

# Learning to constrain new physics

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# LHC legacy measurements

- What's hiding in the electroweak sector?  
⇒ precision constraints on dimension-6 EFT operators  
(or Pseudo-Observables, non-linear EFT, ...)

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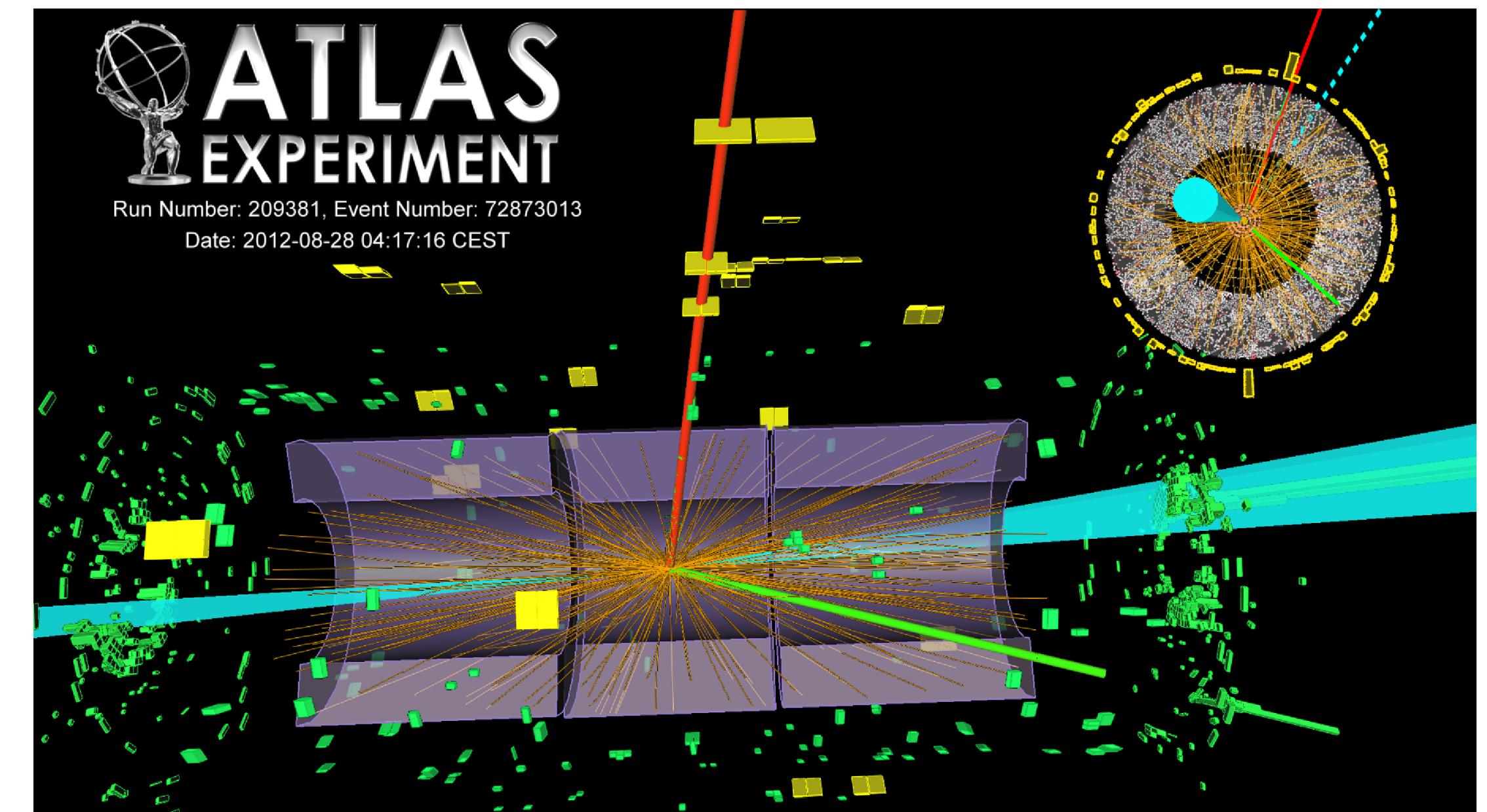
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(or Pseudo-Observables, non-linear EFT, ...)
- These measurements are difficult!

## 1. Many parameters

$$\begin{aligned} S = \int d^4x \left[ & \mathcal{L}_{\text{SM}} + \frac{f_{\phi,2}}{\Lambda^2} \frac{1}{2} \partial_\mu (\phi^\dagger \phi) \partial^\mu (\phi^\dagger \phi) + \frac{f_{\phi,3}}{\Lambda^2} \frac{1}{3} (\phi^\dagger \phi)^3 \right. \\ & + \frac{f_{GG}}{\Lambda^2} (\phi^\dagger \phi) G_{\mu\nu}^a G^{\mu\nu a} - \frac{f_{BB}}{\Lambda^2} \frac{g'^2}{4} (\phi^\dagger \phi) B_{\mu\nu} B^{\mu\nu} - \frac{f_{WW}}{\Lambda^2} \frac{g^2}{4} (\phi^\dagger \phi) W_{\mu\nu}^a W^{\mu\nu a} \\ & + \frac{f_B}{\Lambda^2} \frac{ig'}{2} (D^\mu \phi)^\dagger D^\nu \phi B_{\mu\nu} + \frac{f_W}{\Lambda^2} \frac{ig}{2} (D^\mu \phi)^\dagger \sigma^a D^\nu \phi W_{\mu\nu}^a \\ & + \frac{f_\ell}{\Lambda^2} (\phi^\dagger \phi) \bar{L}_L \phi \ell_R + \frac{f_u}{\Lambda^2} (\phi^\dagger \phi) \bar{Q}_L \tilde{\phi} u_R + \frac{f_d}{\Lambda^2} (\phi^\dagger \phi) \bar{Q}_L \phi d_R \\ & \left. + \frac{f_{G\widetilde{G}}}{\Lambda^2} (\phi^\dagger \phi) G_{\mu\nu}^a \widetilde{G}^{\mu\nu a} - \frac{f_{B\widetilde{B}}}{\Lambda^2} \frac{g'^2}{4} (\phi^\dagger \phi) B_{\mu\nu} \widetilde{B}^{\mu\nu} - \frac{f_{W\widetilde{W}}}{\Lambda^2} \frac{g^2}{4} (\phi^\dagger \phi) W_{\mu\nu}^a \widetilde{W}^{\mu\nu a} \right] \end{aligned}$$

