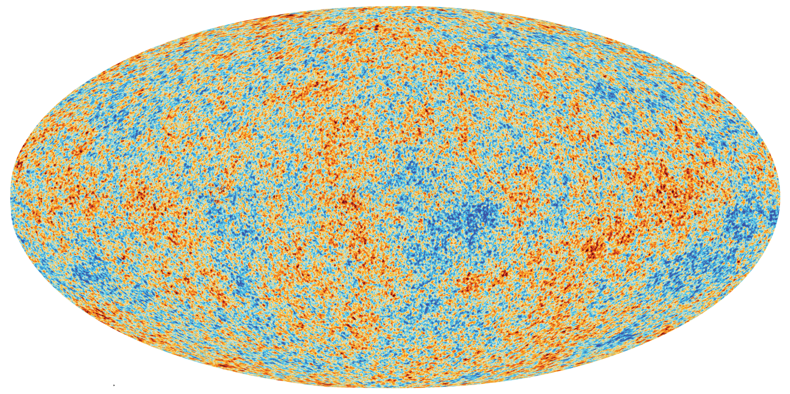
Flames



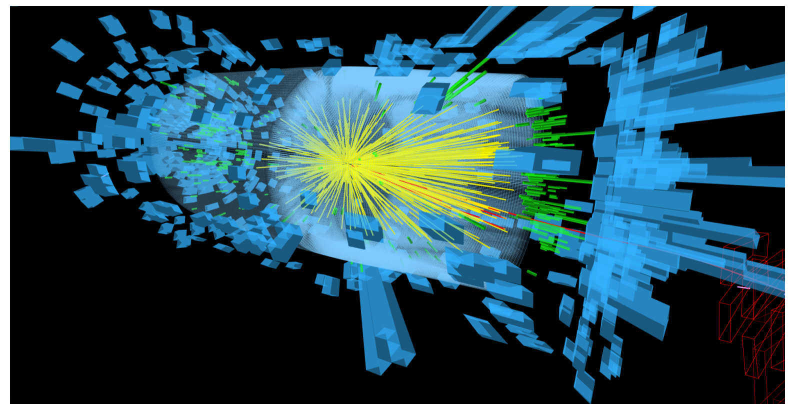
Stellar streams



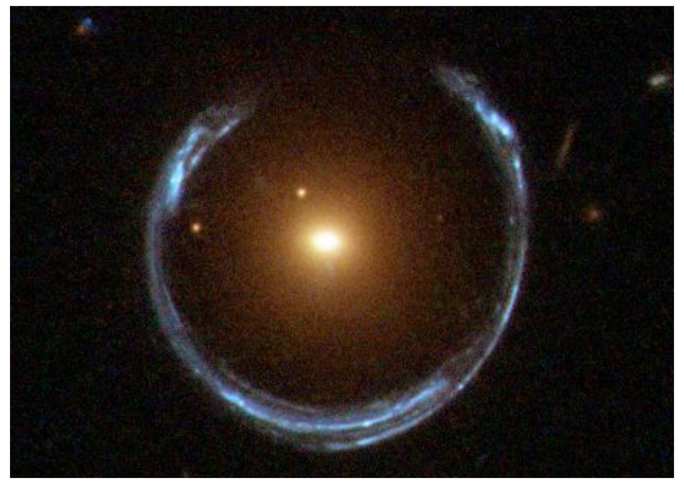
Gravitational waves



Evolution of the Universe



Collider experiments



Gravitational lensing

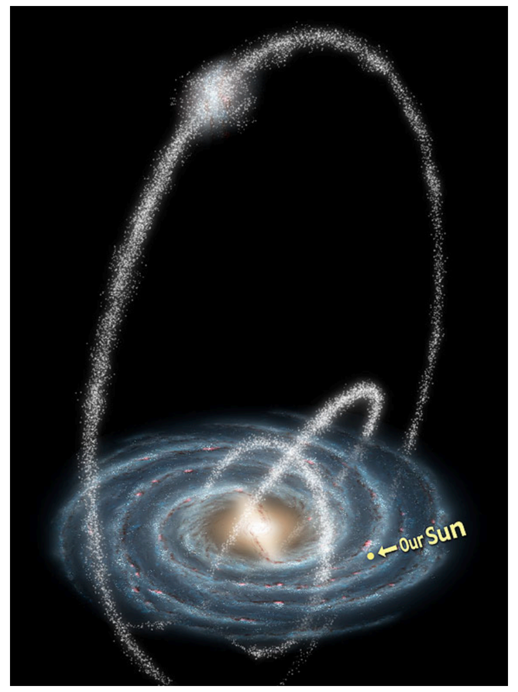
Approximate length scale [m]

[Ask me for image sources]

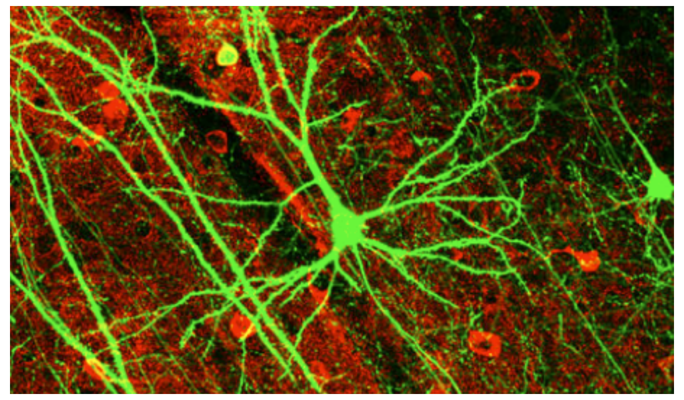
… appear in many fields of science

Chemical reactions

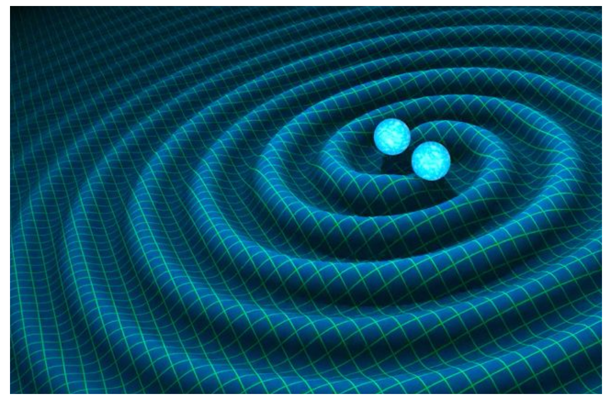
Flames



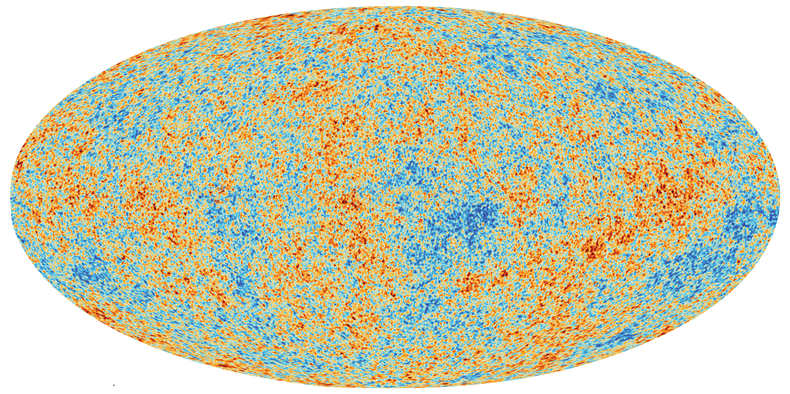
Stellar streams



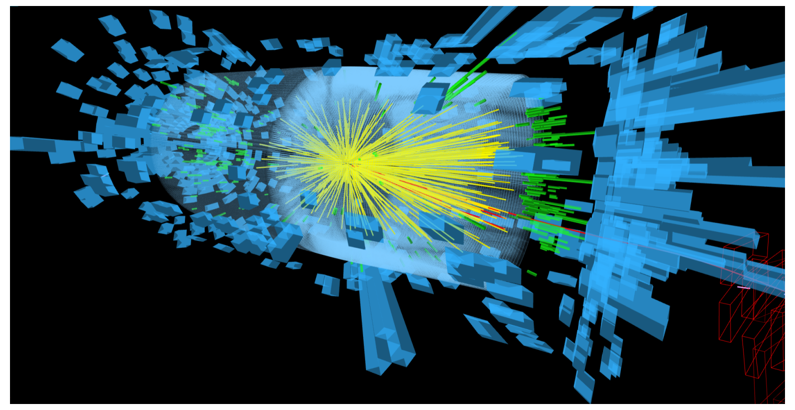
Neurons



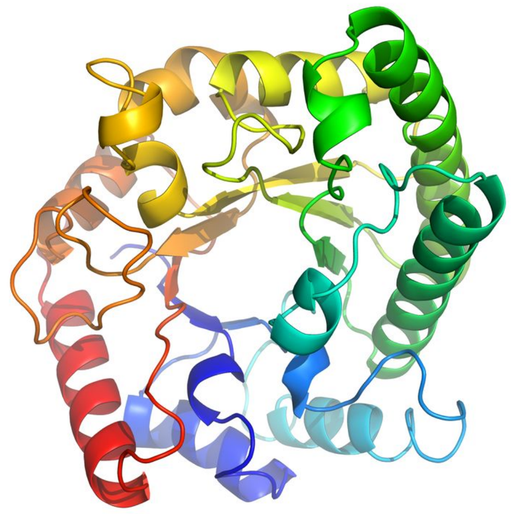
Gravitational waves



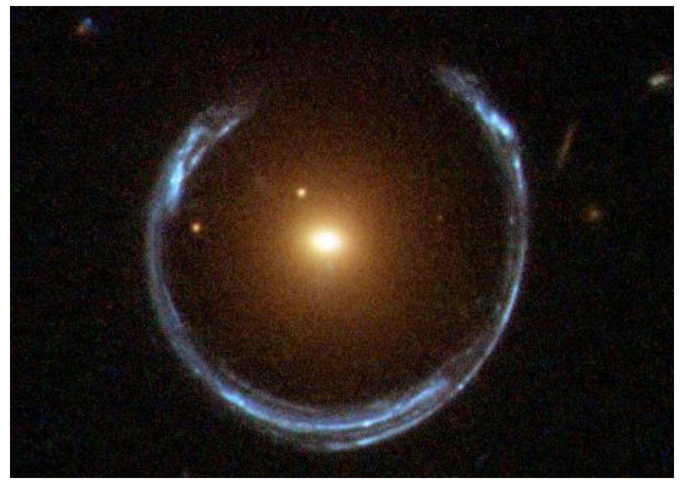
Evolution of the Universe



Collider experiments



Protein networks



Gravitational lensing

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

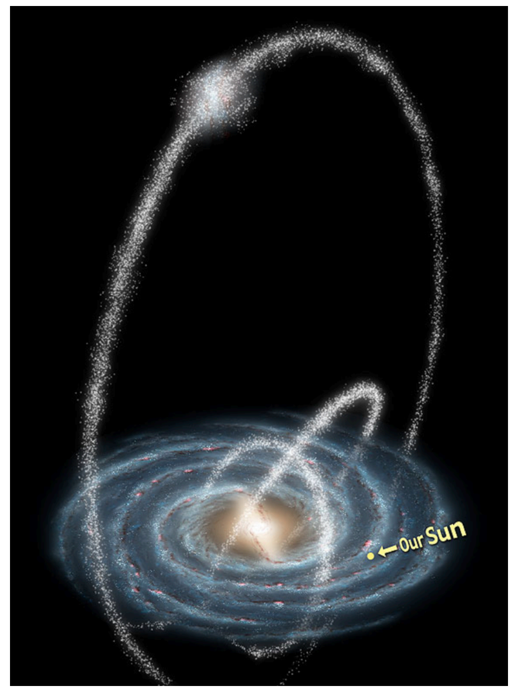
Approximate length scale [m]

[Ask me for image sources]

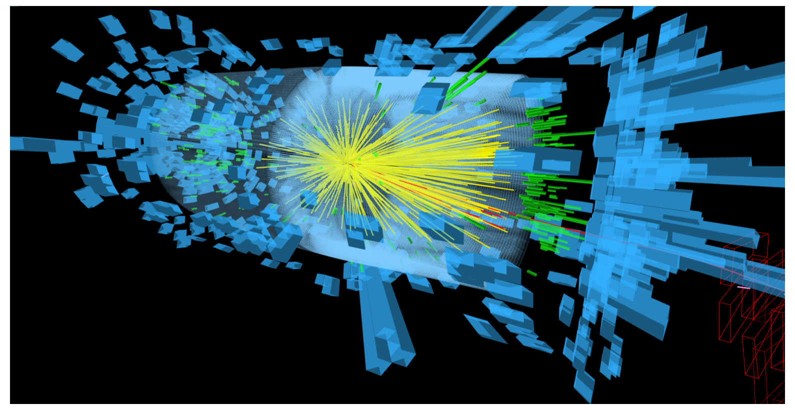
… appear in many fields of science

Chemical reactions

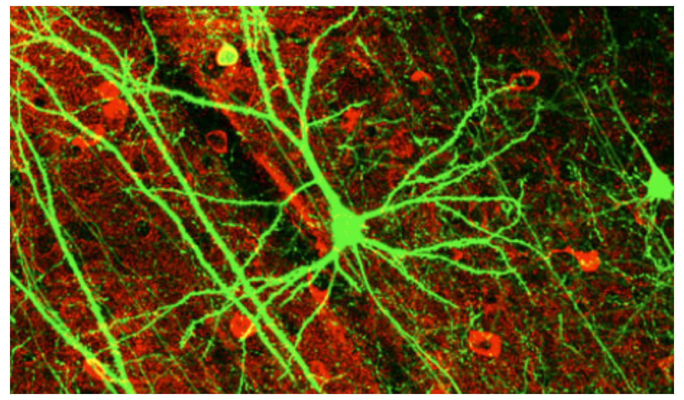
Flames



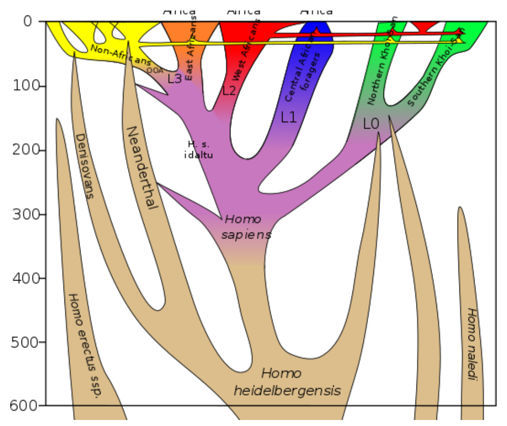
Stellar streams



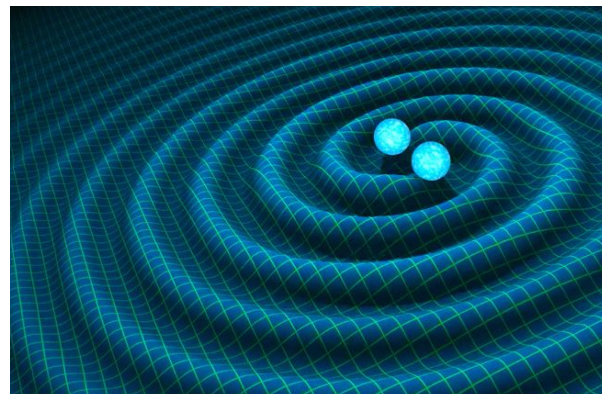
Collider experiments



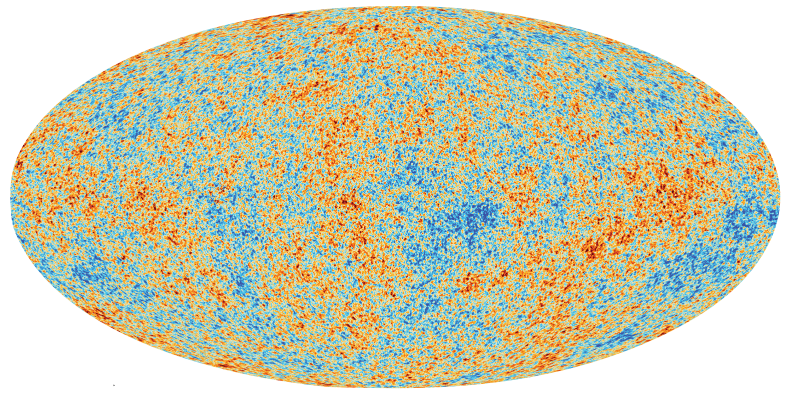
Neurons



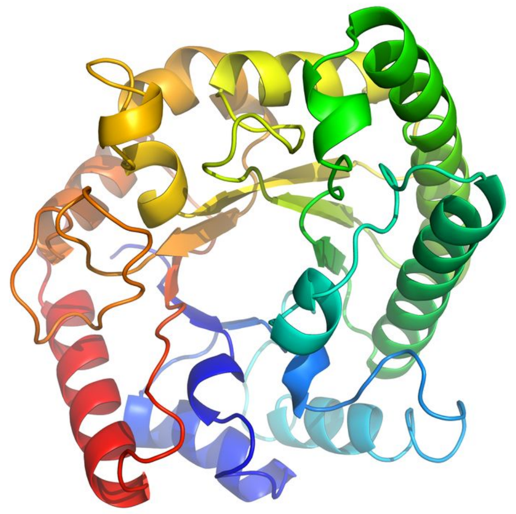
Evolution



Gravitational waves

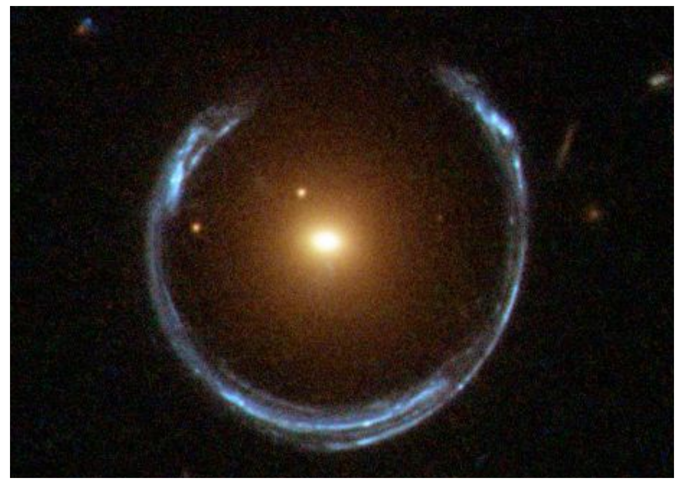


Evolution of the Universe



Protein networks

Ecological systems



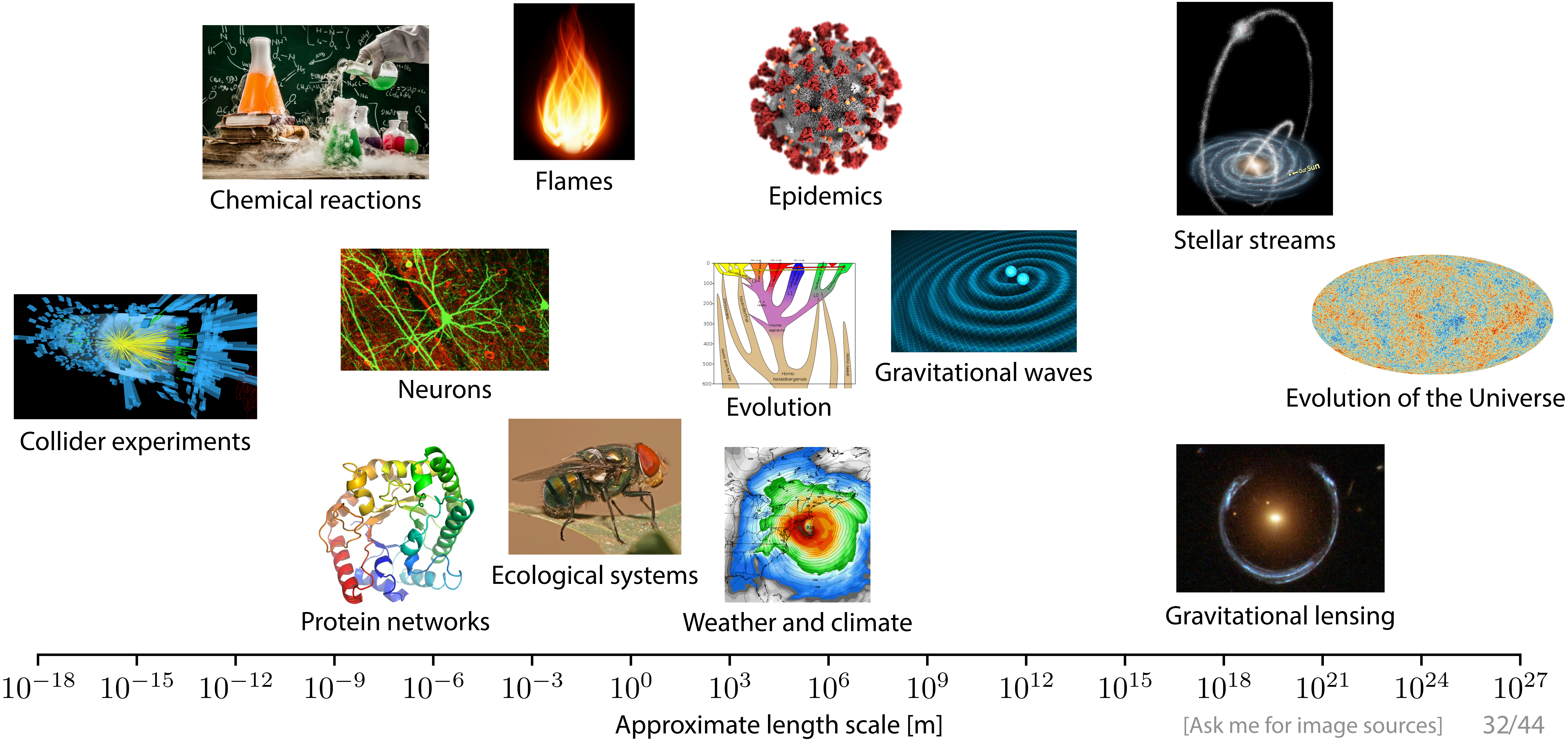
Gravitational lensing

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

Approximate length scale [m]

[Ask me for image sources]

… appear in many fields of science

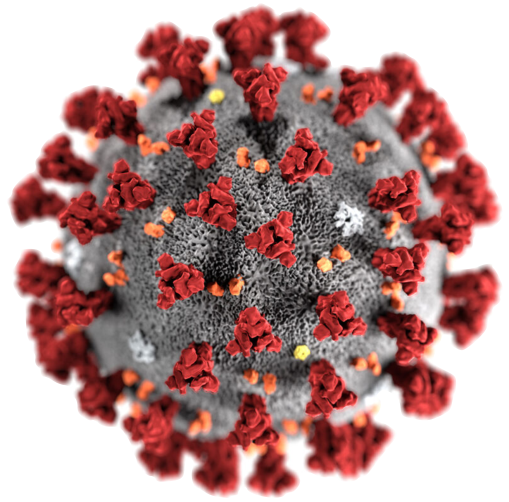


[Ask me for image sources]

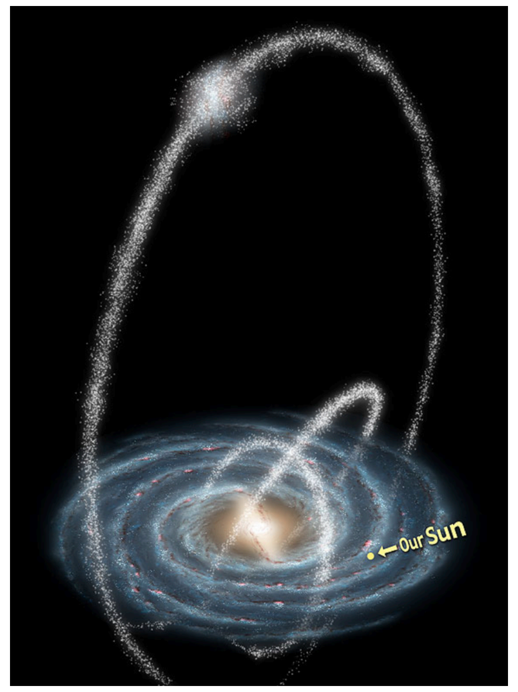
… appear in many fields of science

Chemical reactions

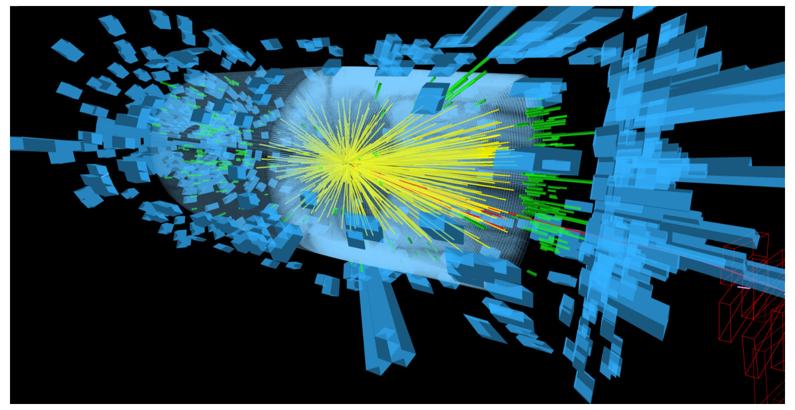
Flames



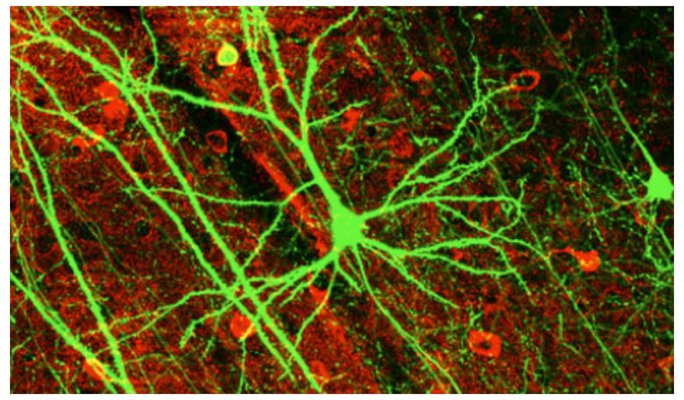
Epidemics



Stellar streams

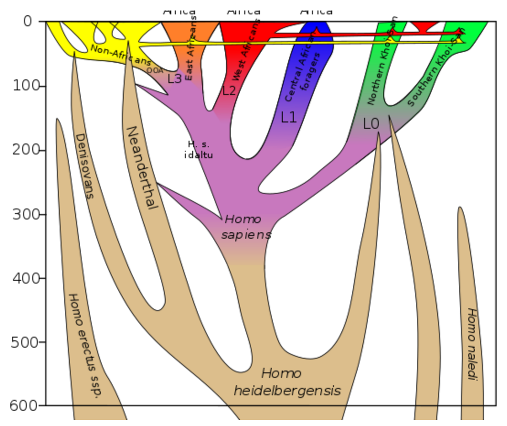


Collider experiments

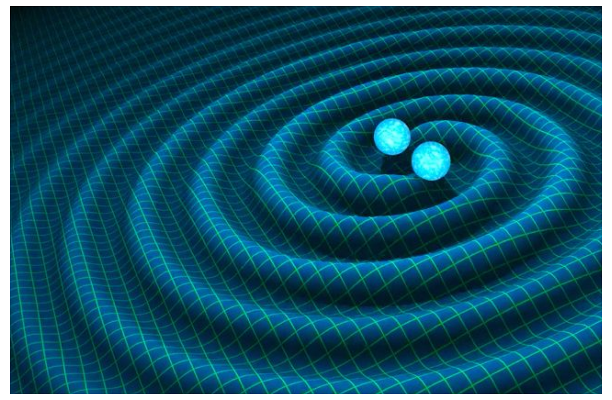


Neurons

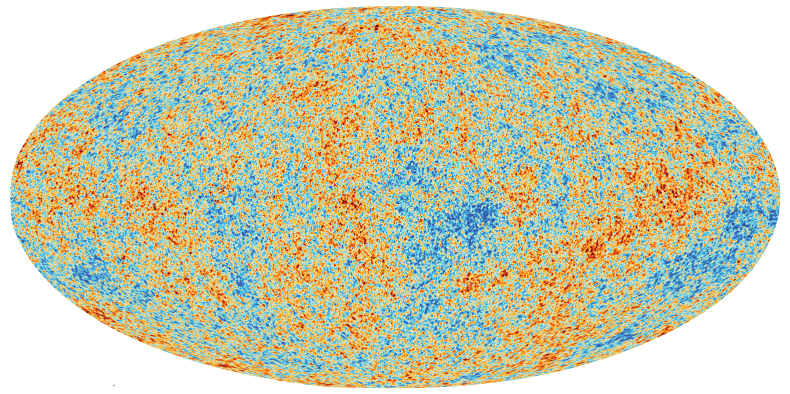
Robotics



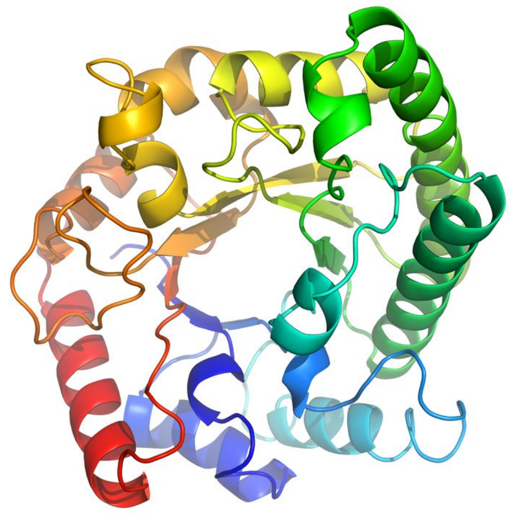
Evolution



Gravitational waves

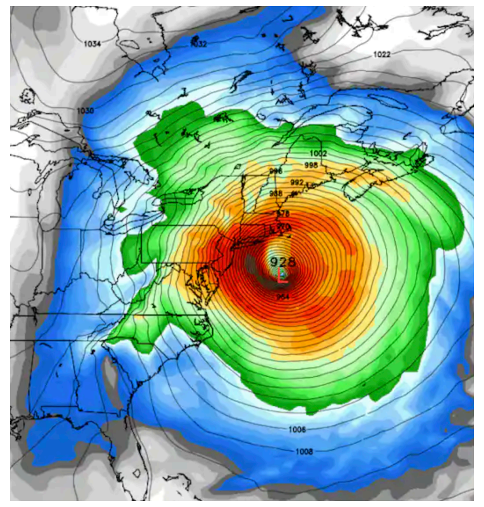


Evolution of the Universe

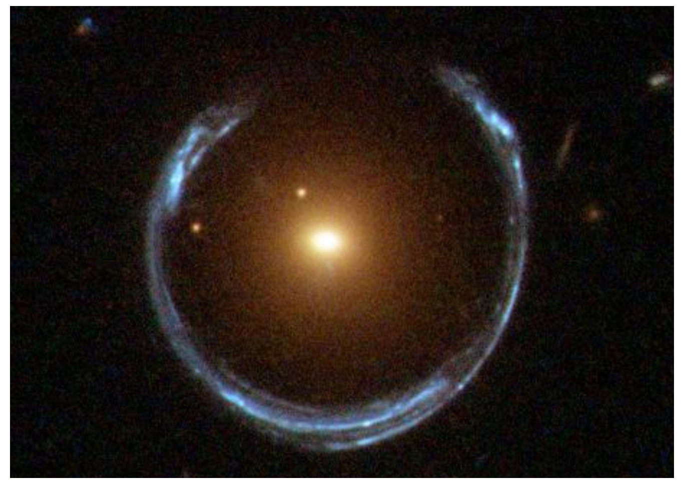


Protein networks

Ecological systems



Weather and climate



Gravitational lensing

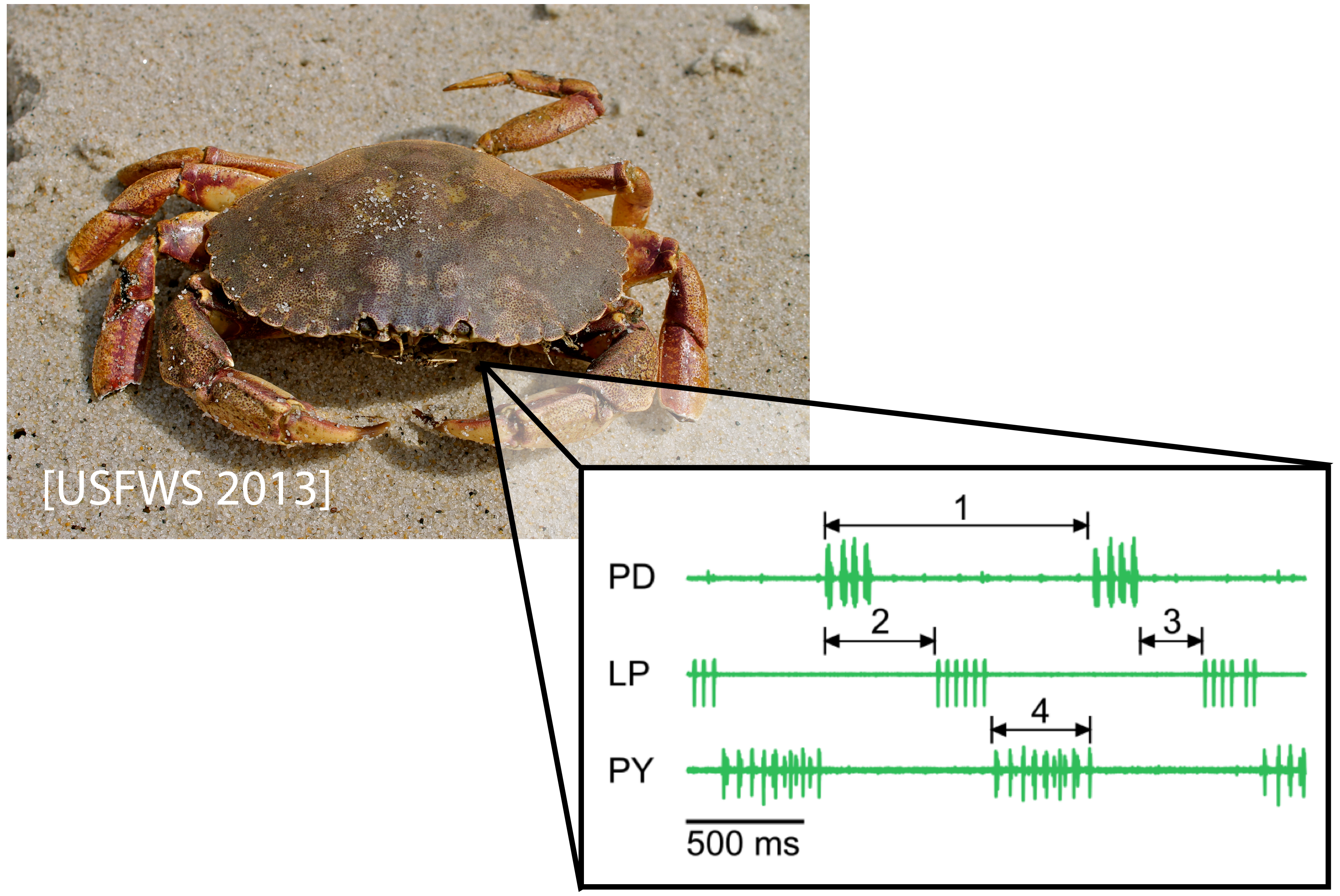
10^{-18} 10^{-15} 10^{-12} 10^{-9} 10^{-6} 10^{-3} 10^{0} 10^{3} 10^{6} 10^{9} 10^{12} 10^{15} 10^{18} 10^{21} 10^{24} 10^{27}

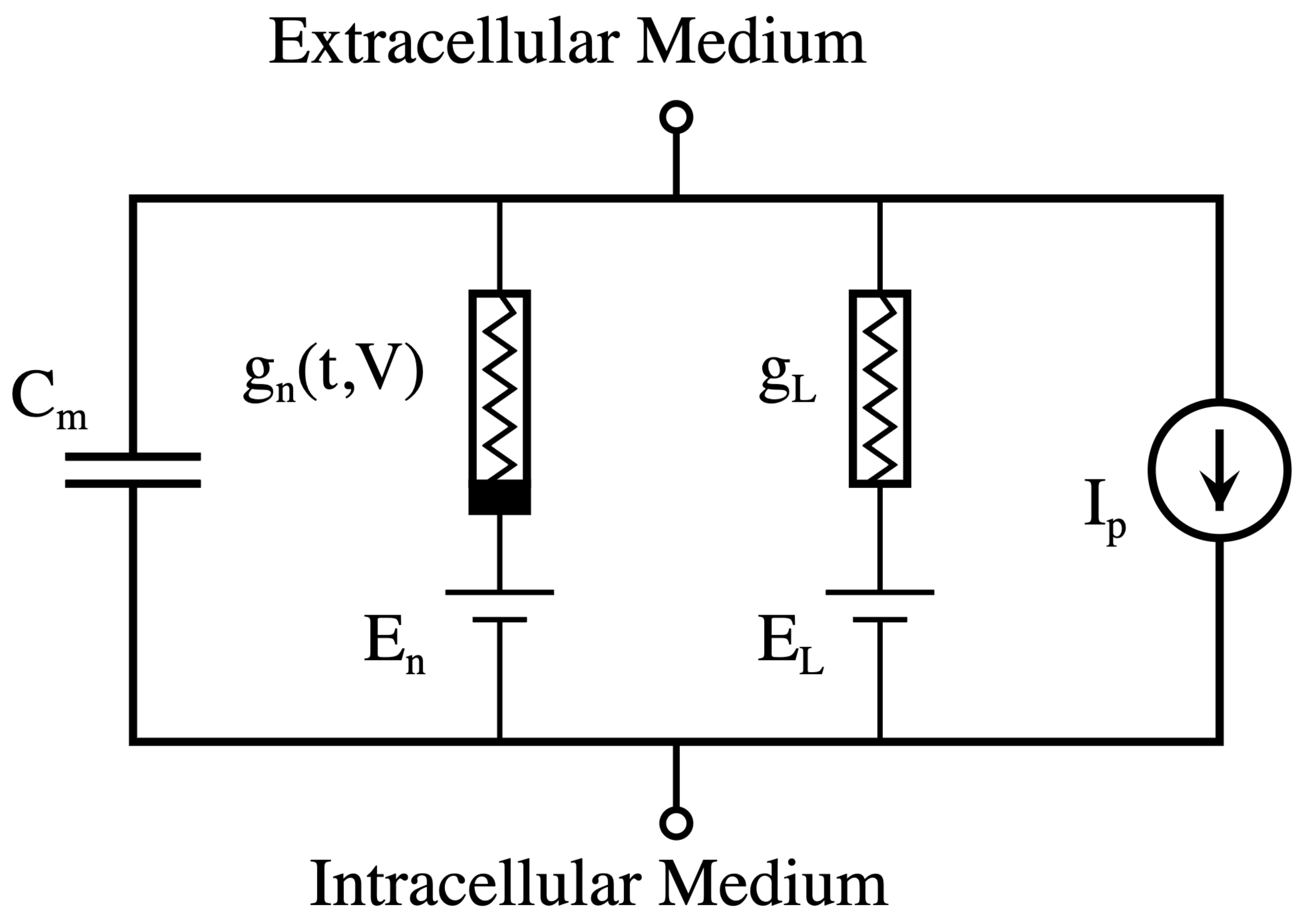
Approximate length scale [m]

[Ask me for image sources]

Neuroscience example

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



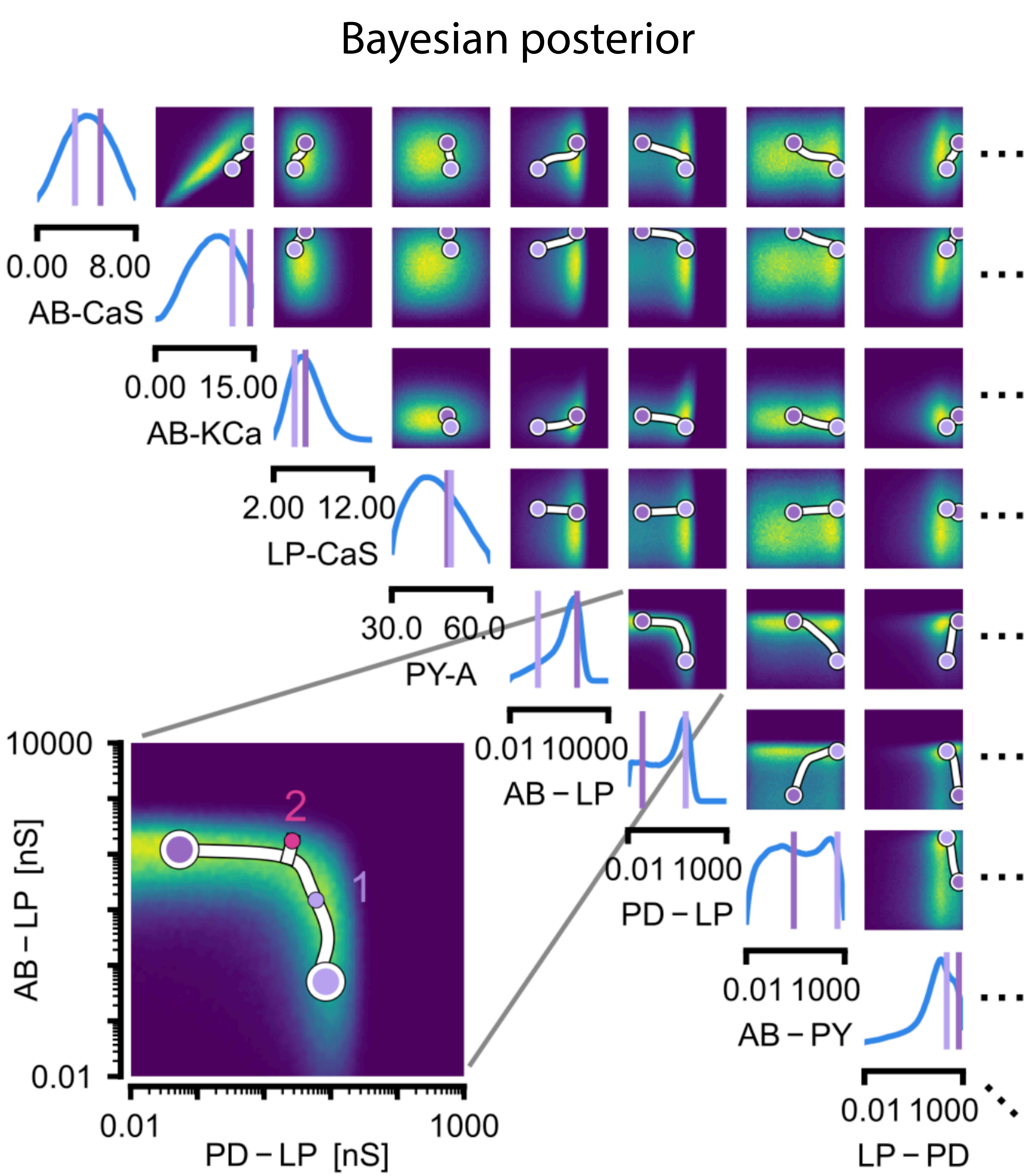


Activity recordings in stomatogastric ganglion nerve cells in Jonah Crabs

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

Crab results

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



Gravitational lensing example

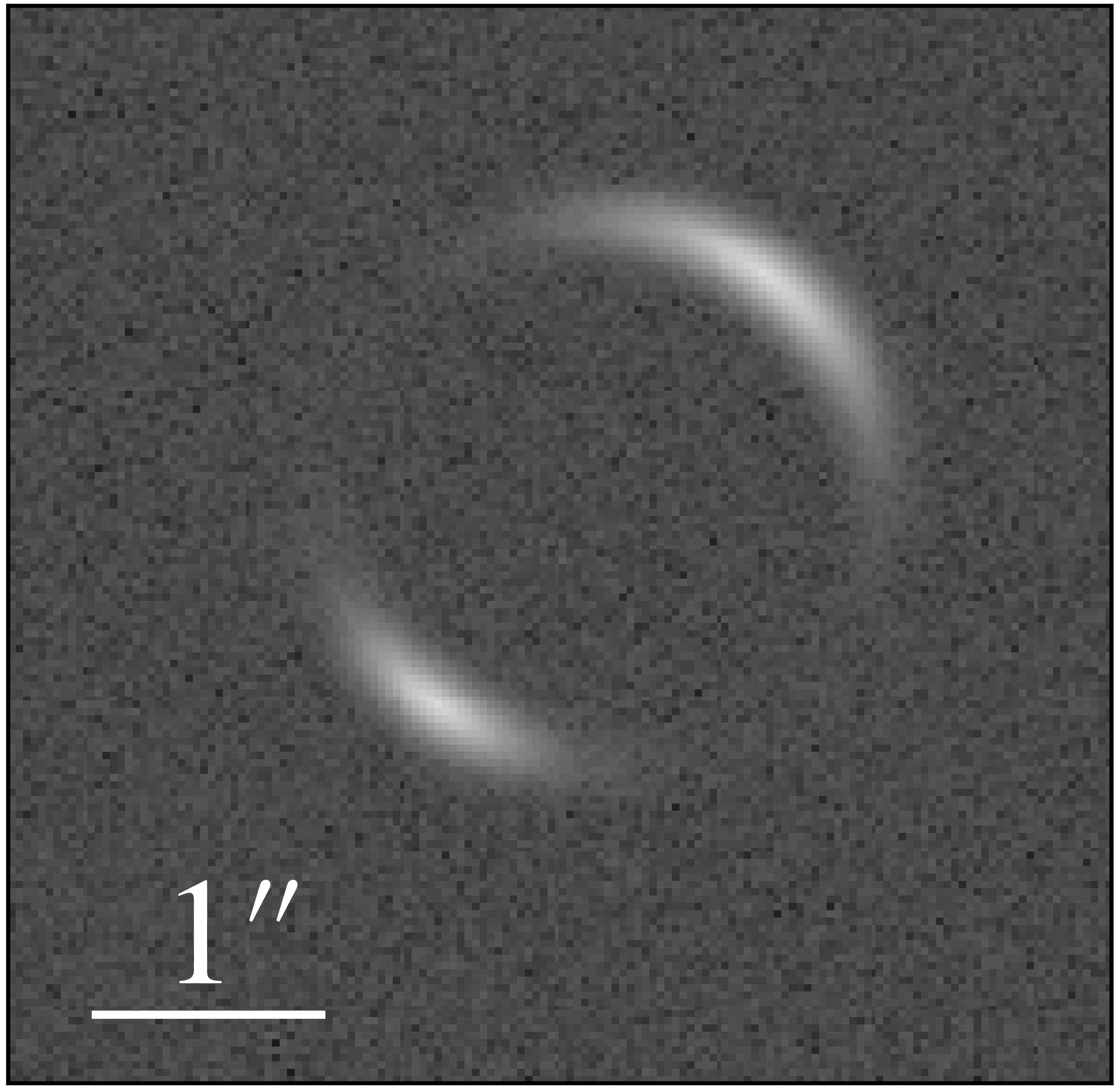
[T. Brown, J.Tumlinson]