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(or Pseudo-Observables, non-linear EFT, ...)
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  1. Many parameters
  2. Many observables



[ATLAS 1501.04943]

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[M. Yao, idea for analogy: K. Cranmer]

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  4. The likelihood function of high-dimensional observables cannot be calculated

# LHC legacy measurements

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  2. Many observables
  3. Subtle kinematic effects
  4. The likelihood function of high-dimensional observables cannot be calculated
- Established data analysis methods struggle...  
**New ideas can improve the sensitivity to new physics!**

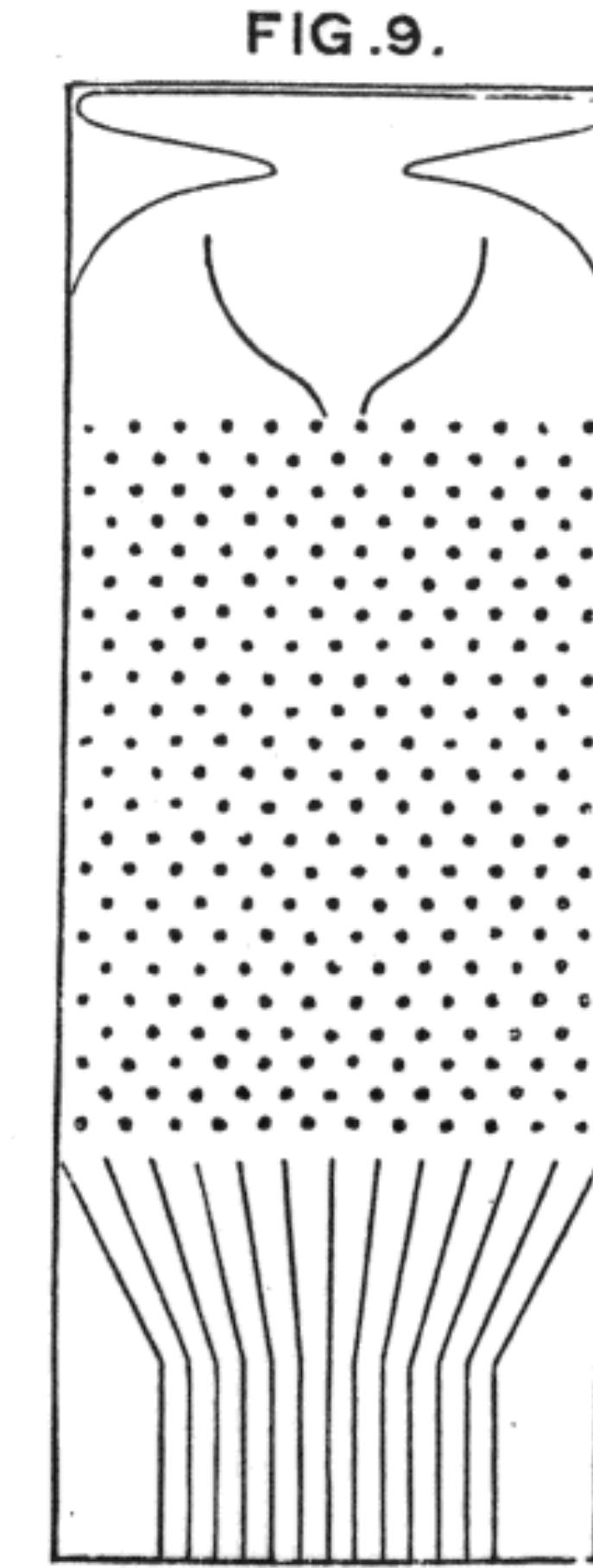
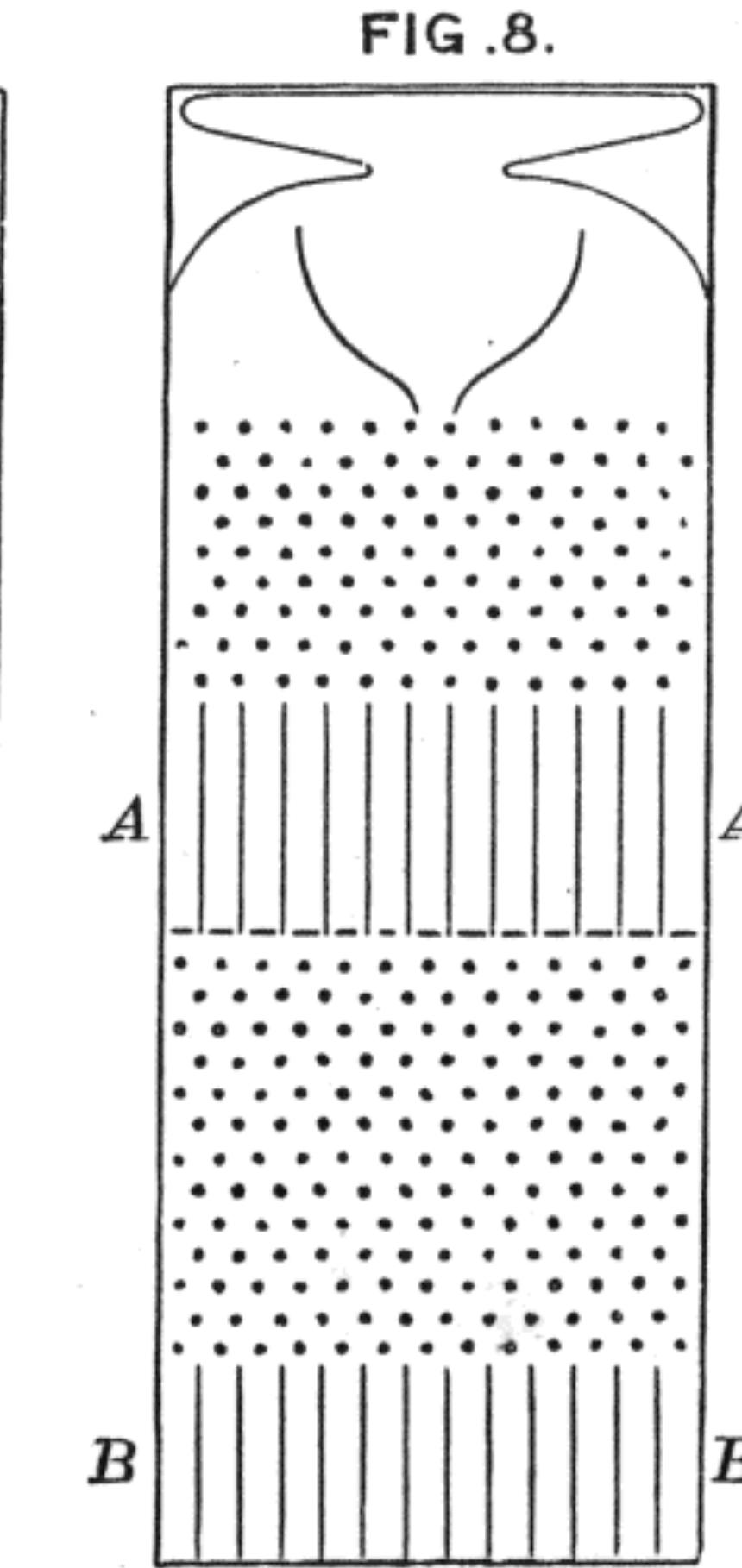
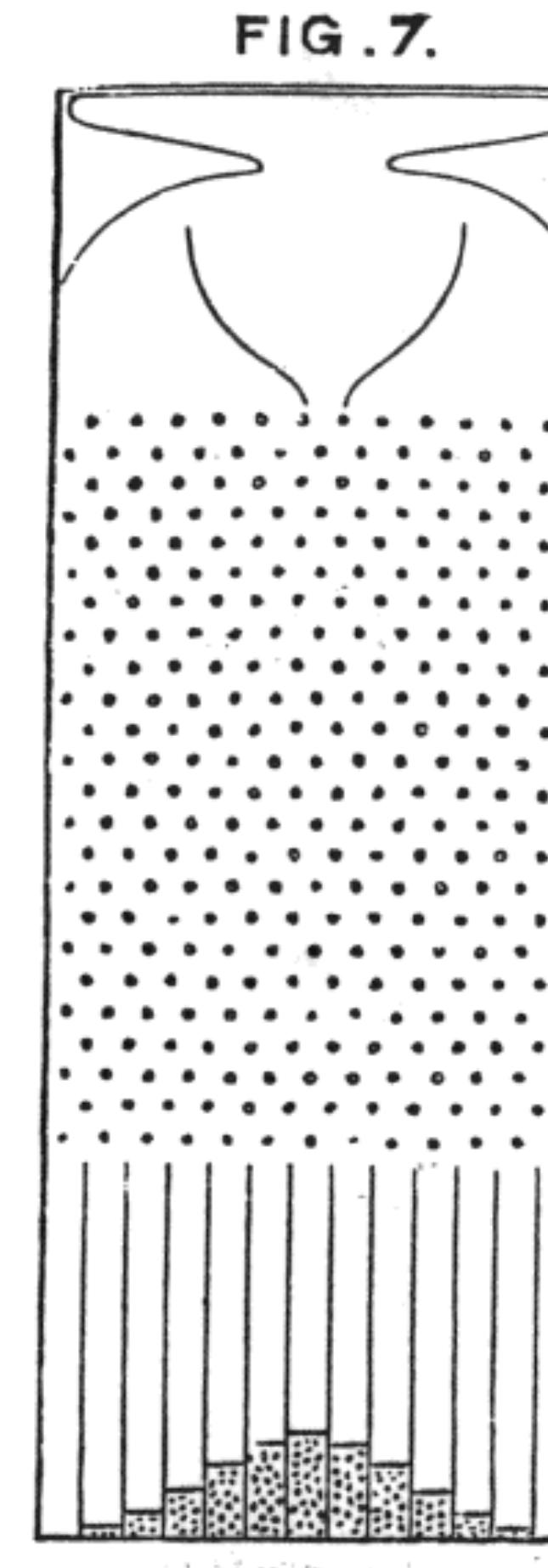
# Likelihood-free inference