[NASA/ESA; Abe Books]


[Hubble Space Telescope]

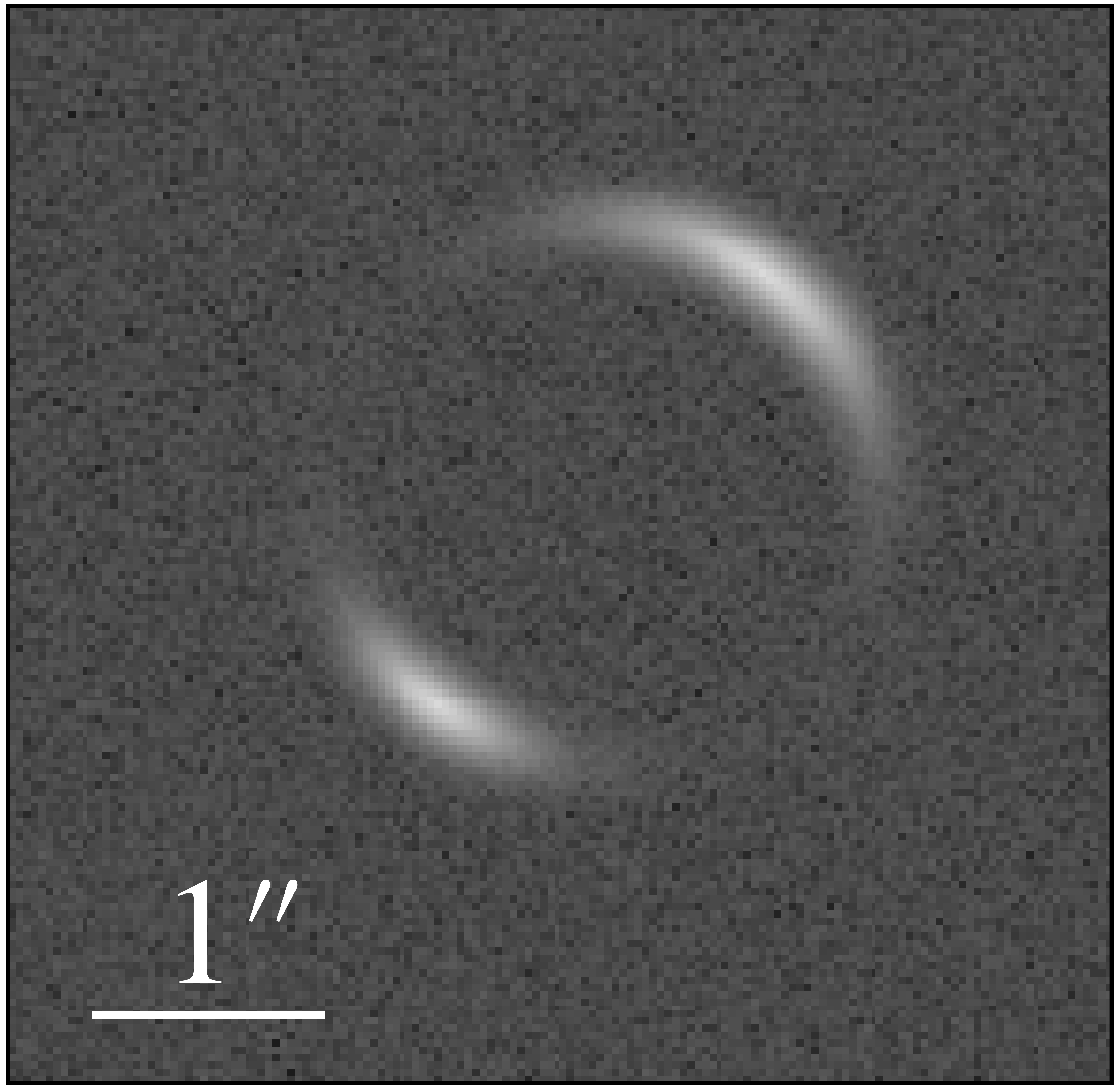
Subhalos affect strong lensing

Smooth halo only

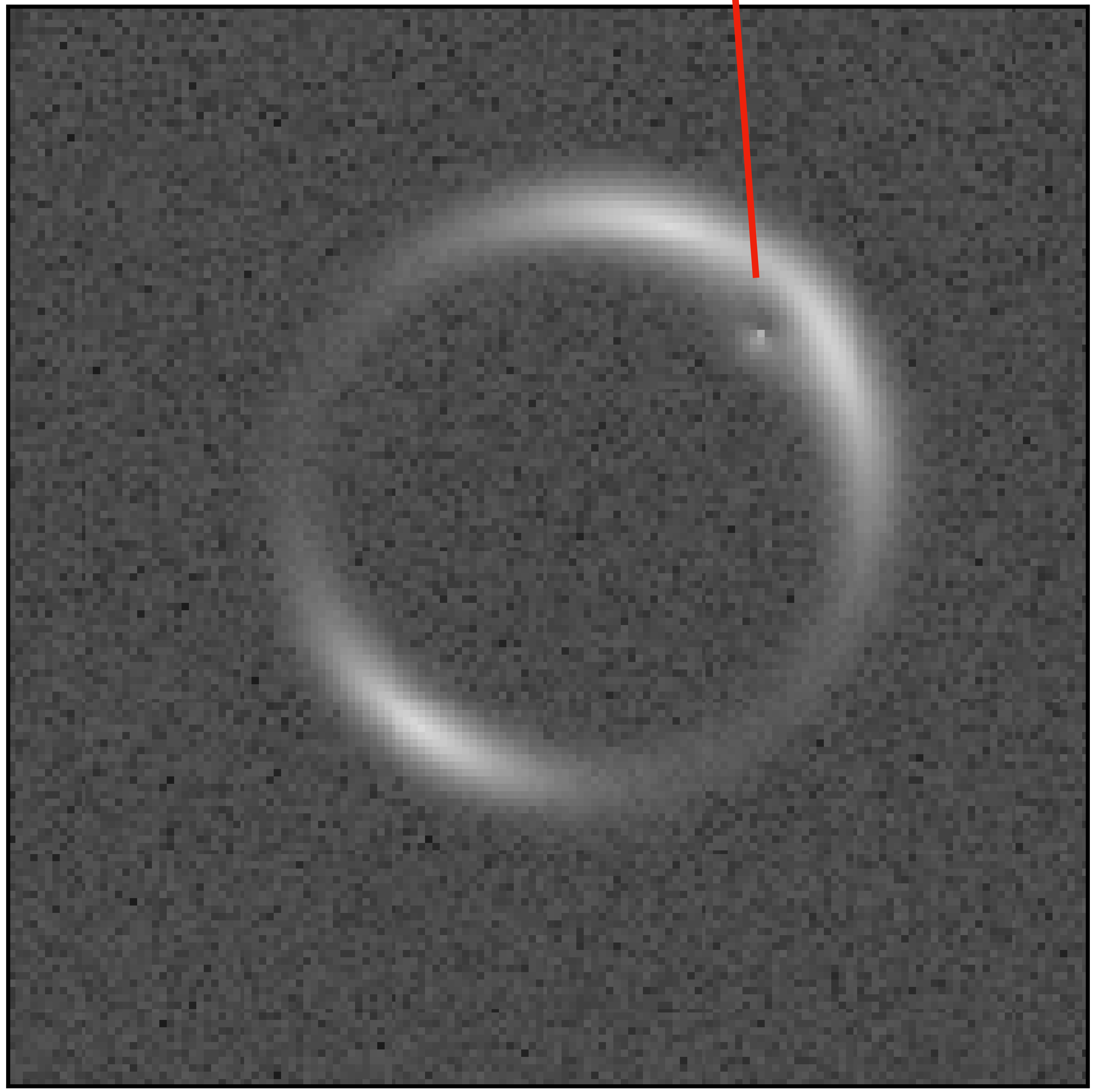


Subhalos affect strong lensing

Smooth halo only

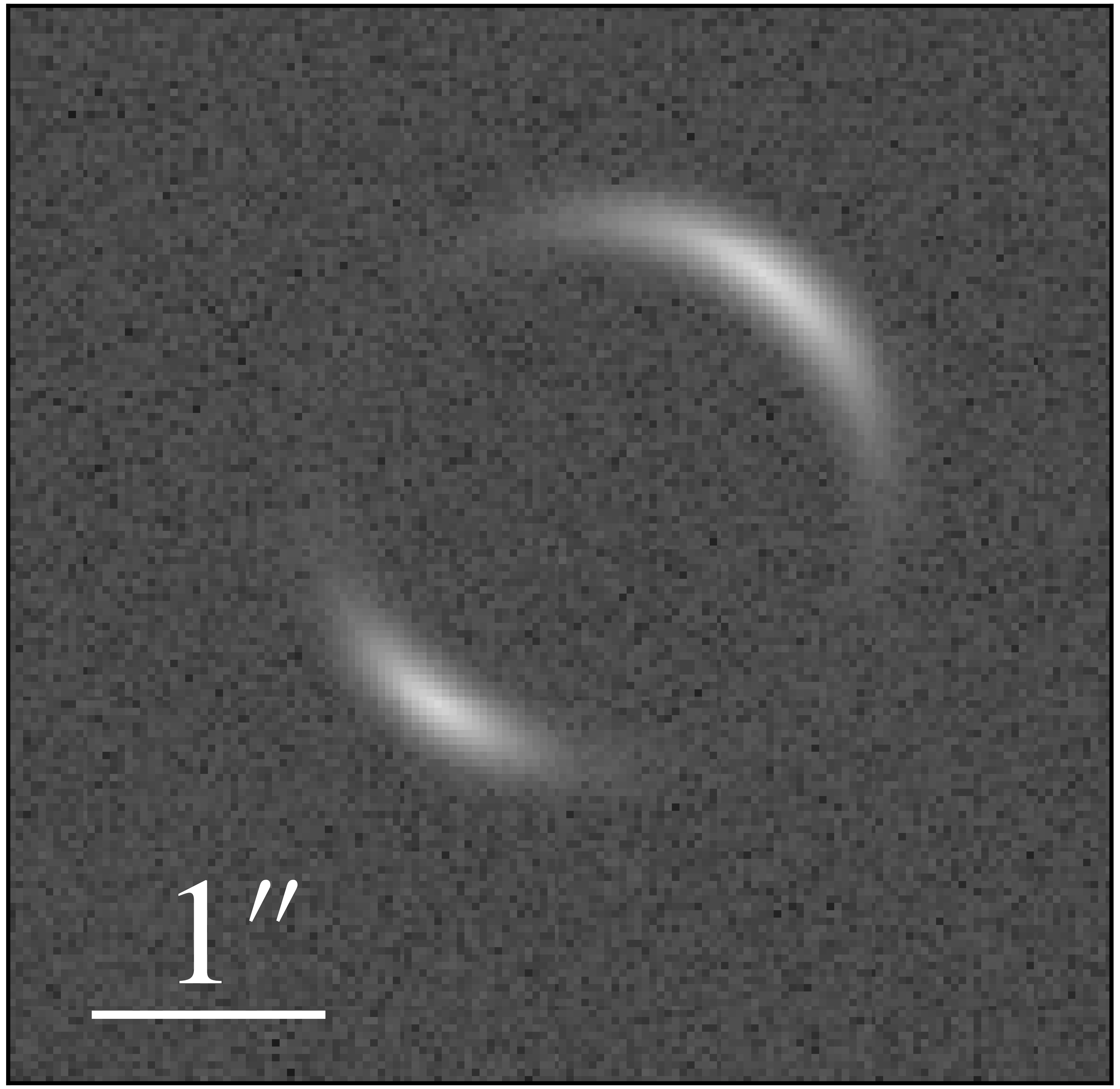


Smooth halo + subhalo

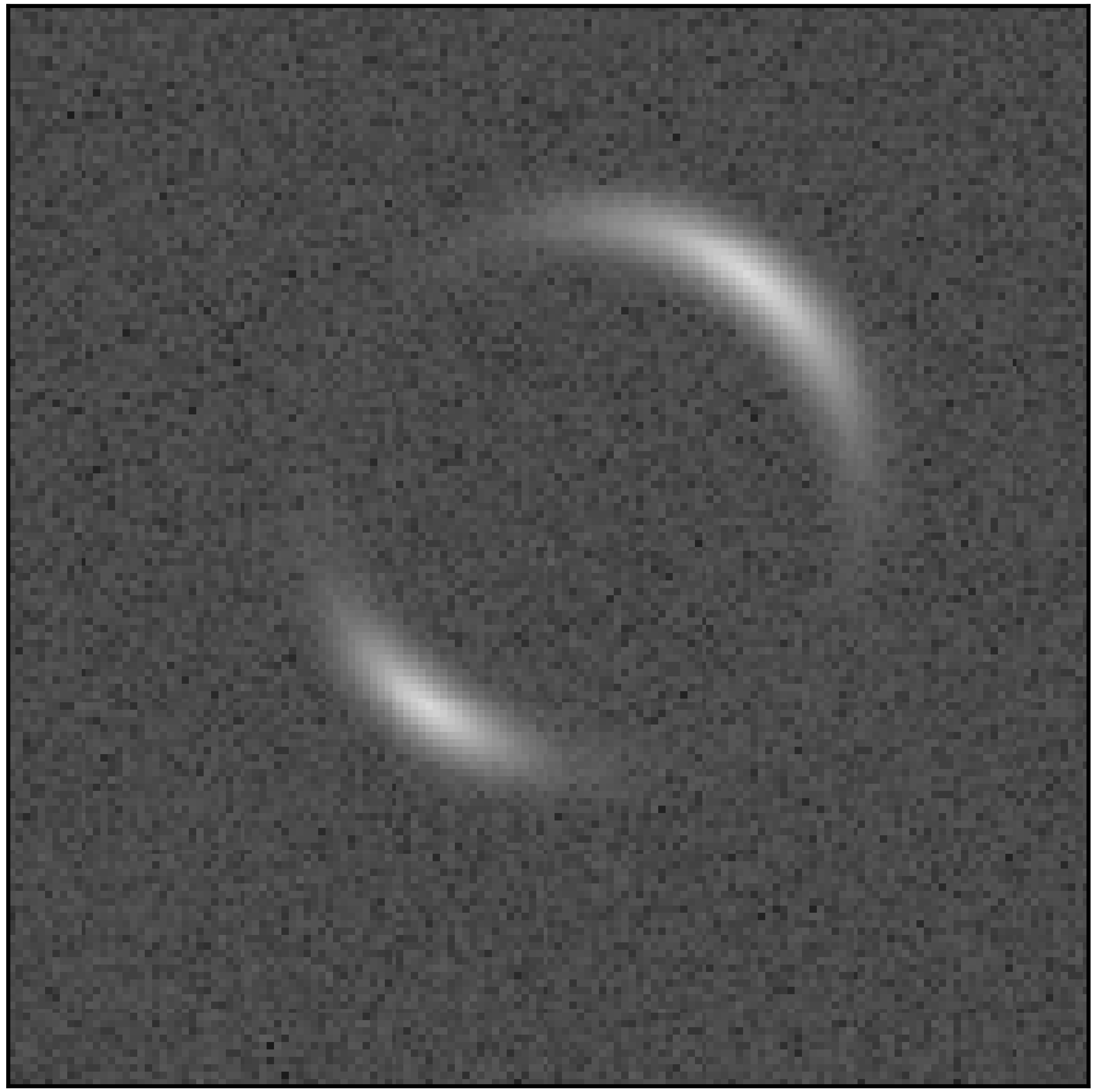


Subhalos affect strong lensing… realistically

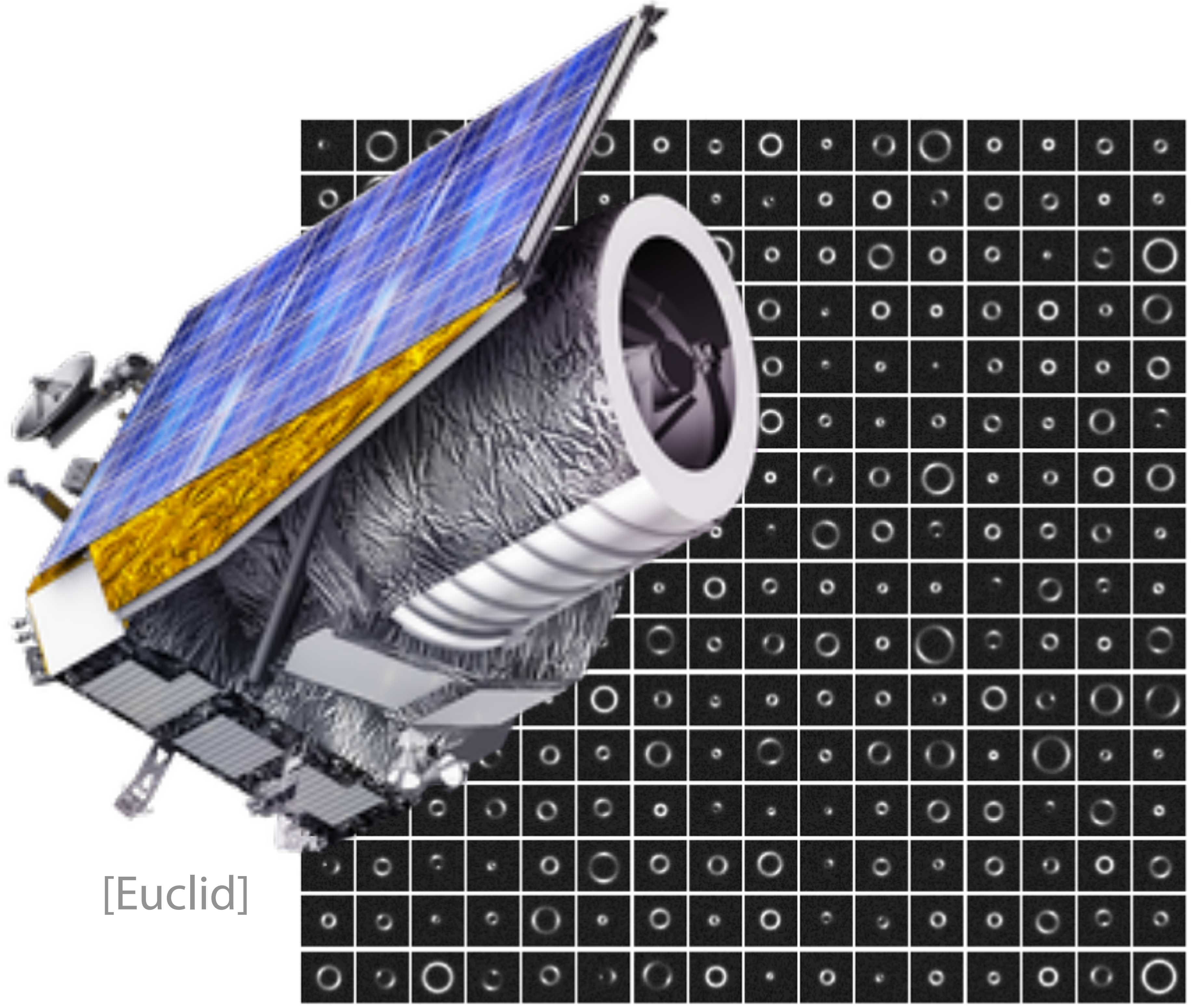
Smooth halo only

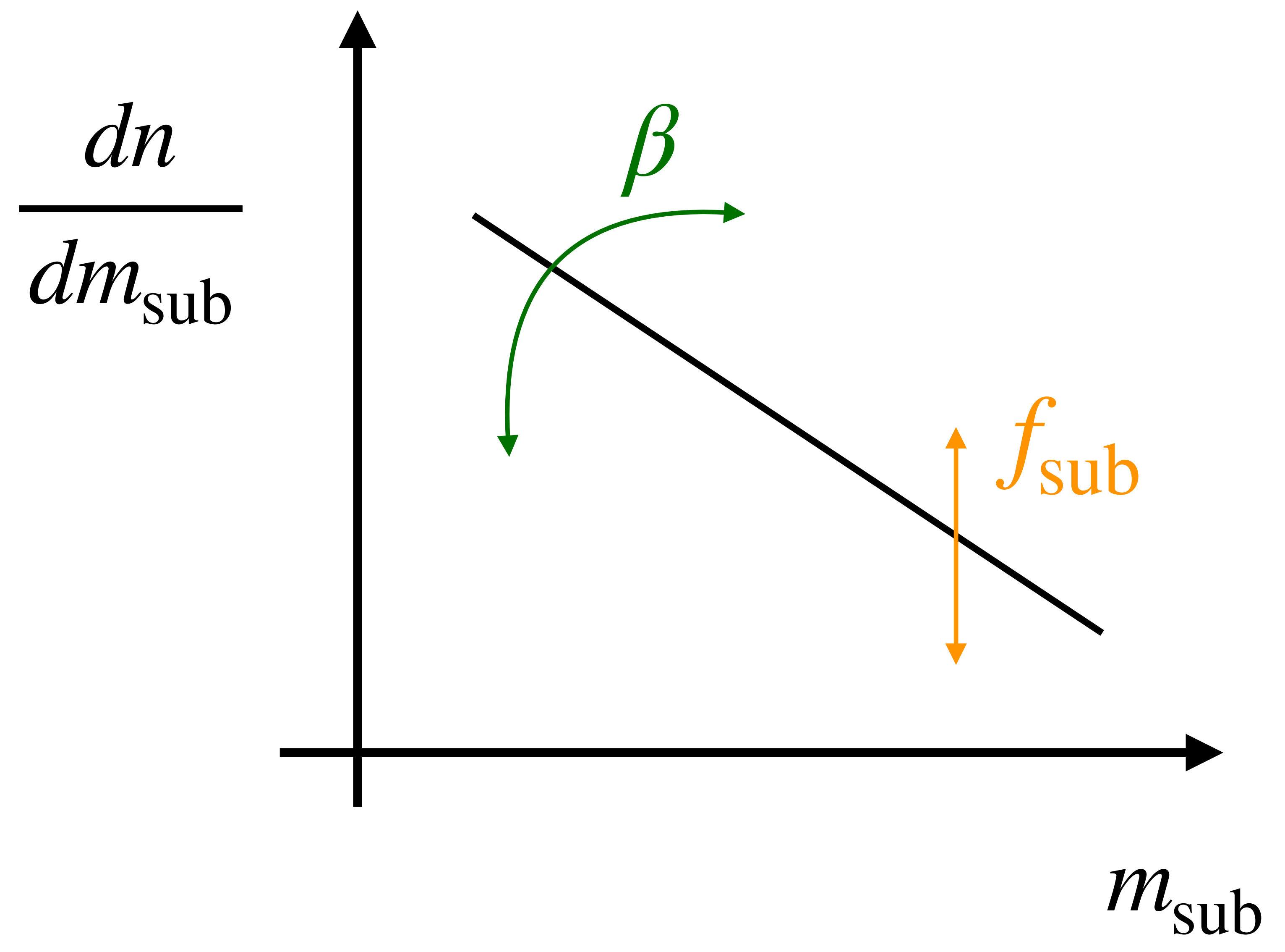


Smooth halo + subhalos



Scalable inference for small subhalos



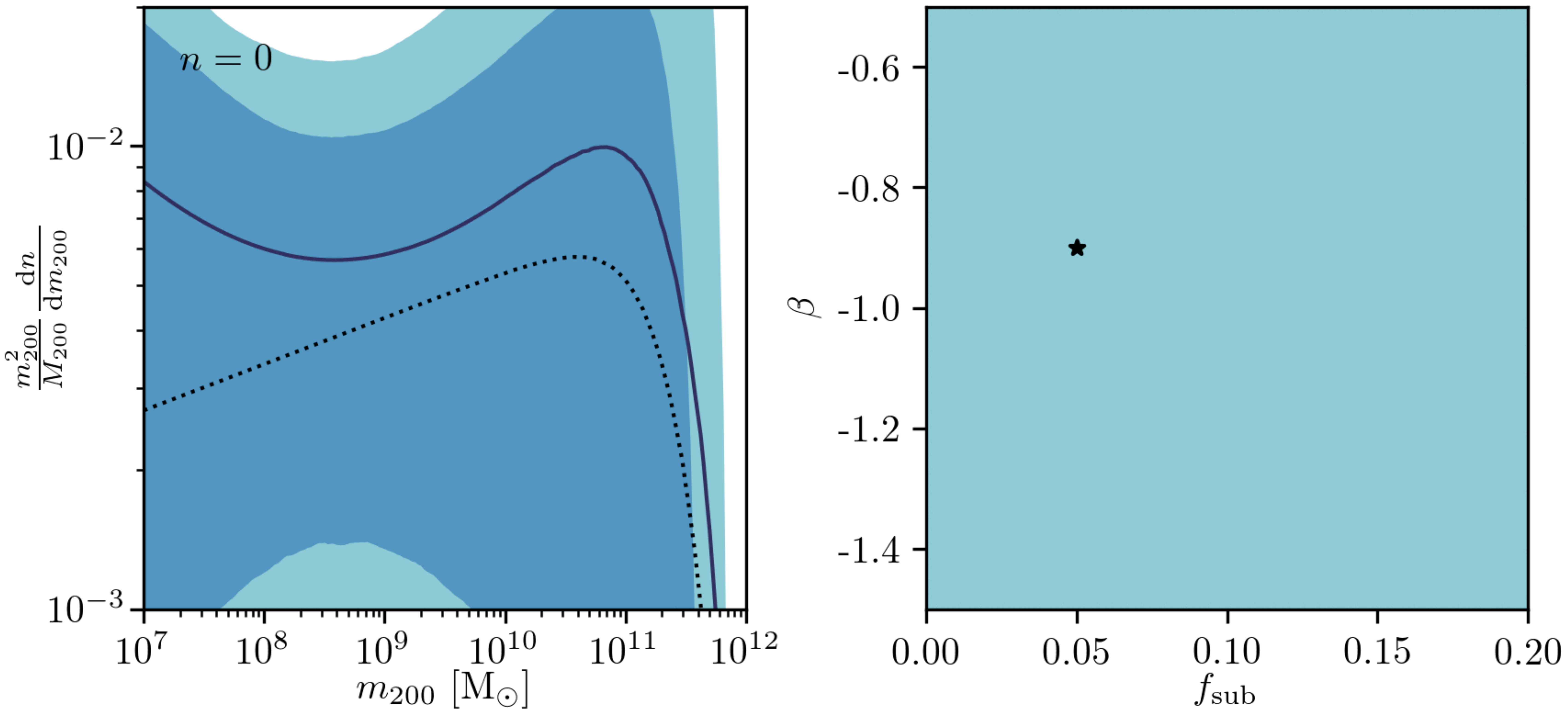


Near-future telescopes and satellites will collect hundreds of lensing images [Collett et al 1507.02657]

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

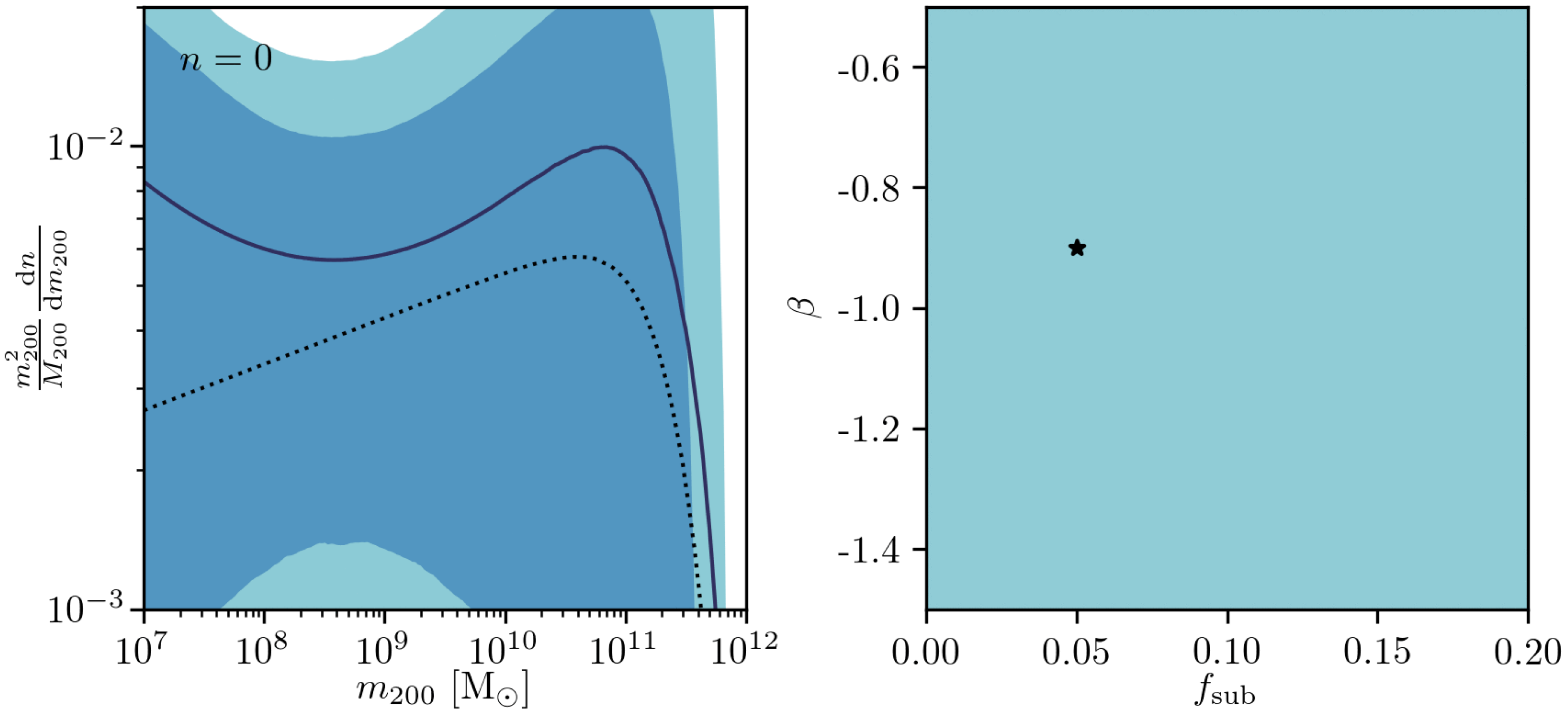
ML-based Bayesian inference

[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

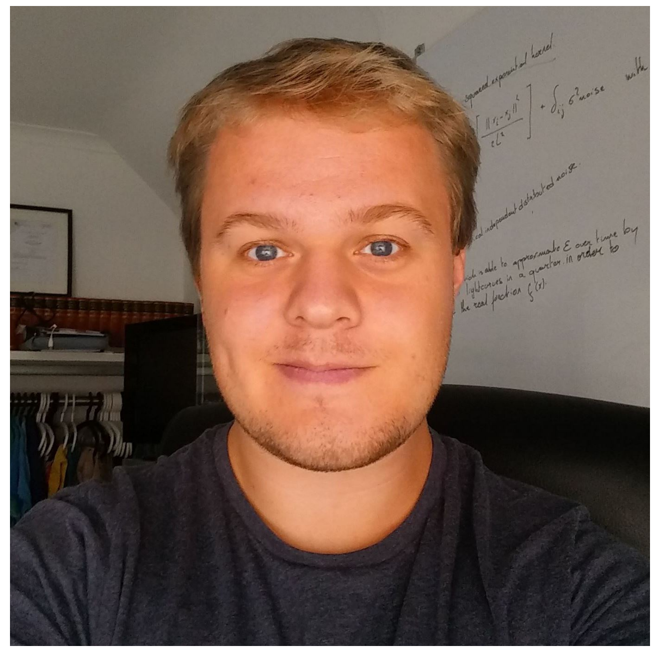

Markus Stoye


Felix Kling

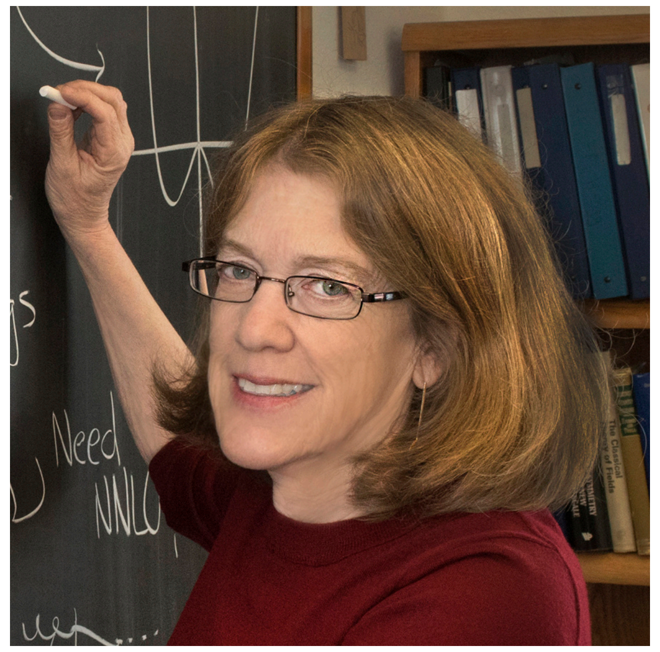

Irina Espejo


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

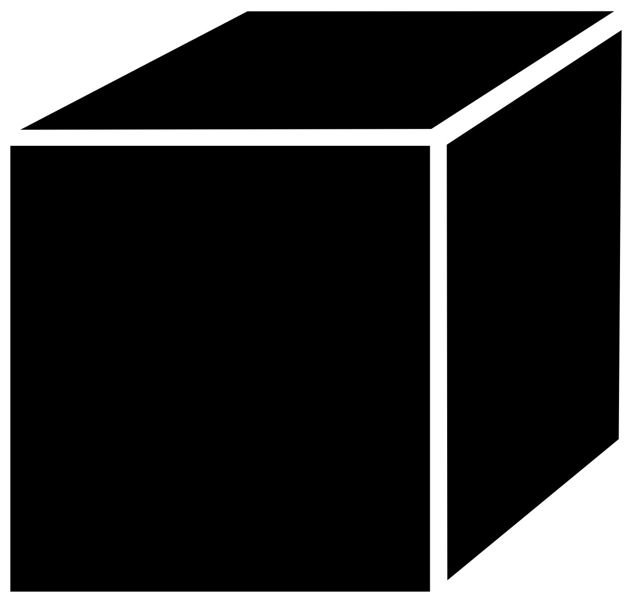
NYU

MSDSE
Moore - Sloan
Data Science Environments

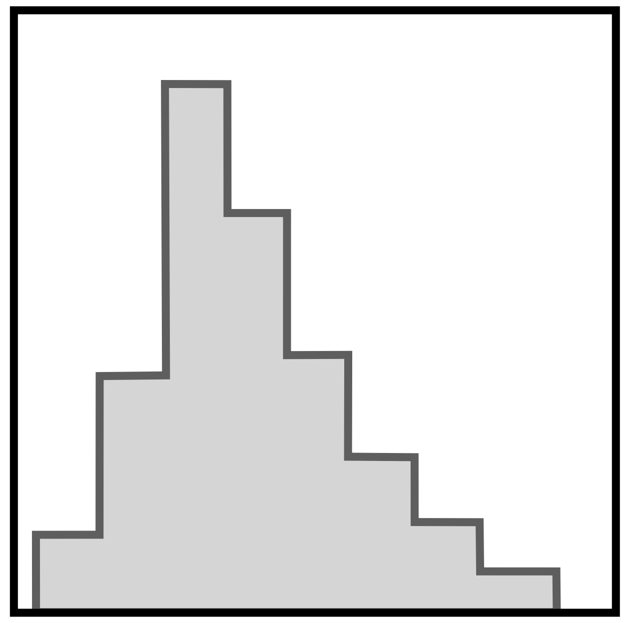
dianahep

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

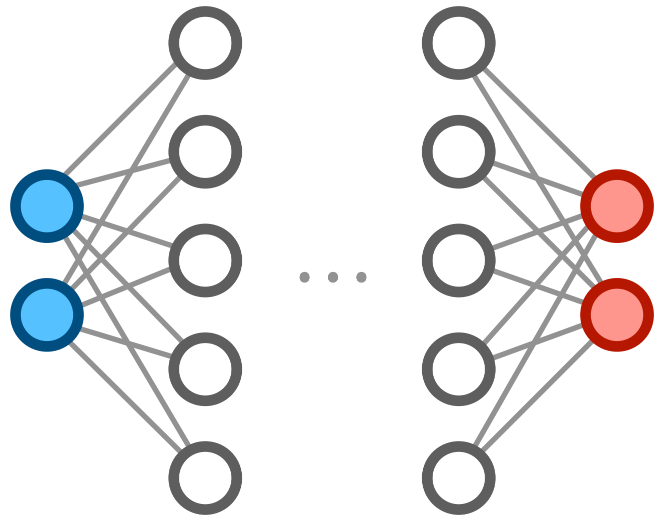
The SCAILFIN Project
scailfin.github.io



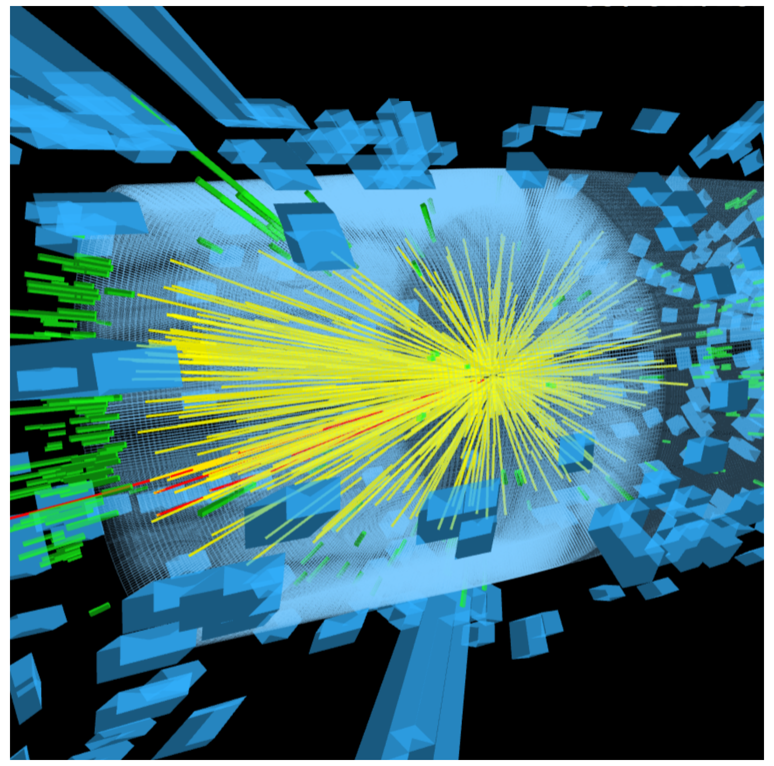
Simulators make precise predictions, but inference is challenging.



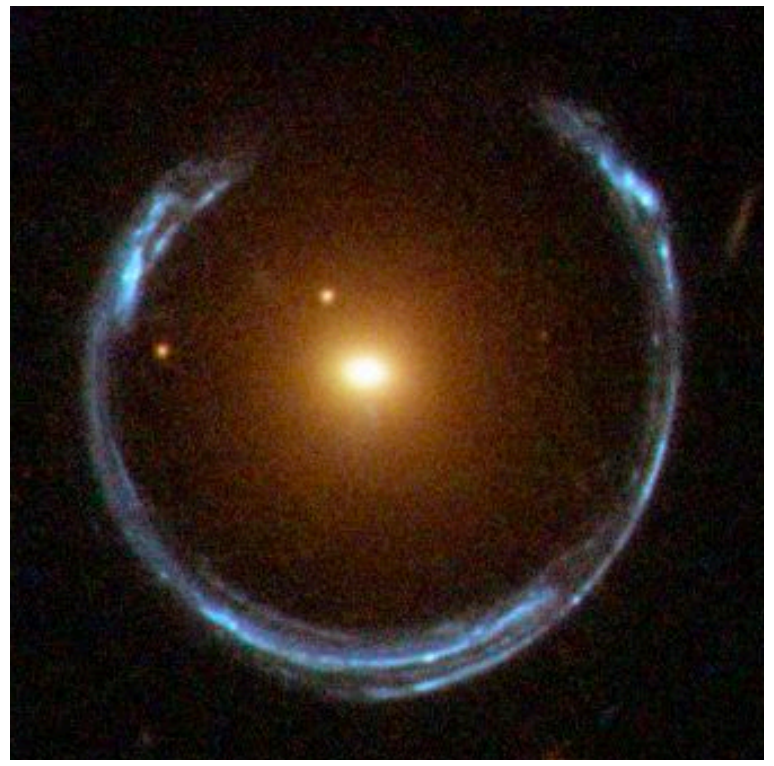
Scientists have side-stepped this problem with summary statistics.