# The Galton board



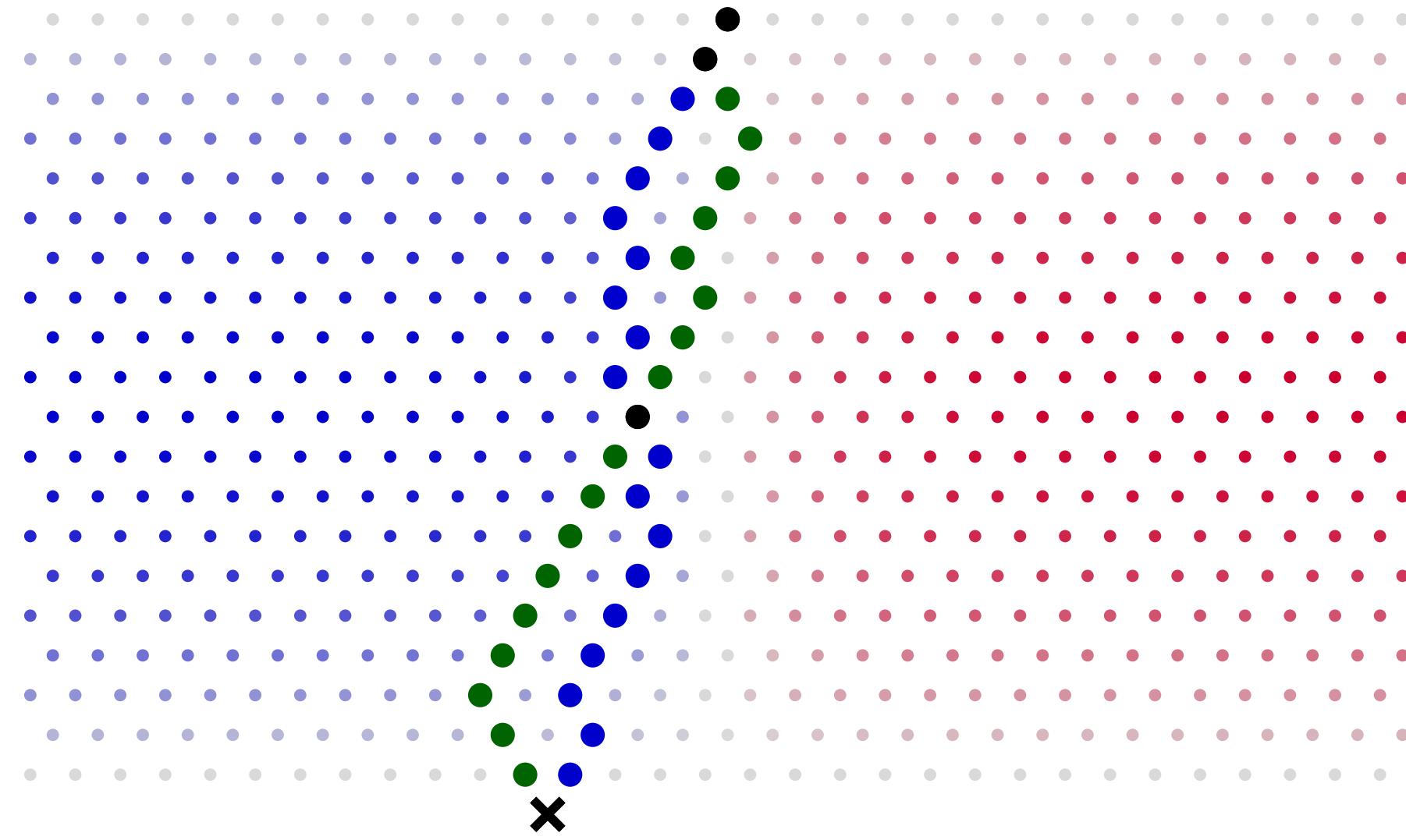
[galtonboard.com]

# The Galton board



[F. Galton 1889]

# Probabilities from integrating trajectories



Probability of ending in bin  $x$  :  $p(x) = \int dz p(x, z)$

Sum over  
all trajectories  
("latent variables")

Probability of  
each path  $z$   
from start to  $x$

# The generalized Galton board

What if probability to go left at a nail is not always 0.5, but some (known) function of some parameters  $\theta$  ?

- **Prediction:** given  $\theta$ , generate samples of observations  $\{x_i\}$ .

Simple: just drop balls!

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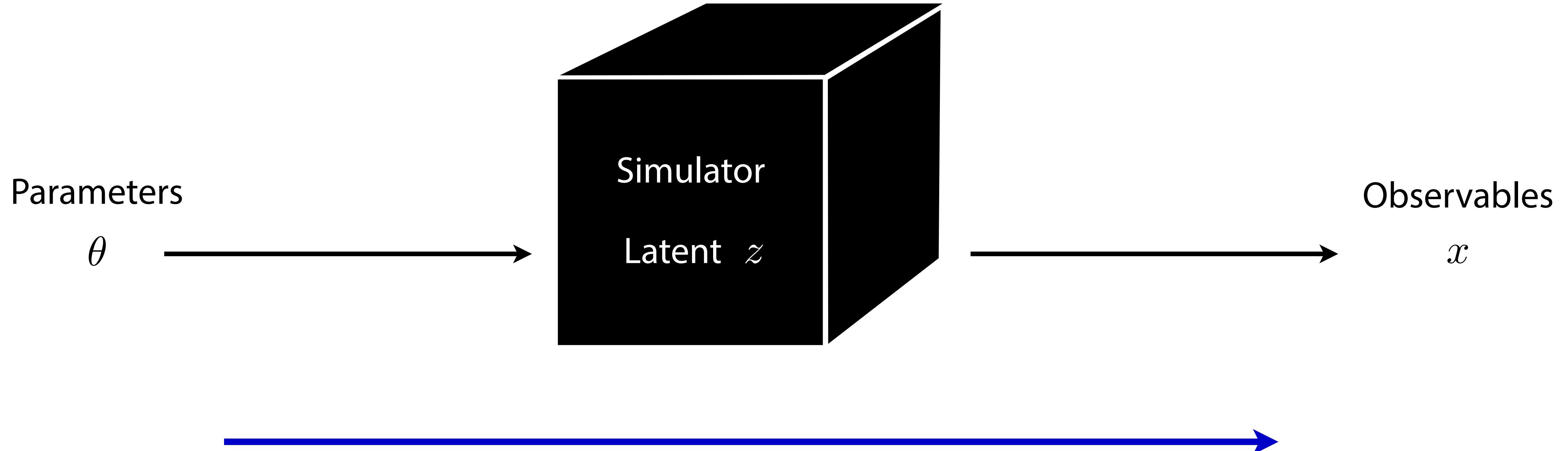
- **Inference:** given observations  $\{x_i\}$ , what are the most likely values for  $\theta$  ?

“Easy” problem if we can evaluate likelihood

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

But the number of possible **paths**  $z$  can be huge, and it becomes impossible to calculate the integral!