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

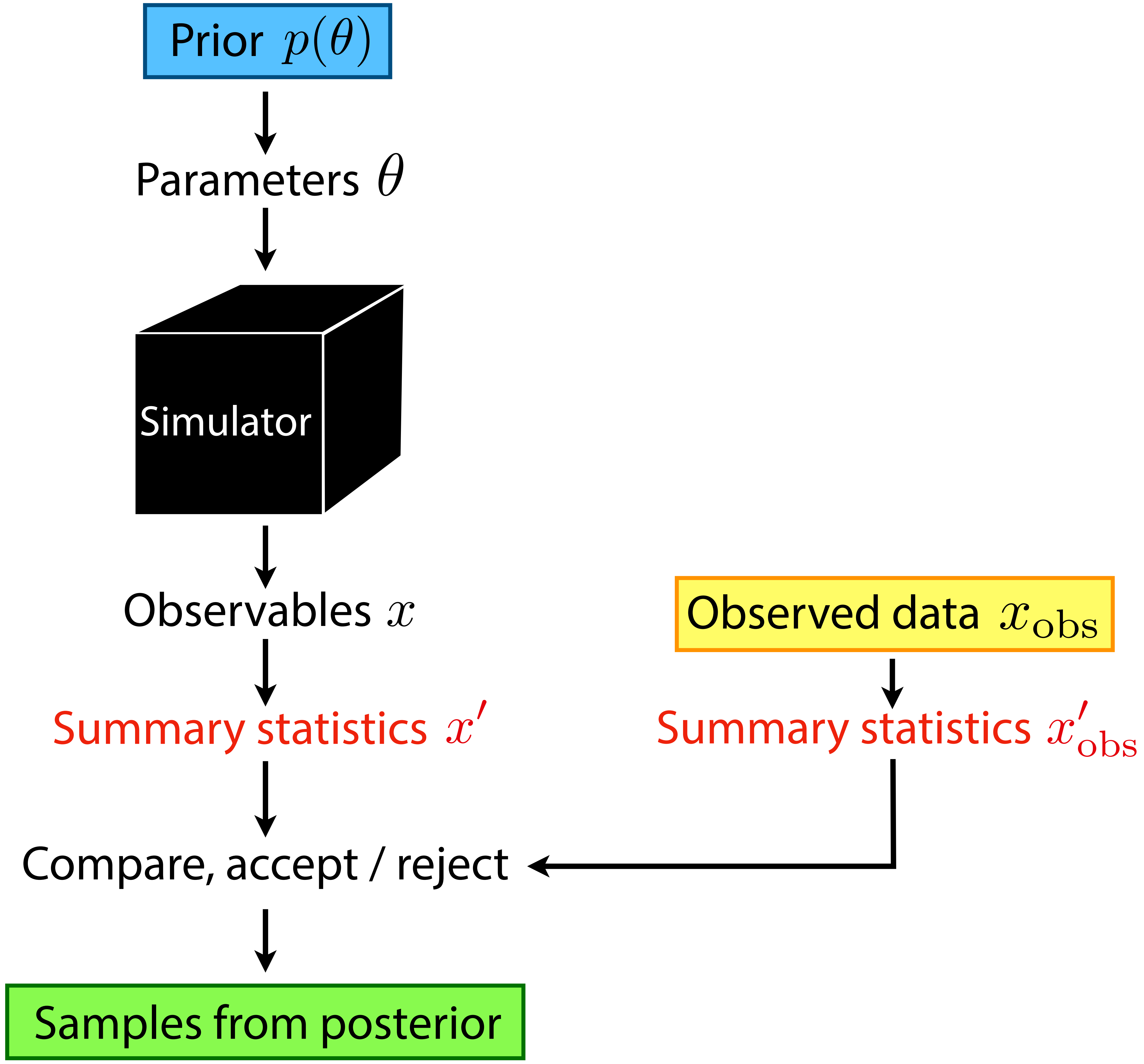
Astrophysics

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

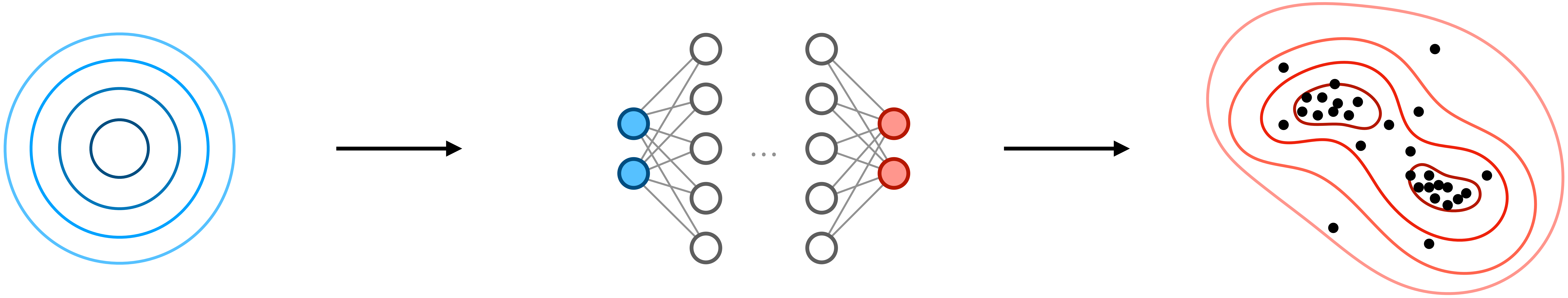
Approximate Bayesian Computation (ABC)

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

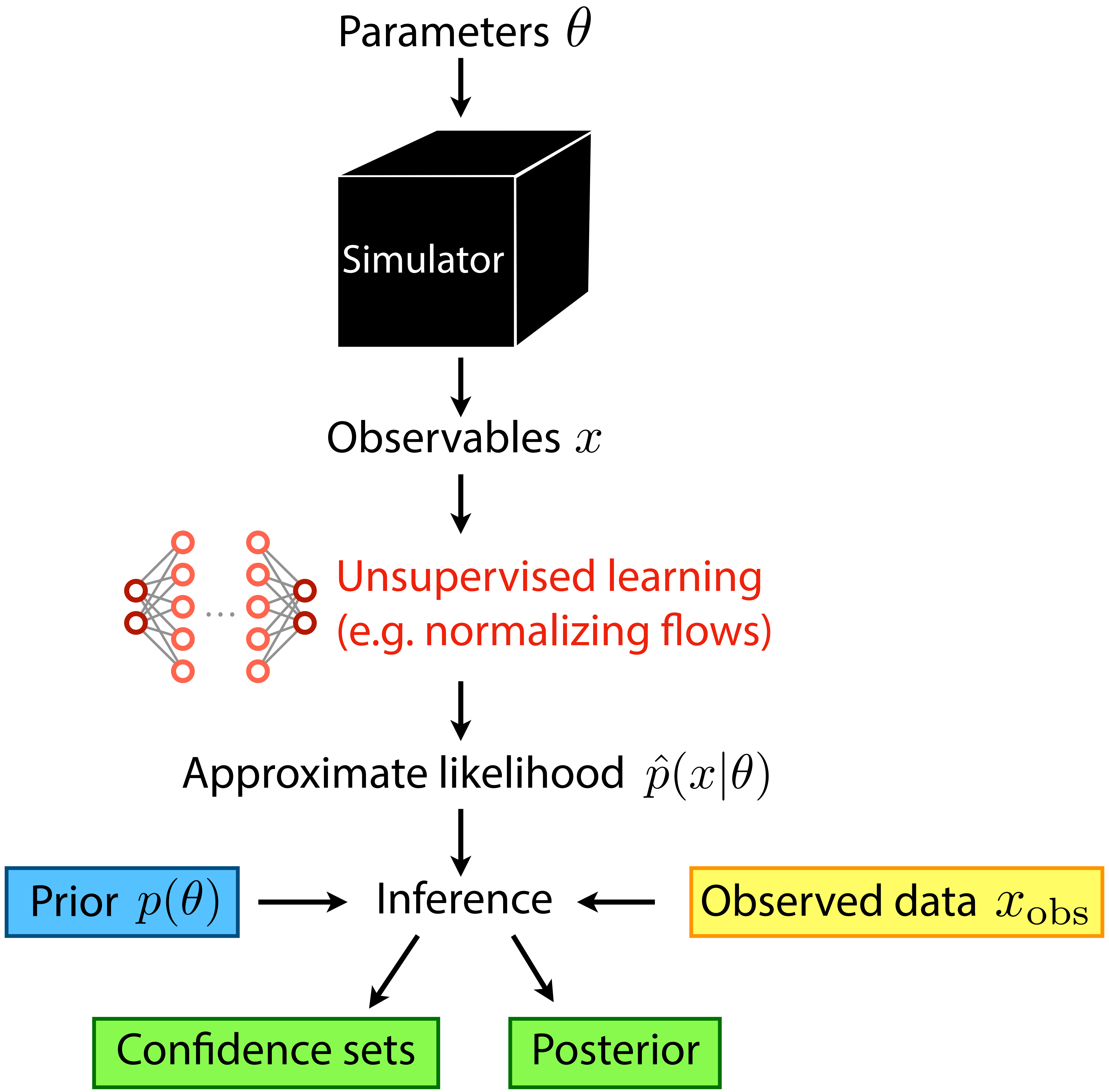
Train transformation by maximizing $\log \hat{p}(x)$

Transformation can depend on θ 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

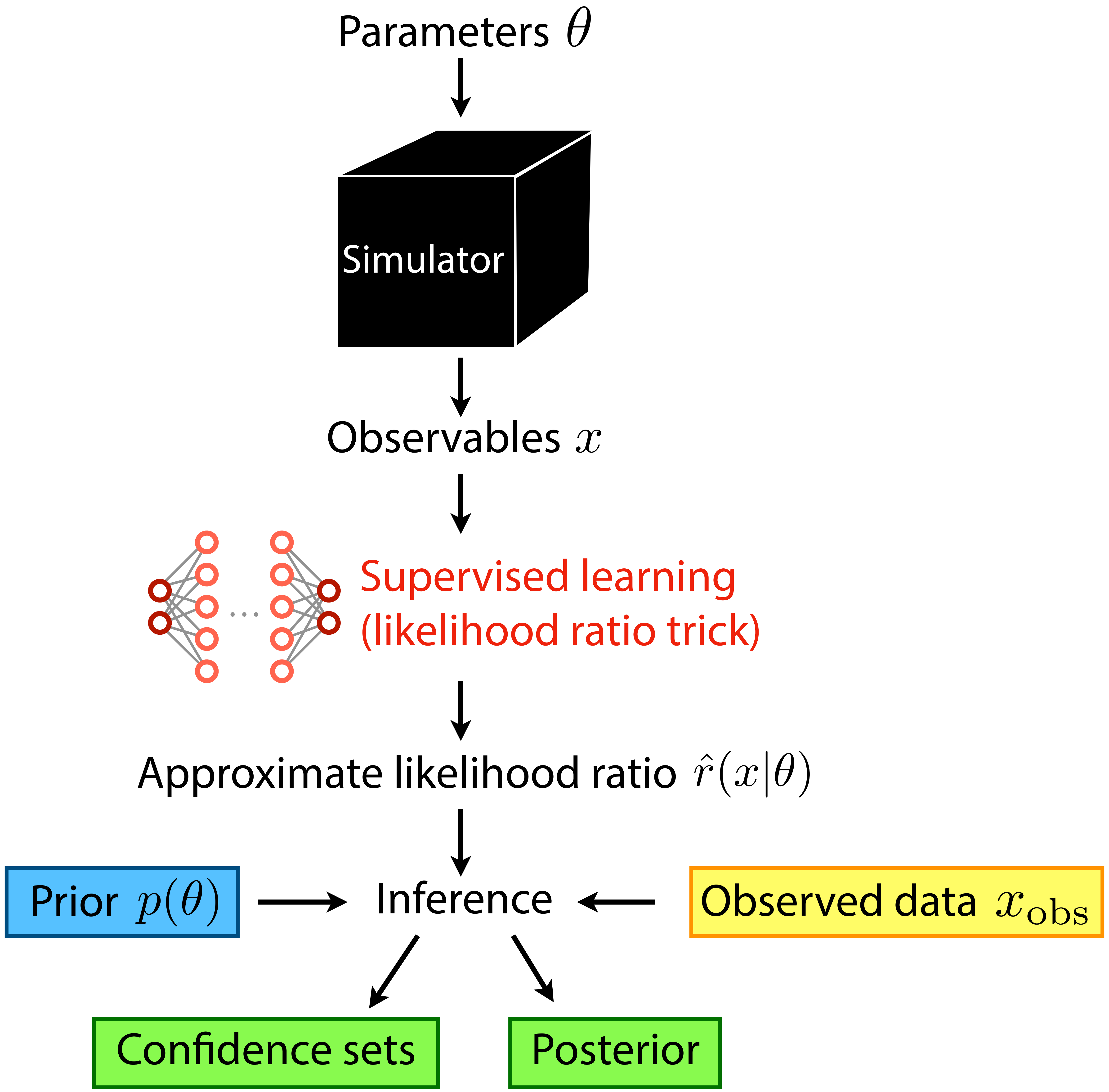
[G. Papamakarios, D. Sterrart, I. Murray 1805.07226;
J.-M. Lueckmann, G. Bassetto, T. Karaletsos, J. Macke 1805.09294]



- 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 $\hat{p}(\theta|x_{\text{obs}})$
  [G. Papamakarios et al 1605.06376;
  J.-M. Lueckmann et al 1711.01861]

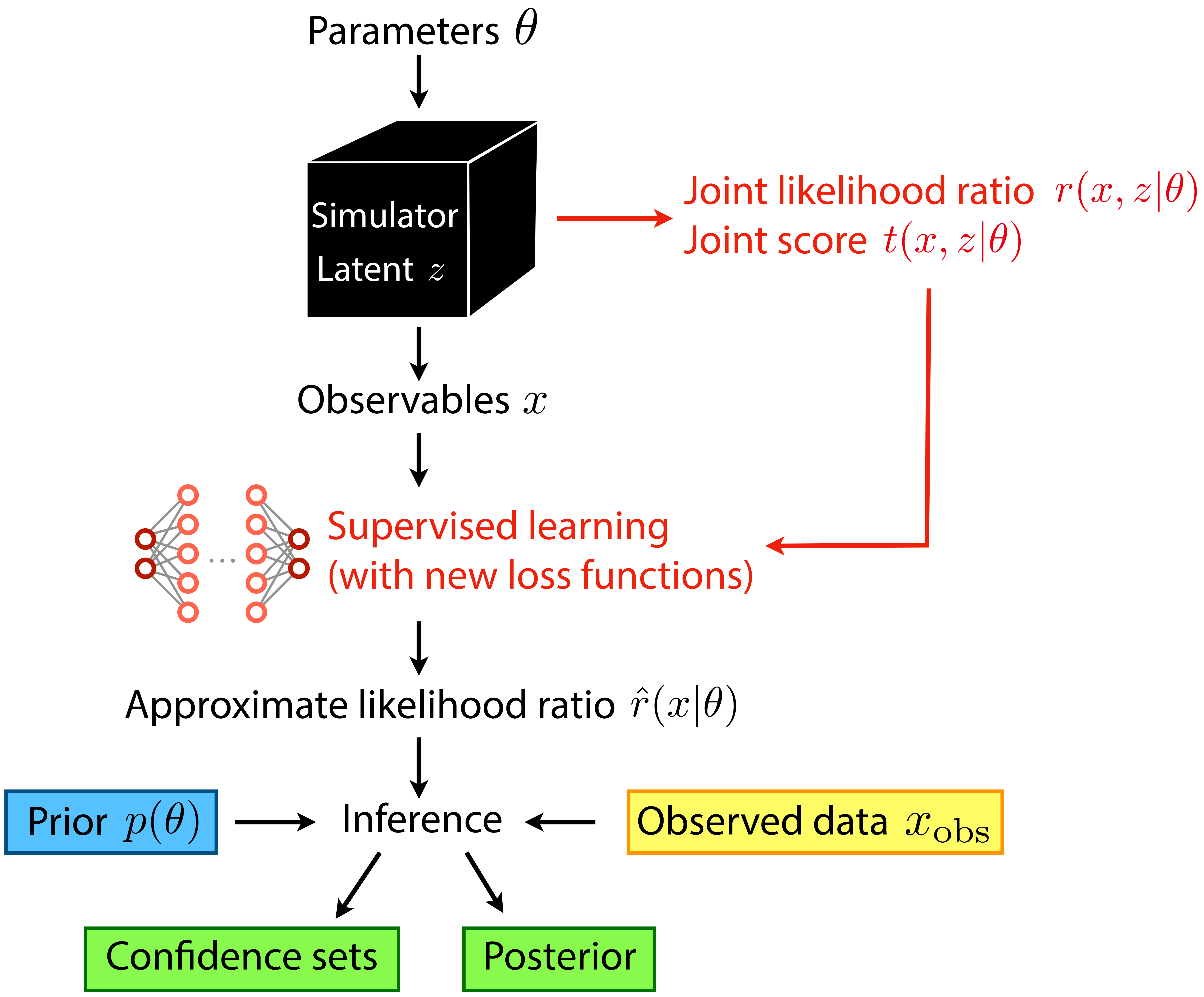
Inference by likelihood ratio trick

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



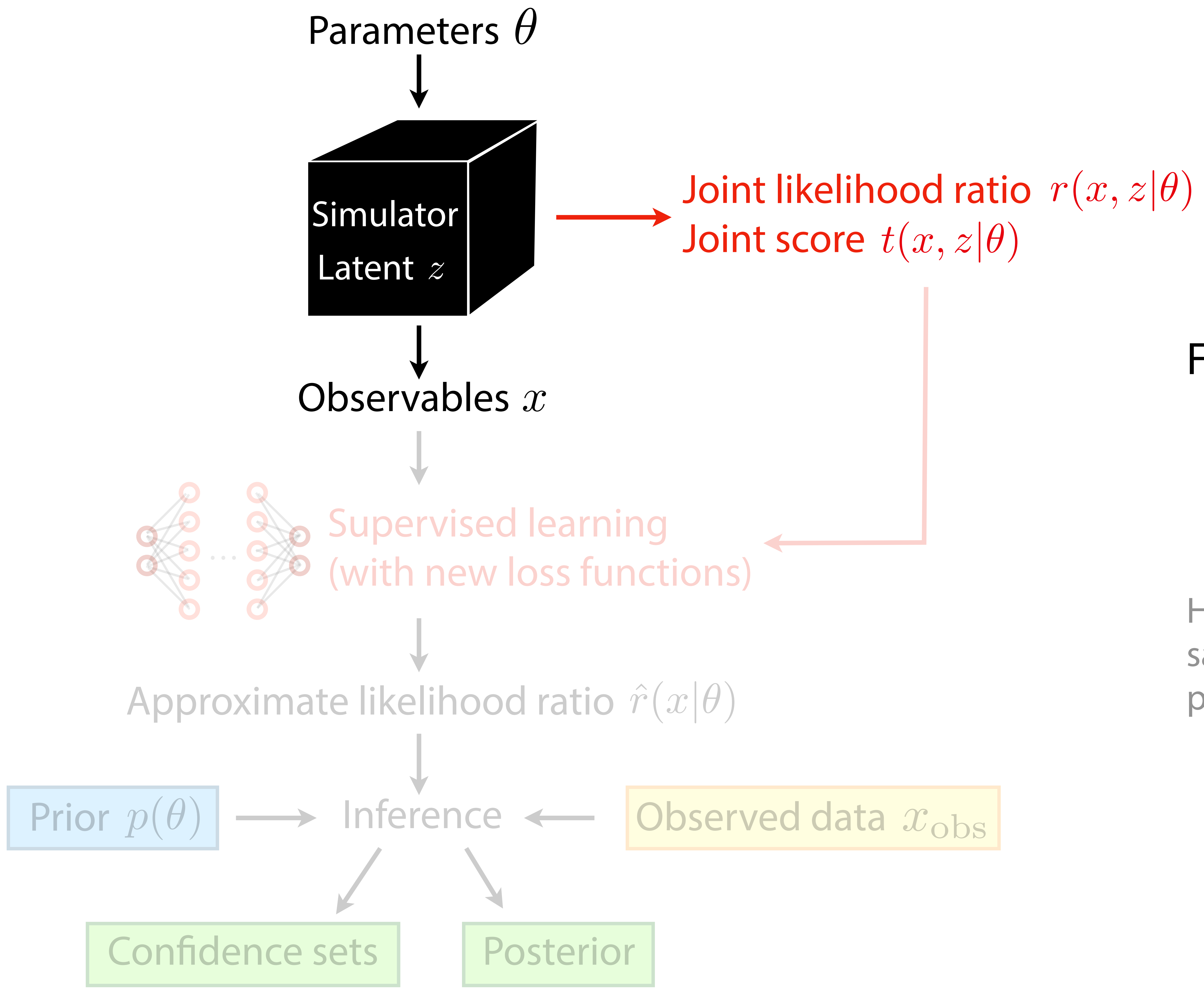
- For inference, likelihood and likelihood ratio are interchangeable
- Advantage: Learning the likelihood ratio can be a simpler task than learning the likelihood
- Disadvantage: Cannot sample from likelihood ratio

Mining gold



Parameters θ
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_{obs}
Confidence sets
Posterior

Step 1: Extracting more information from simulations

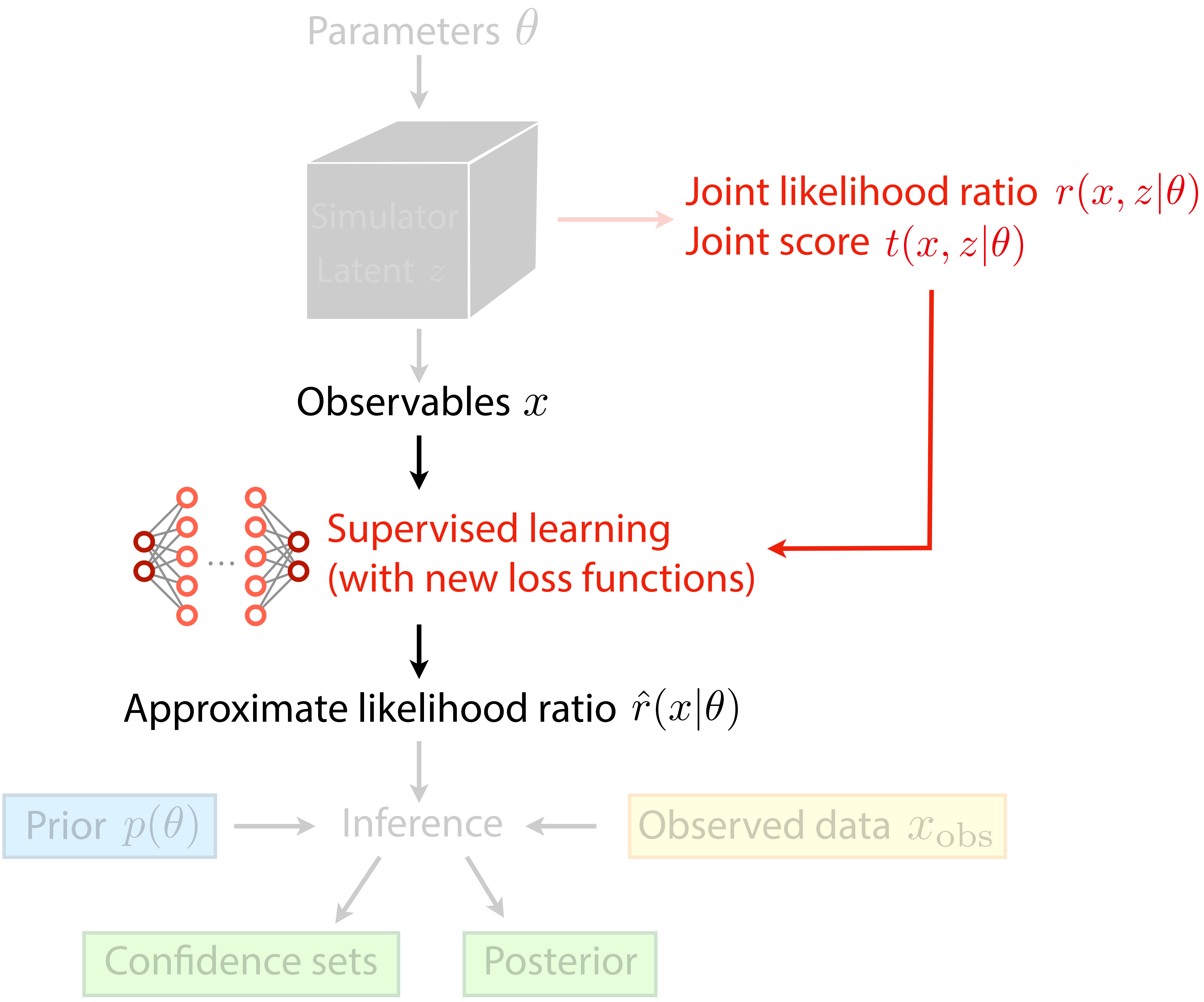


For each simulated event, calculate

- 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

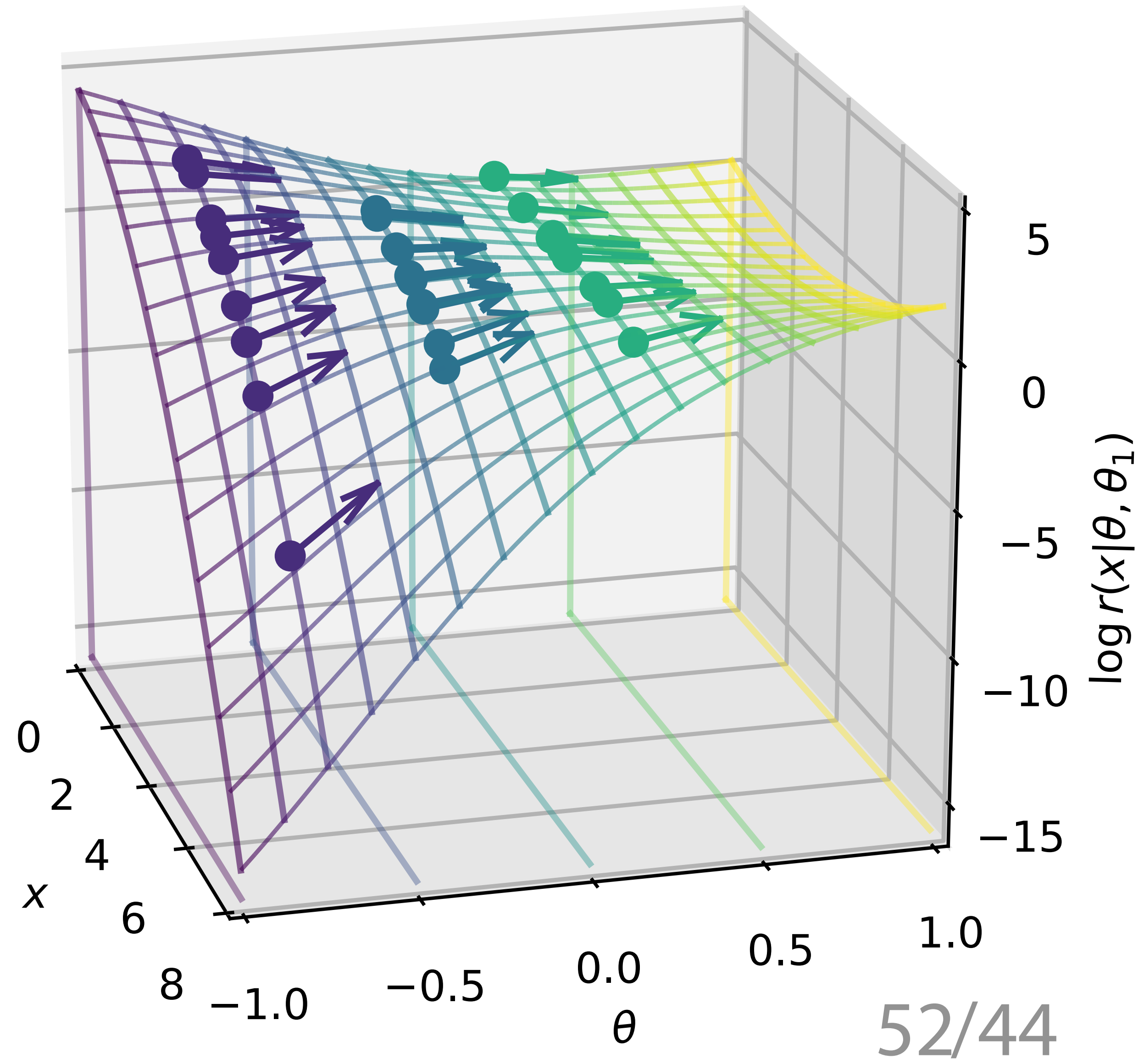
$$L[g] = \frac{1}{N} \sum_i |g(x_i, \theta_i) - r(x_i, z_i|\theta_i)|^2$$

- The network will converge to

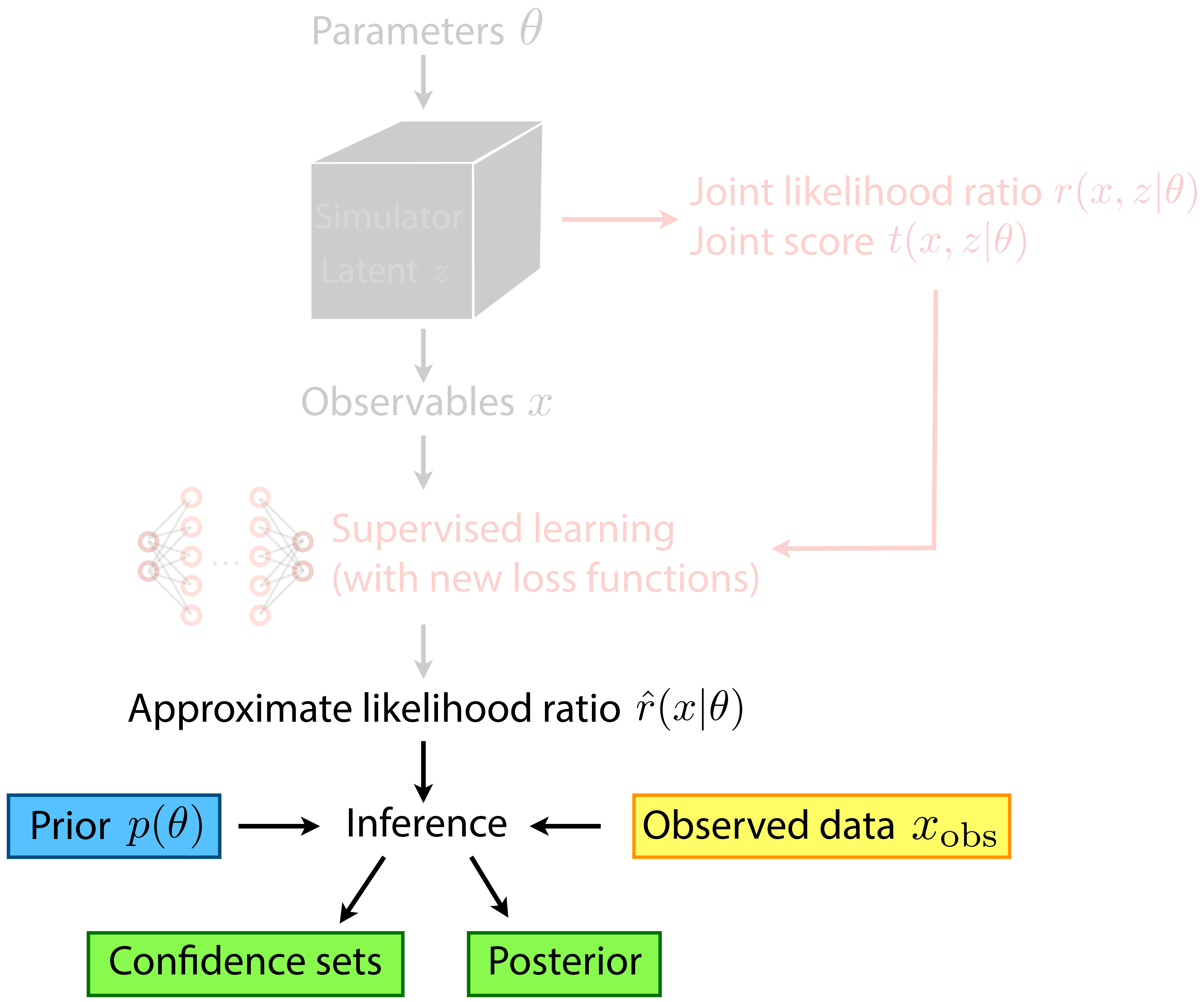
$$g(x, \theta) \to \arg\min L[g] = r(x|\theta) = \frac{p(x|\theta)}{p_{\text{ref}}(x)} \;!$$

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

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



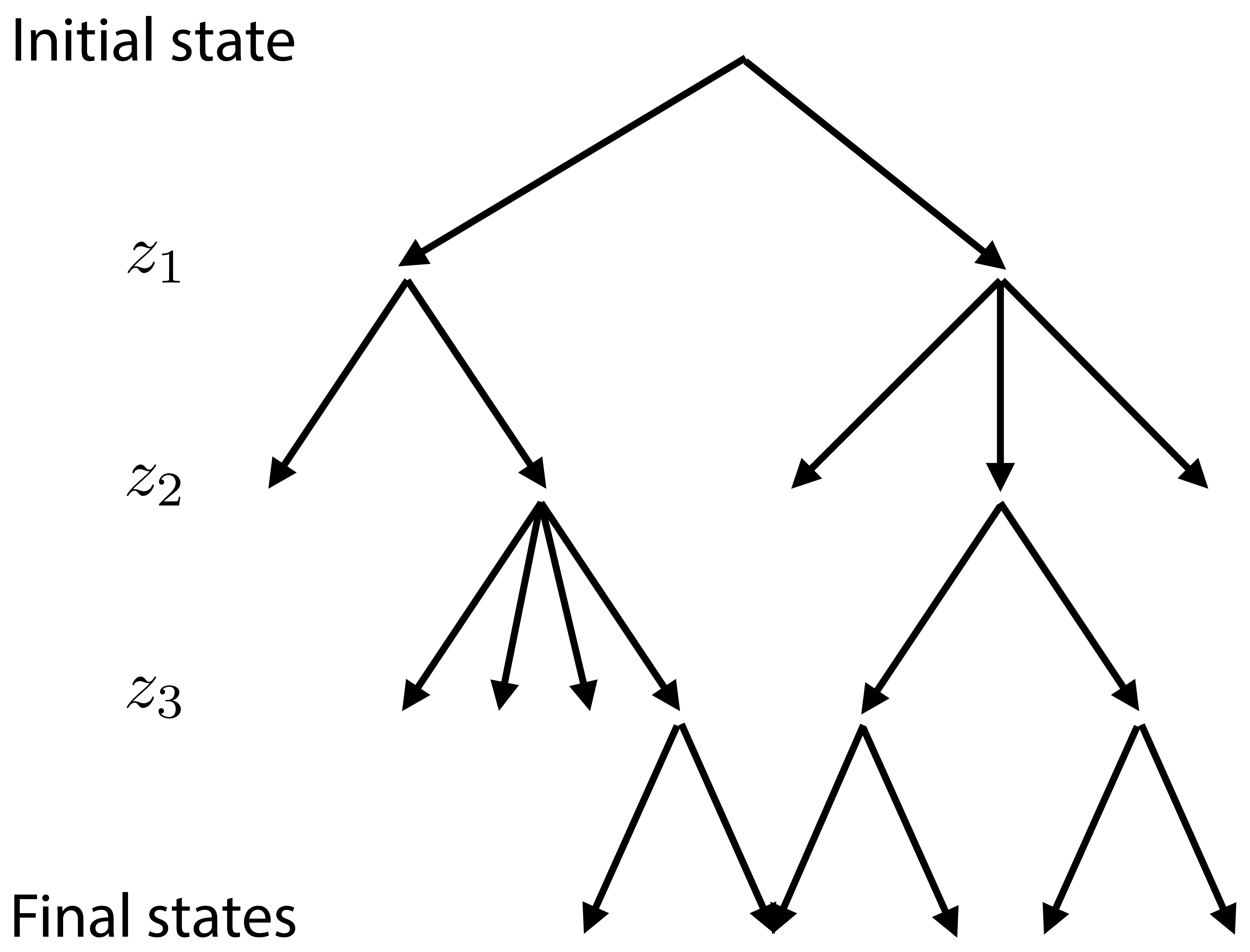
Step 3: Inference



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()
```



Mining gold from any simulation

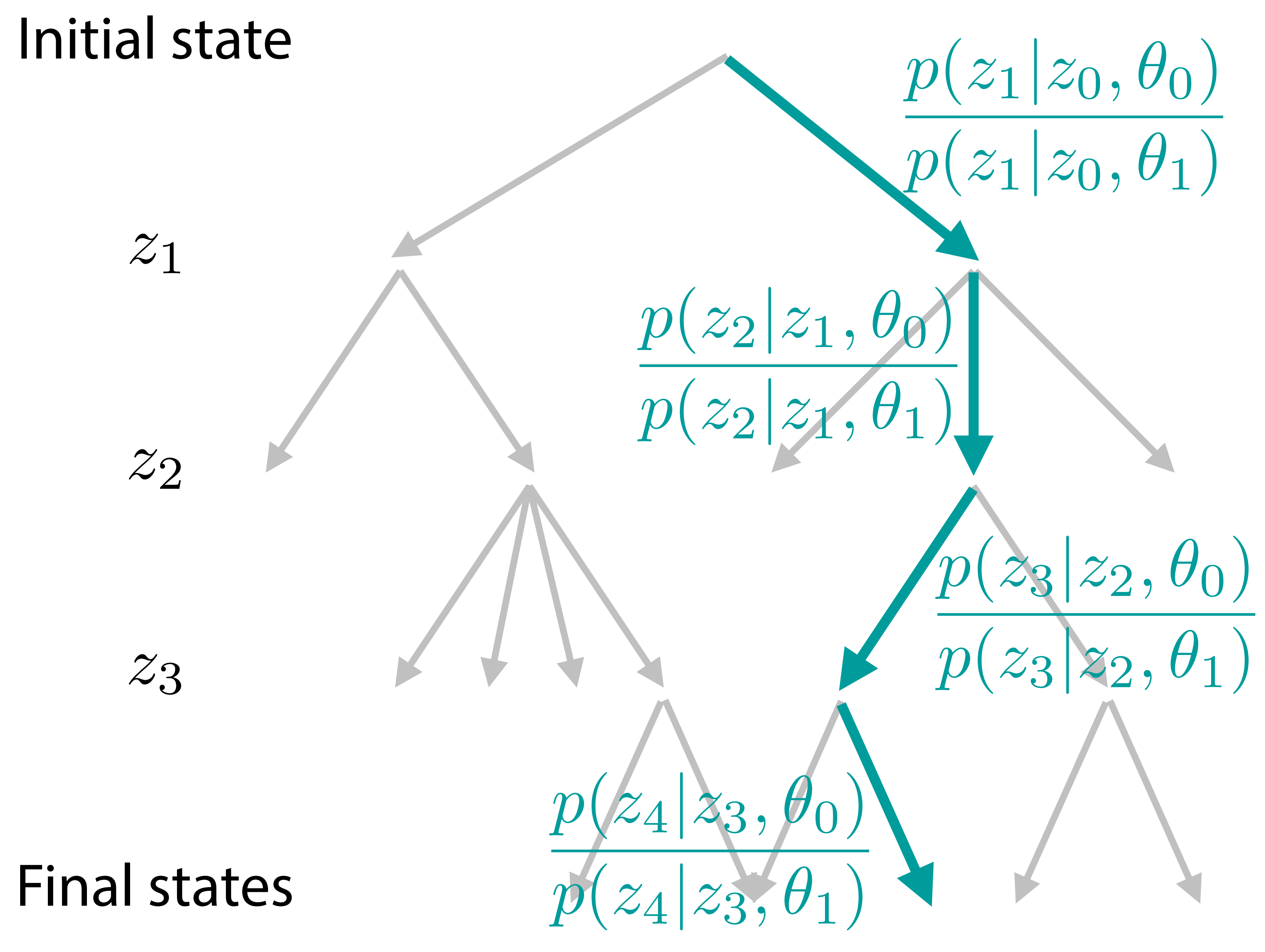
- Computer simulation typically evolve along a tree-like structure of successive random branchings

- 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()
```

- 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

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

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.)

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 $r(x|\theta_0,\theta_1)$!

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

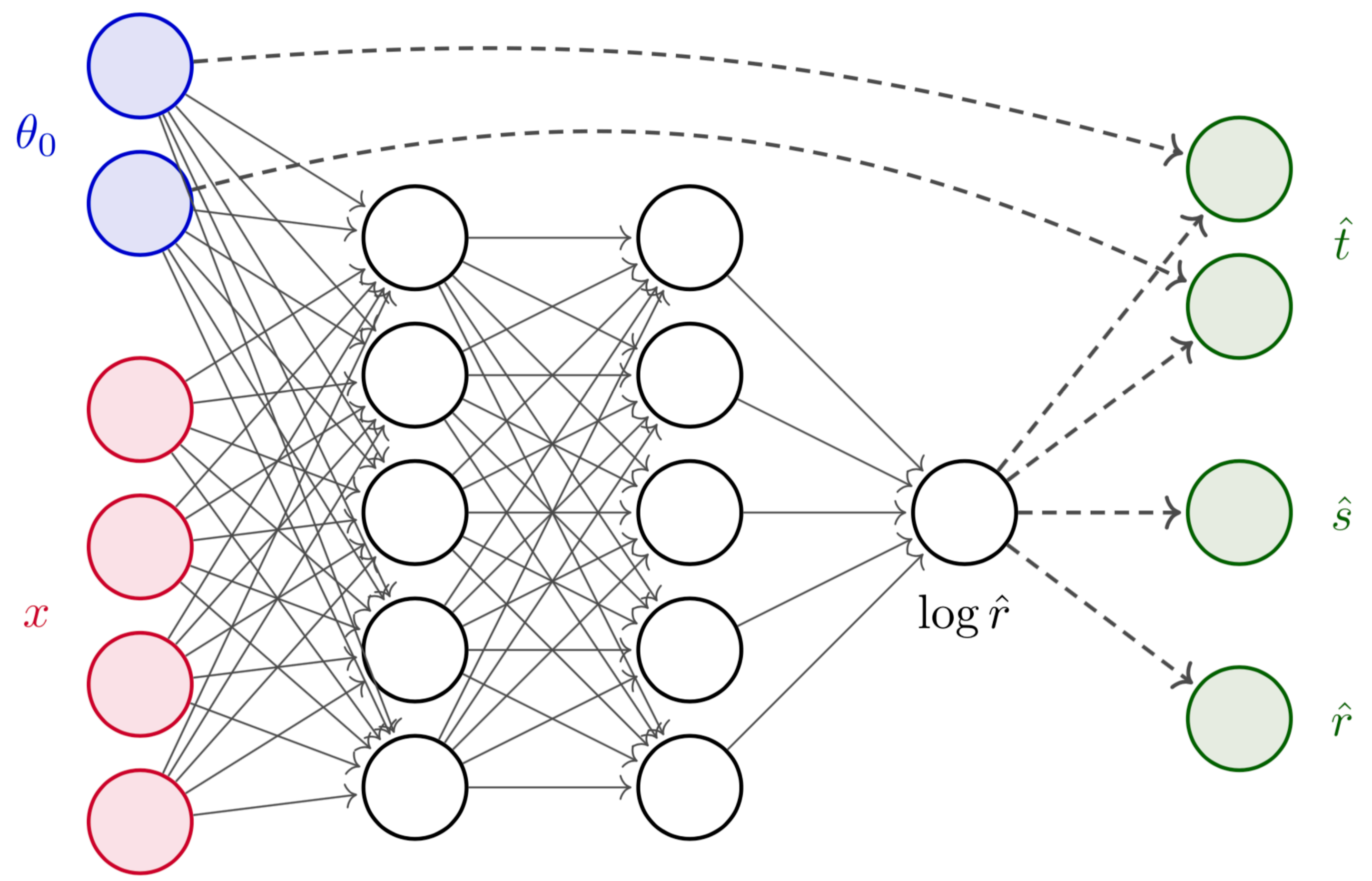
$$r(x|\theta_0,\theta_1) = \arg\min_{\hat{r}(x|\theta_0,\theta_1)} L_r[\hat{r}(x|\theta_0,\theta_1)]$$

Loss function with
finite sum over samples

Stochastic gradient descent

This is where machine learning comes in!

Neural network



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

The local model

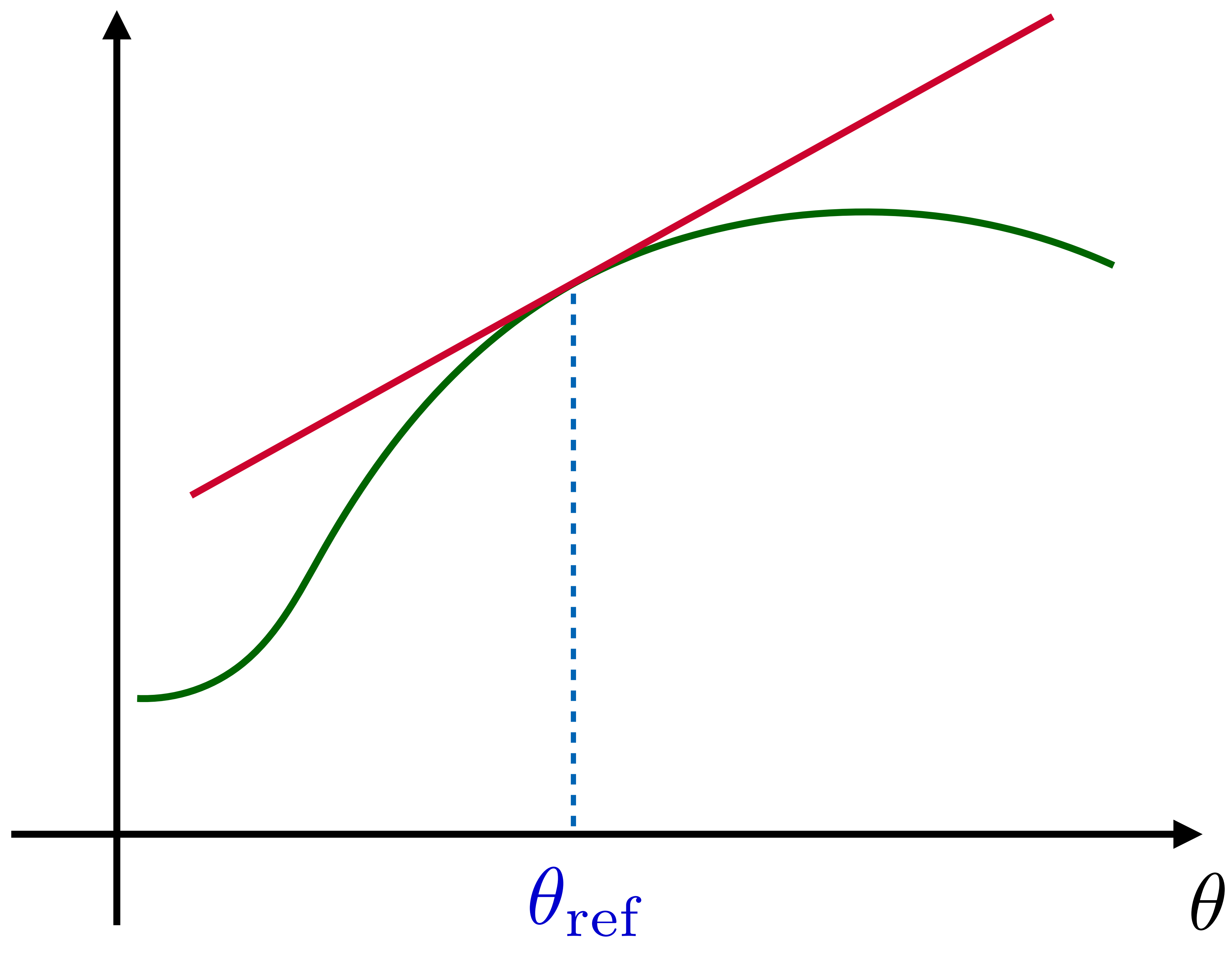
[see also J. Alsing, B. Wandelt 1712.00012; J. Alsing, B. Wandelt. S. Freeney 1801.01497; P. de Castro, T. Dorigo 1806.04743; J. Alsing, B. Wandelt 1903.01473]

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

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

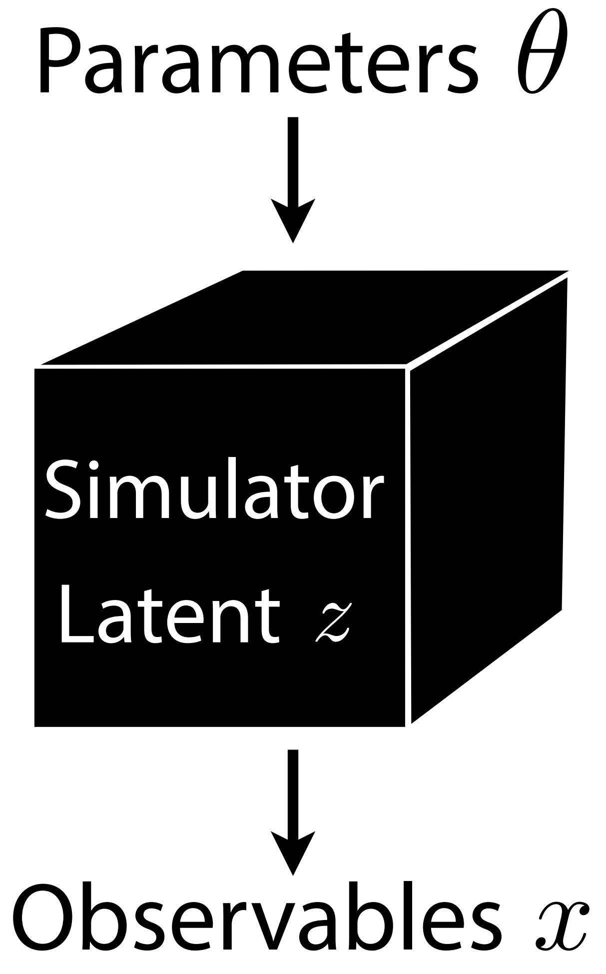
In the neighborhood of θ_{ref}:

- 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

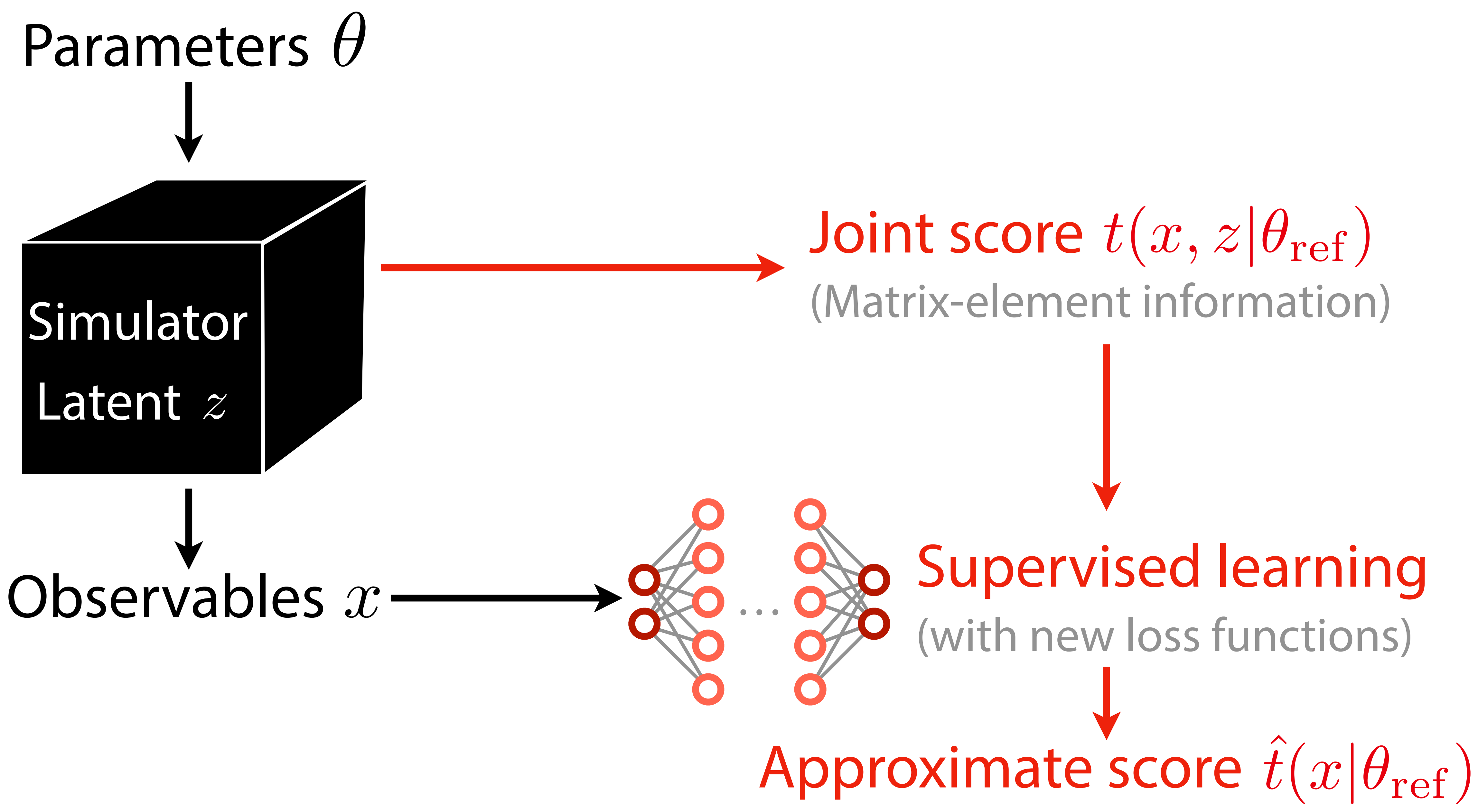


The score itself is intractable. But we can use the same trick as for the likelihood ratio!