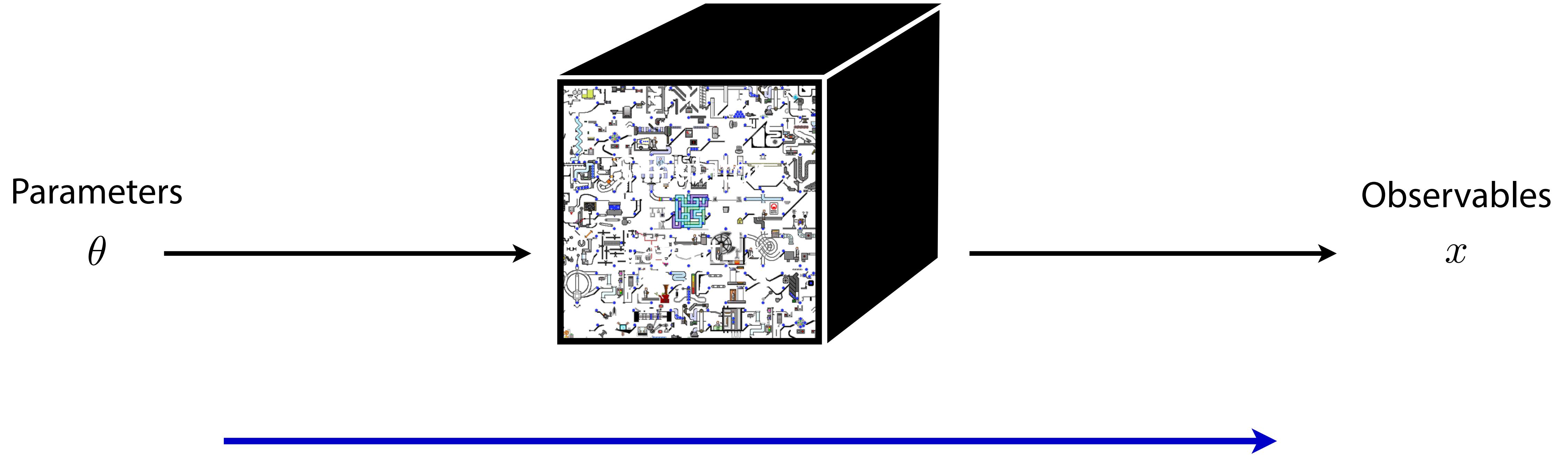
# “Likelihood-free inference”



Prediction:

- Well-understood mechanistic model
- Simulator can generate samples

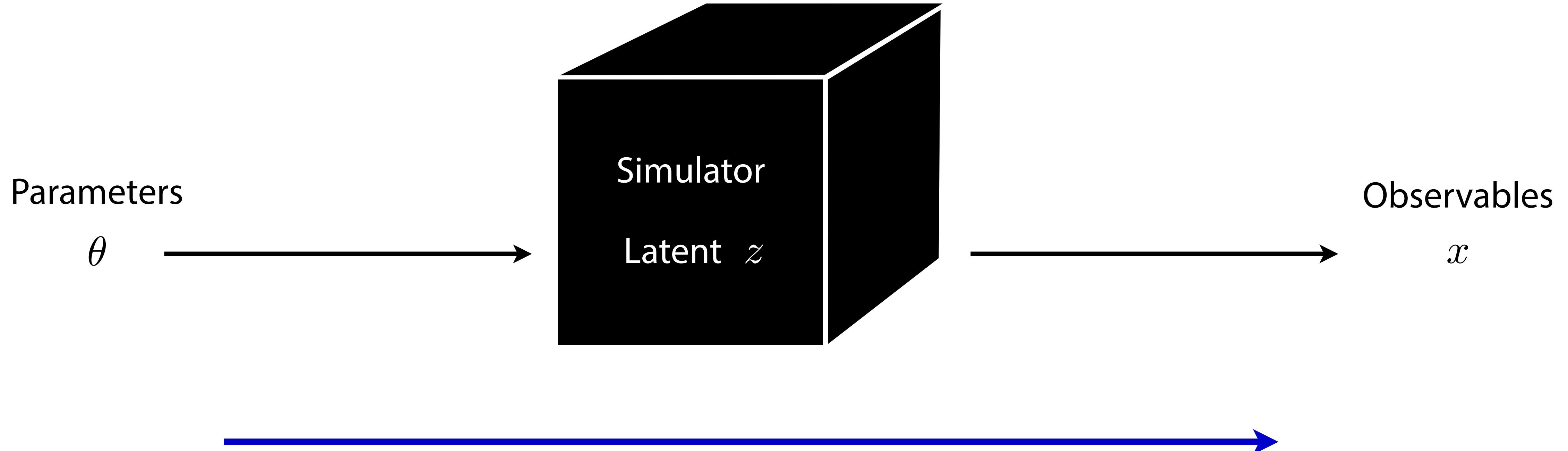
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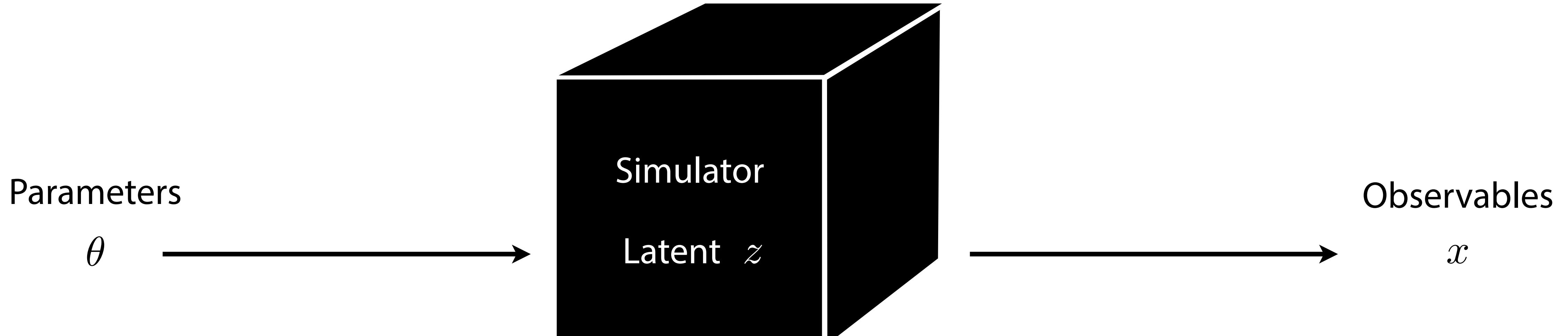