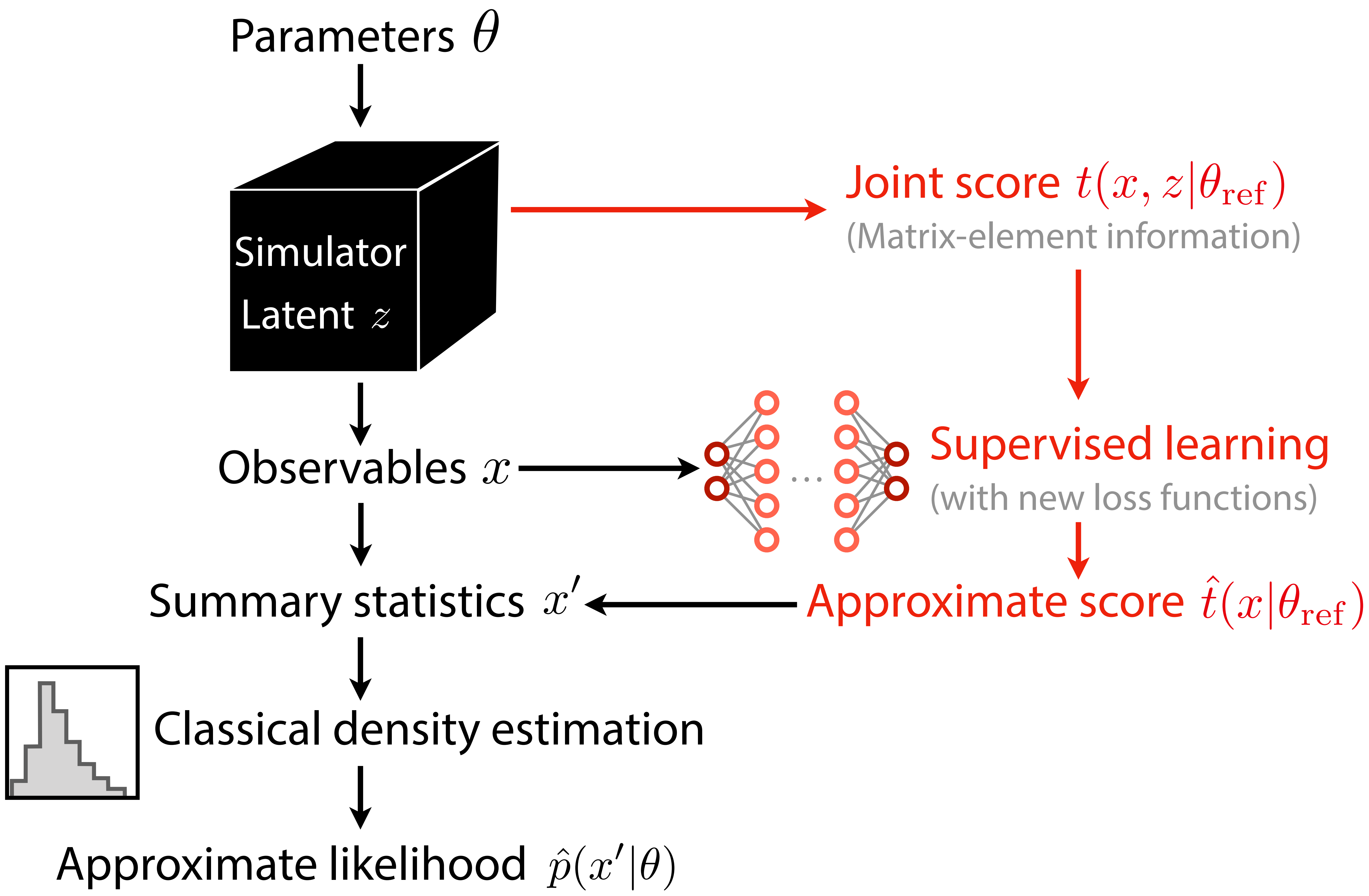
Neural optimal observables (SALLY)



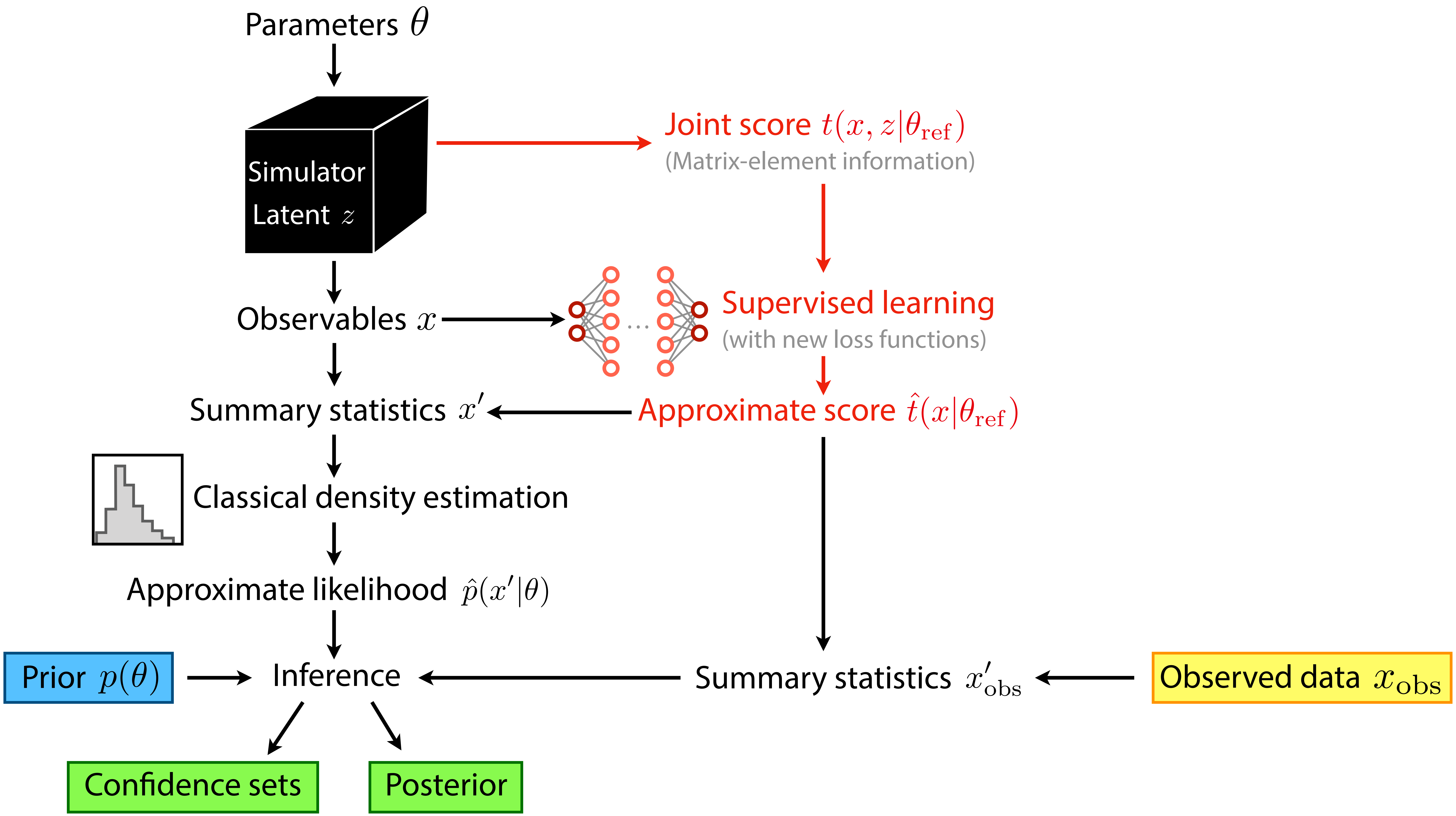
Neural optimal observables (SALLY)



Neural optimal observables (SALLY)



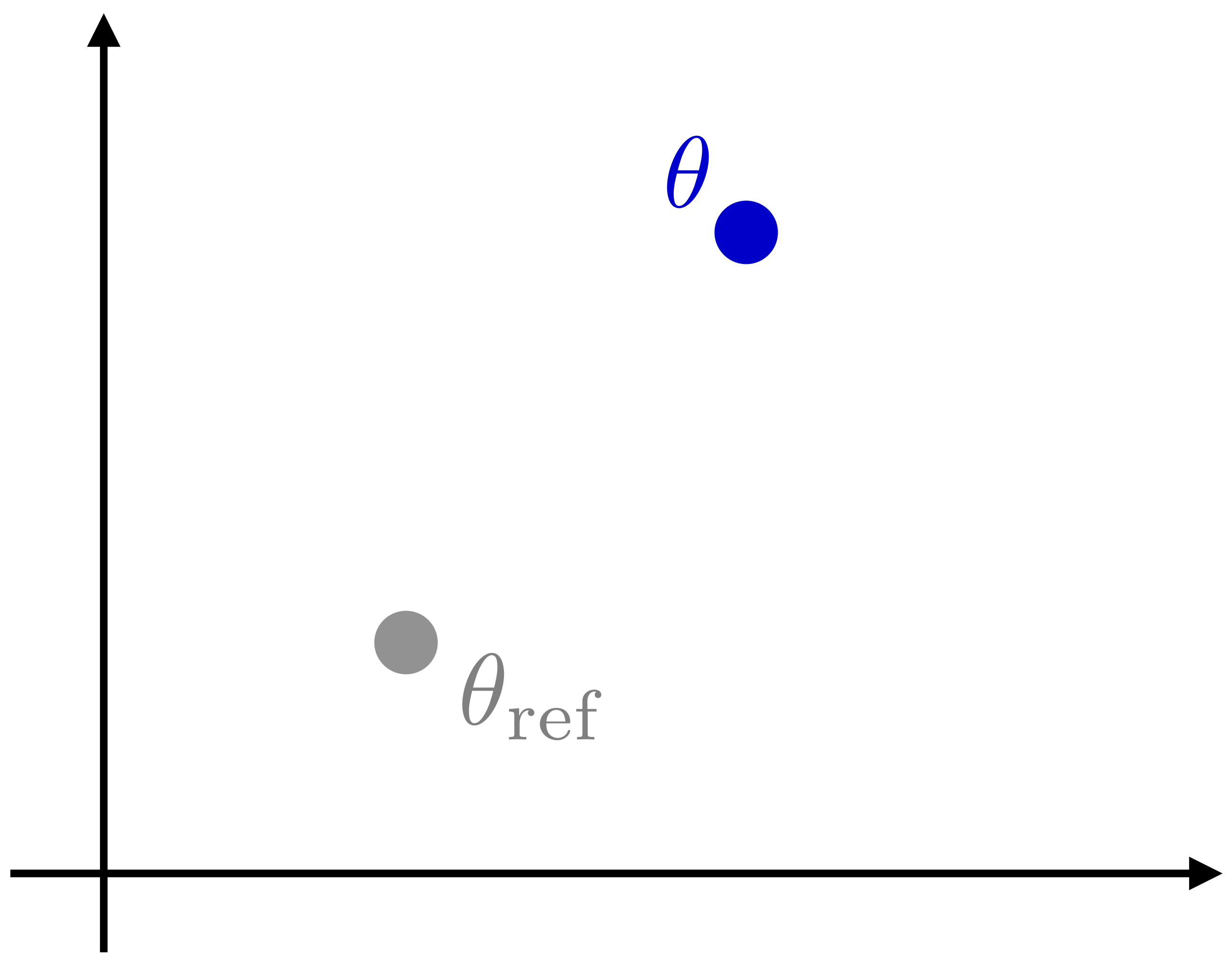
Neural optimal observables (SALLY)



Frequentist inference

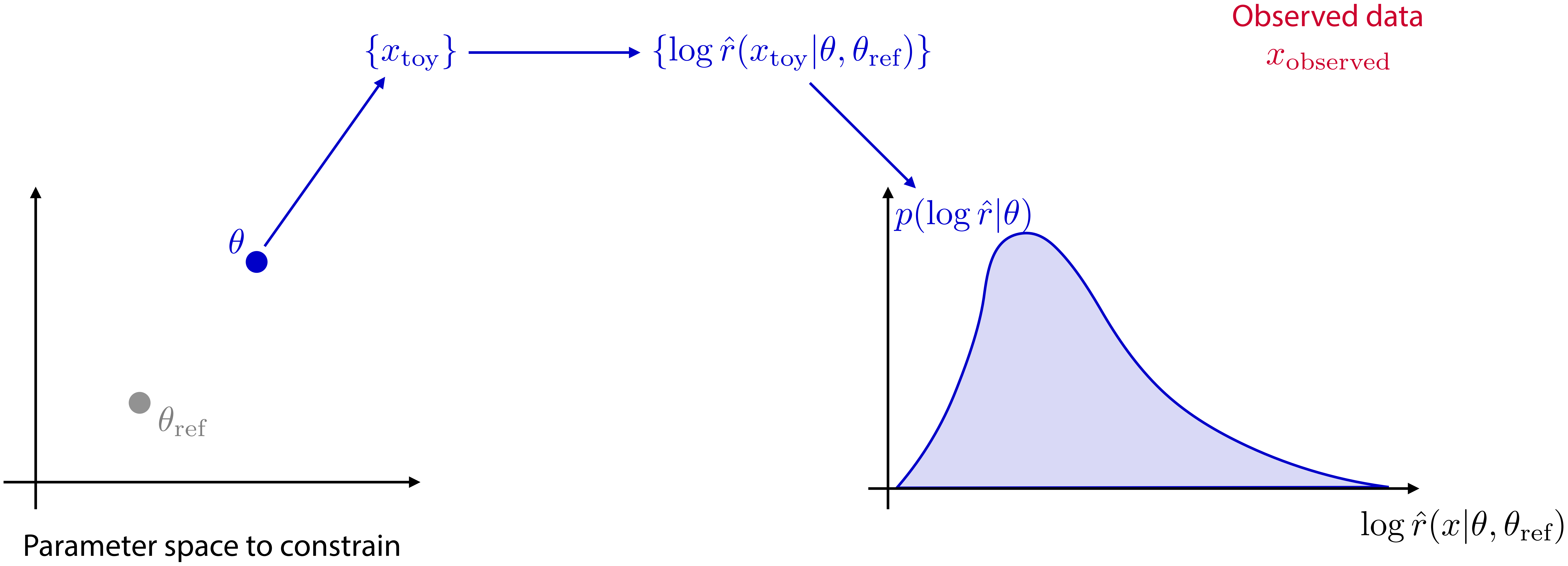
Observed data

x_{observed}

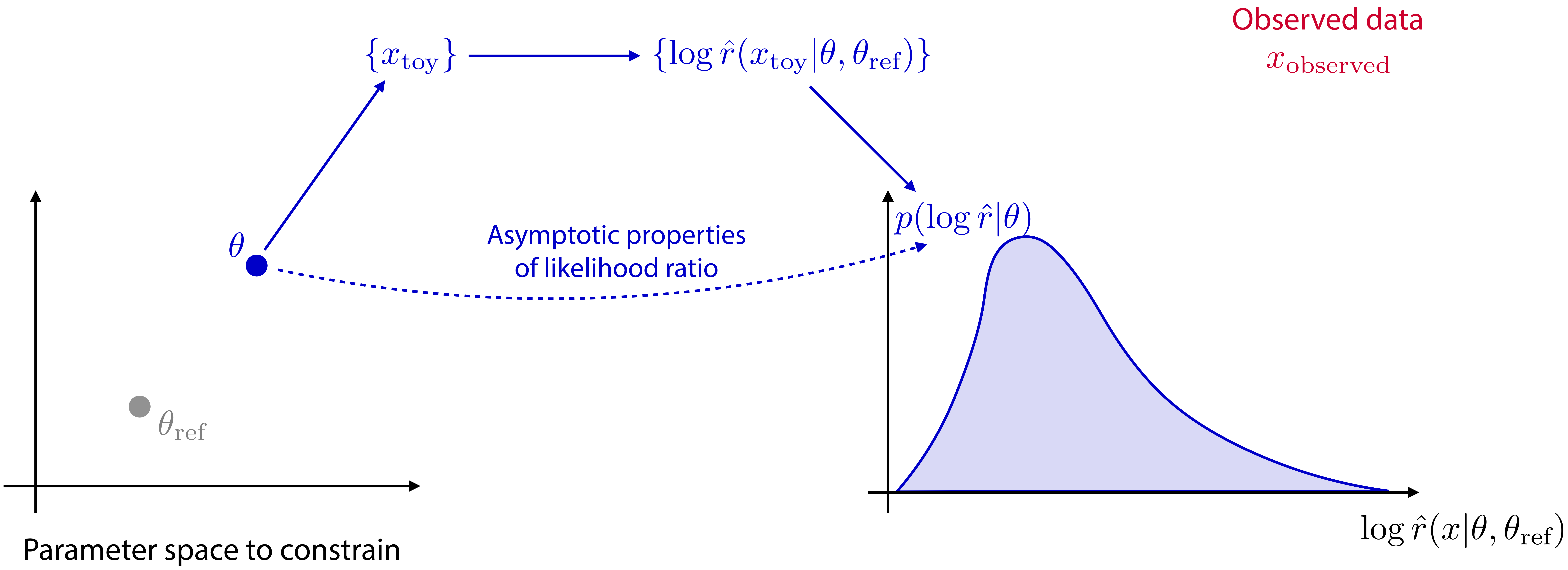


Parameter space to constrain

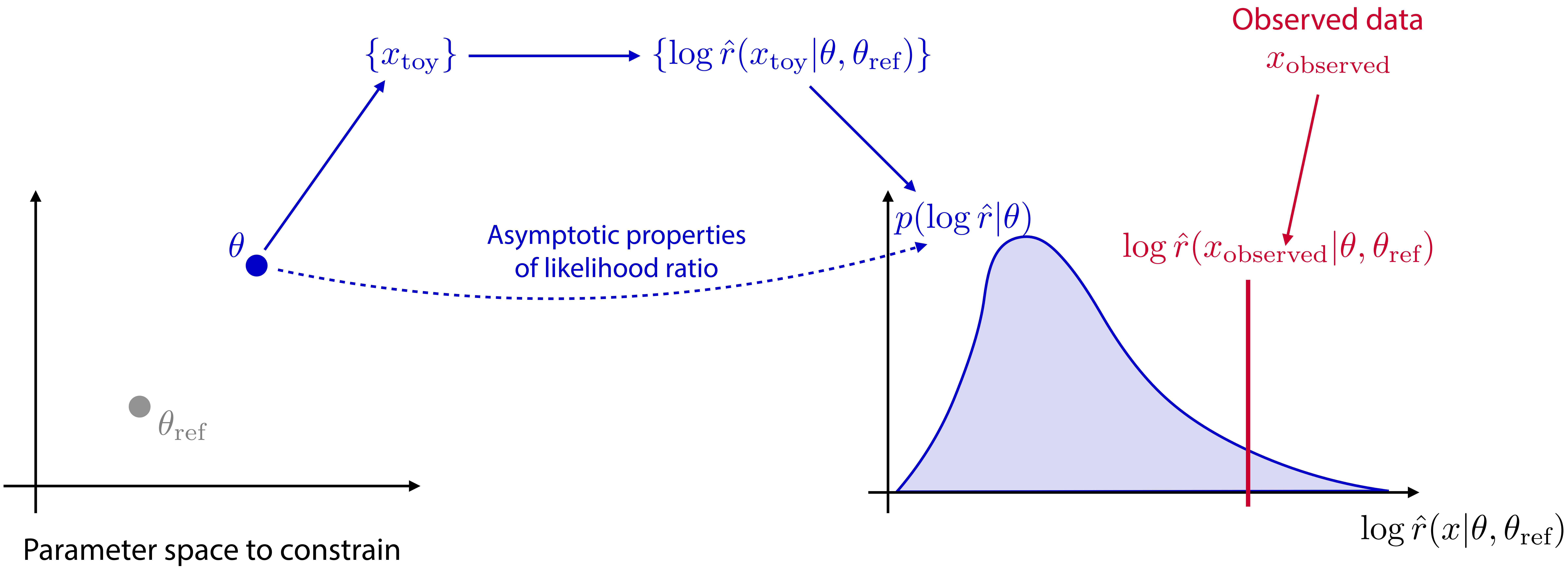
Frequentist inference



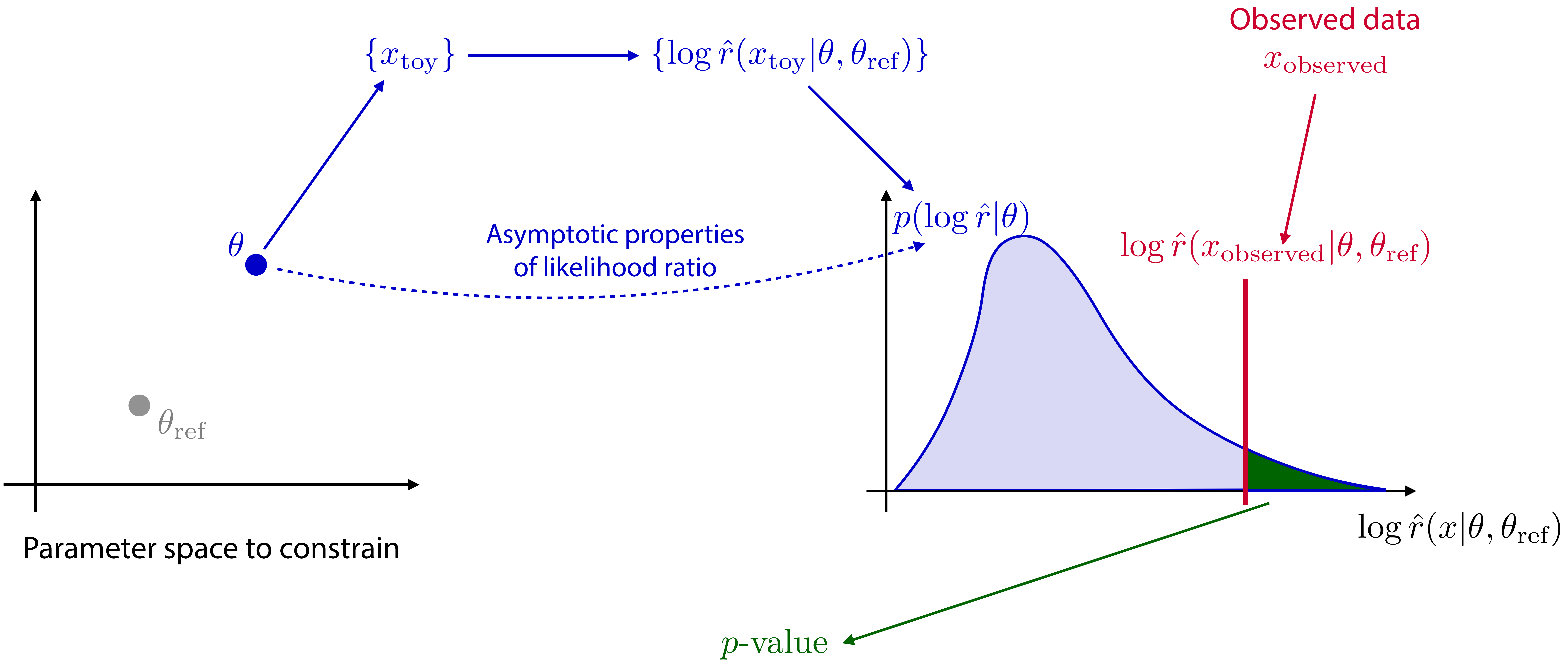
Frequentist inference



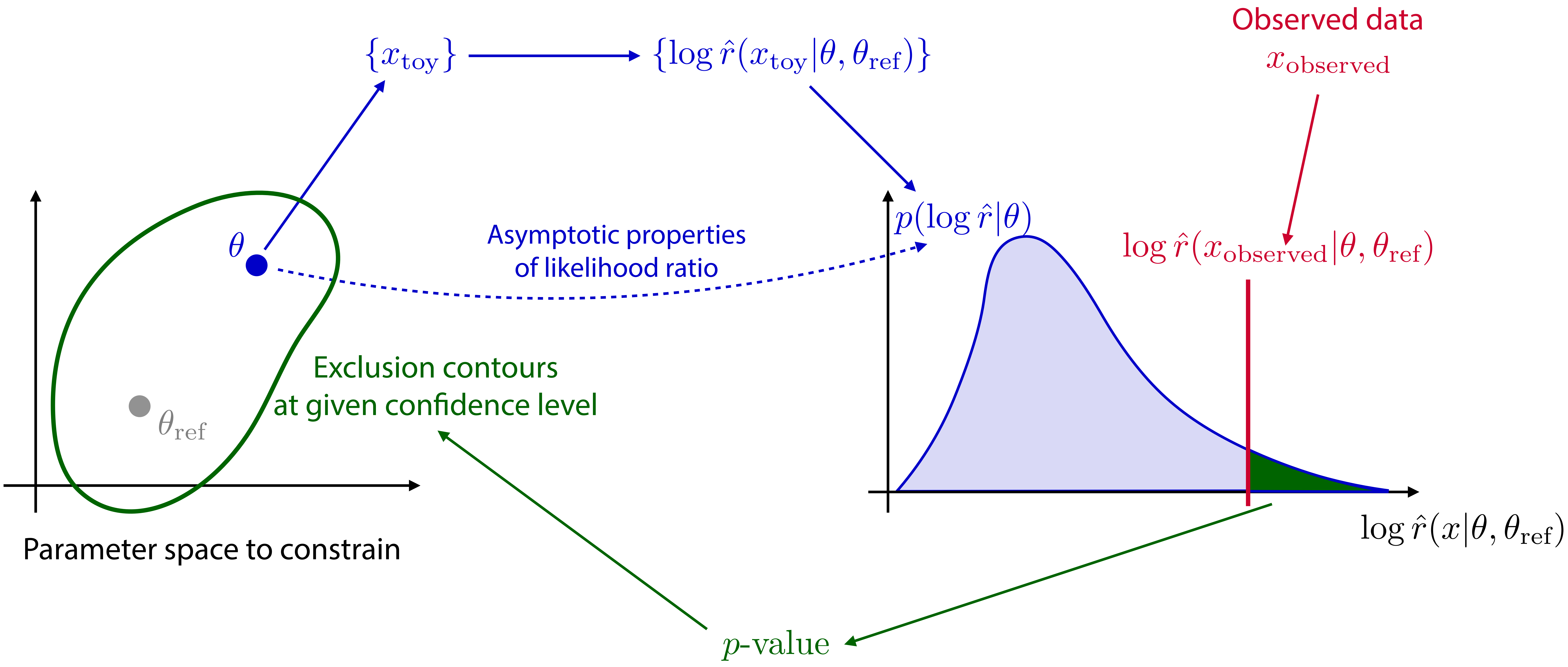
Frequentist inference



Frequentist inference



Frequentist inference

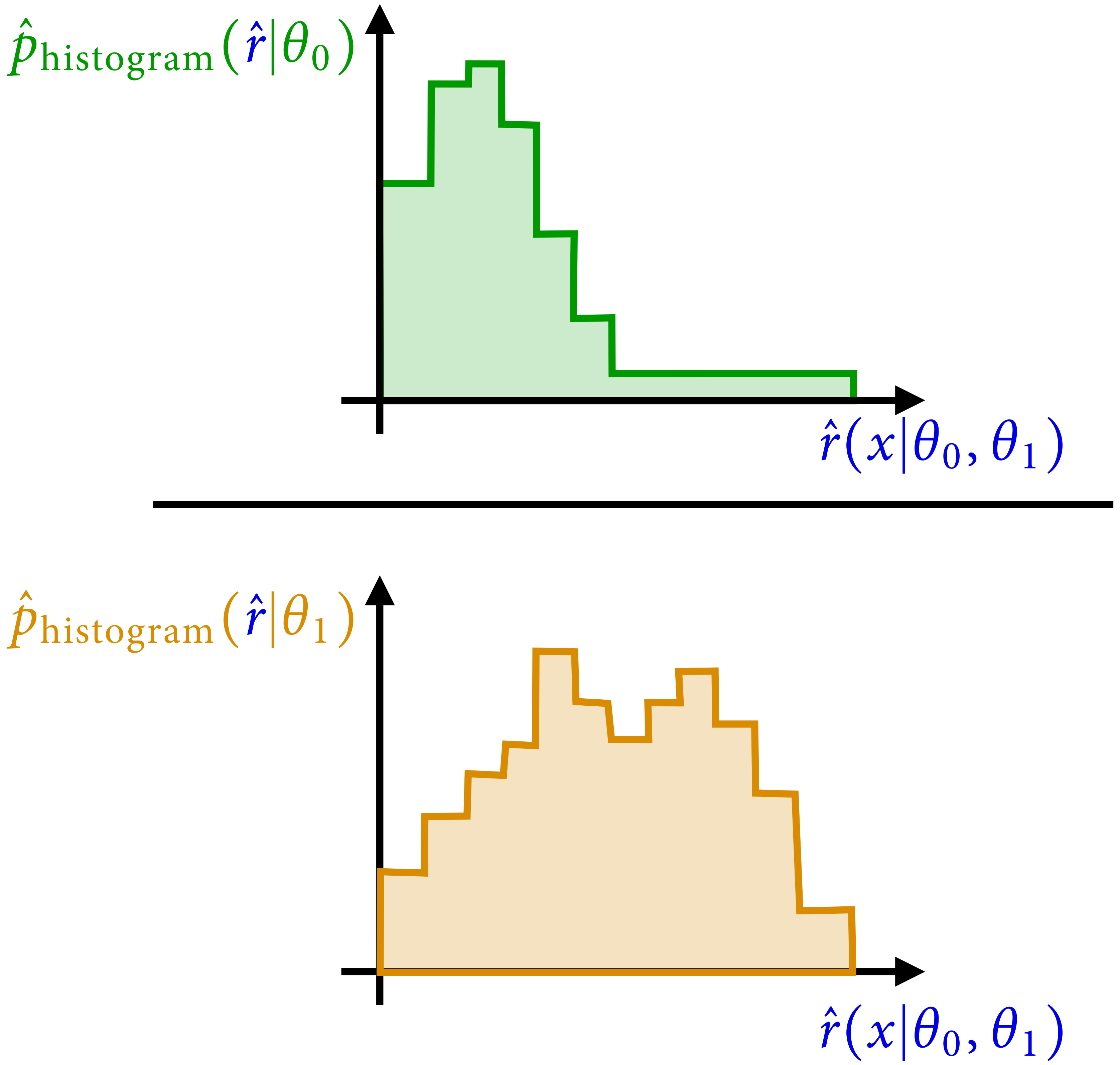


Calibration

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

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

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

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

Modelling particle physics processes

Theory
parameters
θ

Evolution

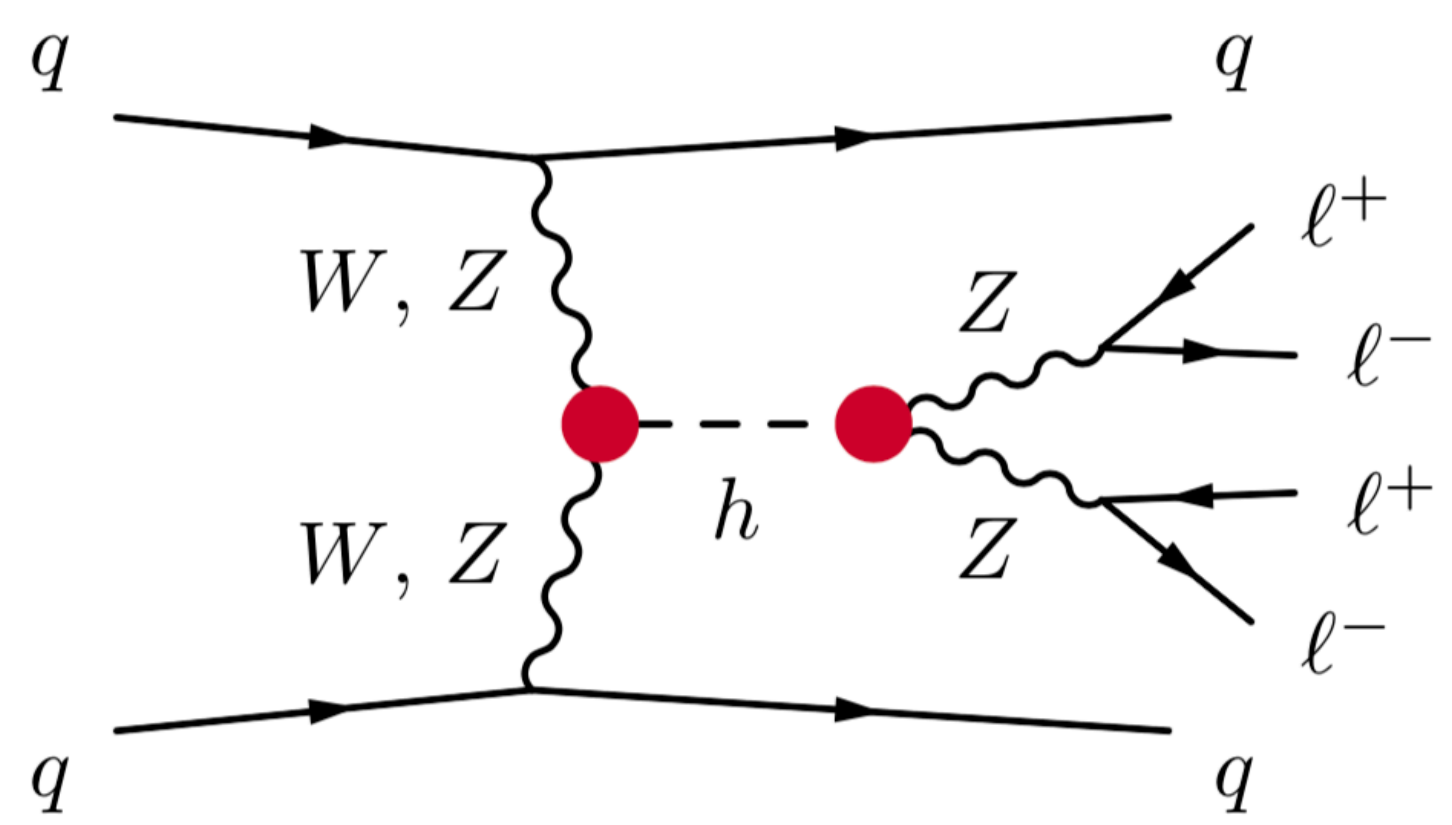
Modelling particle physics processes

Latent variables

Parton-level momenta

Theory parameters

$z_p \longleftarrow \theta$

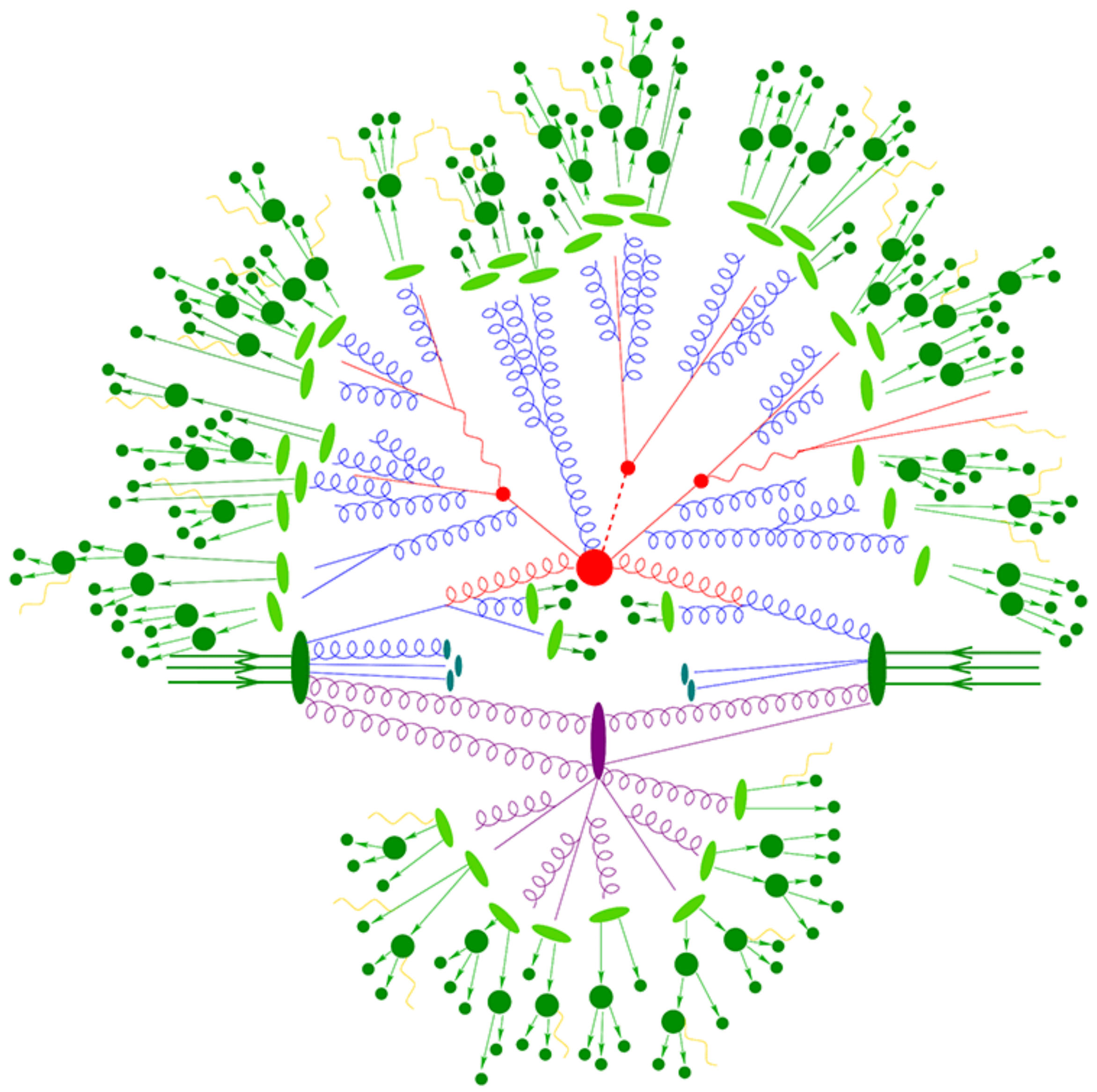


Evolution

Modelling particle physics processes

Latent variables

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



[F. Krauss]

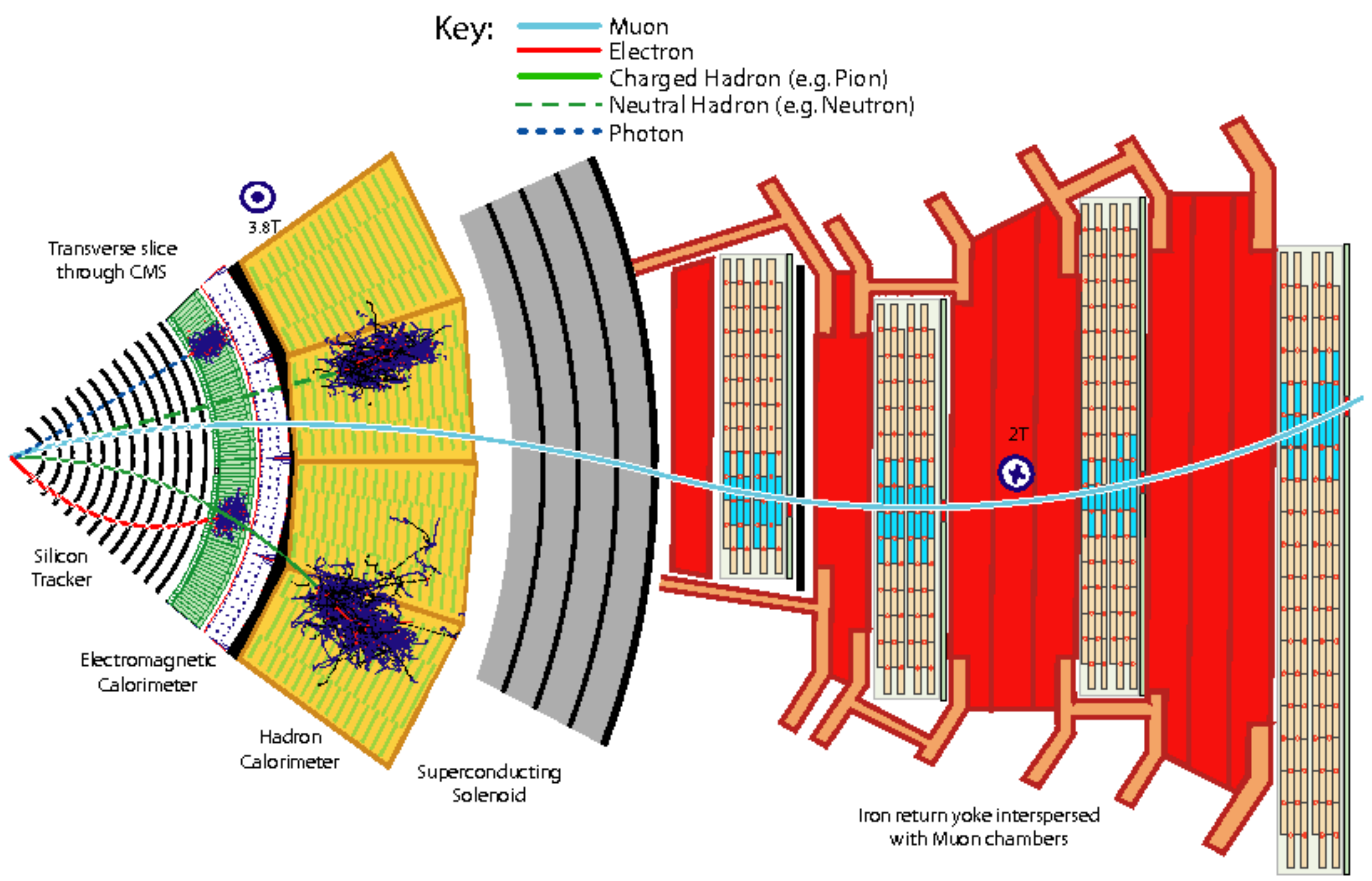
Evolution

Modelling particle physics processes

Latent variables

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

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



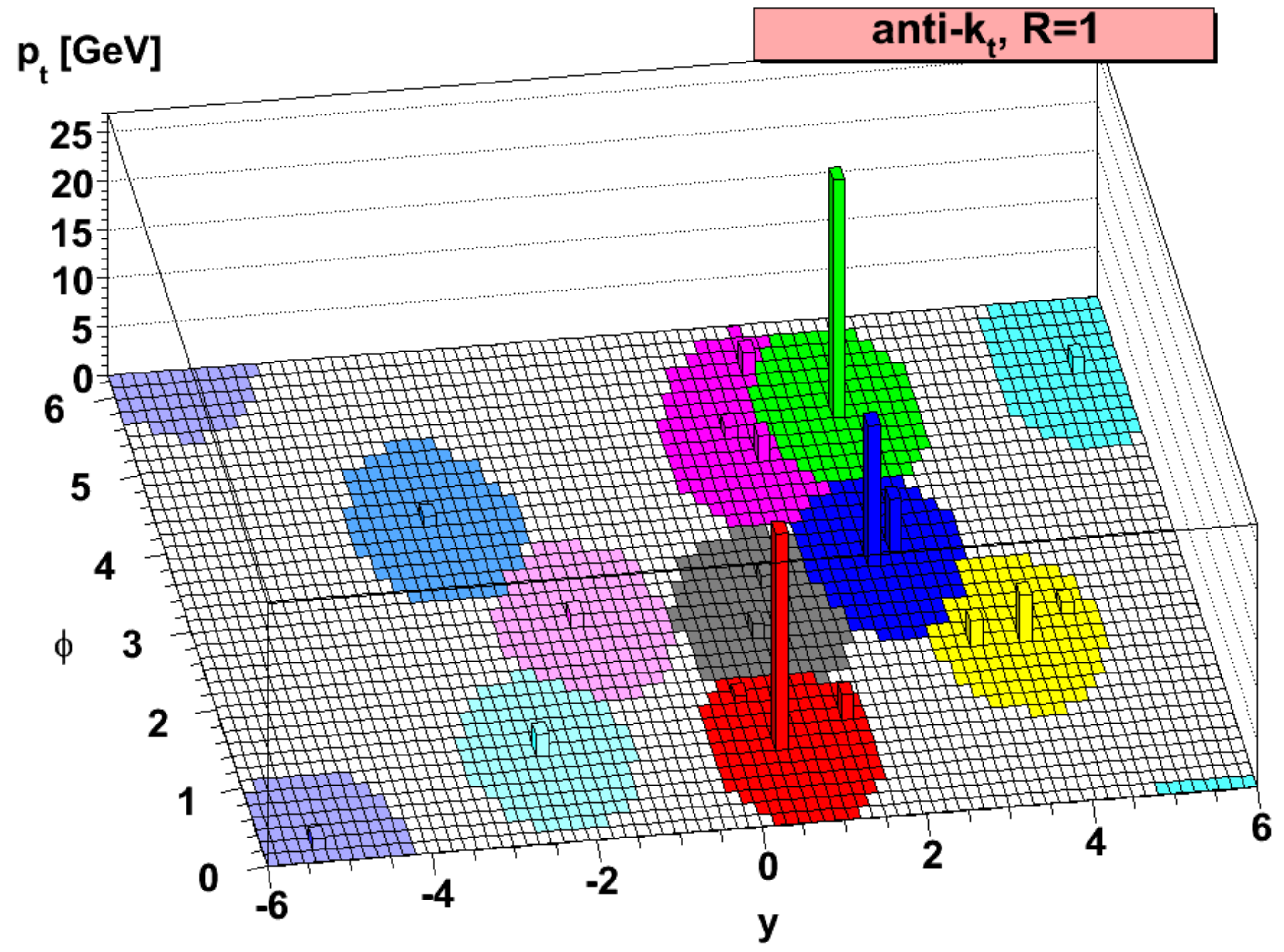
[CMS]

Evolution

Modelling particle physics processes

Latent variables

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



[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	$\longleftarrow$	θ

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

GEANT4 A SIMULATION TOOLKIT

MADGRAPH5_aMC@NLO

$\longleftarrow$

Prediction (simulation)

Modelling particle physics processes

Latent variables

Observables		Detector interactions	Shower splittings	Parton-level momenta	Theory parameters

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

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

Inference

Modelling particle physics processes

Latent variables

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

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

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

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

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

Intractable integrals

Mining gold from the simulator

Latent variables

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

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

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

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 θ_0 compared to θ_1?")

$$\downarrow$$

We want the likelihood ratio function

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

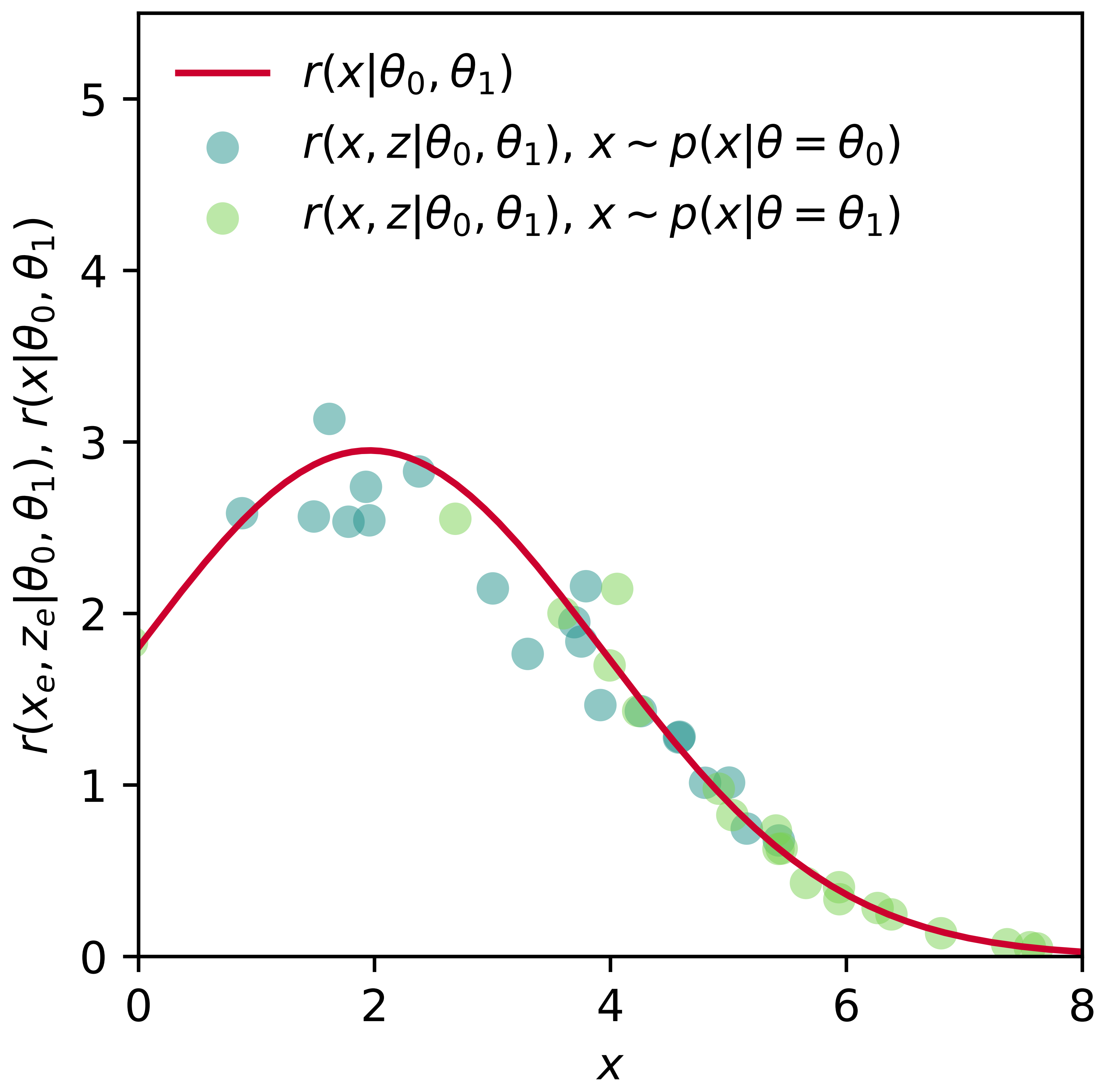
("How much more likely is the observation x for θ_0 compared to θ_1?")

The value of gold

We can calculate the joint likelihood ratio

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

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



We want the likelihood ratio function

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

The value of gold

We can calculate the joint likelihood ratio

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

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.)

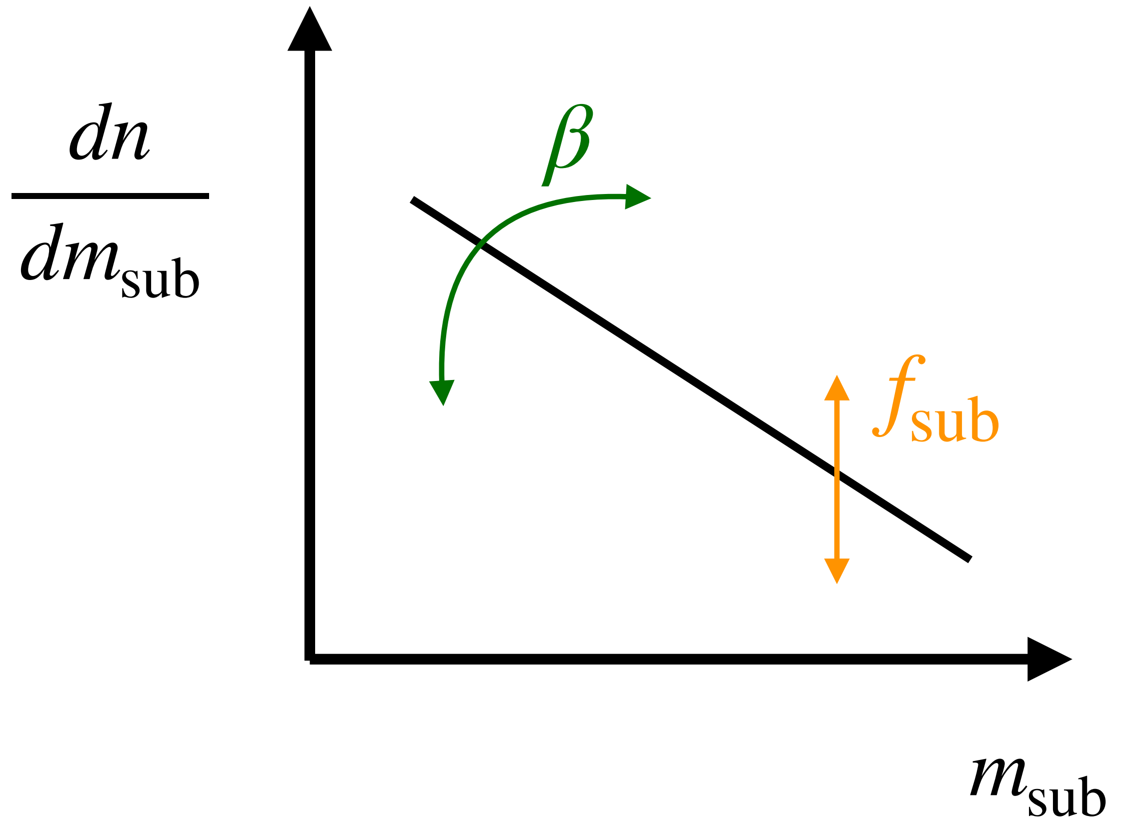
We want the likelihood ratio function

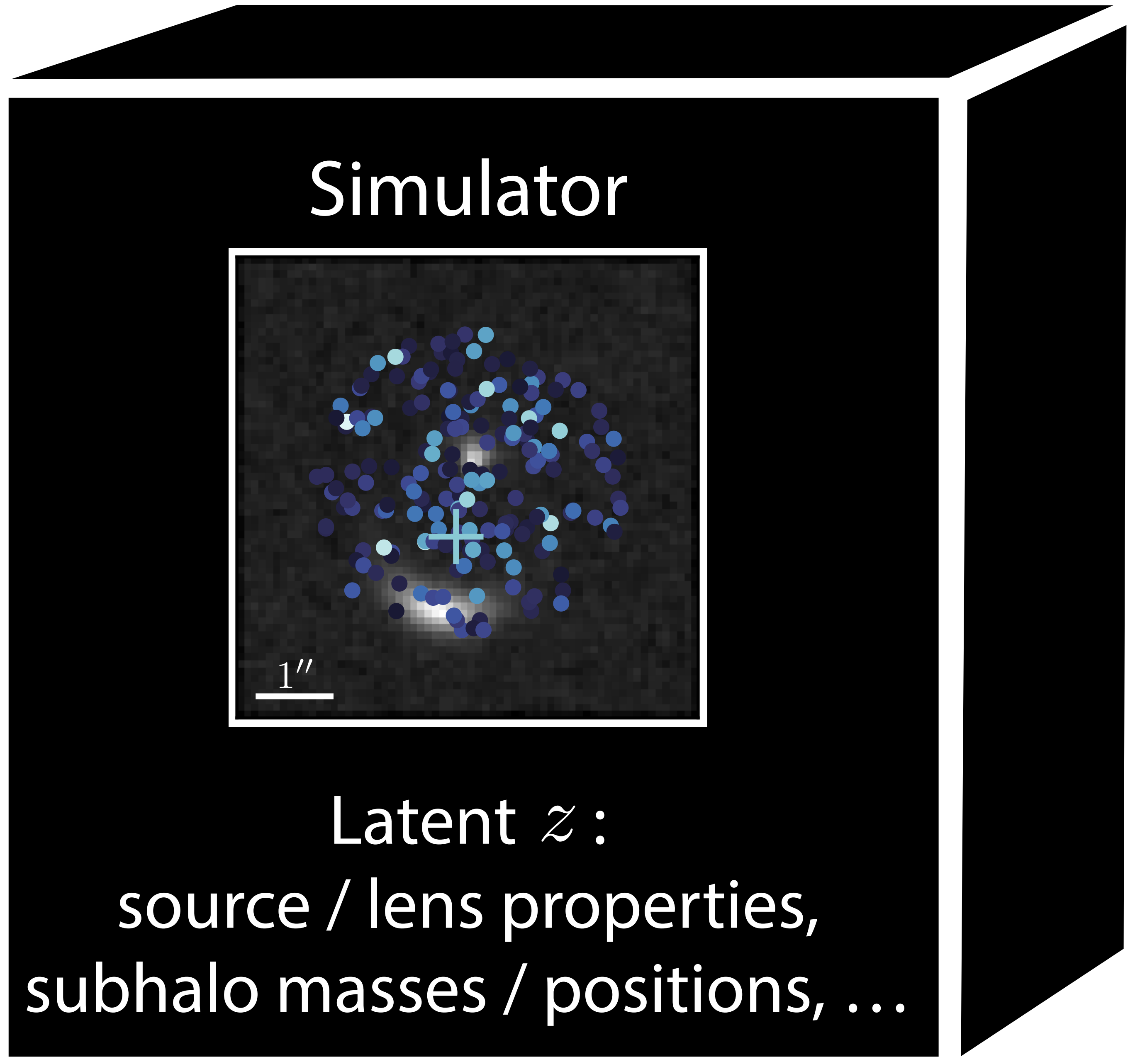
$$r(x|\theta_0, \theta_1) \equiv \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

Bonus material: gravitational lensing

Overview

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





64^2 observables x

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

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

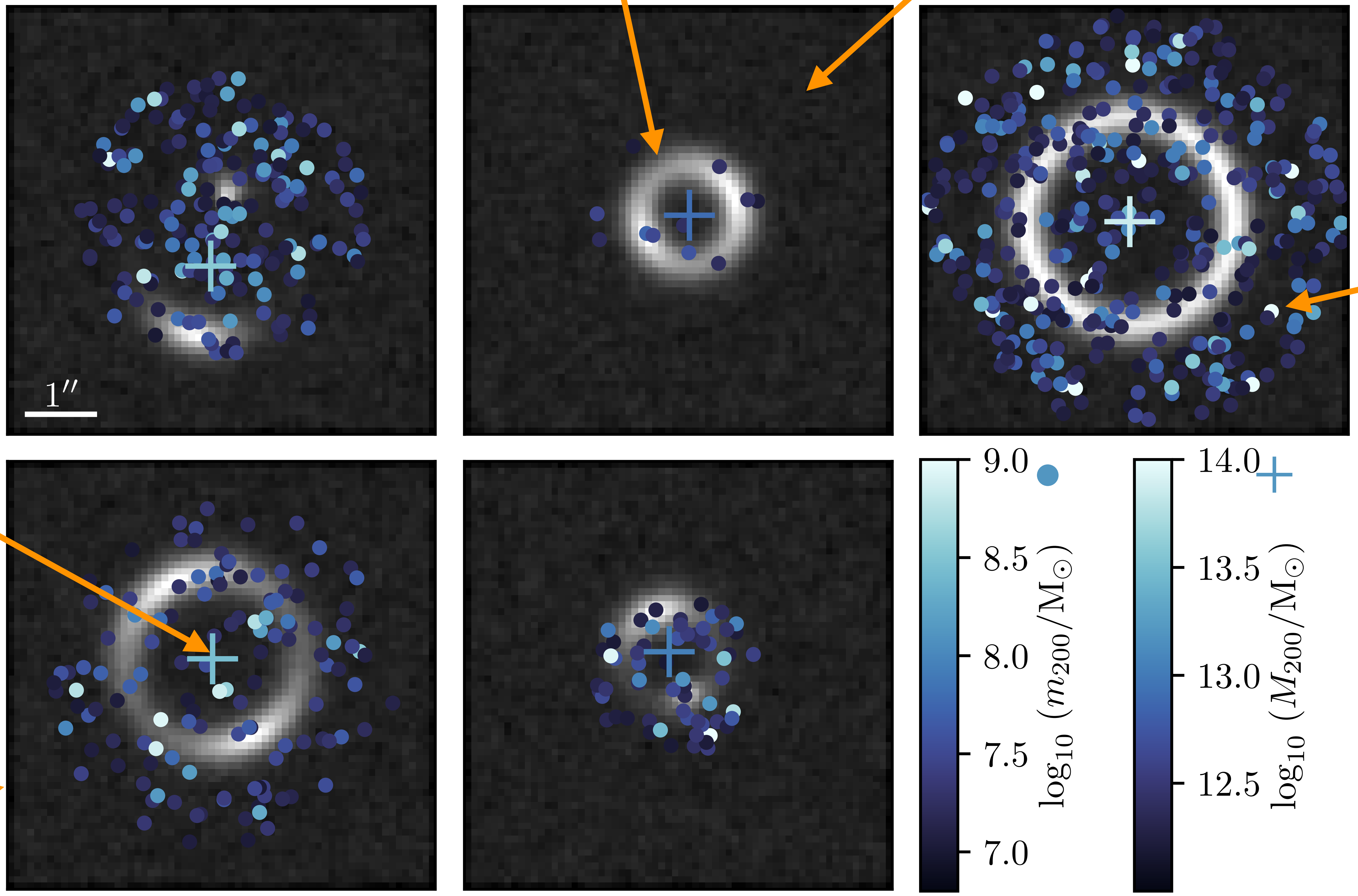
Proof-of-principle simulator

[following T. Collett 1507.02657]

Spherical lensing host galaxies
at redshift ~0.5…1

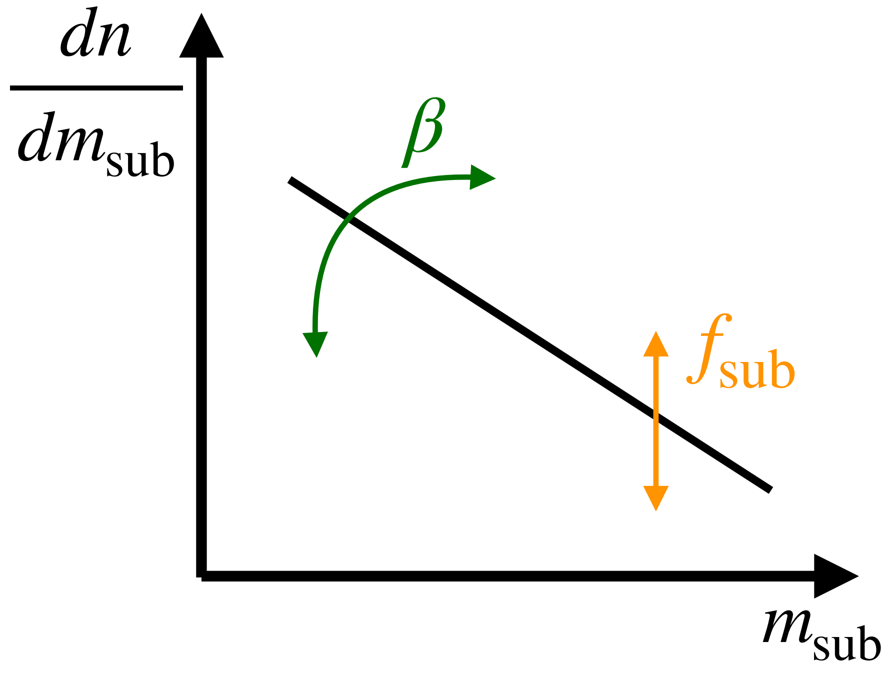
Poisson fluctuations

Extended galaxy sources
at redshift 1.5

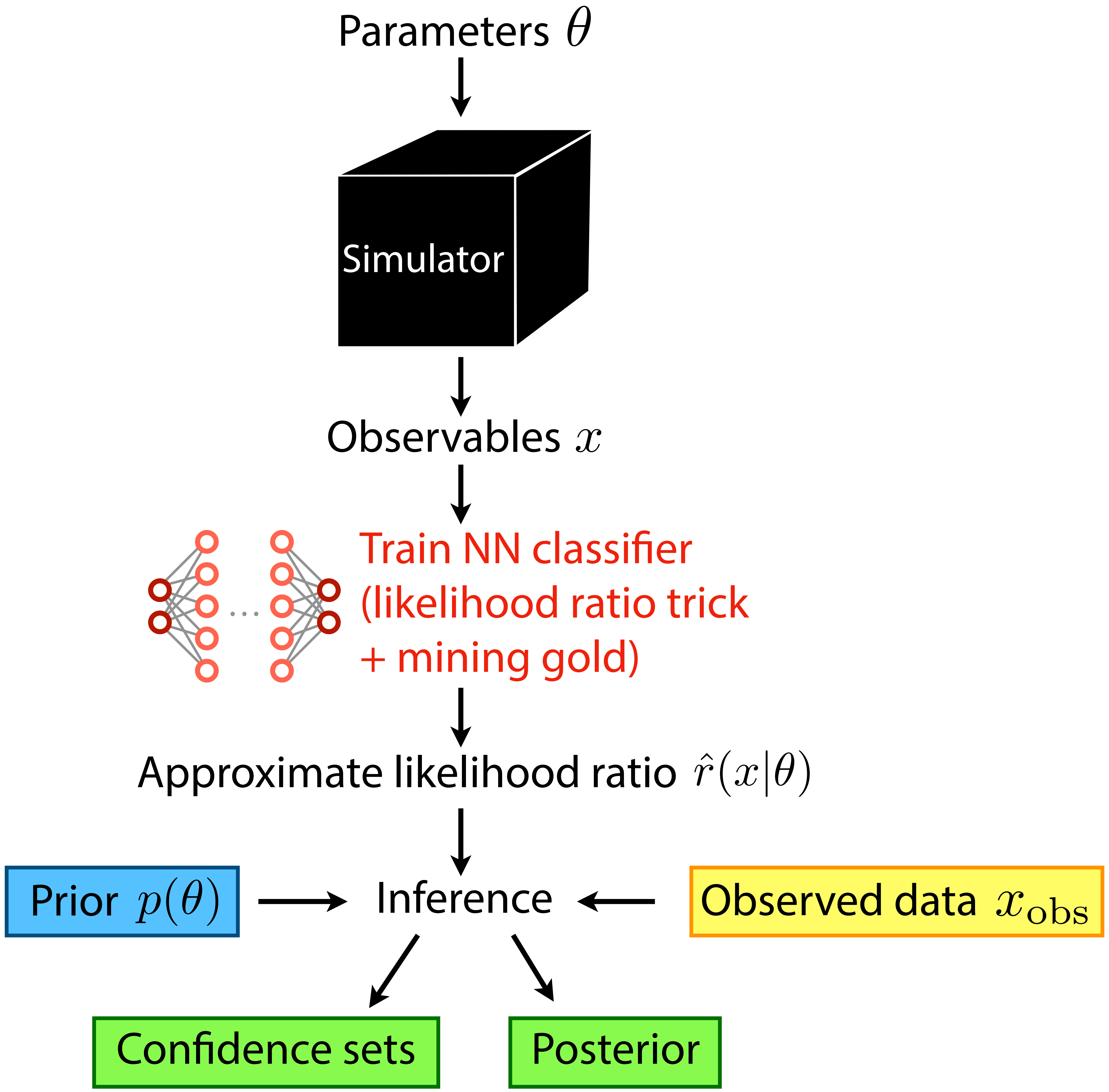


Euclid detector model
(single optical band,
64^2 pixel, Gaussian PSF)

Subhalos follow mass distribution with two parameters



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:

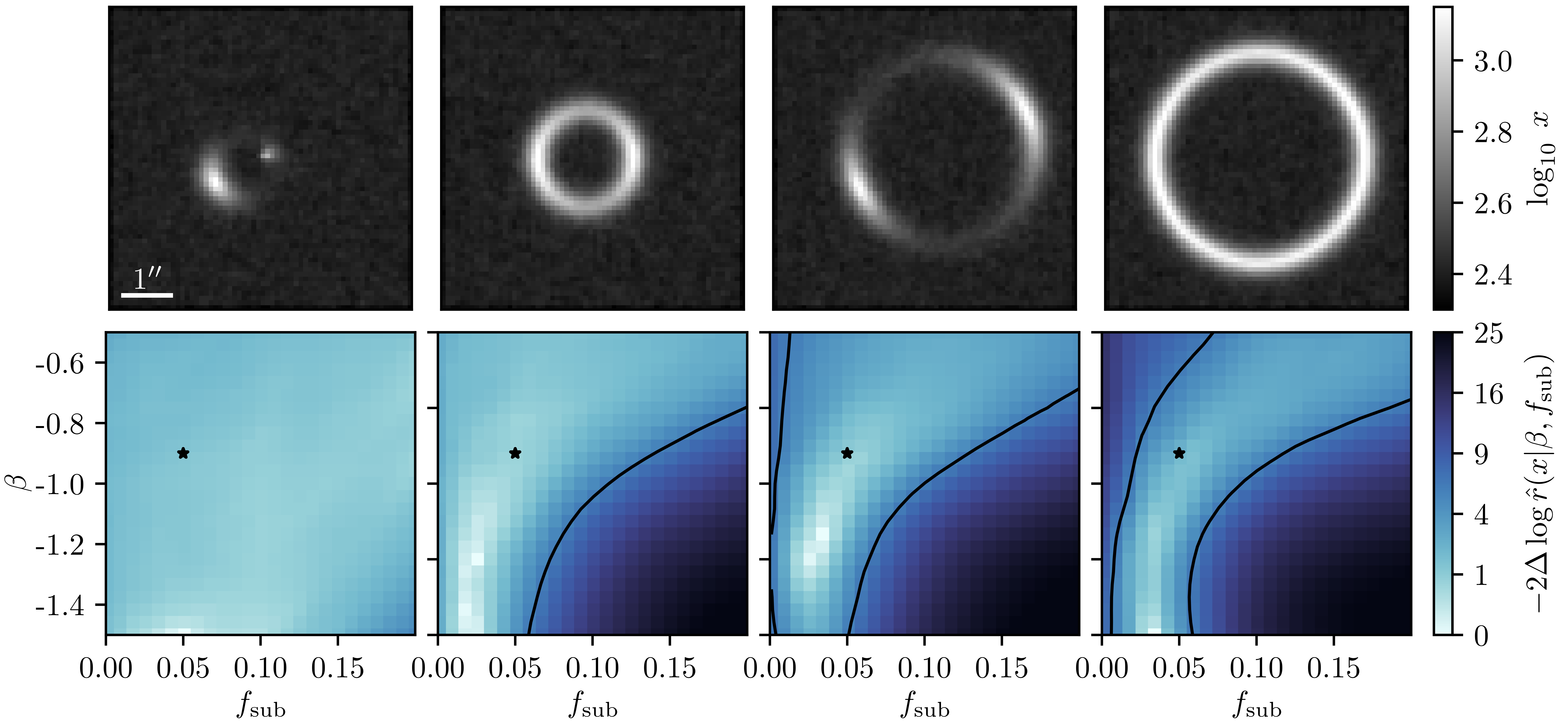
- How likely is it to observe n events after cuts?
- "Easy" to compute
- For simplicity, we ignore this part in this talk

Kinematic term for each event:

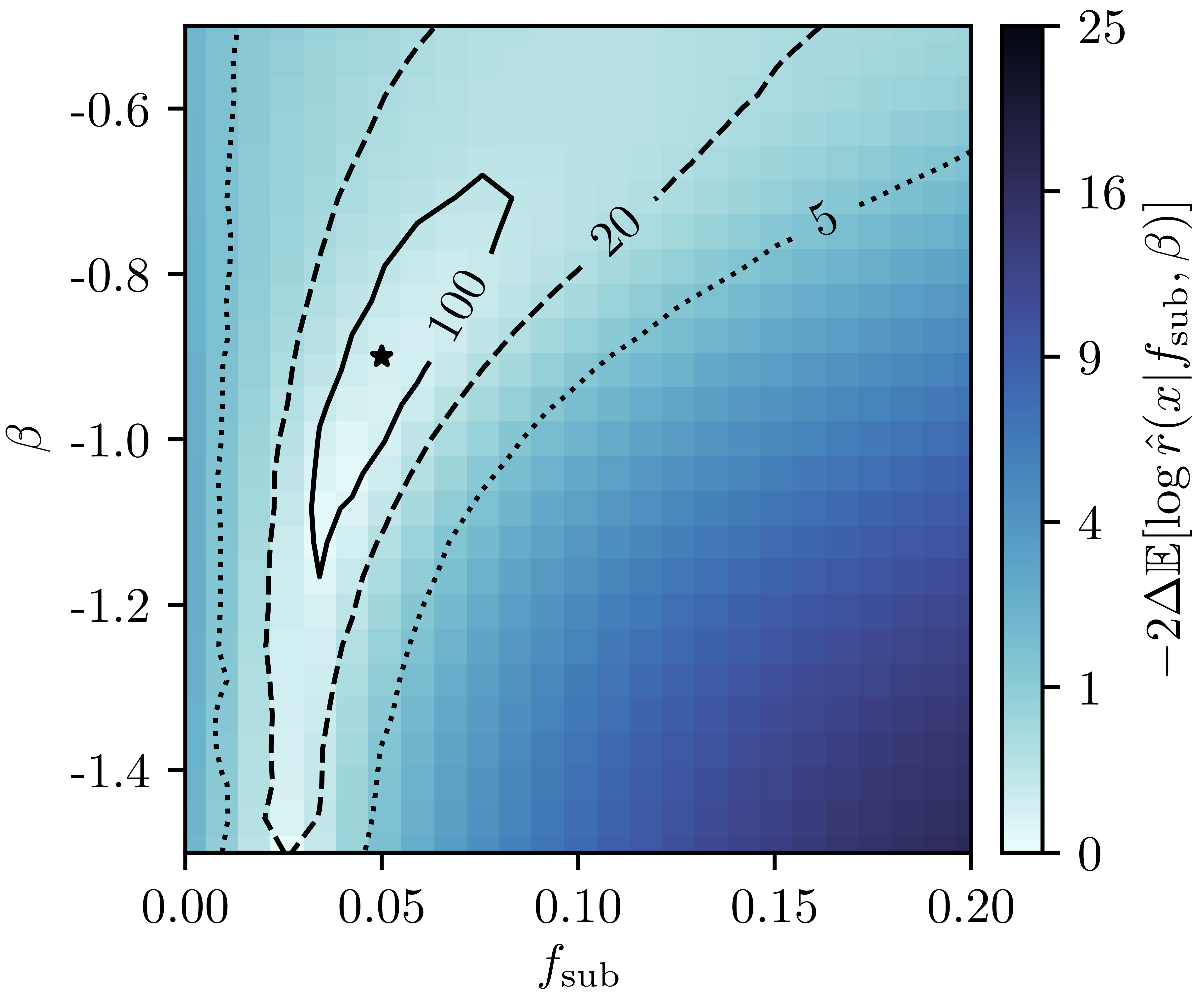
- How likely is it that an event looks like it does?
- ~ normalized differential xsec
- This is the intractable part of the likelihood
- Focus of this talk

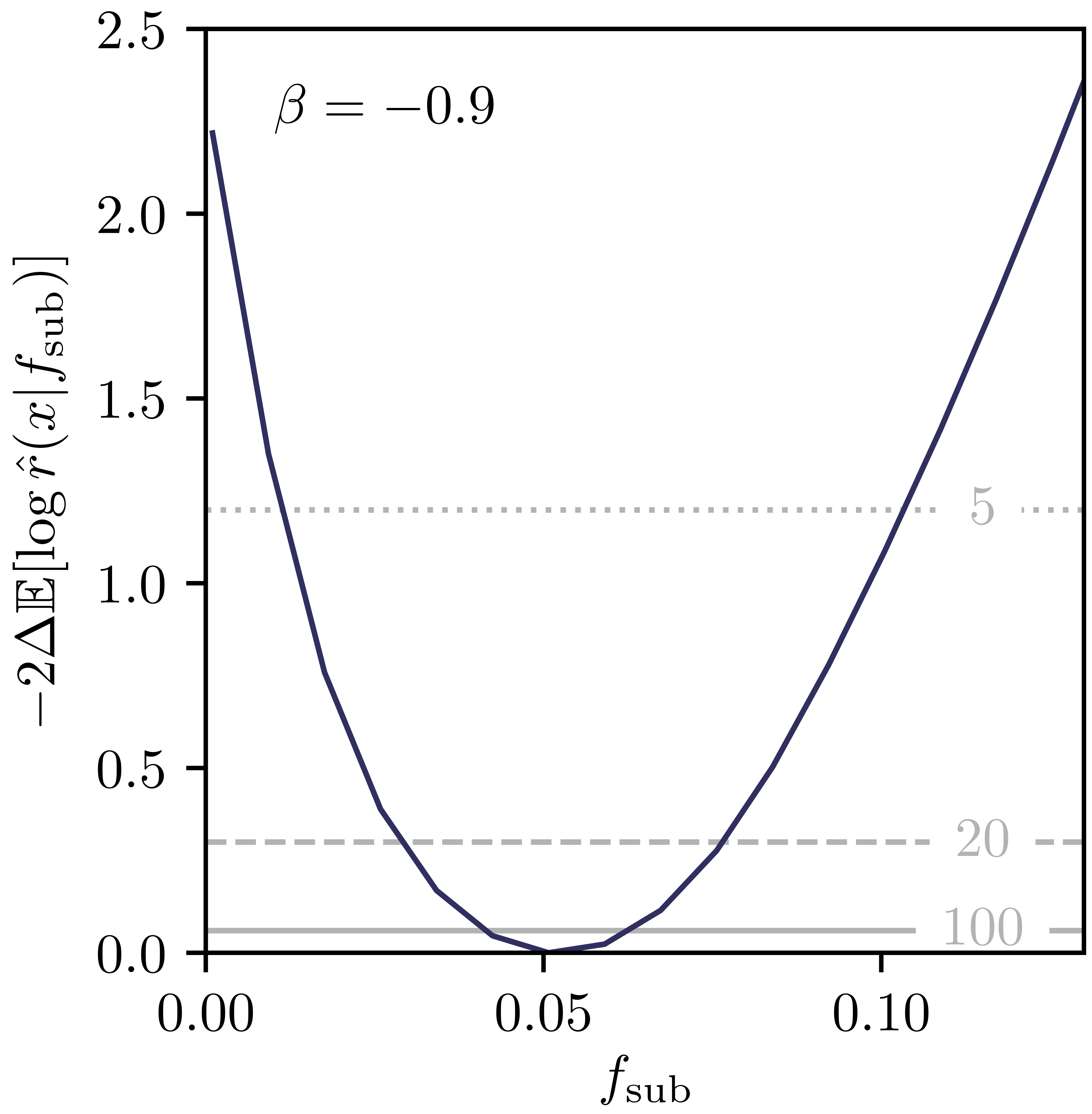
- Event selection:
  - Choice of cuts shifts information between rate and kinematic part
  - "Good" cuts depend on inference strategy
  - This talk: assume fixed event selection

Inferring parameters from individual images



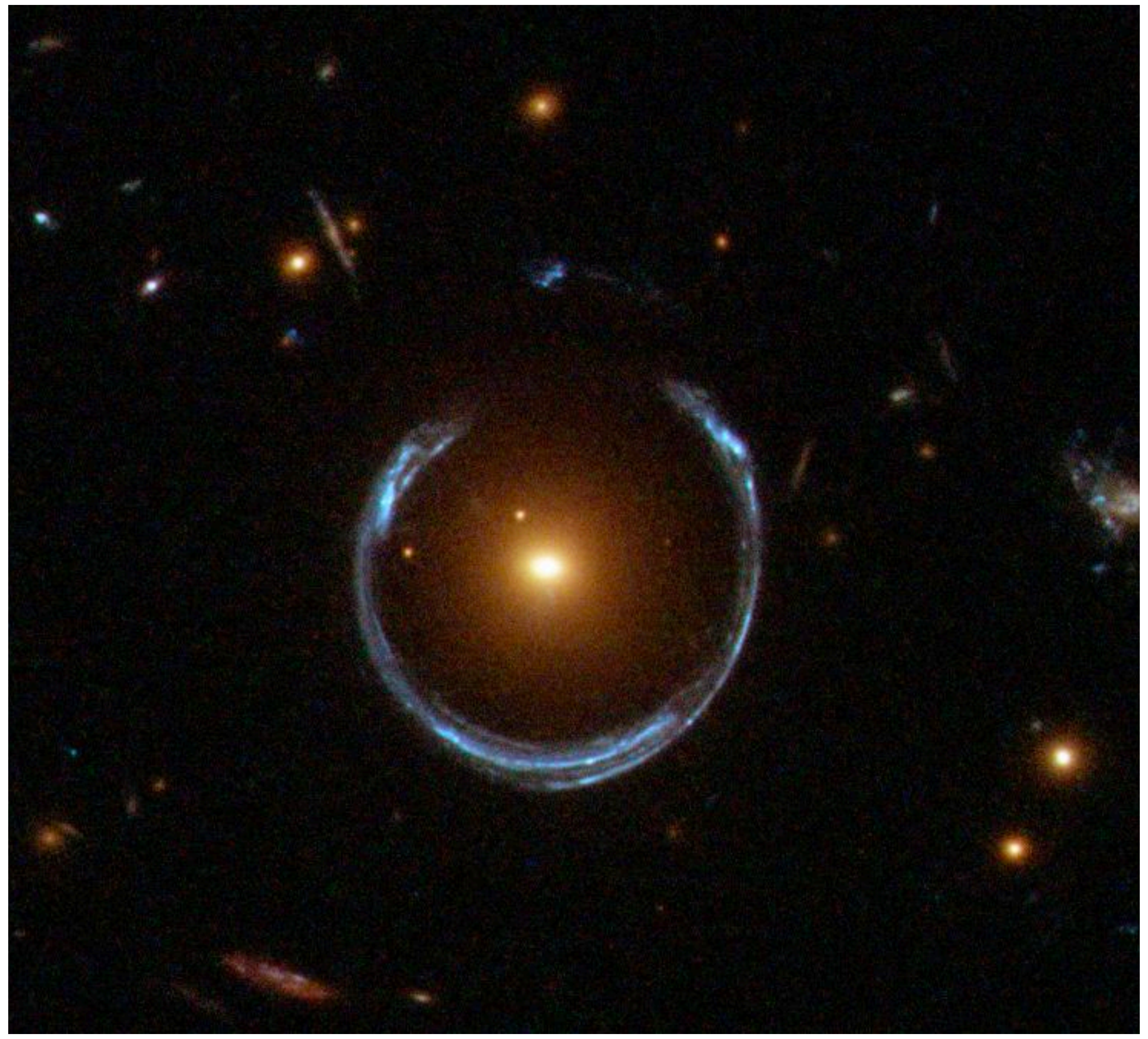
Expected likelihood ratio map





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

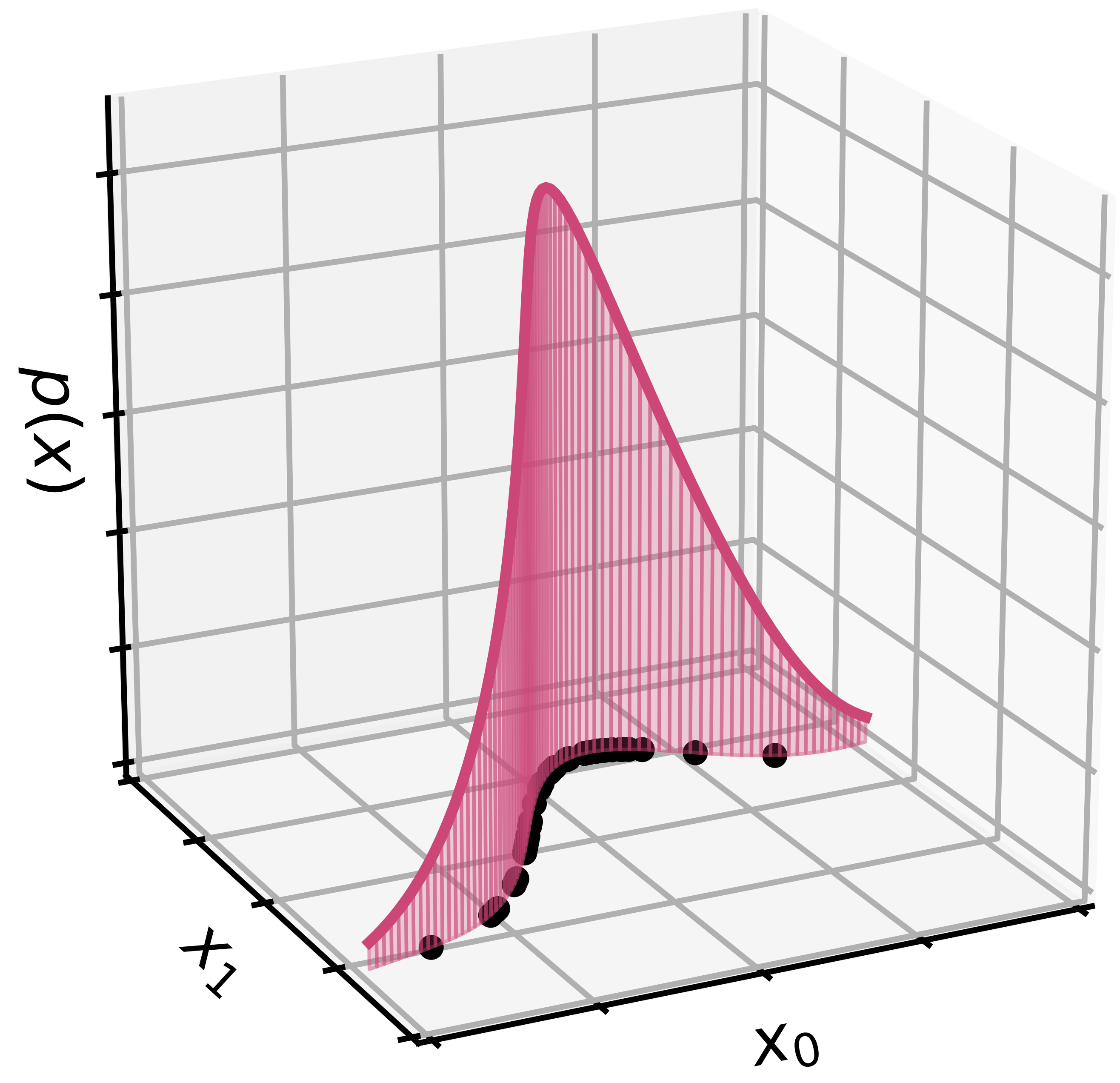
$\mathcal{M}$-flows

[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



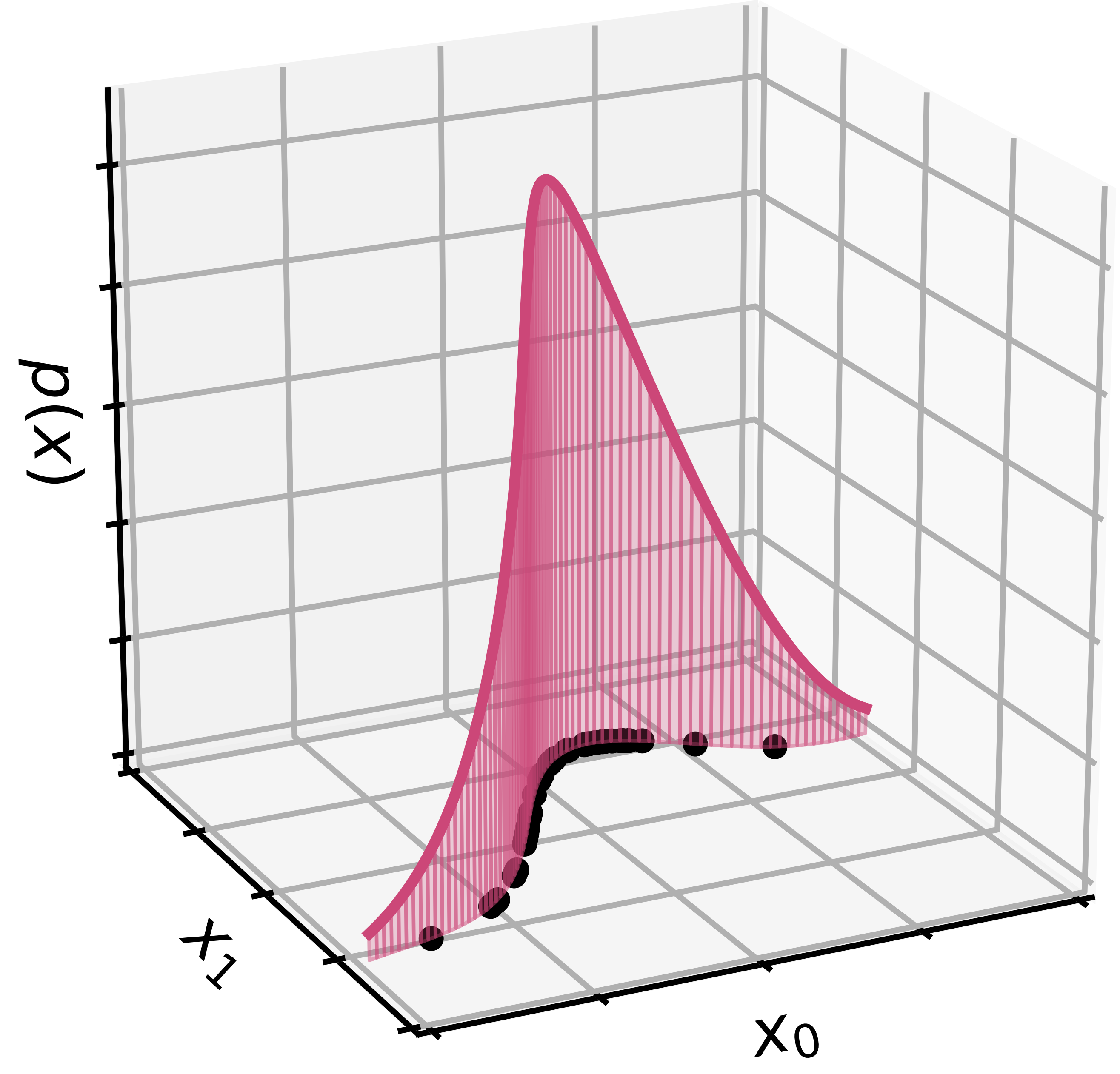
$\mathcal{M}$-flows

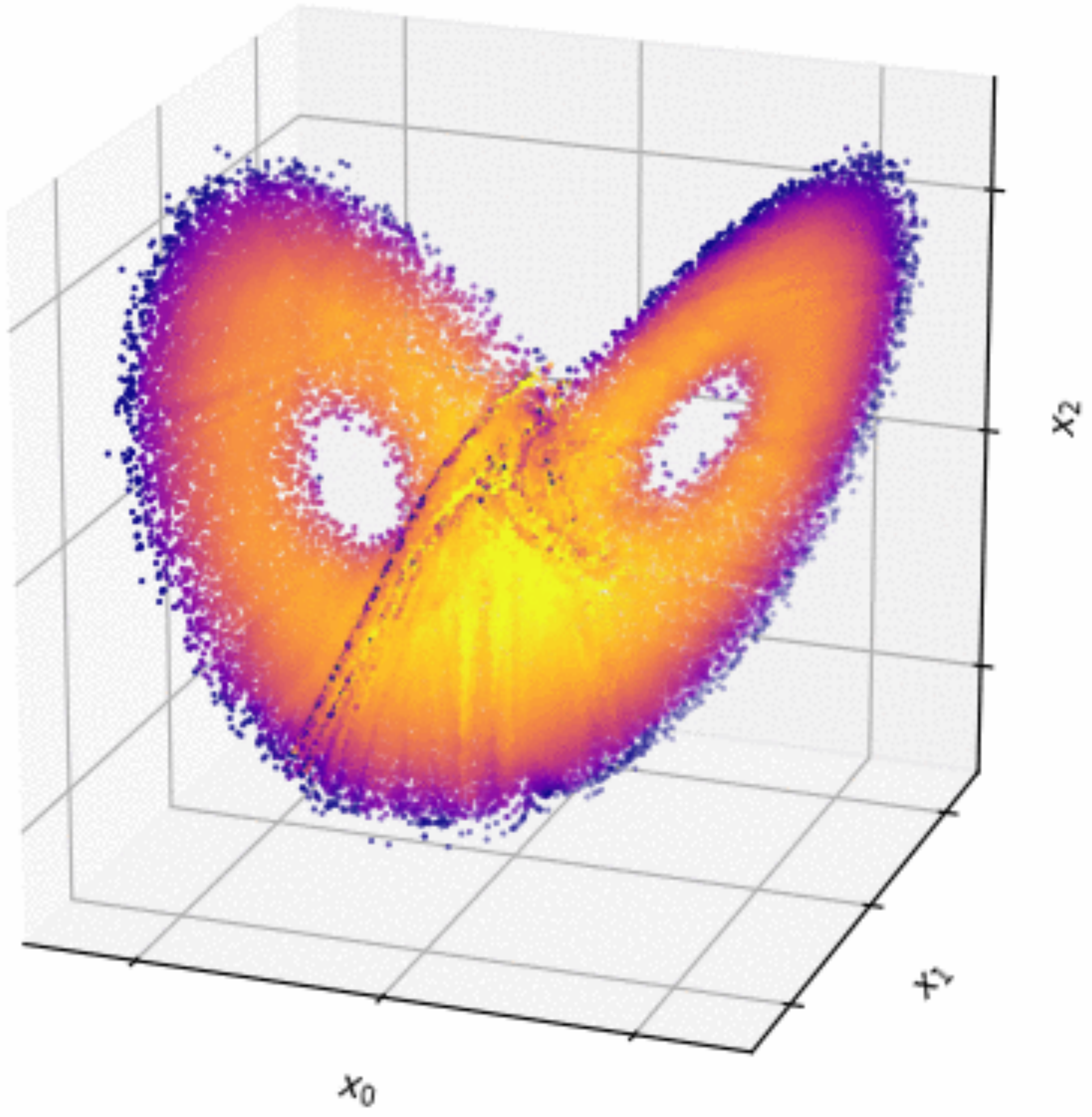
[JB, K. Cranmer 2003.13913]