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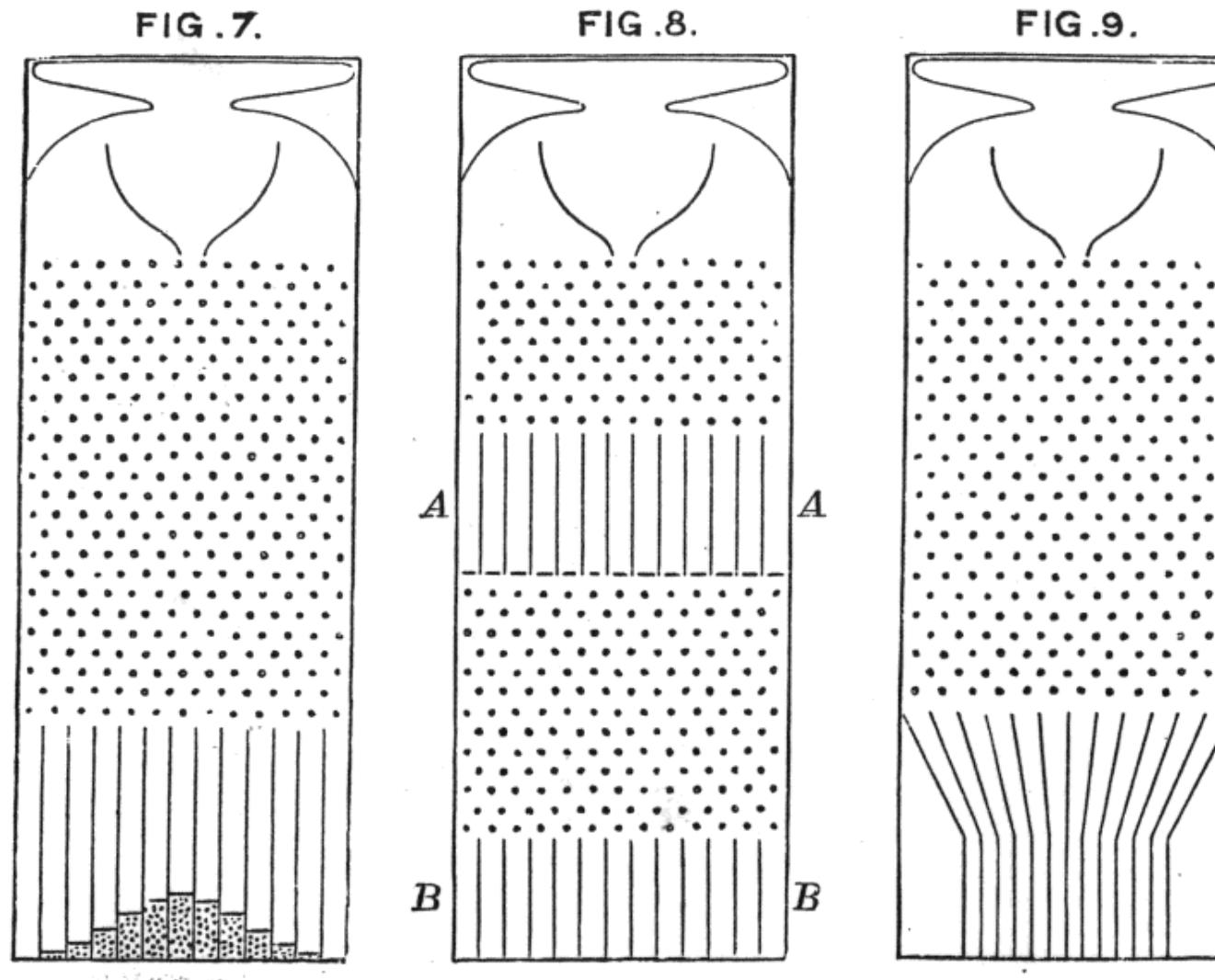
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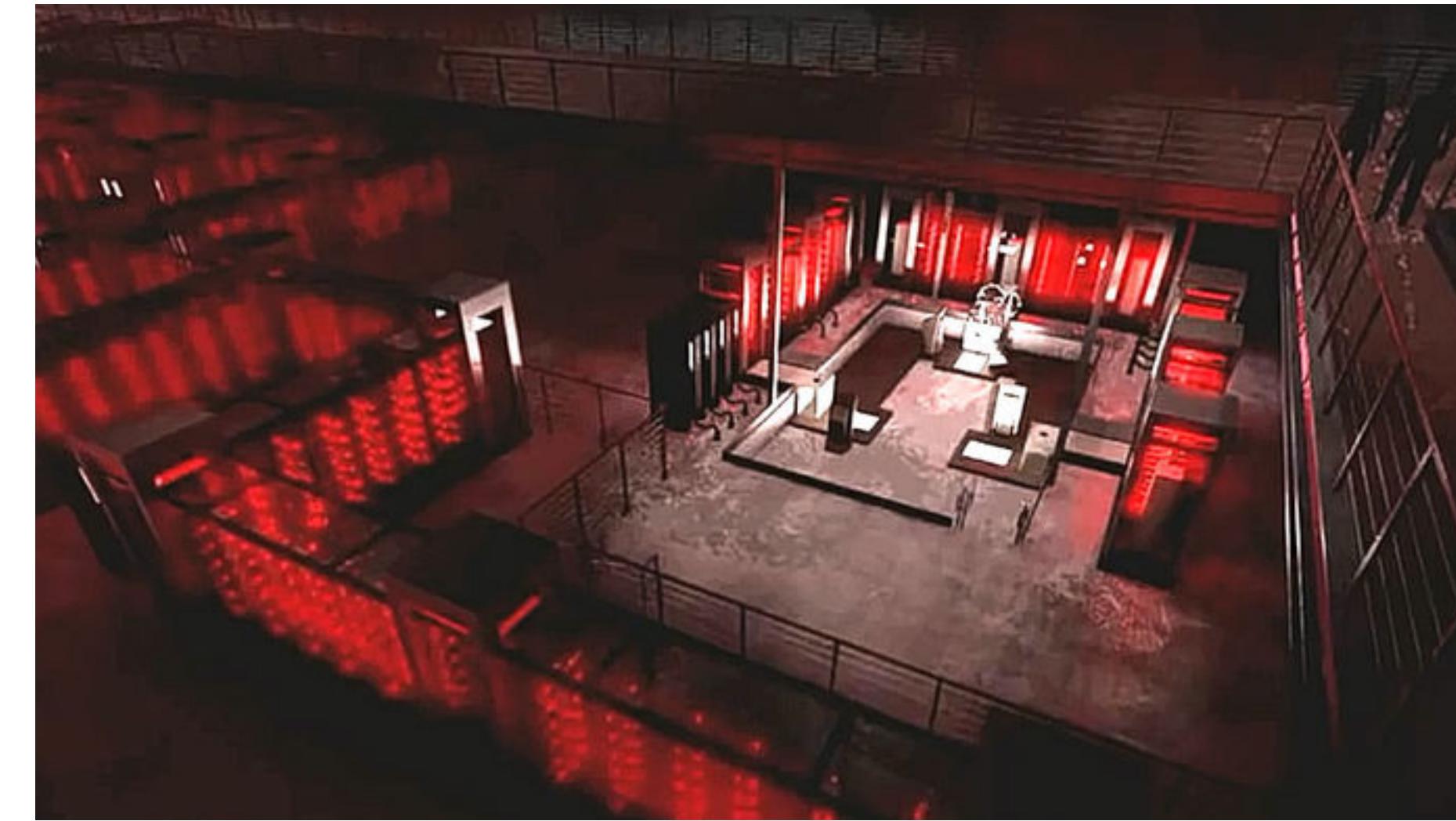
Inference:

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

# Galton board: metaphor for simulator-based science



[F. Galton 1889]



[HBO 2018]

Galton board device



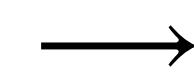
Computer simulation

Parameters  $\theta$



Model parameters  $\theta$

Bins  $x$



Observables  $x$

Path  $z$



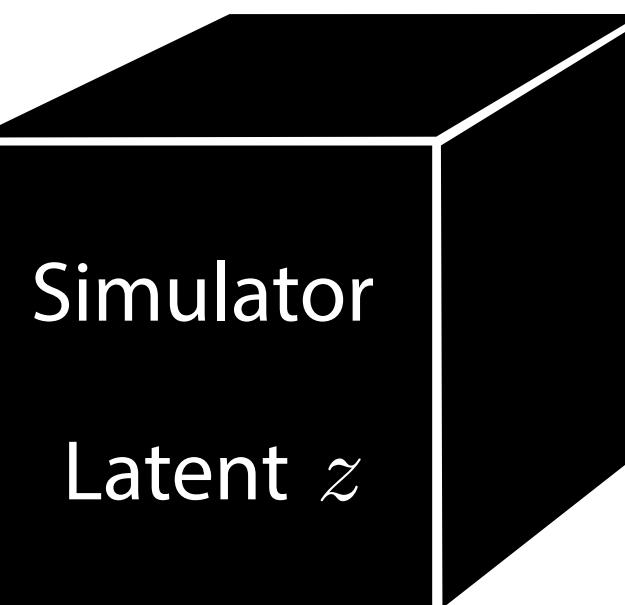
Latent variables  $z$

(stochastic execution trace through simulator)