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





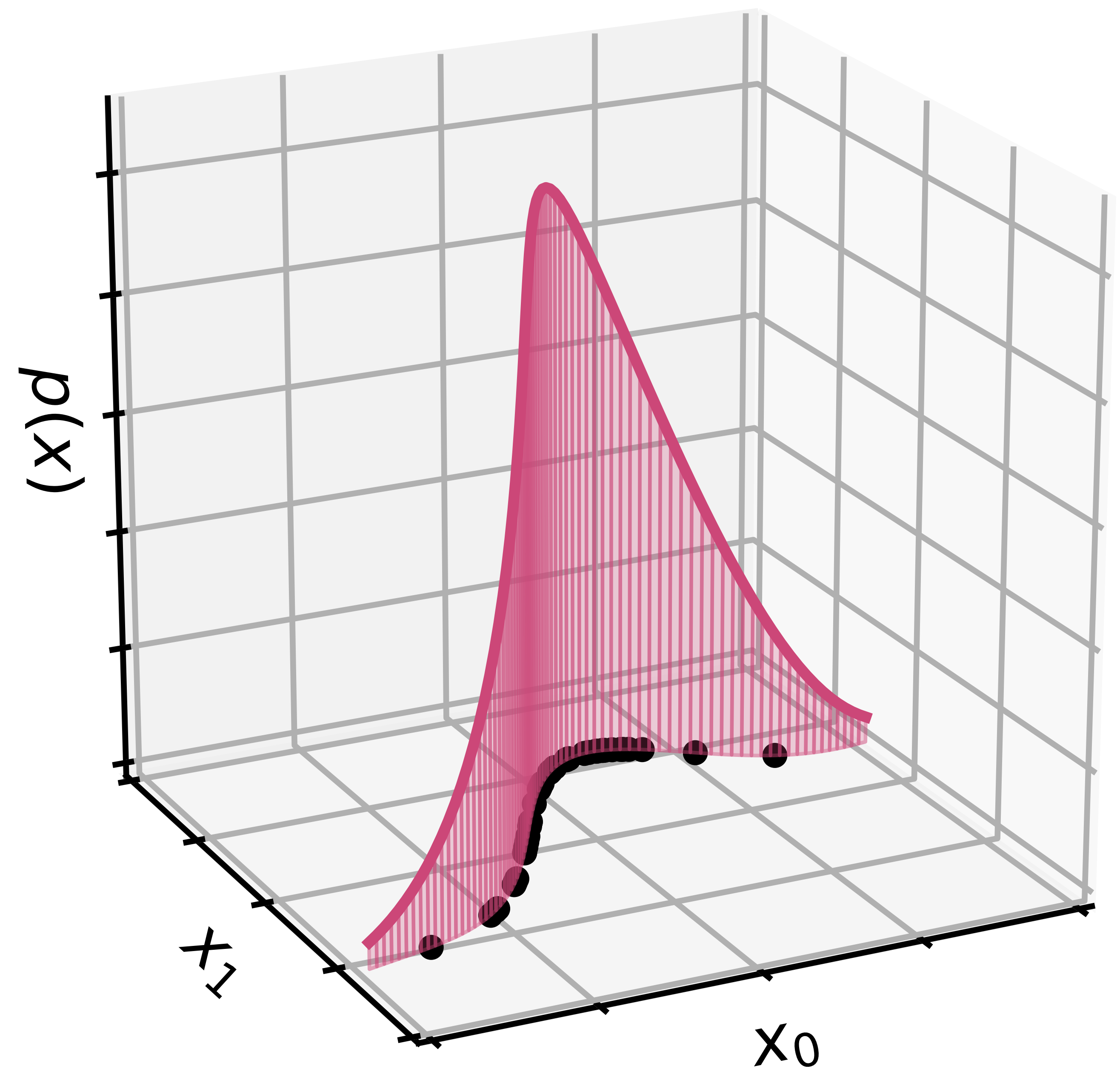
$\mathcal{M}$-flows

[JB, K. Cranmer 2003.13913]

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

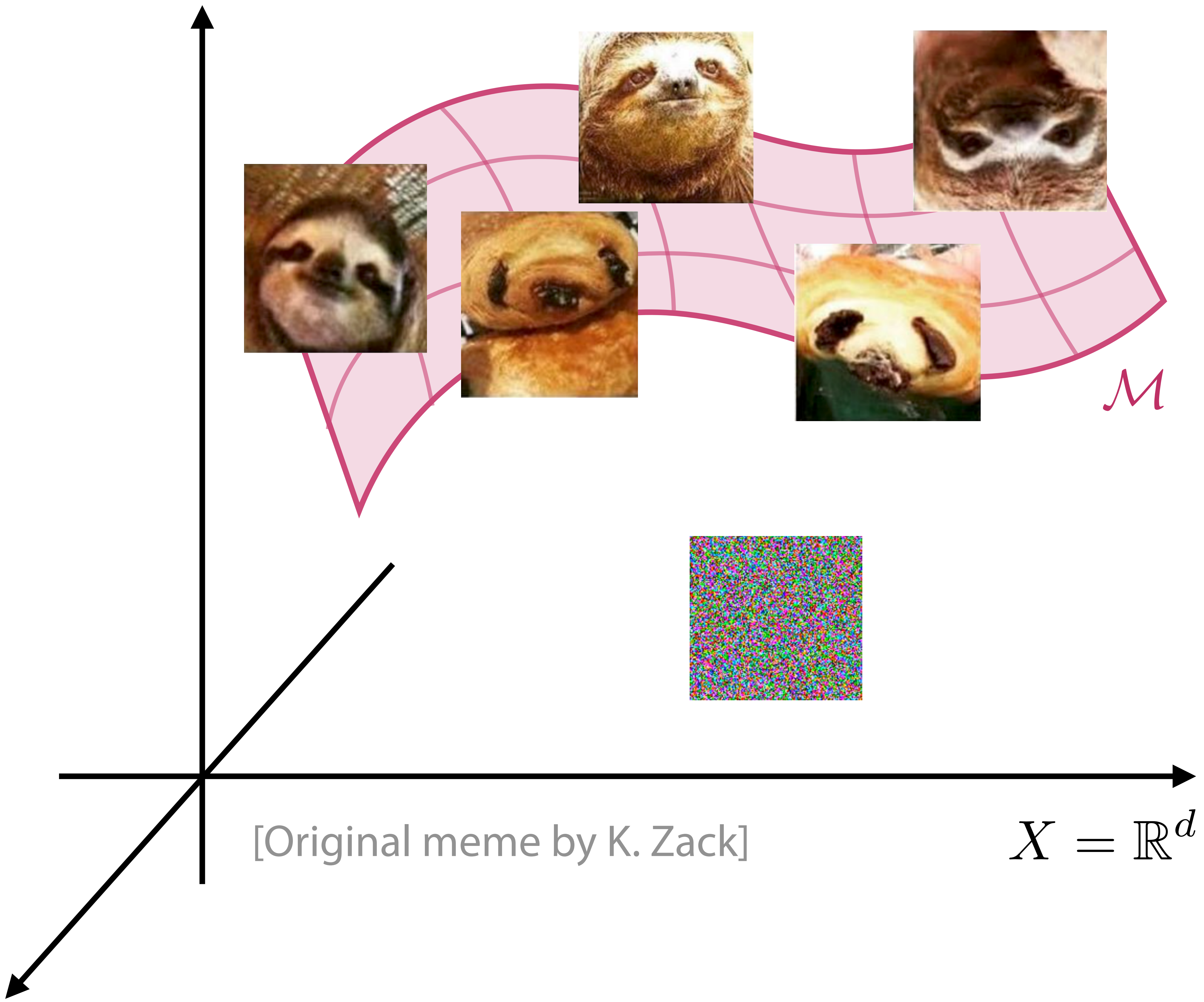
$\mathcal{M}$-flows are a new probabilistic / generative model that

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



The manifold hypothesis

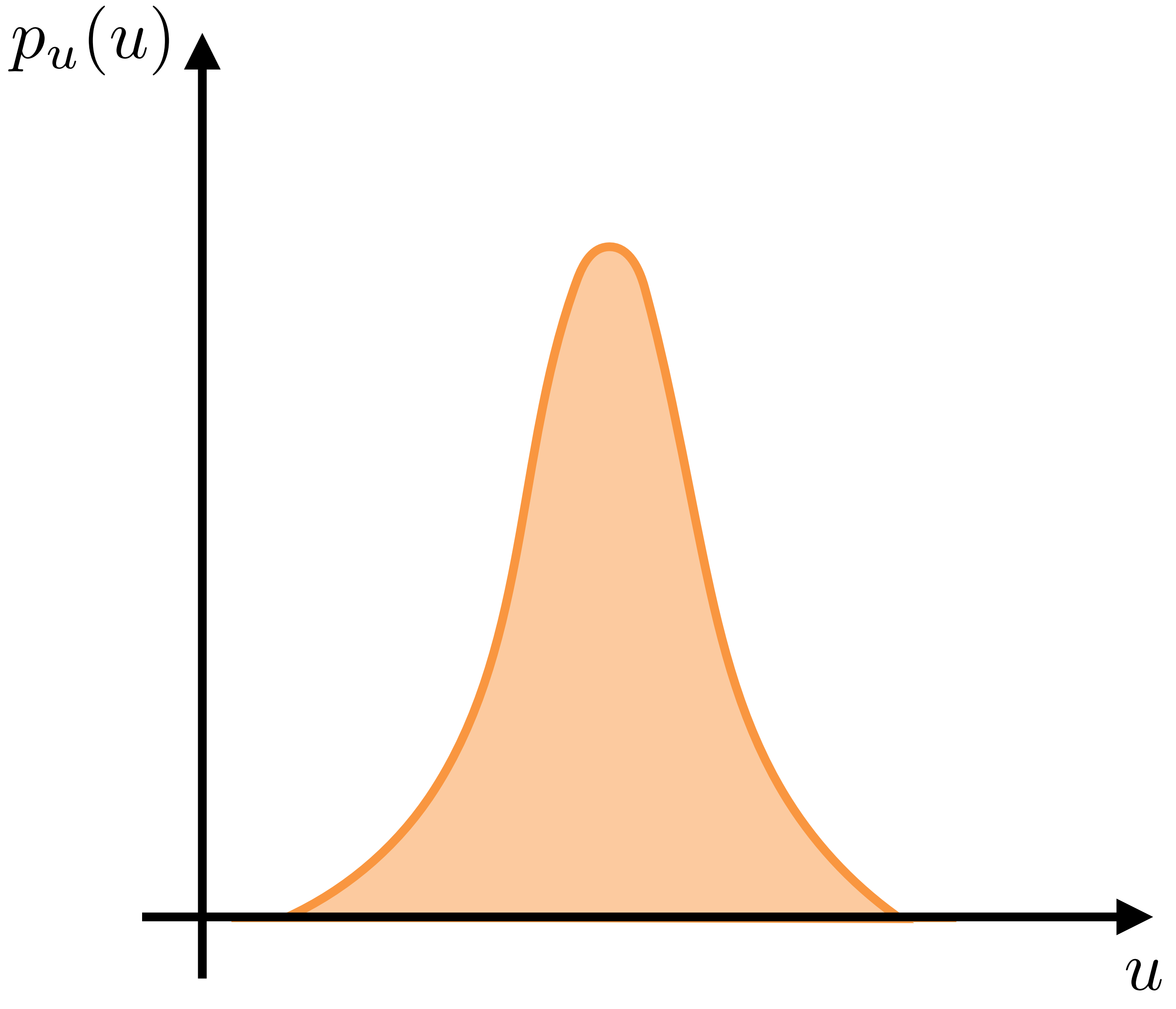
Data often live on a n-dimensional manifold embedded in the d-dimensional ambient space



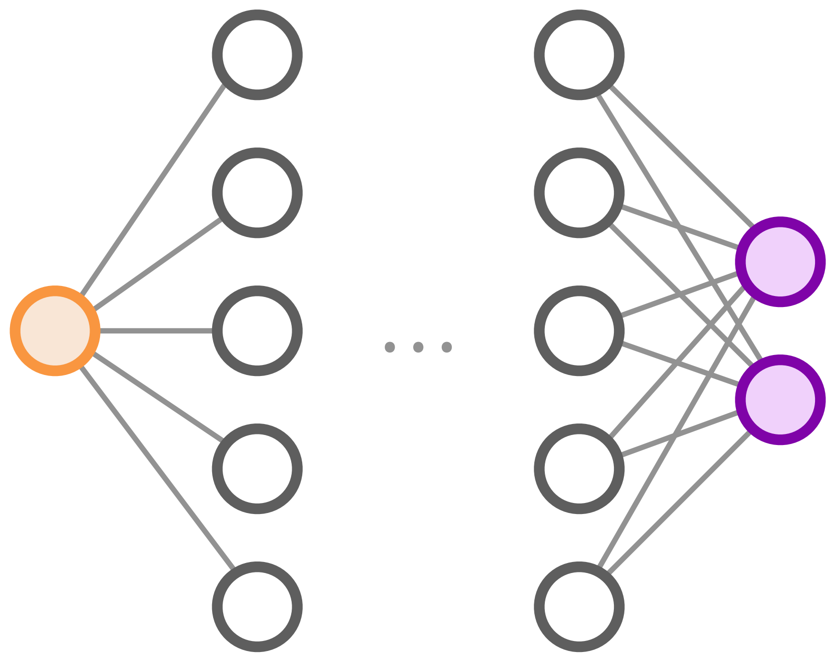
- Robot arms, molecules: limited degrees of freedom
- Particle physics: energy-momentum conservation, on-shell conditions, redundant observables
- Many other high-dimensional datasets (e.g. images): empirical evidence for (approximate) data manifold
  [L. Cayton 2005; …]

Generative adversarial networks (GANs)

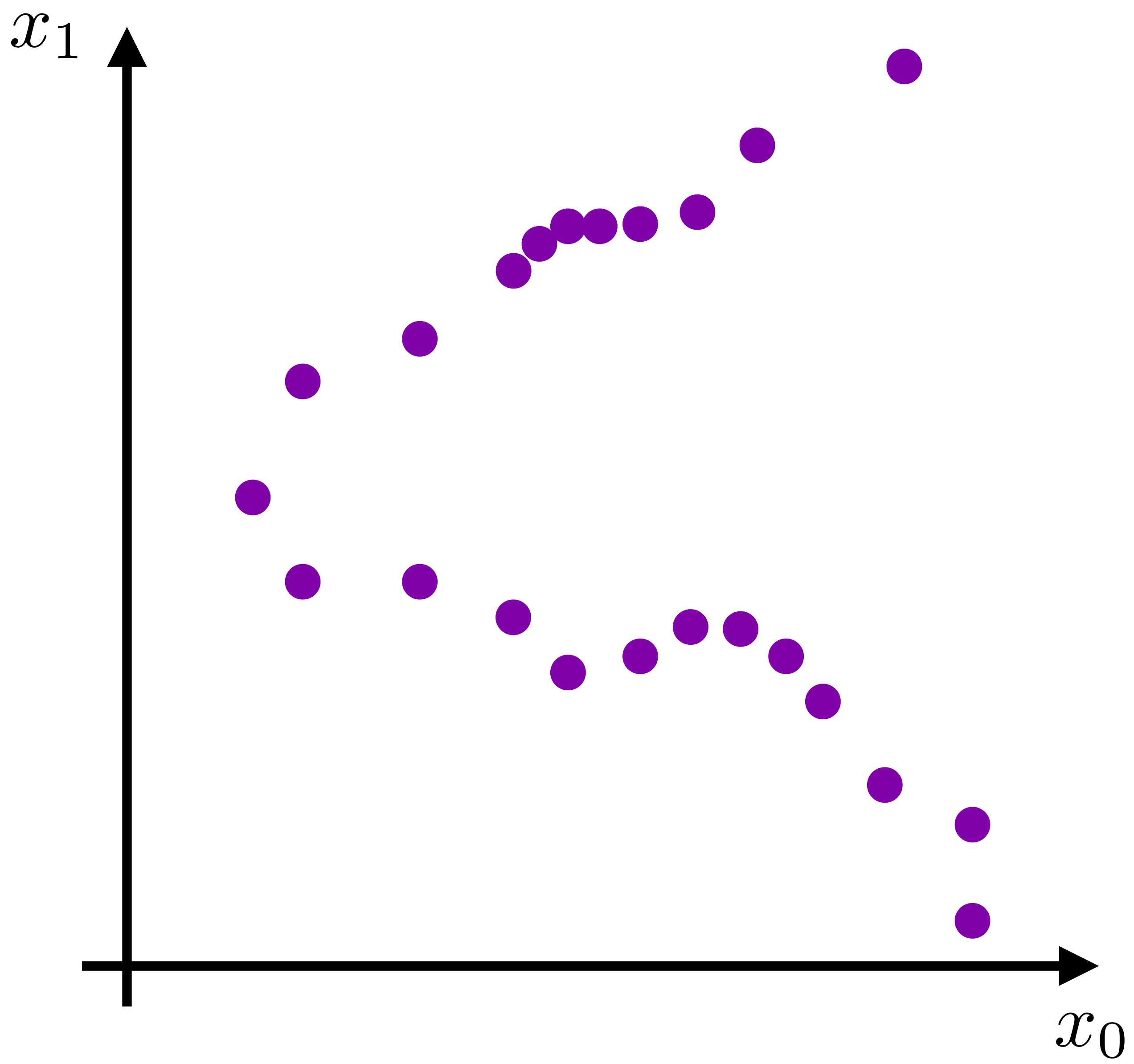
[I. Goodfellow et al 1406.2661]



$u \sim p_u(u)$



g



x

n-dim. latent variables

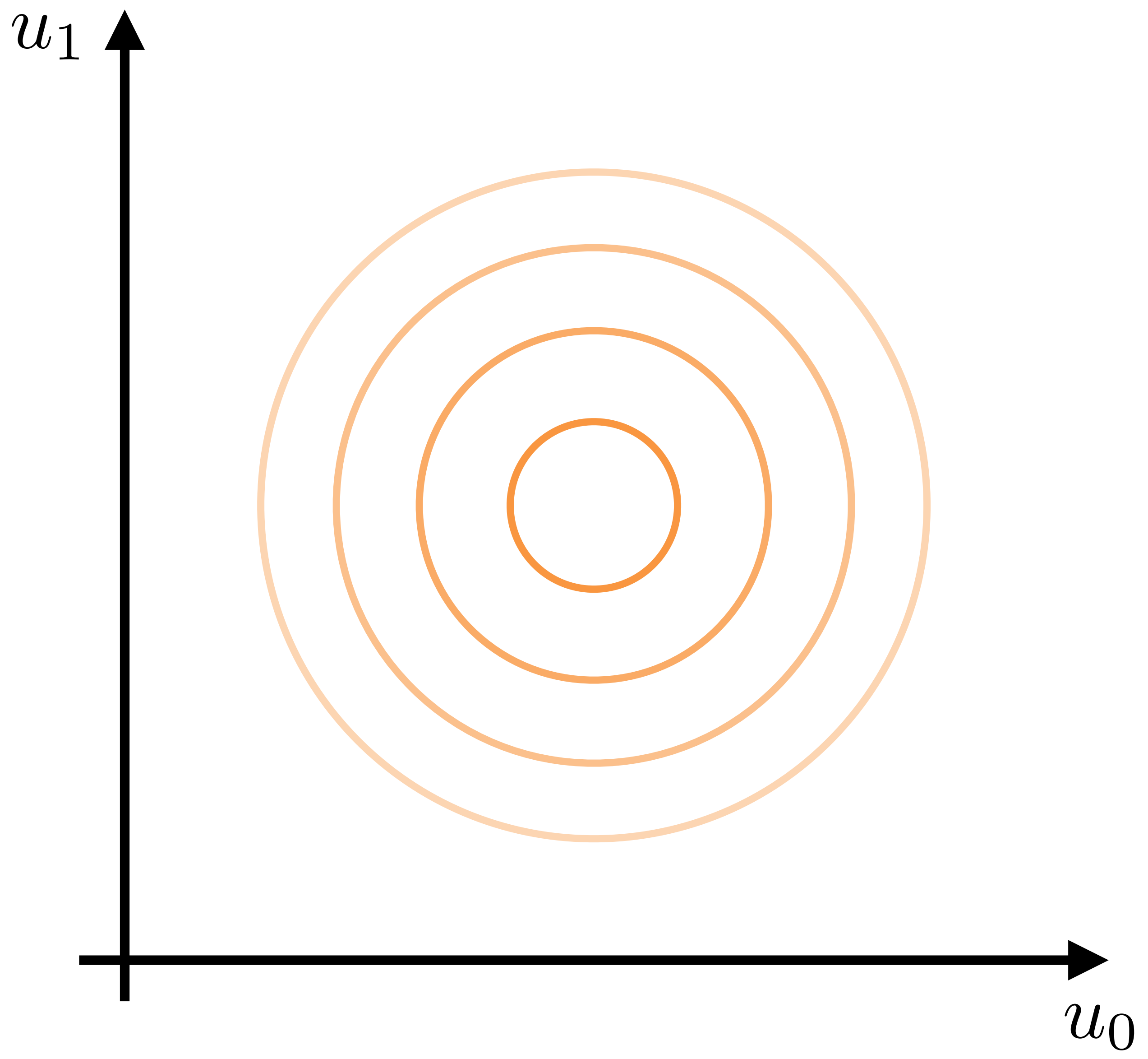
unconstrained NN

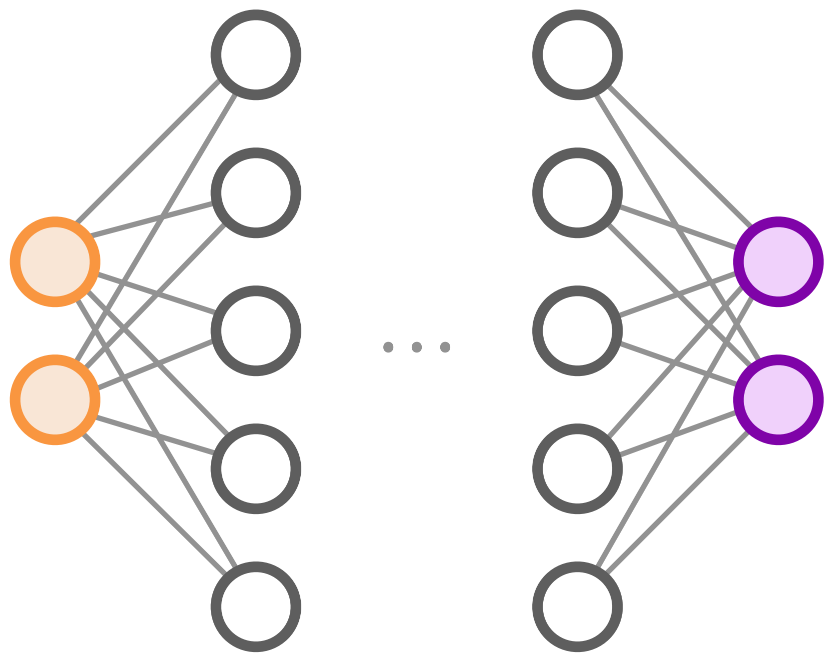
implicit density over $\mathcal{M}$

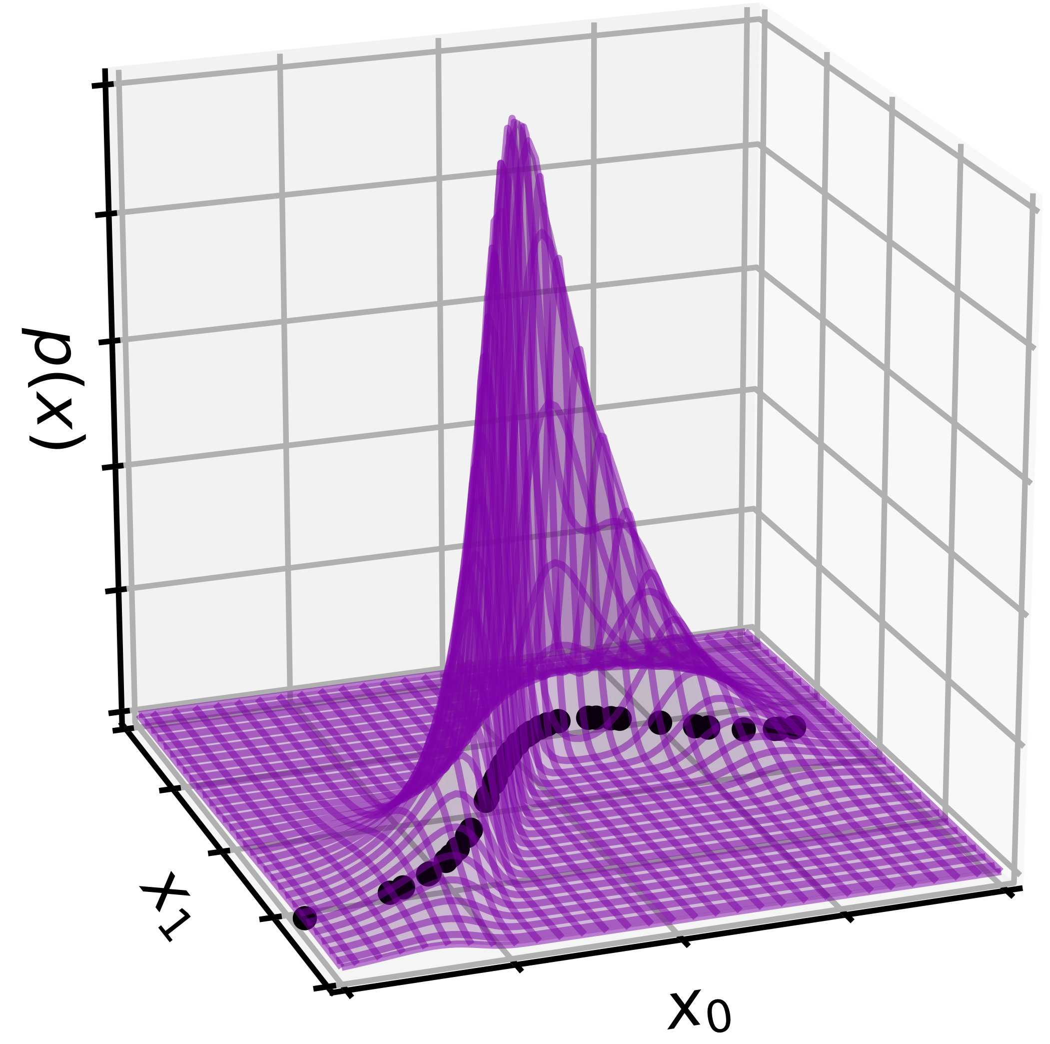
$p_{\mathcal{M}}(x)$ intractable

Normalizing flows in the ambient data space

[G. Papamakarios et al 1912.02762]







$u \sim p_u(u)$

f

x

d-dim. latent variables

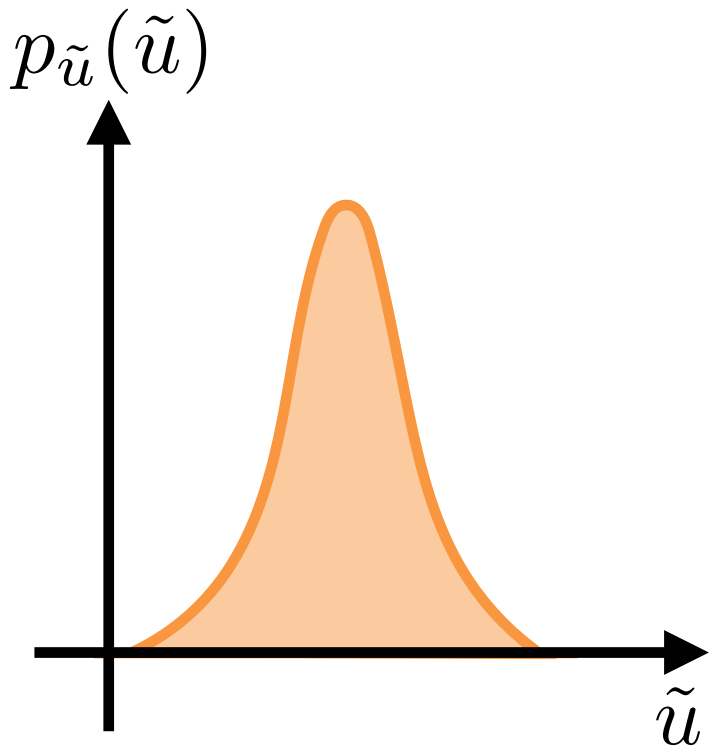
invertible NN

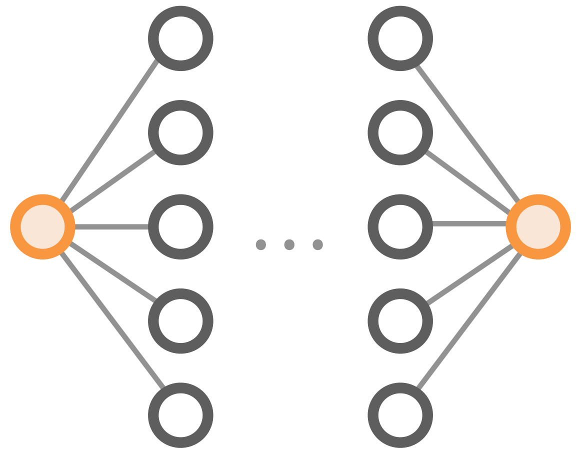
tractable density over ambient data space

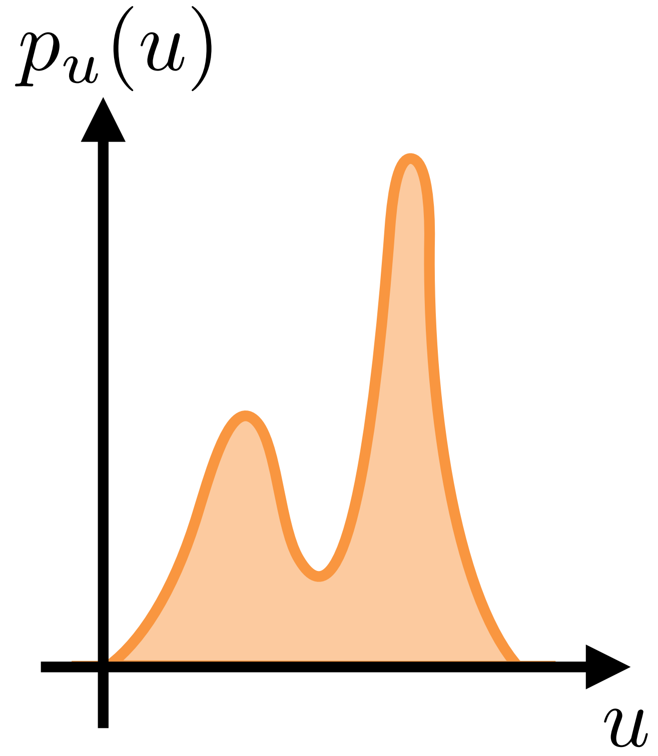
$$p_x(x) = p_u(f^{-1}(x))\,|\det J_f(f^{-1}(x))|^{-1}$$

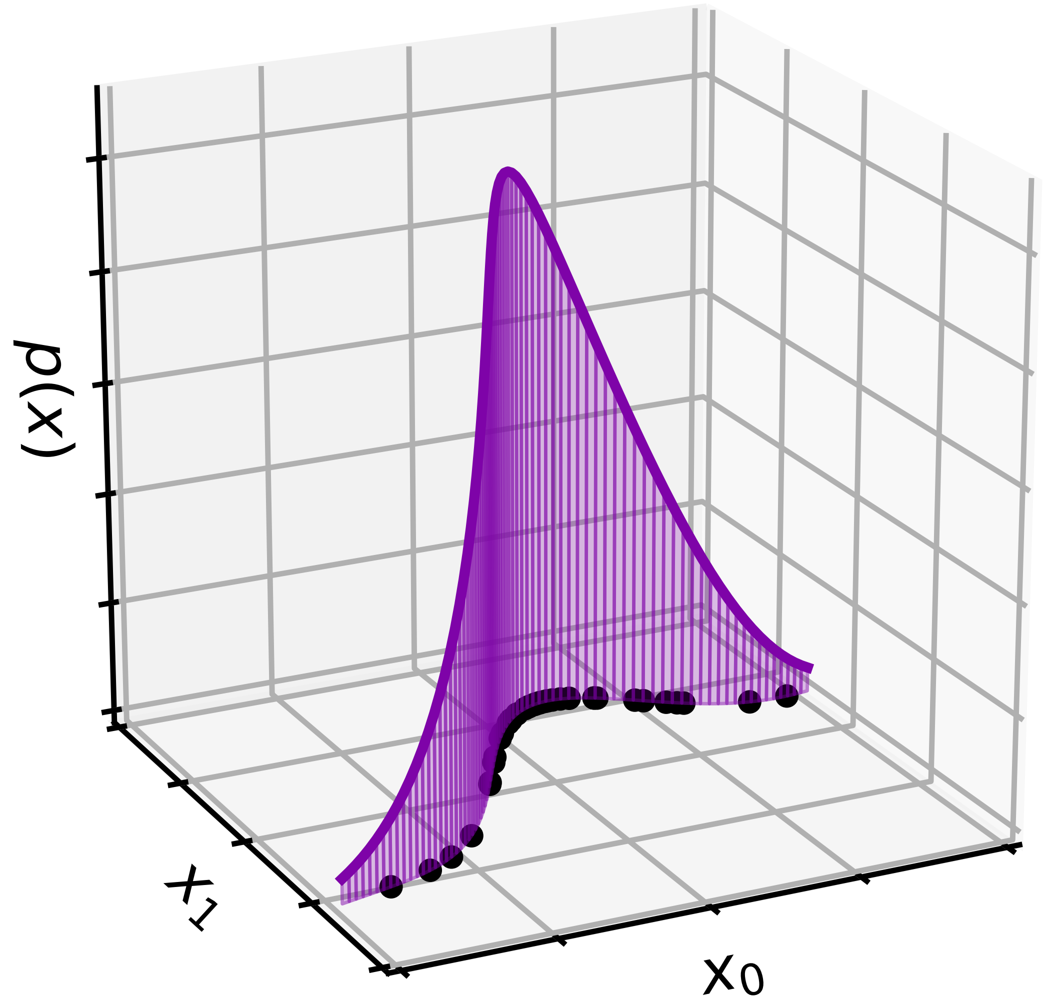
Flows on a prescribed manifold

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









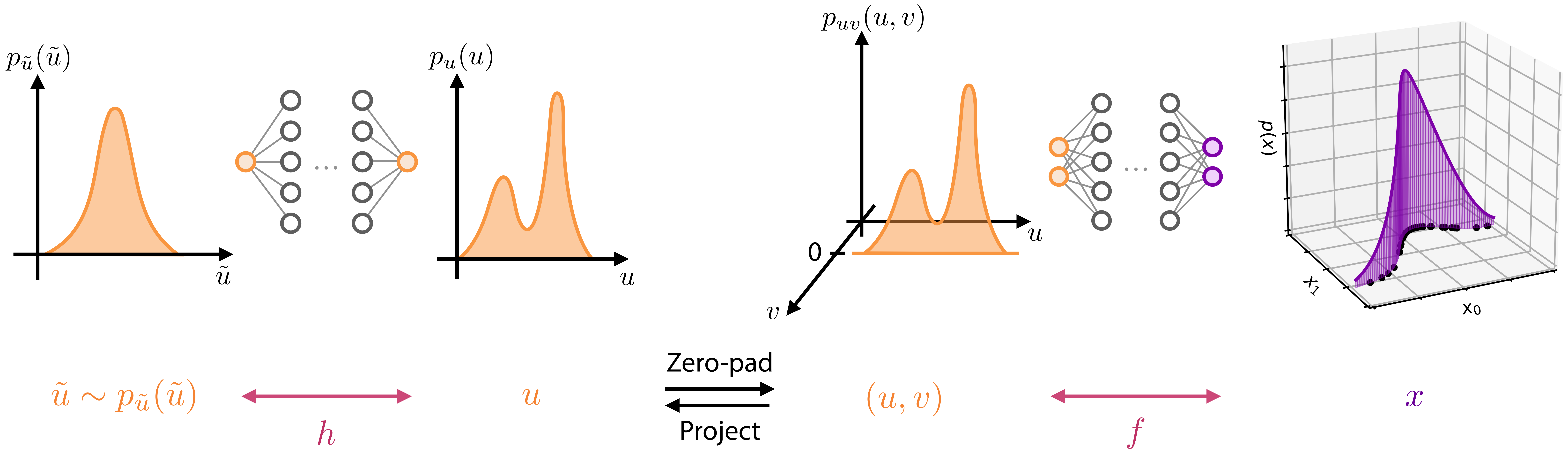
$\tilde{u} \sim p_{\tilde{u}}(\tilde{u})$ $\longleftrightarrow$ h u $\longleftrightarrow$ g^* x

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

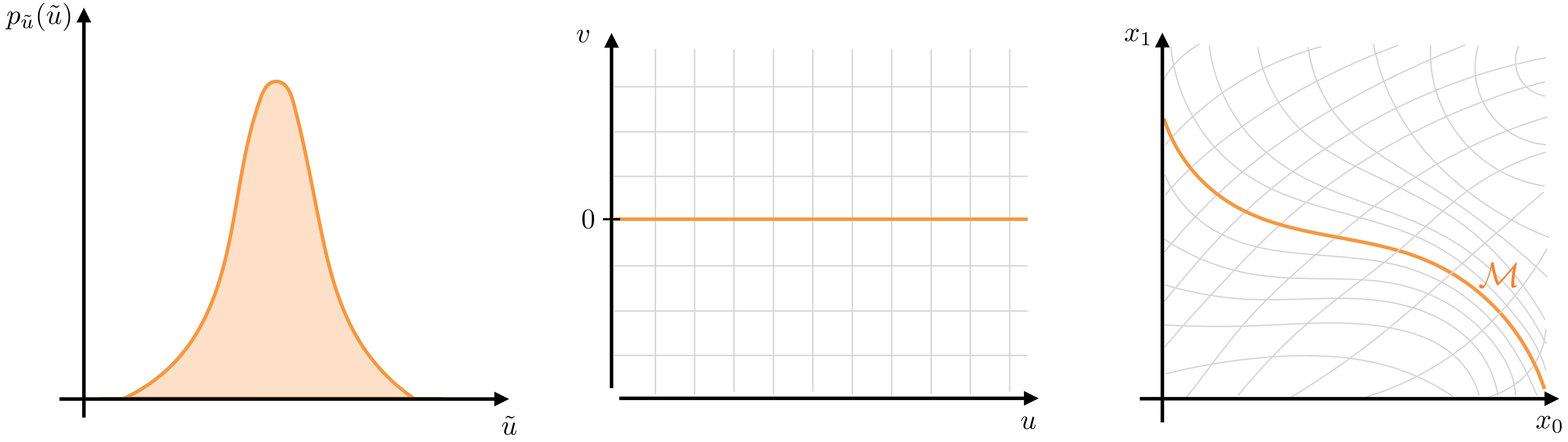
[JB, Kyle Cranmer 2003.13913]



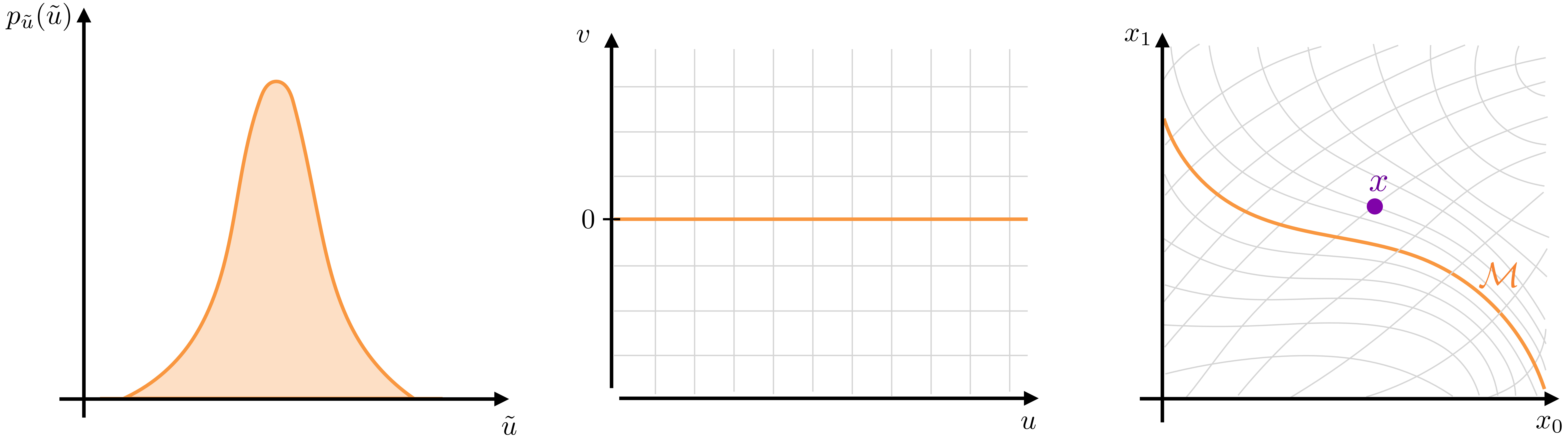
n-dim. latents | inv. NN | n-dim. latents | embed | d-dim. latents | inv. NN | tractable density over $\mathcal{M}$

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

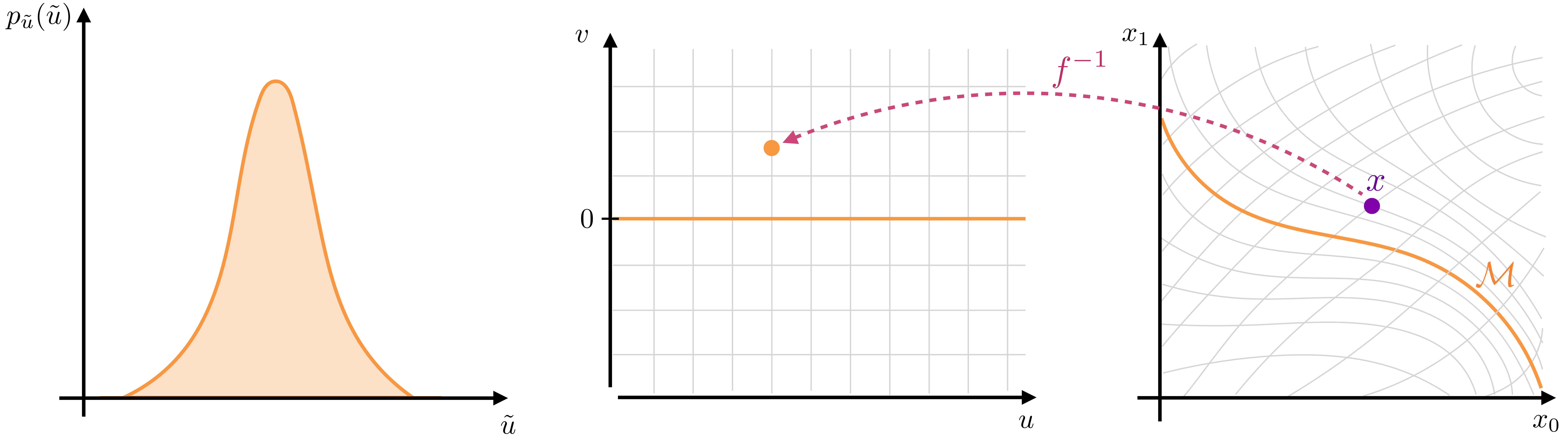
Evaluating data on or off the manifold



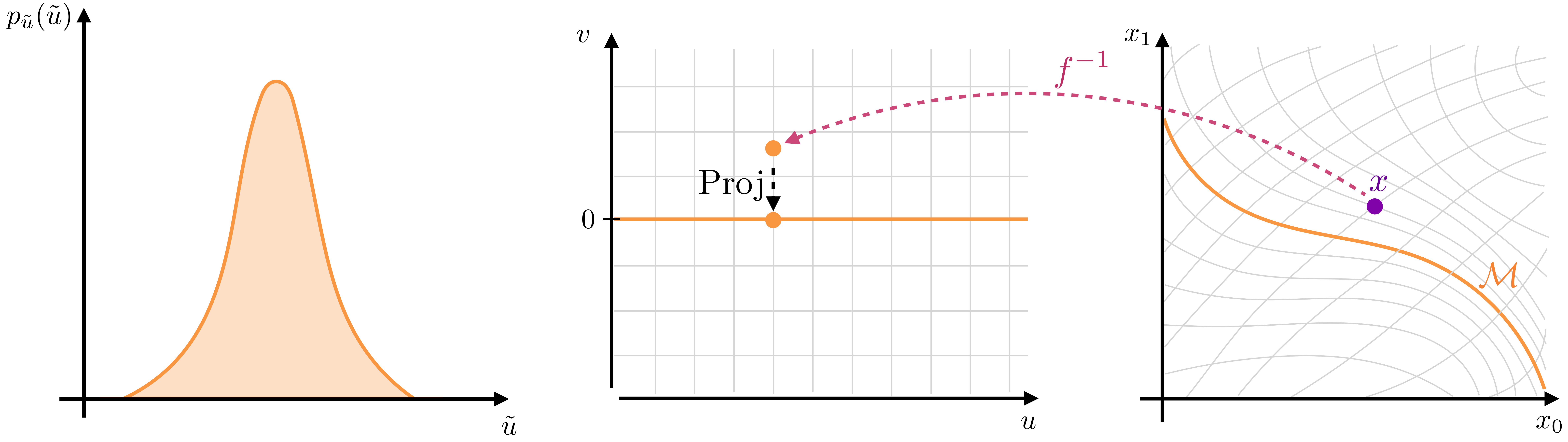
Evaluating data on or off the manifold



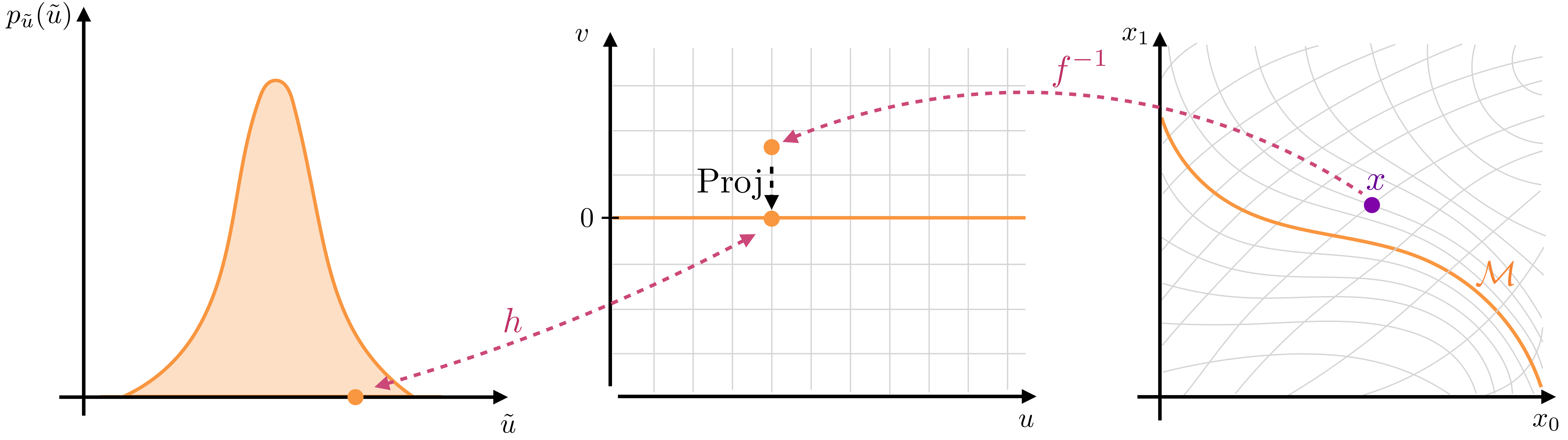
Evaluating data on or off the manifold



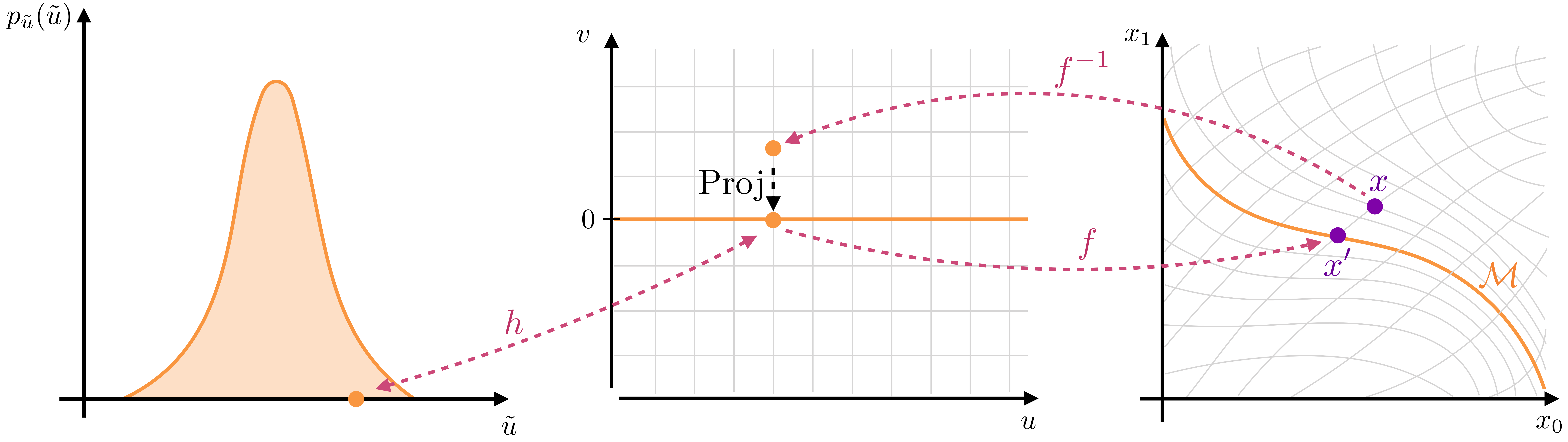
Evaluating data on or off the manifold



Evaluating data on or off the manifold



Evaluating data on or off the manifold



Evaluating data on or off the manifold

Input x

Evaluating data on or off the manifold

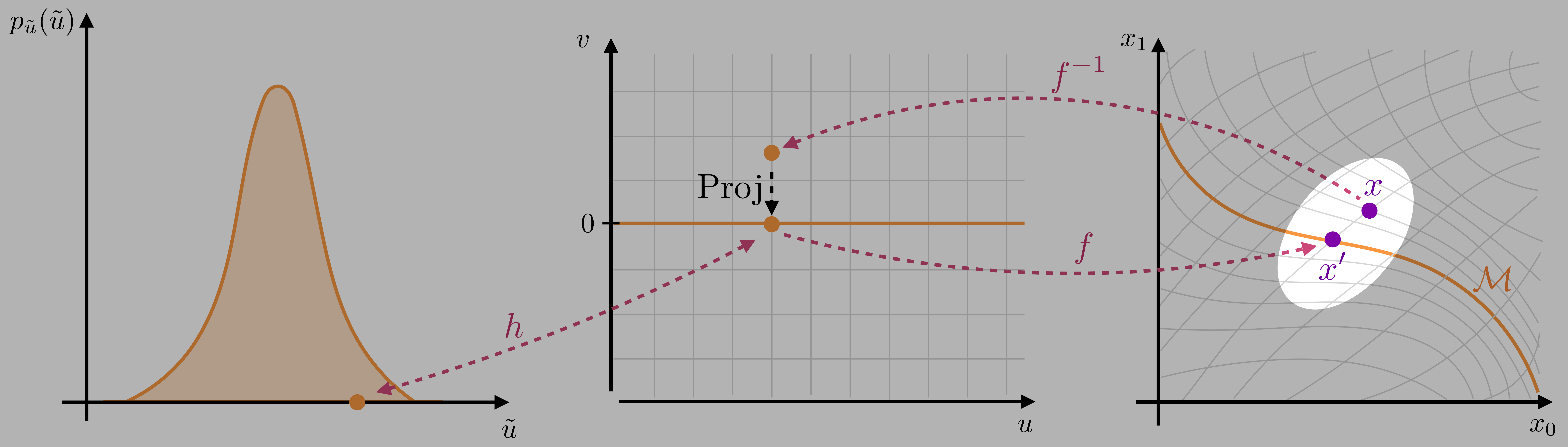
Input x $\rightsquigarrow$ Representation $\tilde{u}$ (dimensionality reduction)

Evaluating data on or off the manifold

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

⇝ Projection to manifold x' (denoising)

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)

Evaluating data on or off the manifold

Input x

- $\rightsquigarrow$ Representation $\tilde{u}$ (dimensionality reduction)
- $\rightsquigarrow$ Projection to manifold x' (denoising)
- $\rightsquigarrow$ Reconstruction error $\|x - x'\|$ (training, OOD detection)
- $\rightsquigarrow$ 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 ϕ_f

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

$\Rightarrow$ Learning ϕ_f by maximum

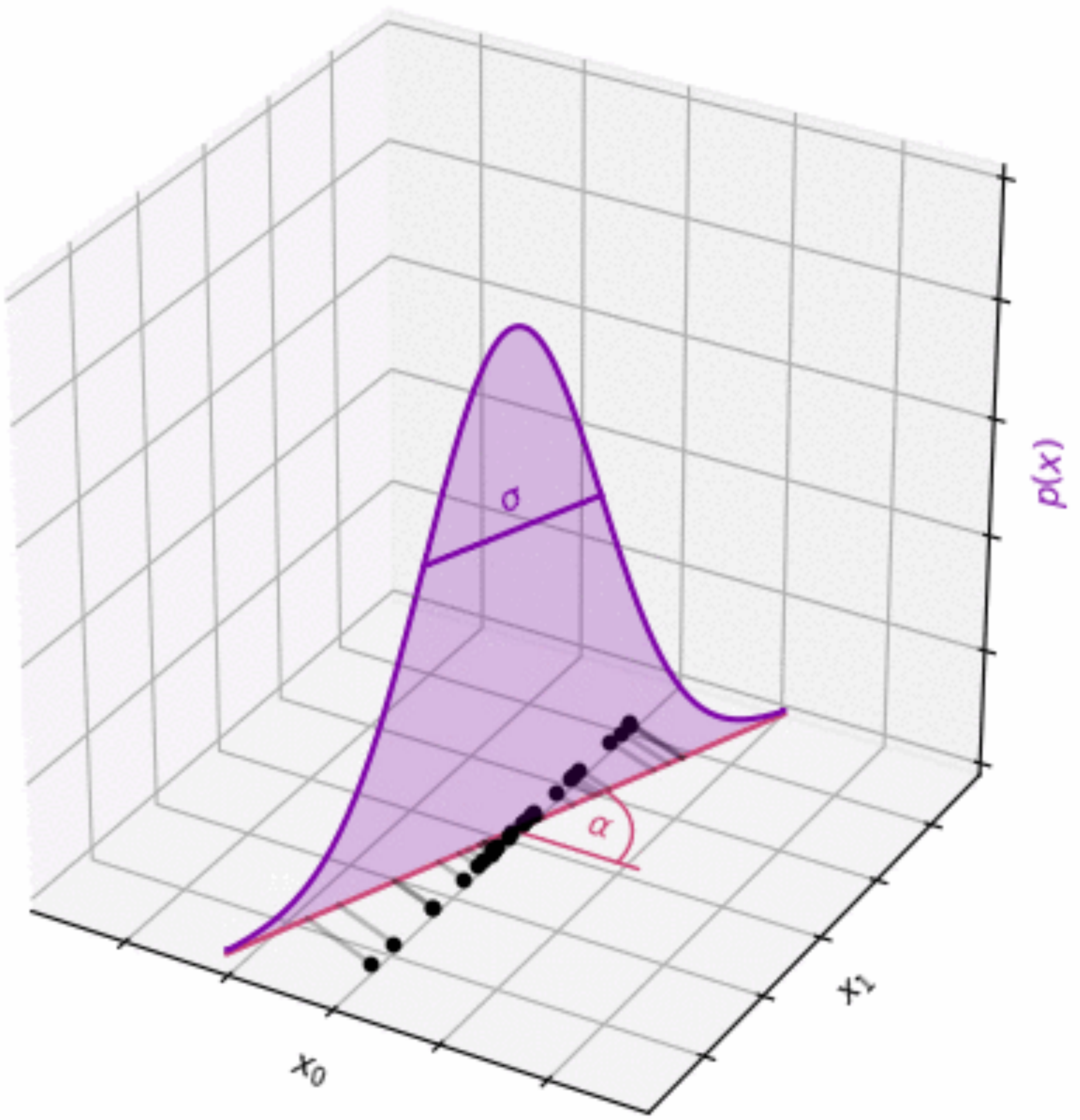
likelihood is unstable

Maximum likelihood is not enough

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

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

⇒ Learning ϕ_f by maximum likelihood is unstable

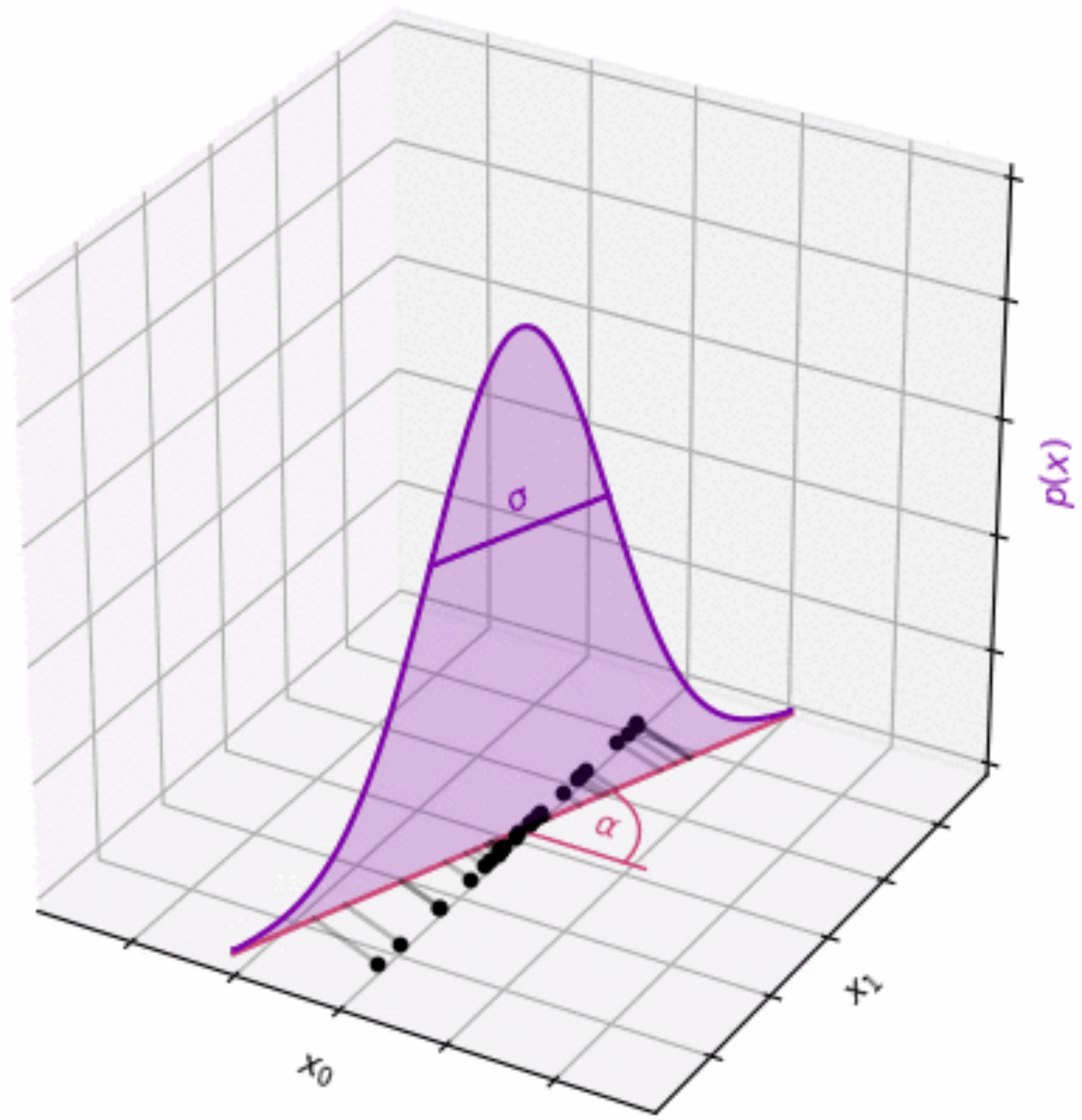


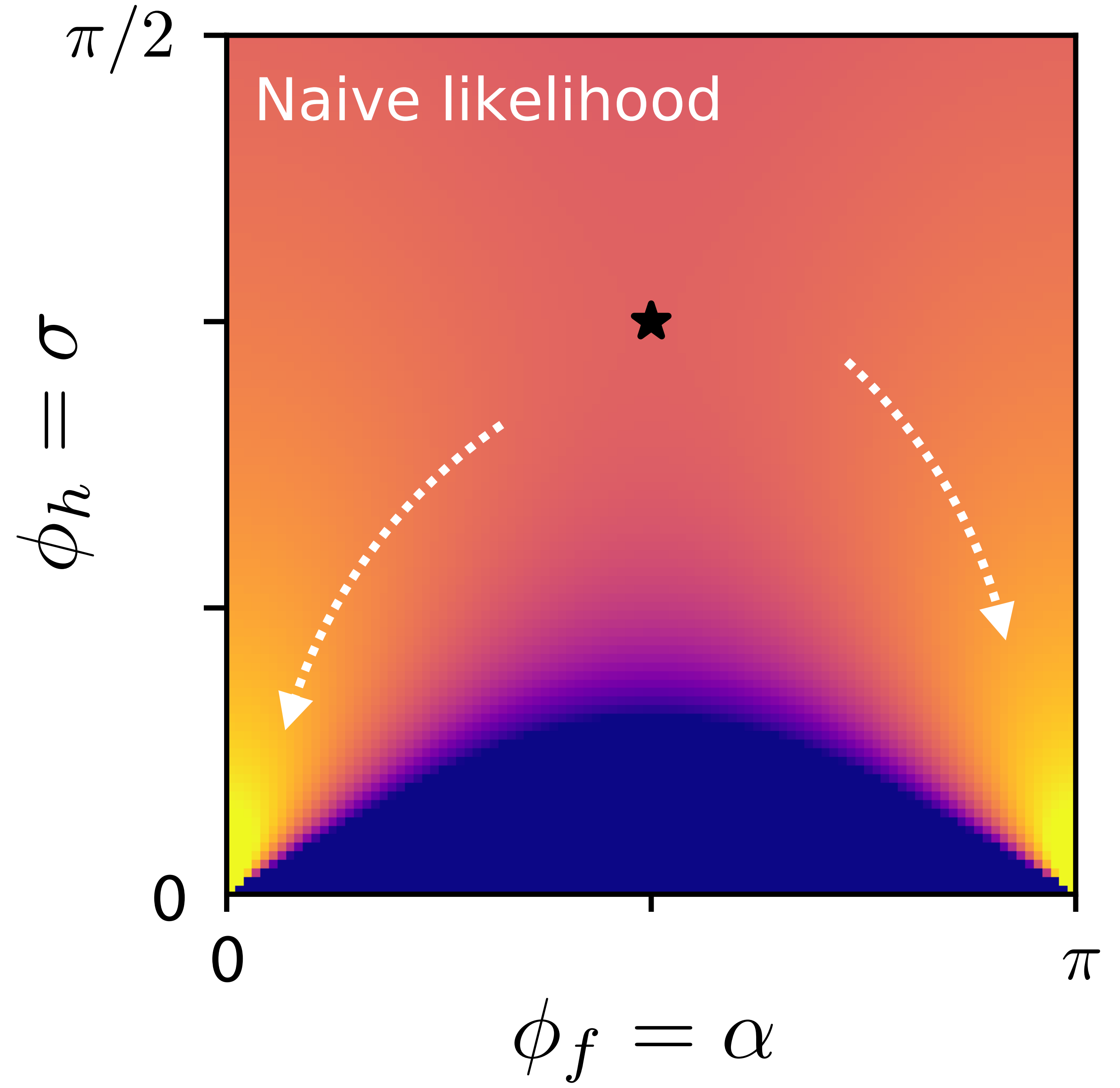
Maximum likelihood is not enough

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

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

⇒ Learning ϕ_f by maximum likelihood is unstable

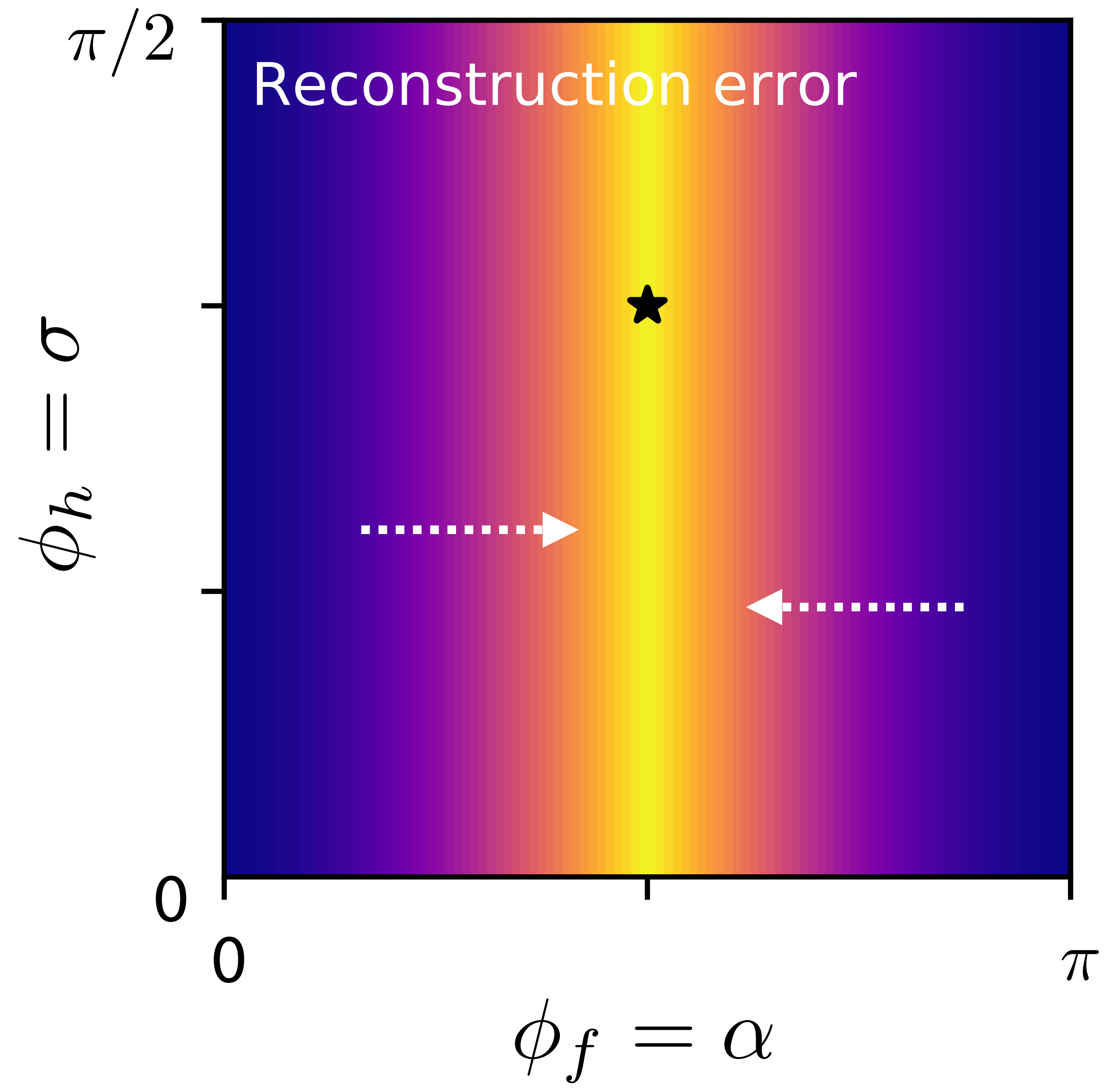




M/D training

Solution: separate training in two phases!

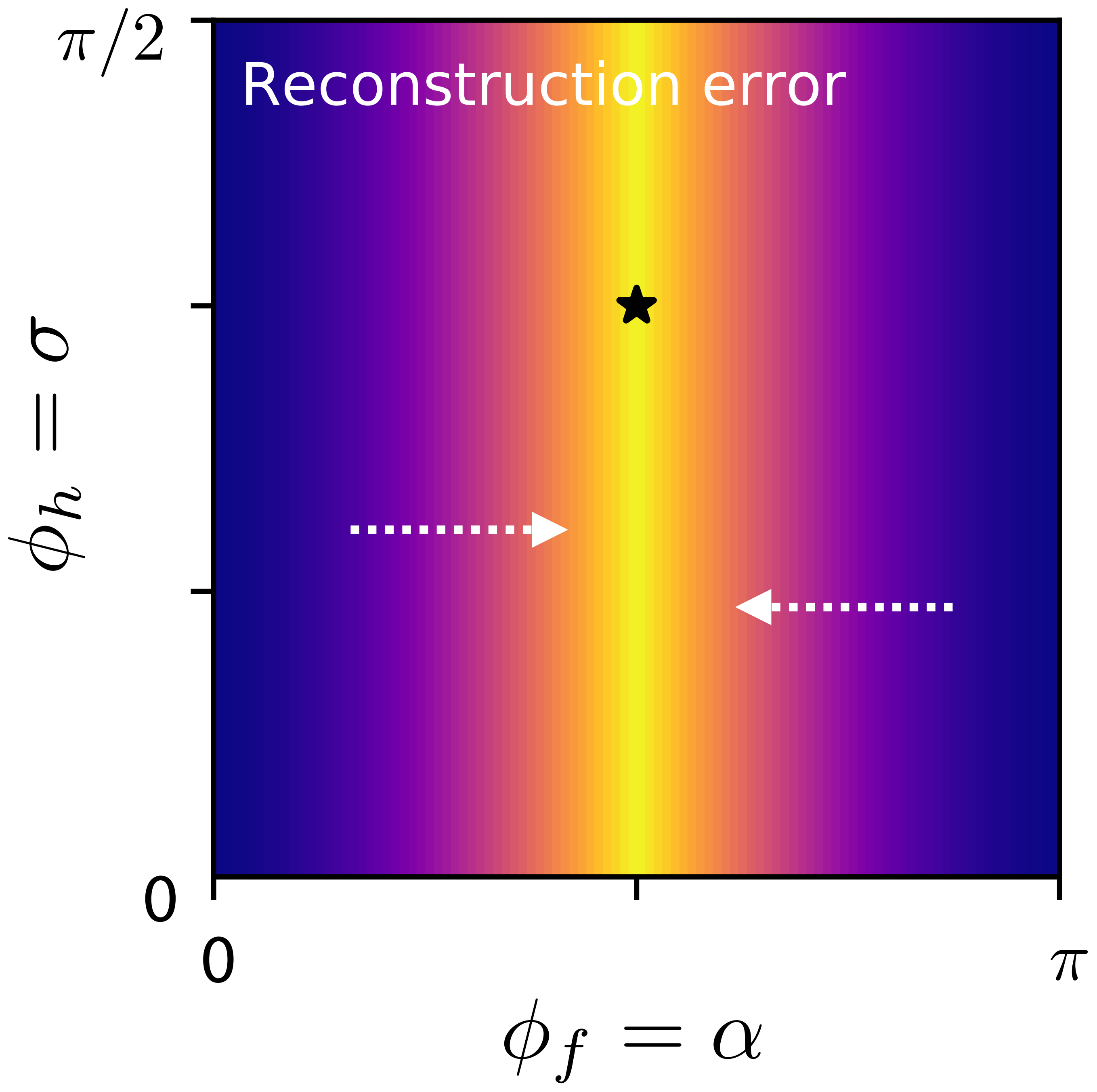
- Manifold phase:
  update ϕ_f (and thus $\mathcal{M}$) by minimizing $\|x - x'\|$



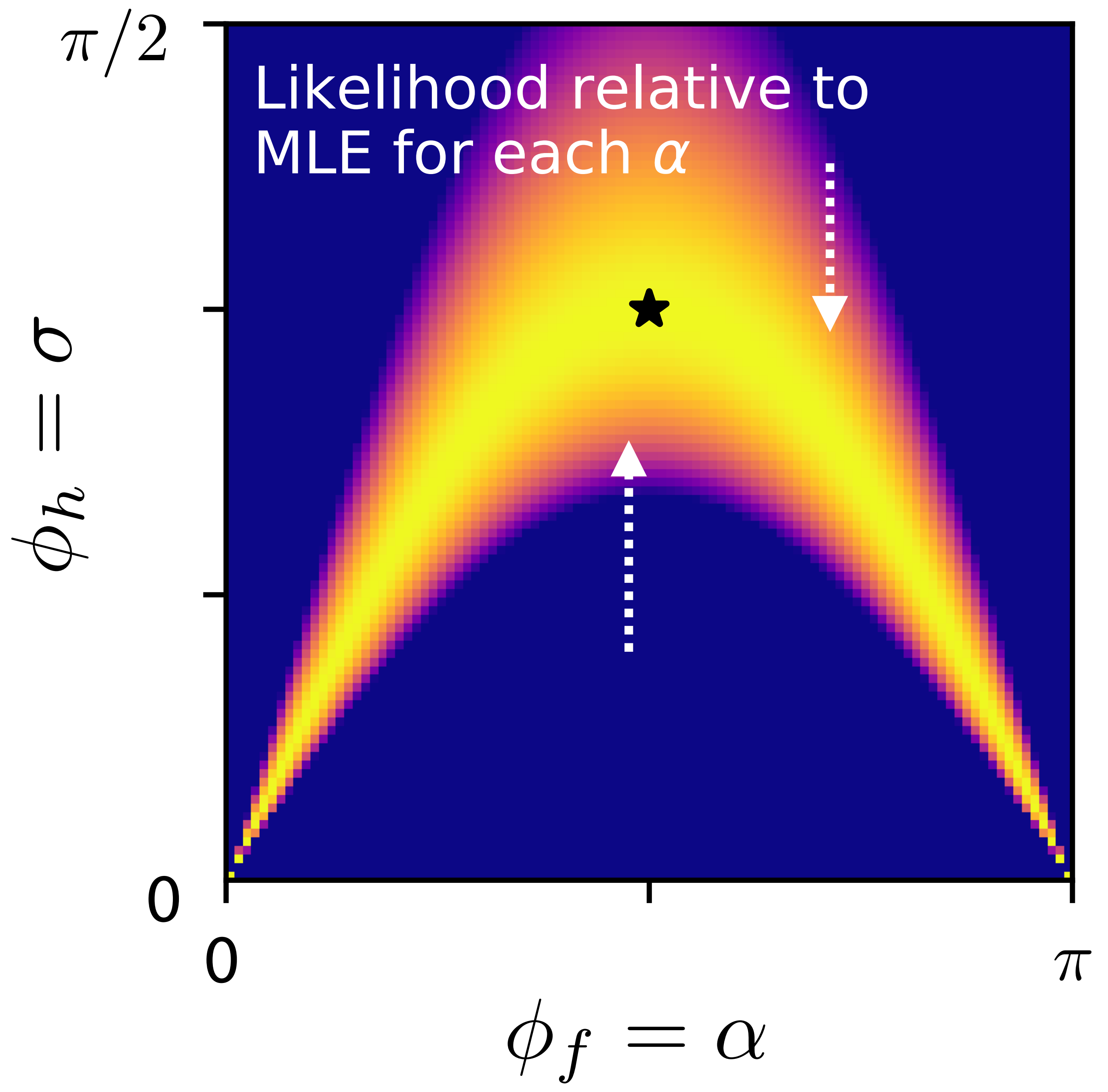
M/D training

Solution: separate training in two phases!

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



- Density phase:
  update ϕ_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:

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

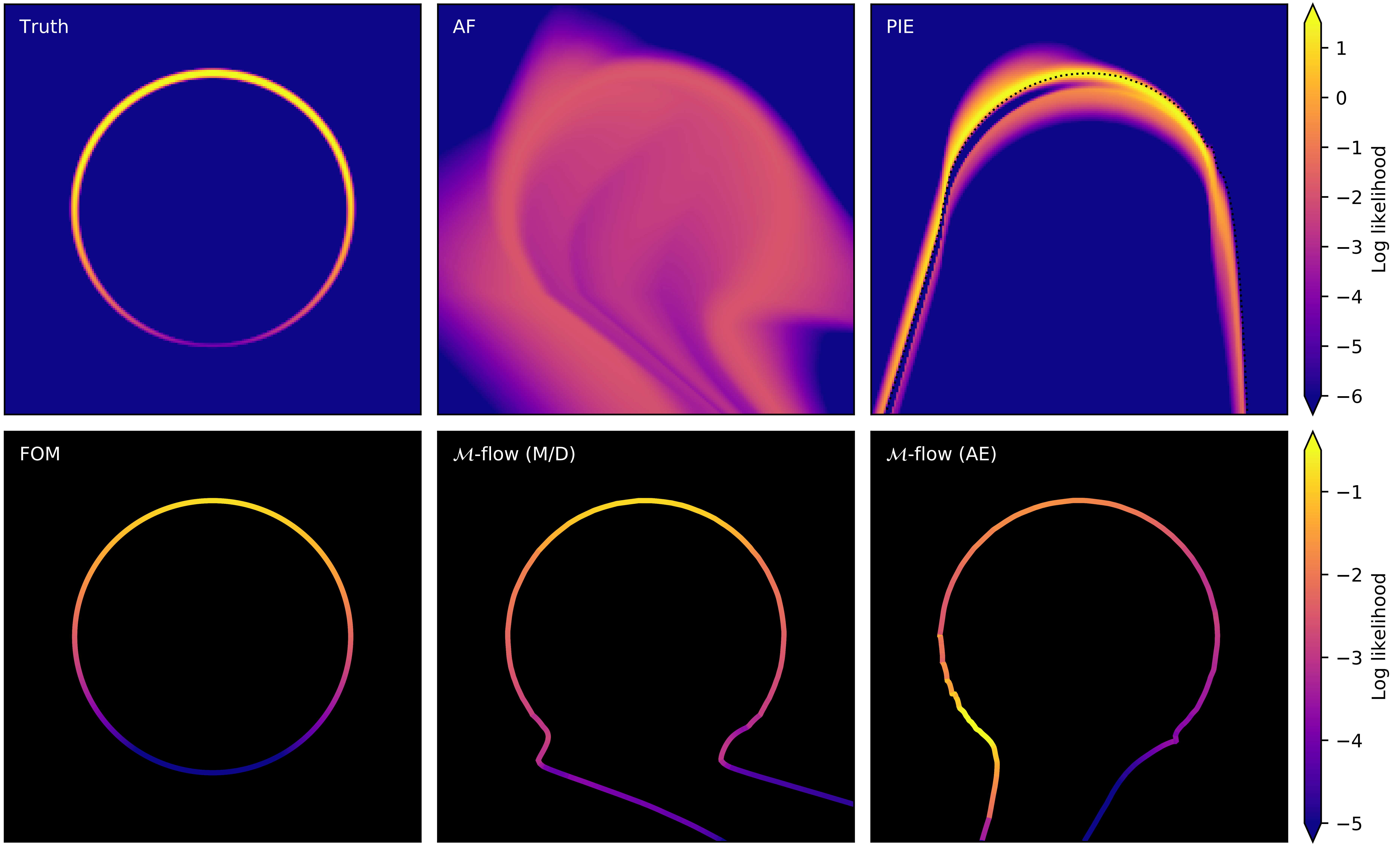
Cannot separate determinant of product of non-square matrices

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

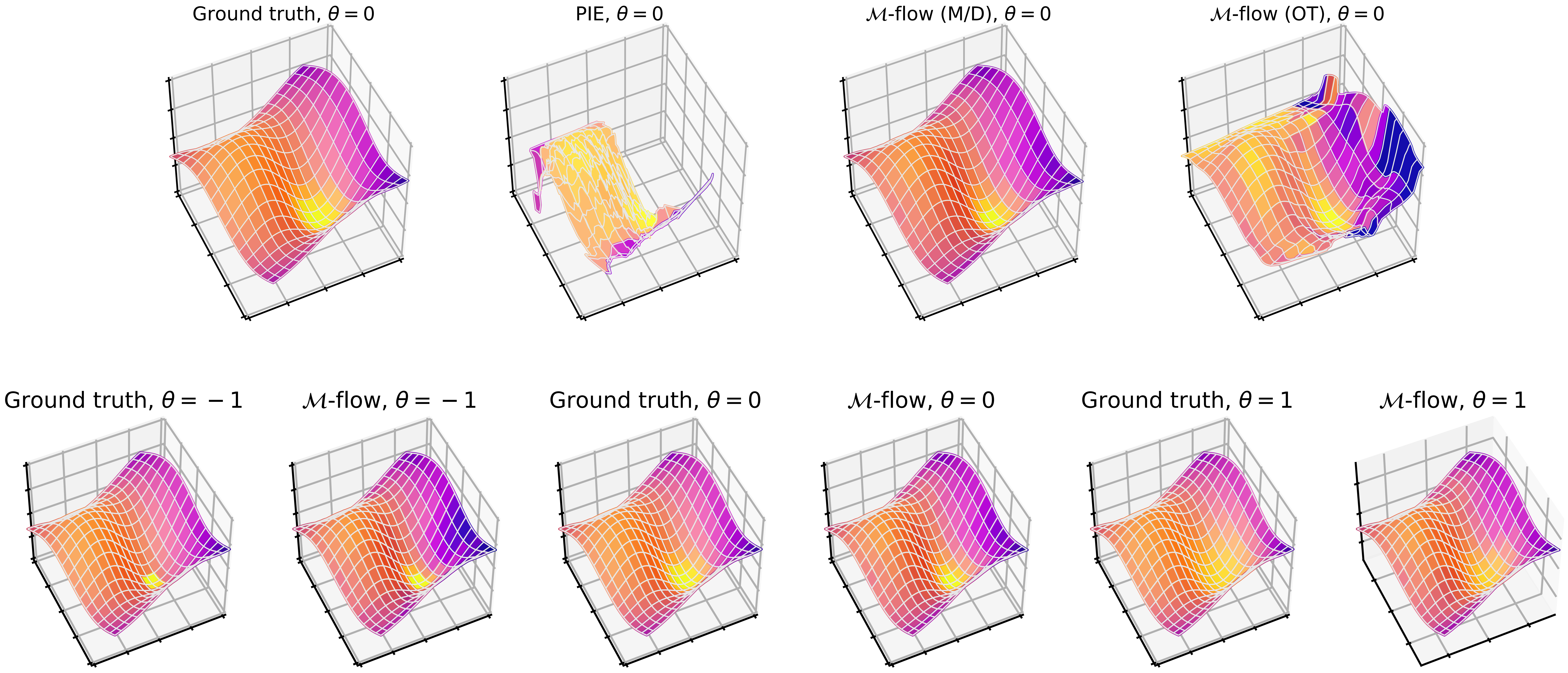
$$\nabla_{\phi_h}\left(\log p_{\mathcal{M}}(x)\right) = \nabla_{\phi_h}\left(\log p_{\tilde{u}}(h^{-1}(u))\right) - \nabla_{\phi_h}\left(\log\det J_h(h^{-1}(u))\right) \underbrace{- \nabla_{\phi_h}\frac{1}{2}\log\det\left[\begin{pmatrix}\mathbb{1} & 0\end{pmatrix} J_f^T(u)\, J_f(u) \begin{pmatrix}\mathbb{1}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

which can be computed efficiently!

Gaussian on a circle

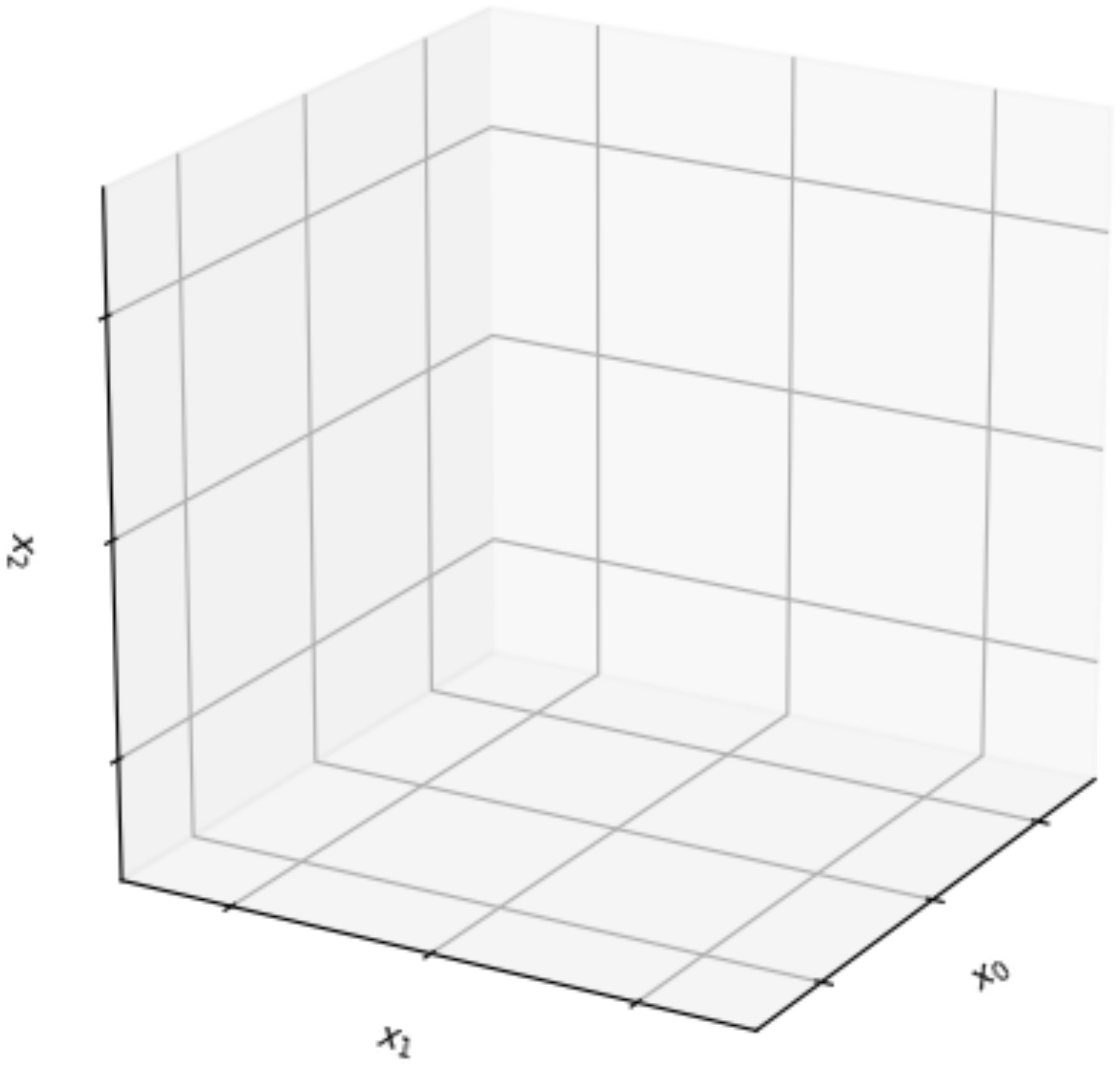


Mixture model on a polynomial surface



Lorenz attractor

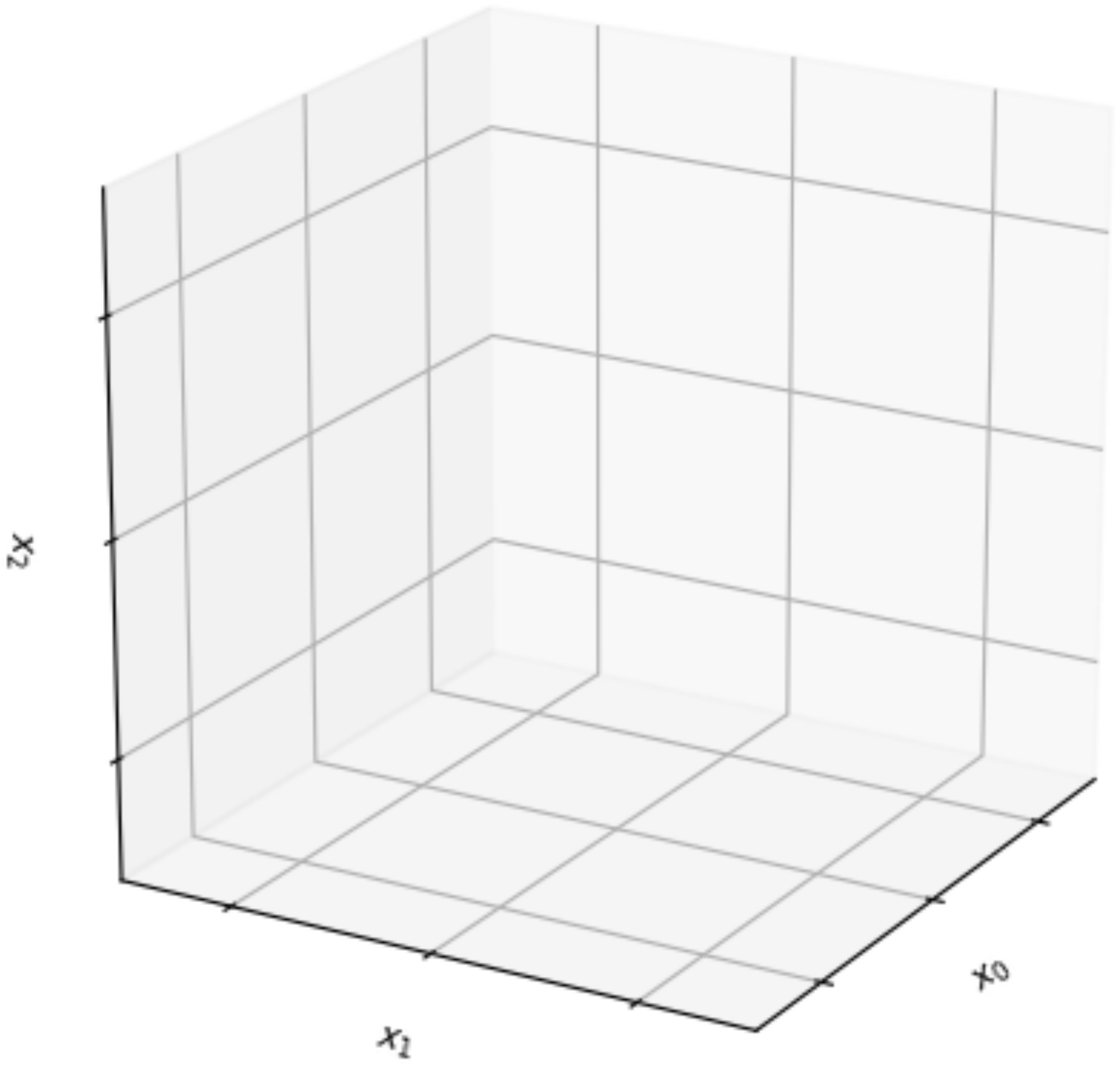
[E. Lorenz 1963]



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

Lorenz attractor

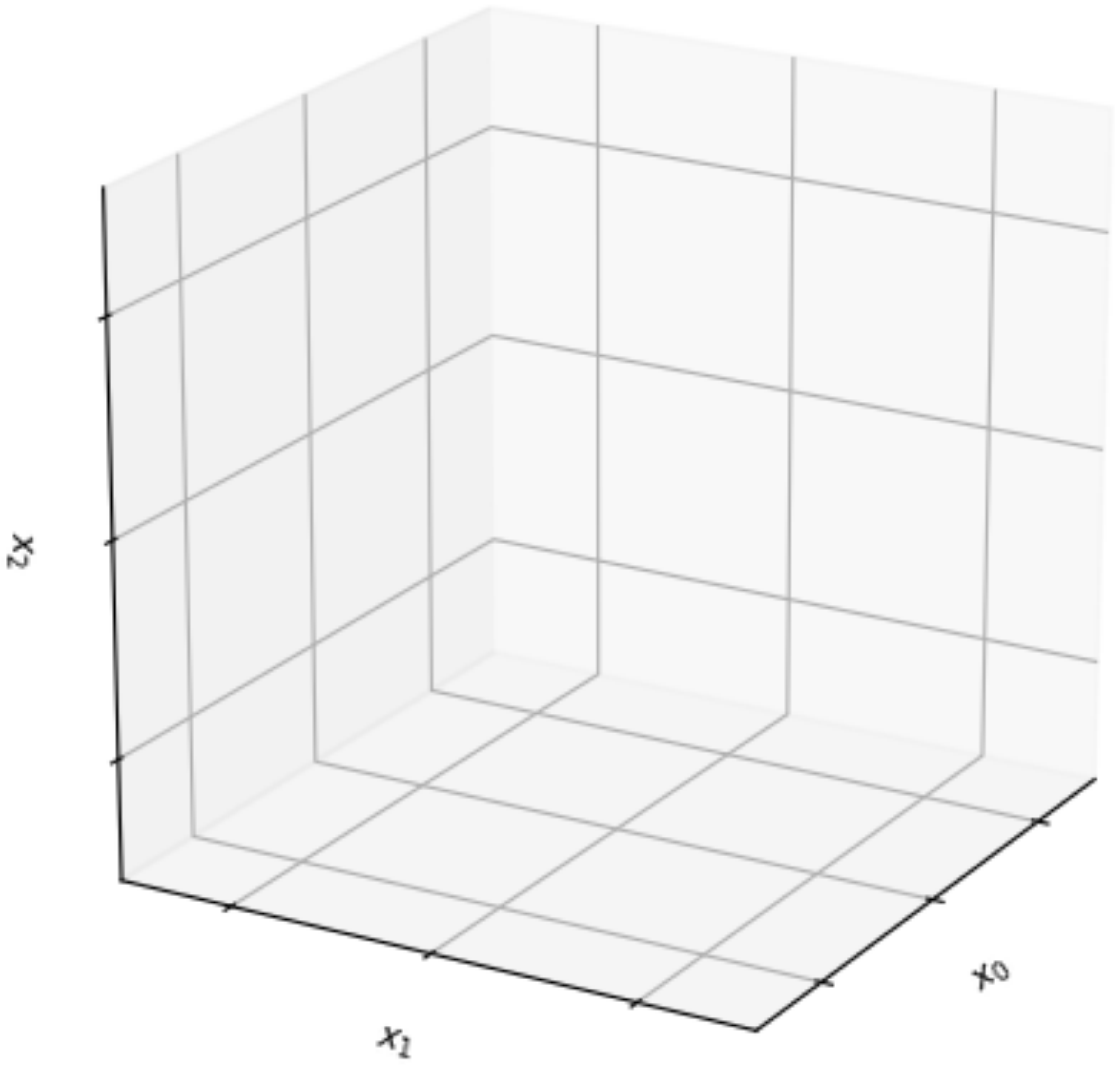
[E. Lorenz 1963]



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

Lorenz attractor

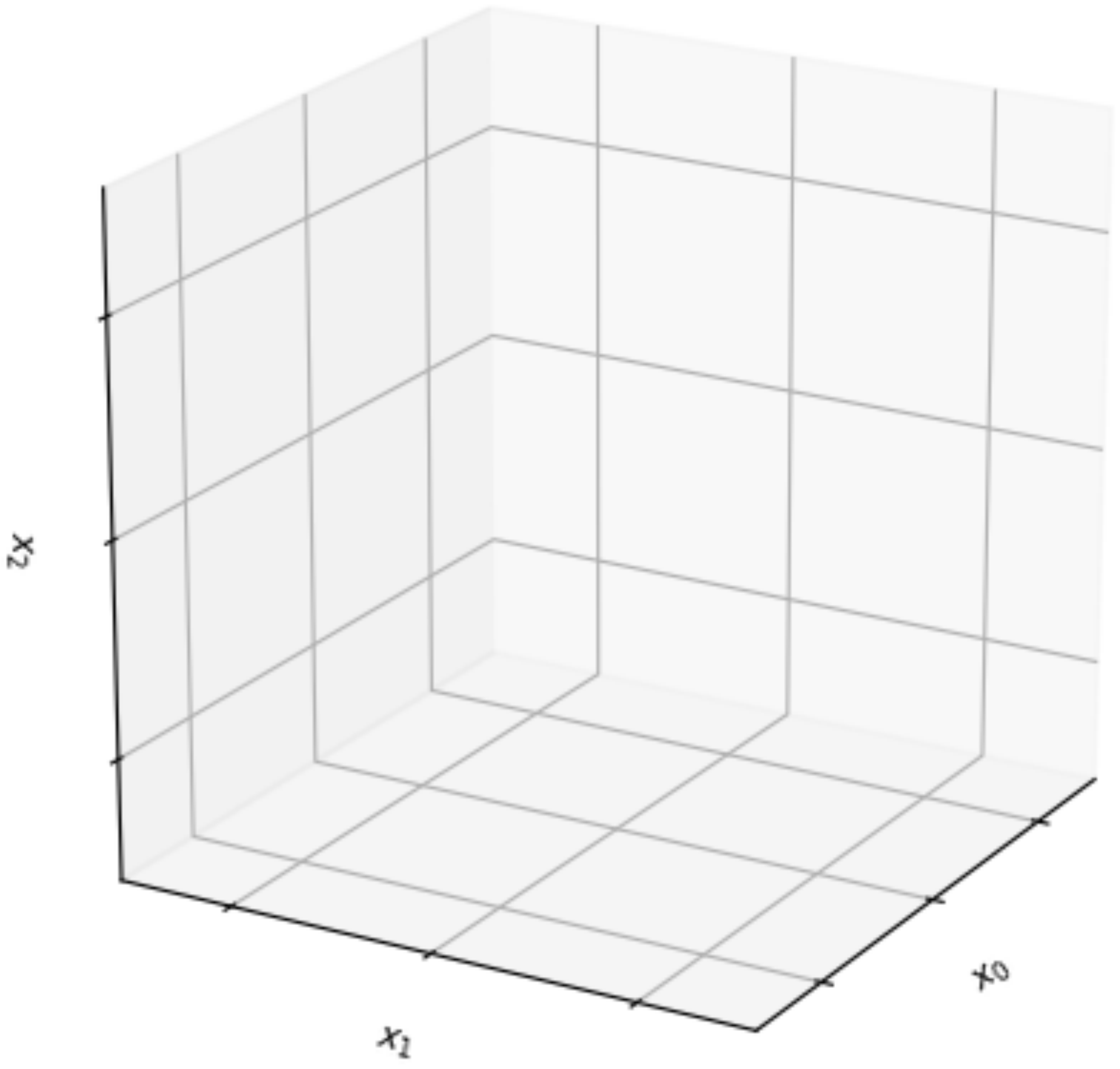
[E. Lorenz 1963]

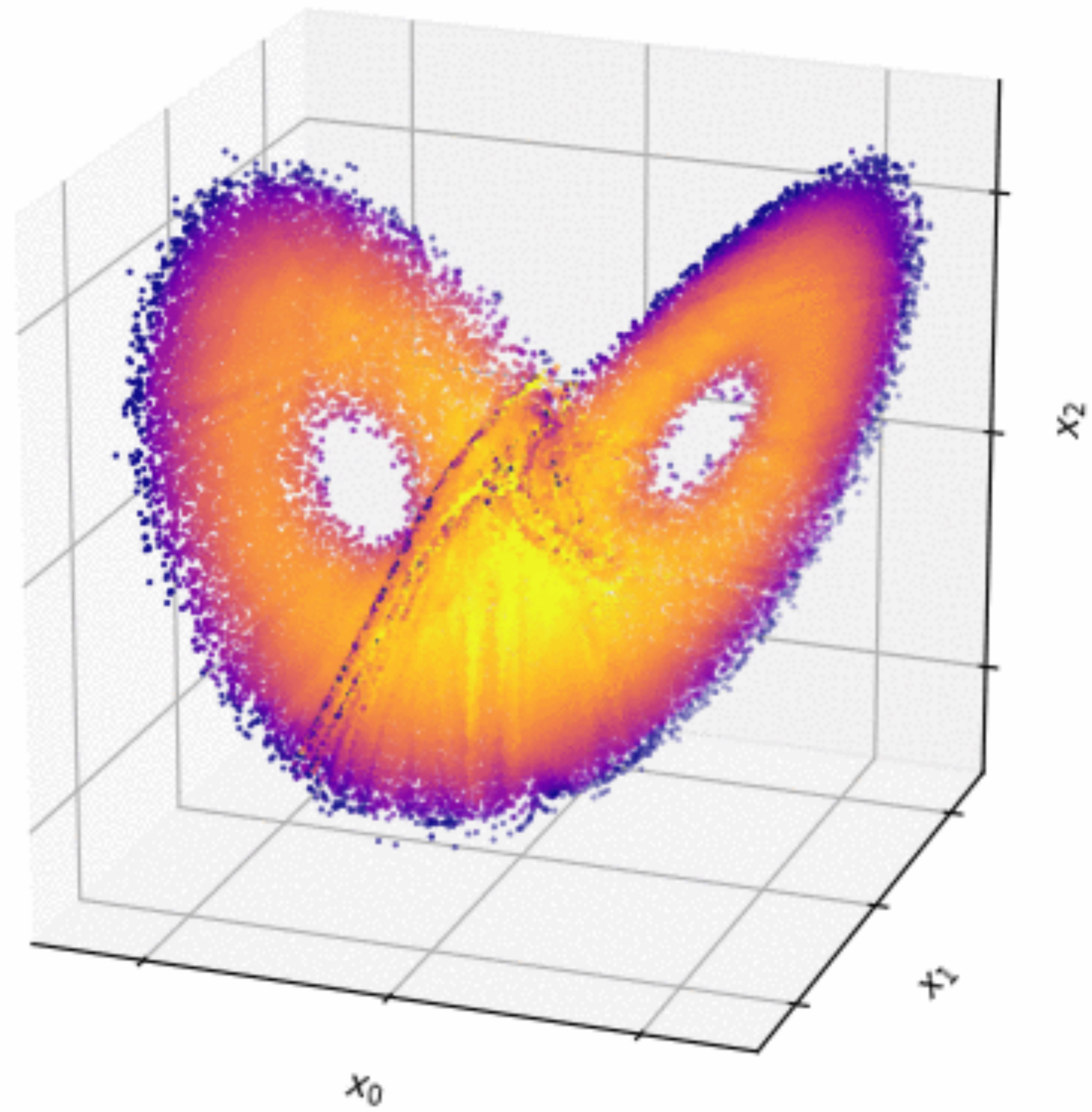


$$\frac{\mathrm{d}x_0}{\mathrm{d}t} = \sigma(x_1 - x_0)\,, \quad \frac{\mathrm{d}x_1}{\mathrm{d}t} = x_0(\rho - x_2) - x_1\,, \quad \frac{\mathrm{d}x_2}{\mathrm{d}t} = x_0 x_1 - \beta x_2\,.$$

Lorenz attractor

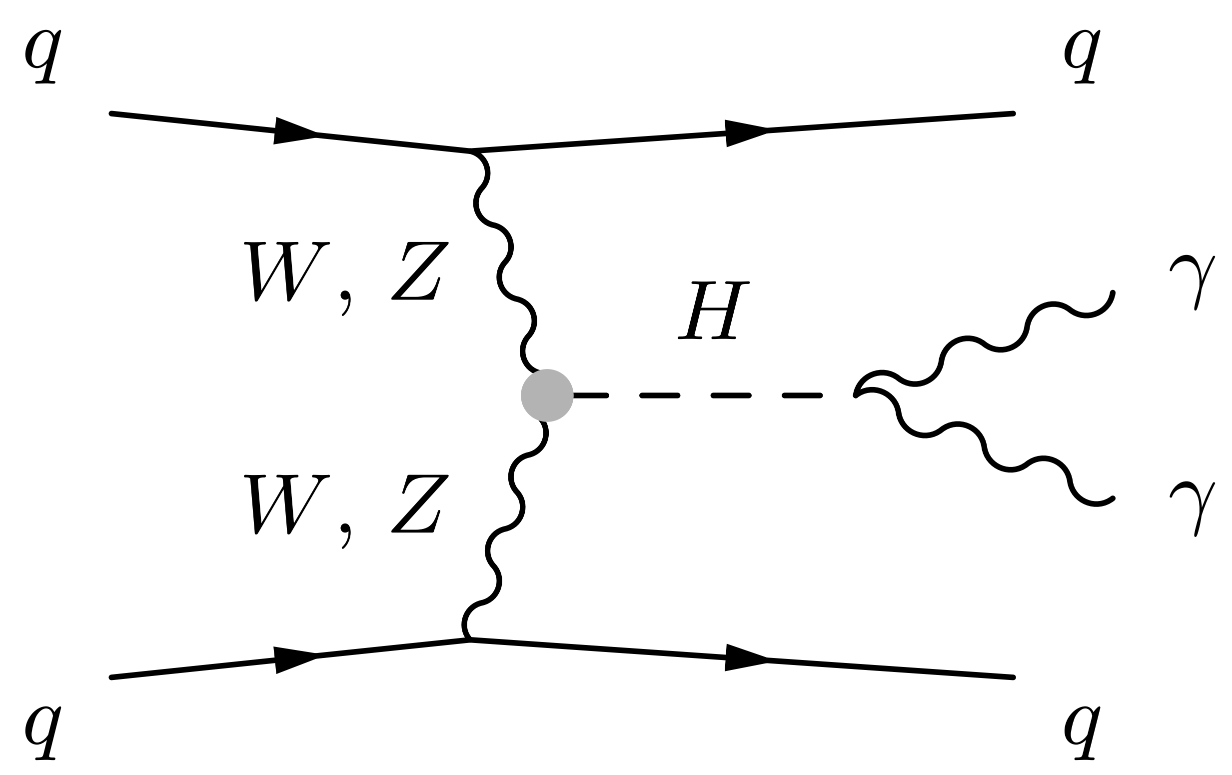
[E. Lorenz 1963]





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

Particle physics: structure

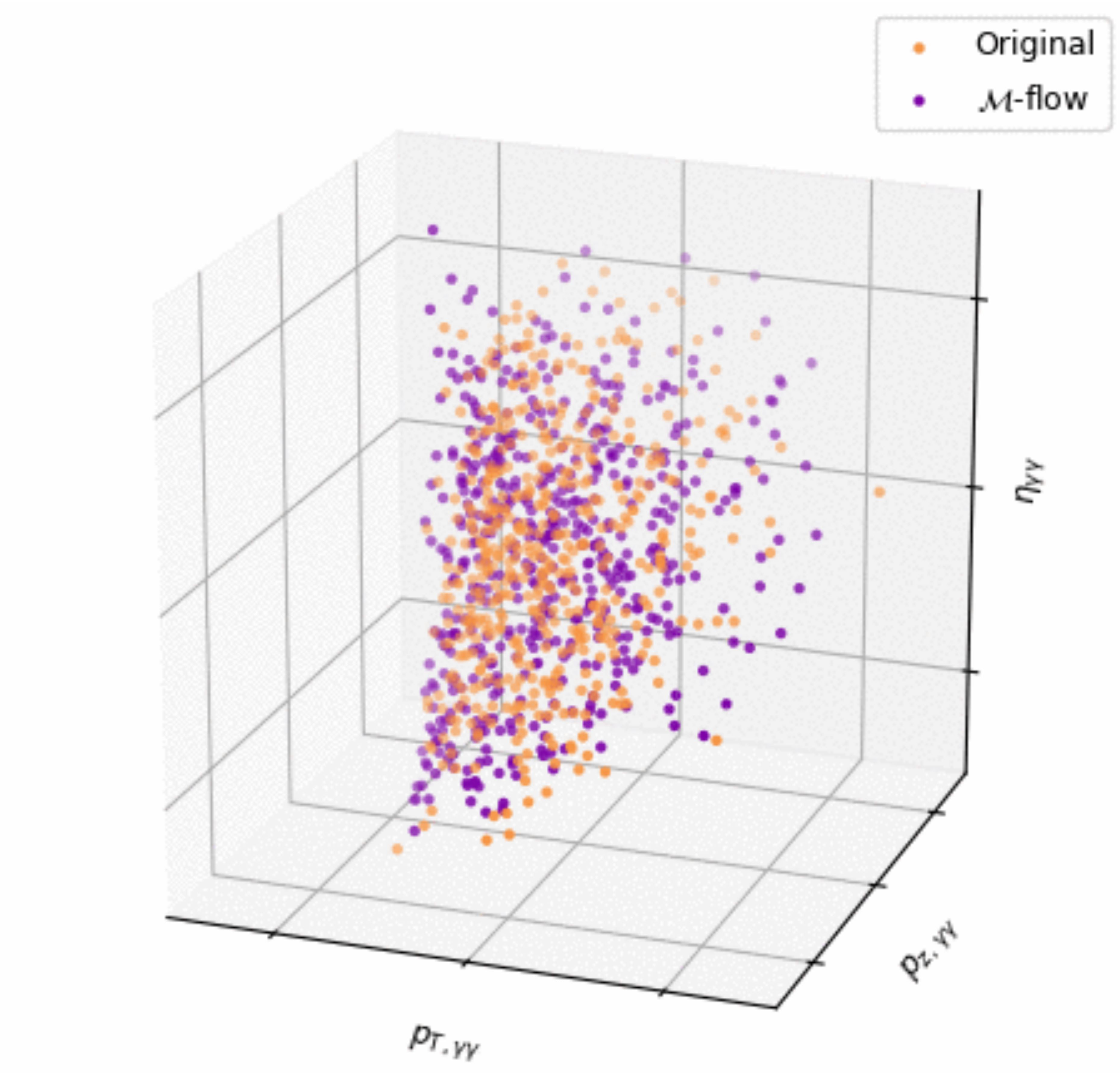


particle masses
("on-shell condition")

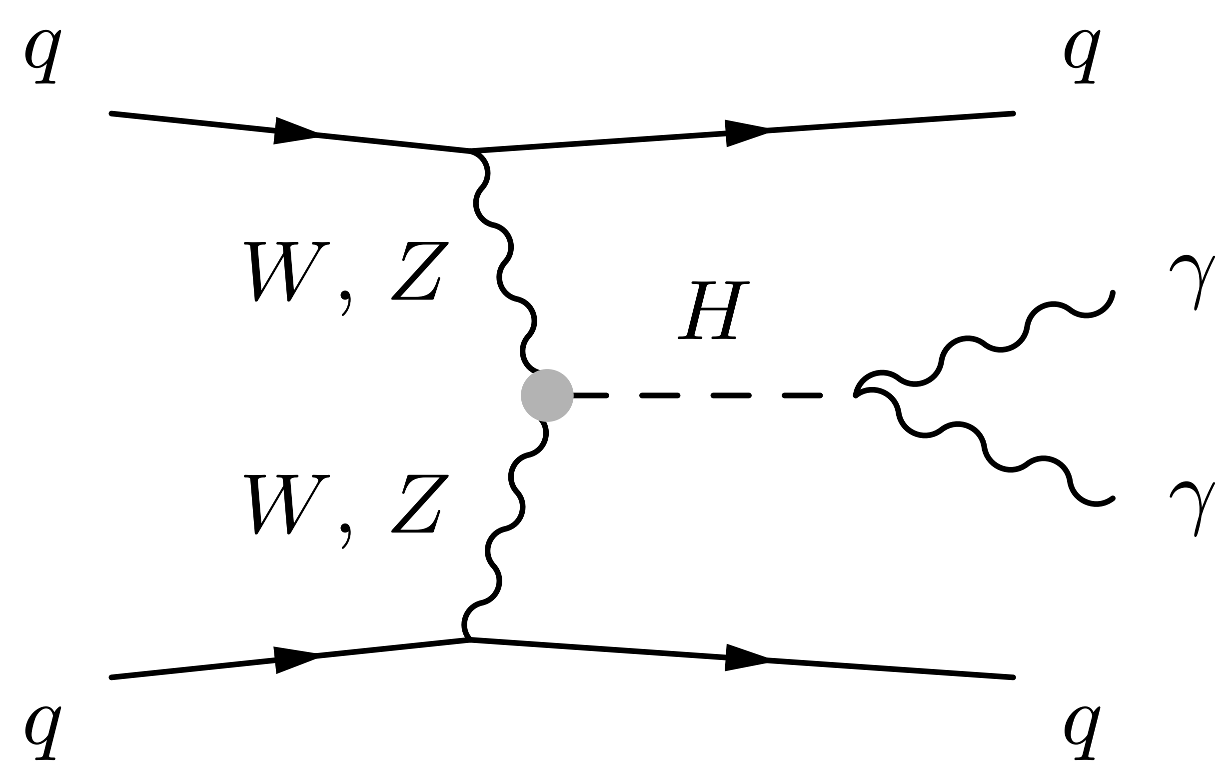
redundant
observables

energy-momentum
conservation

14-dimensional manifold
embedded in 40-dimensional
data space



Particle physics: structure

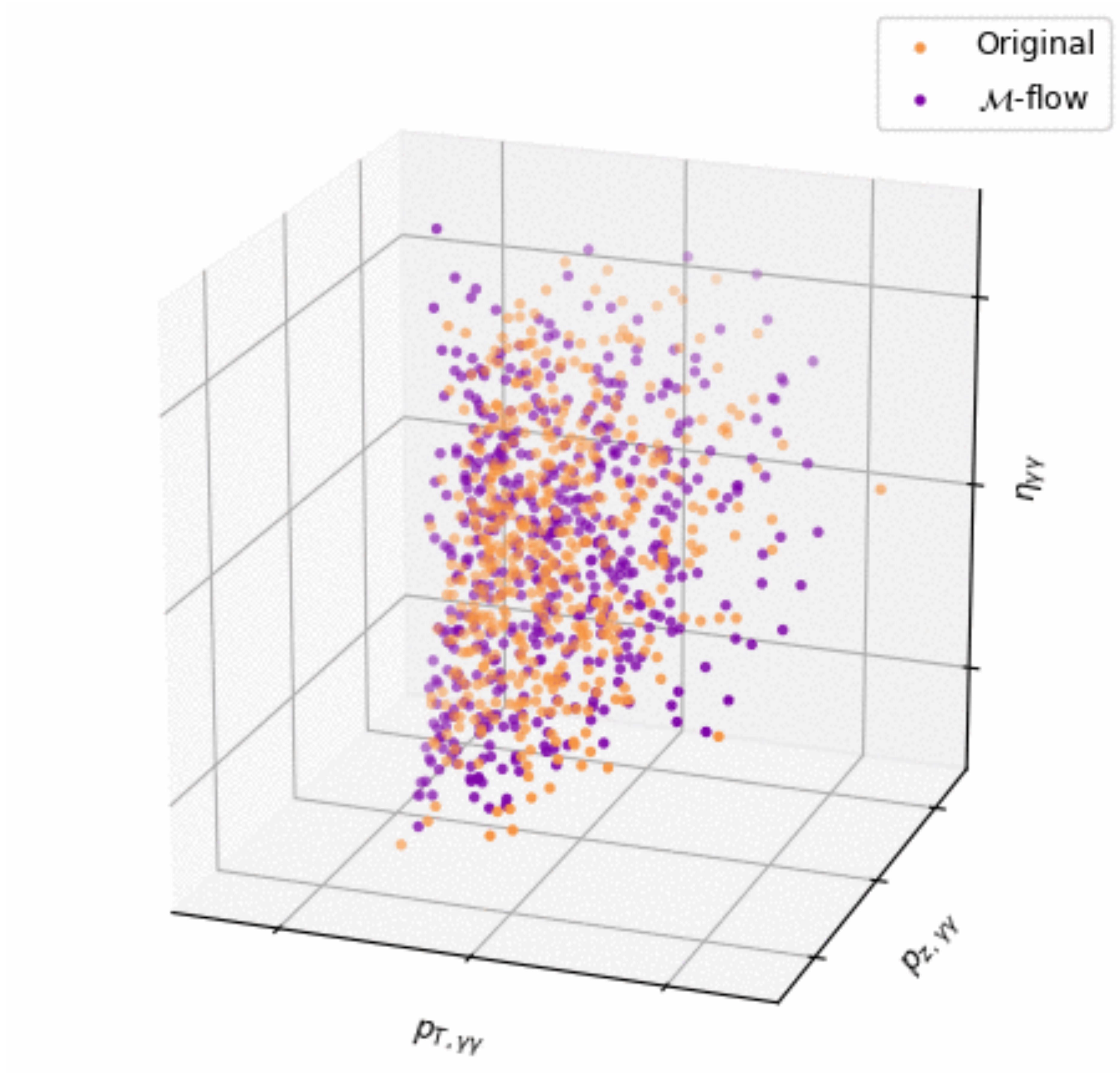


redundant observables

particle masses (“on-shell condition”)

energy-momentum conservation

14-dimensional manifold embedded in 40-dimensional data space



Particle physics: results

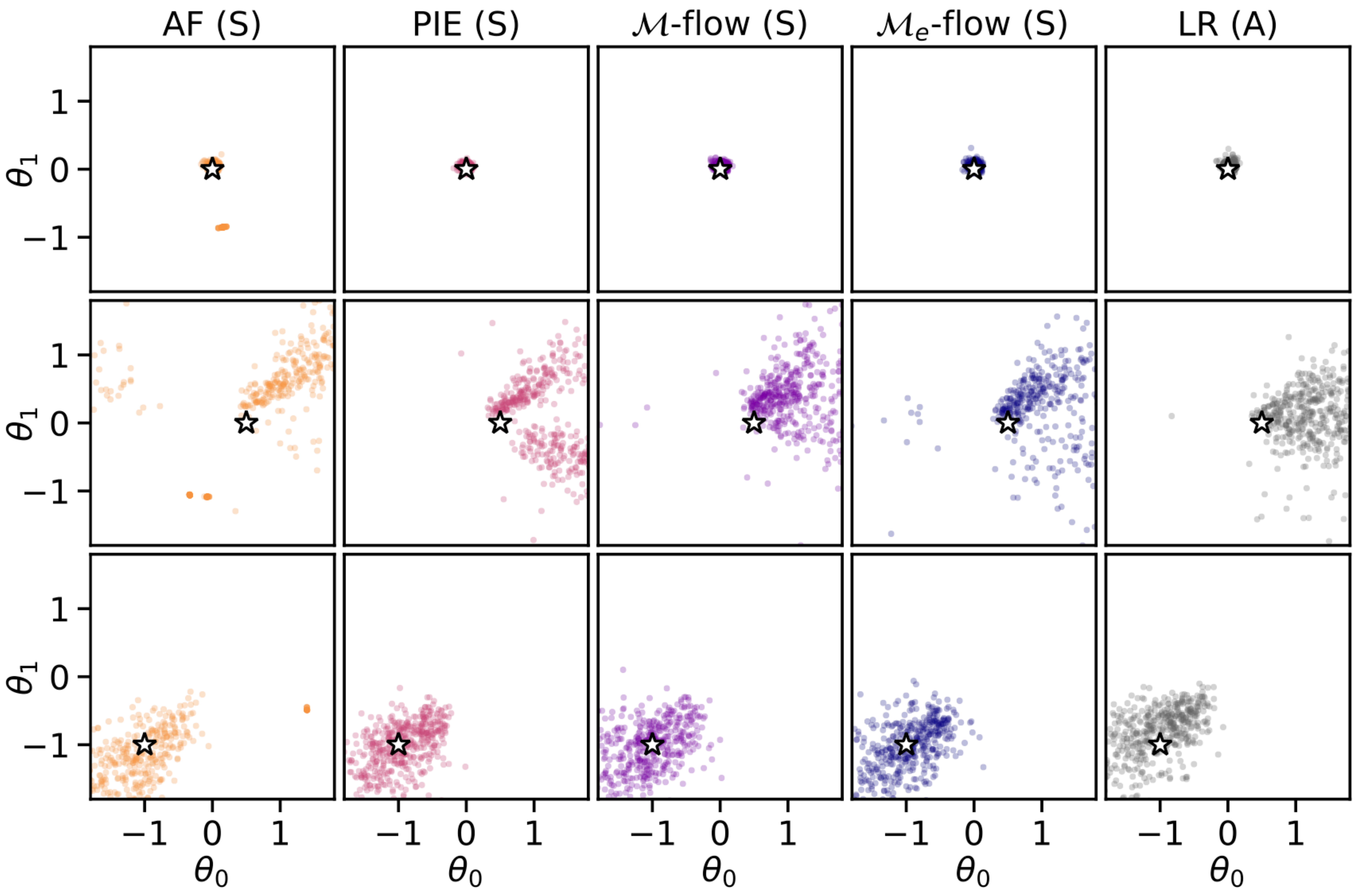
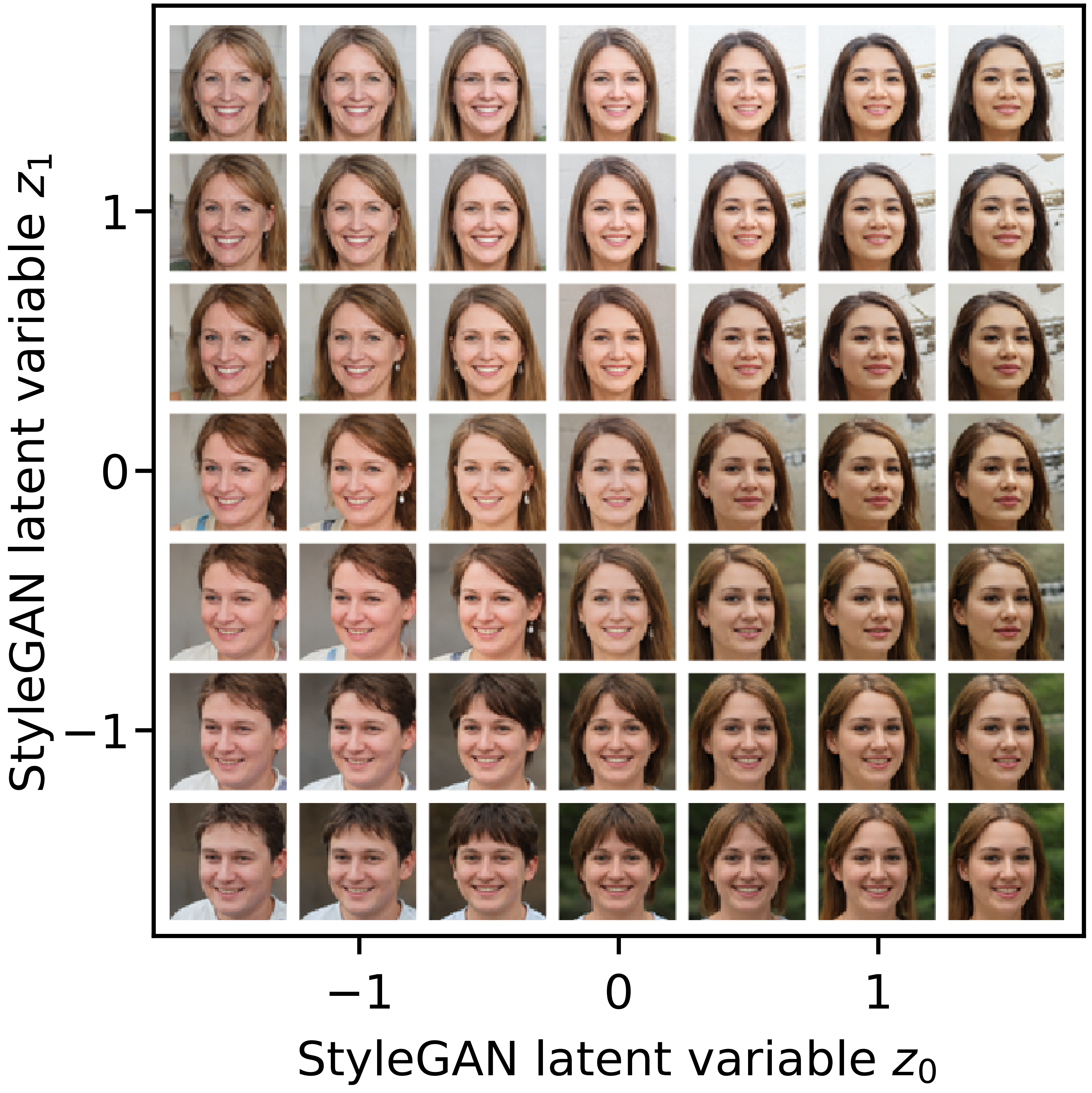


Image manifolds

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

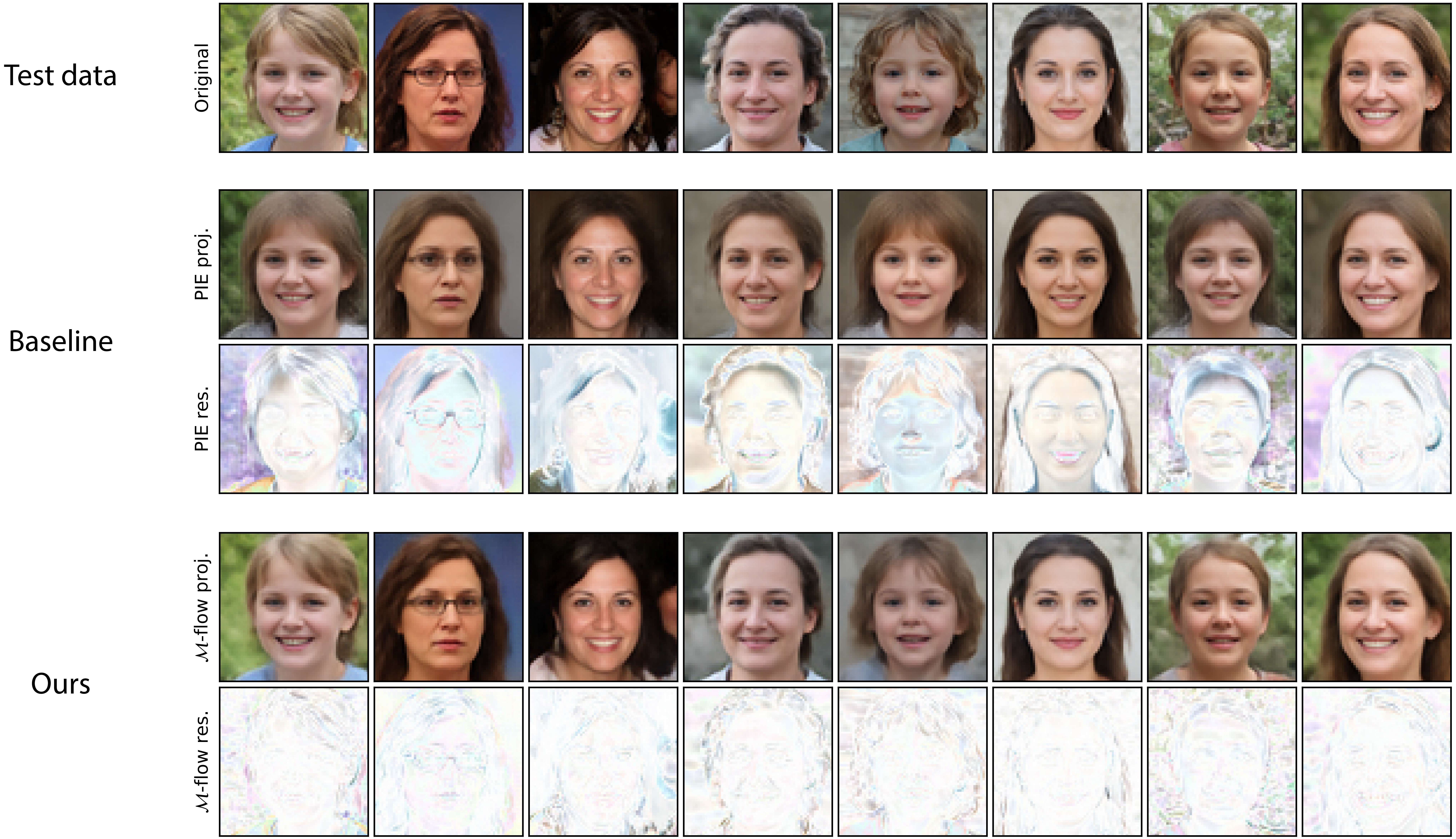
$n = 2$



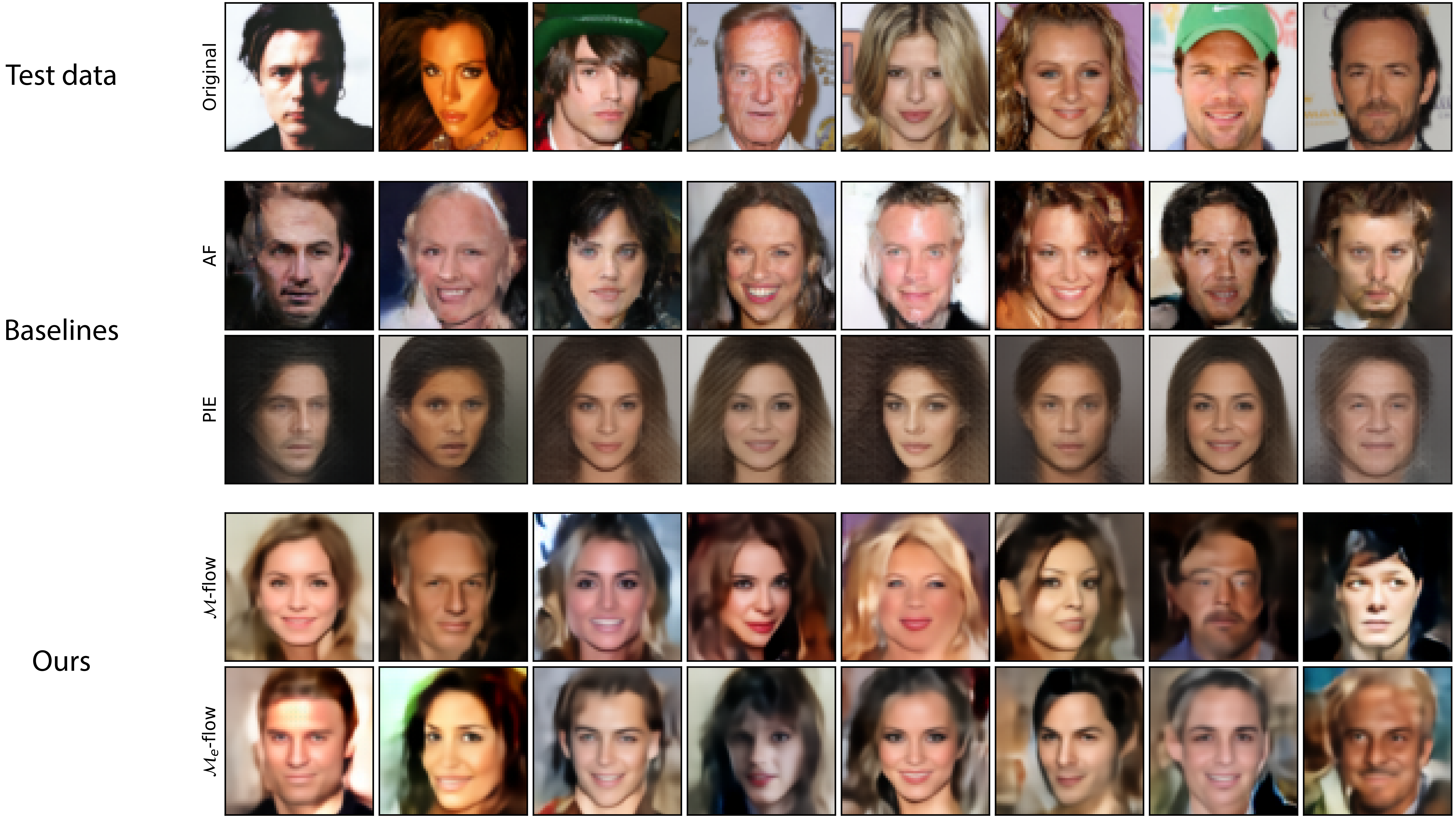
Samples

Test data
Original
Baselines
AF
PIE (manifold)
Ours
$\mathcal{M}$-flow
$\mathcal{M}_e$-flow

Projections to learned manifolds



Real-world images: CelebA samples



CelebA projections