# Cosmological N-body simulations

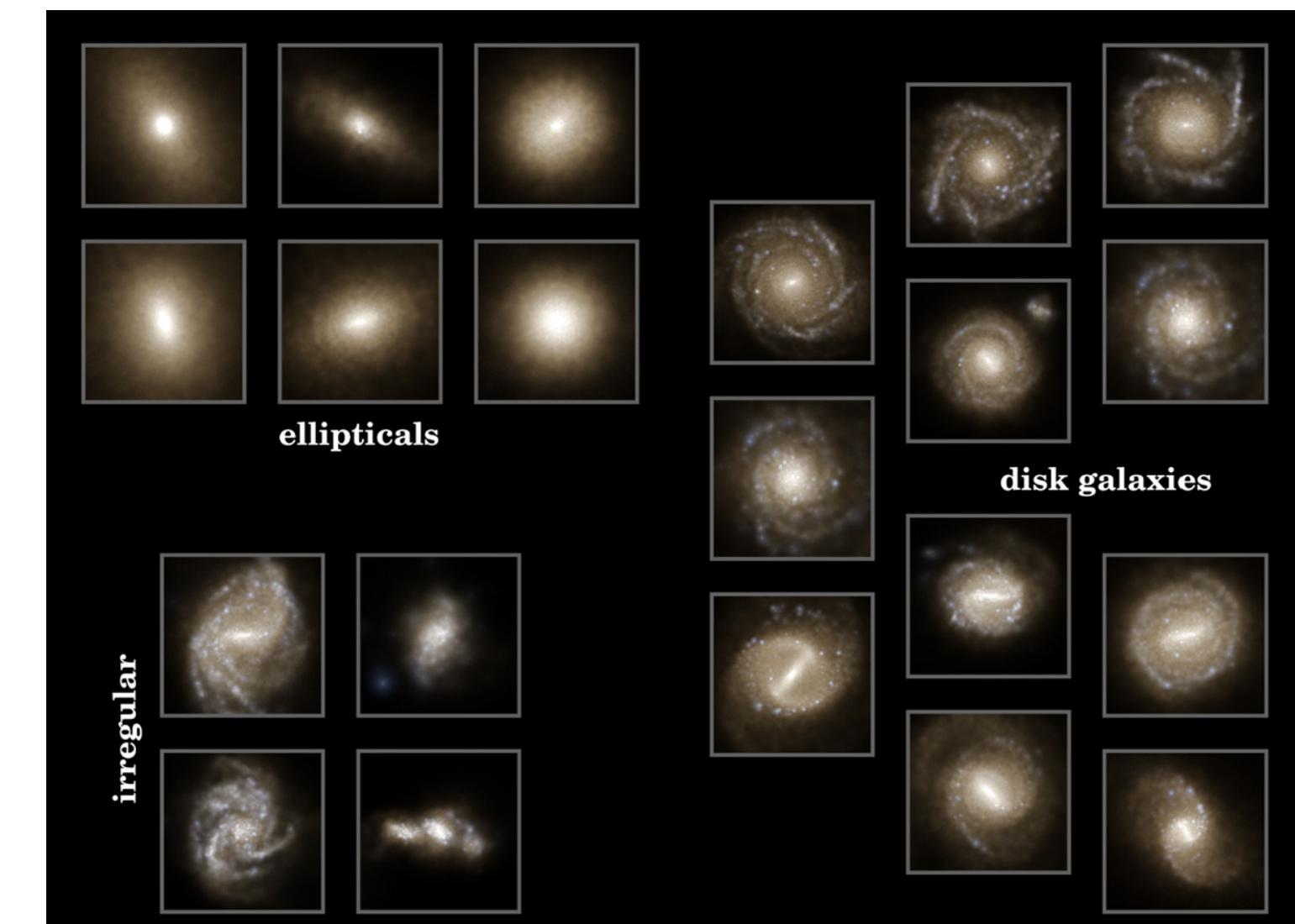
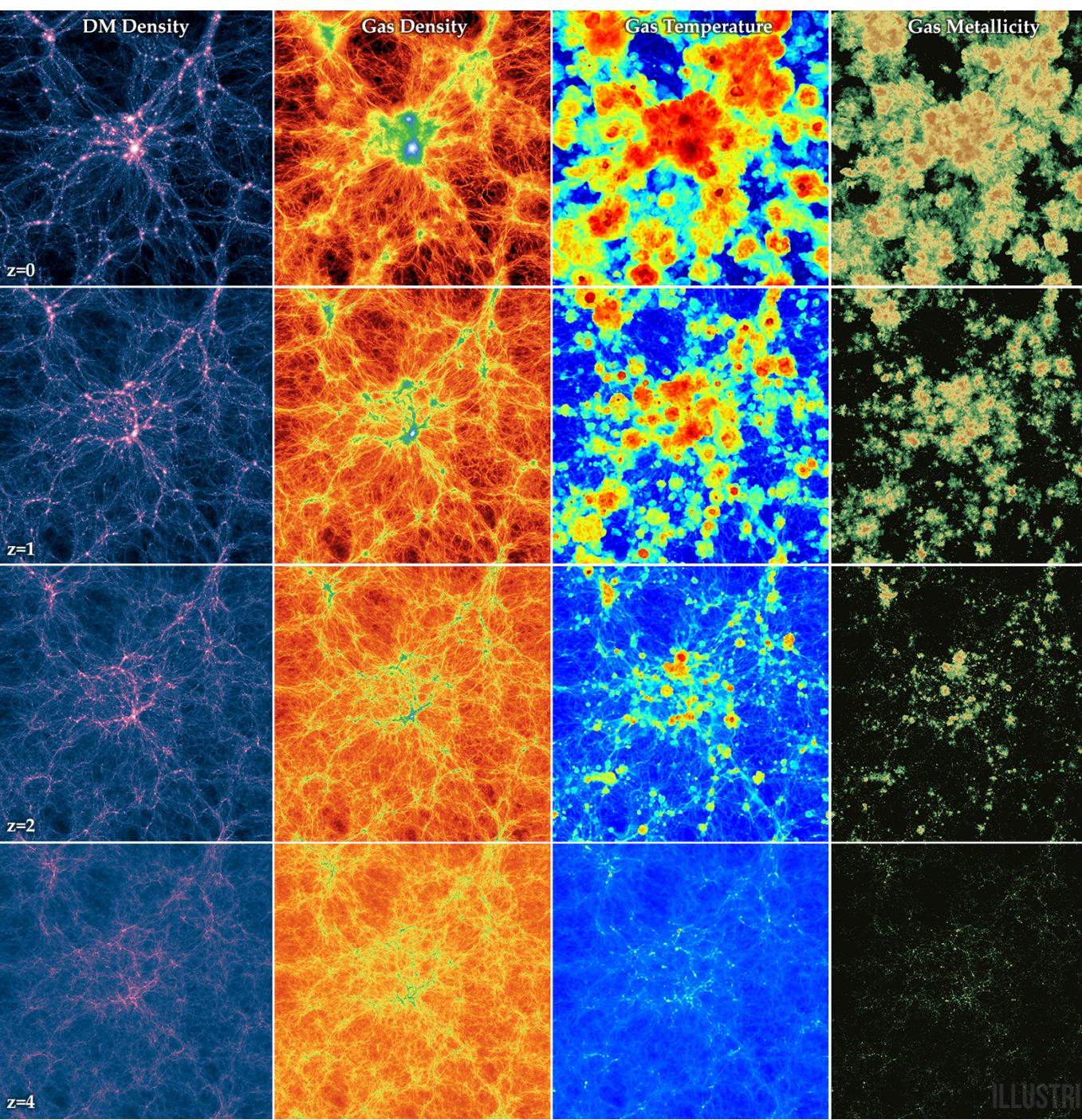
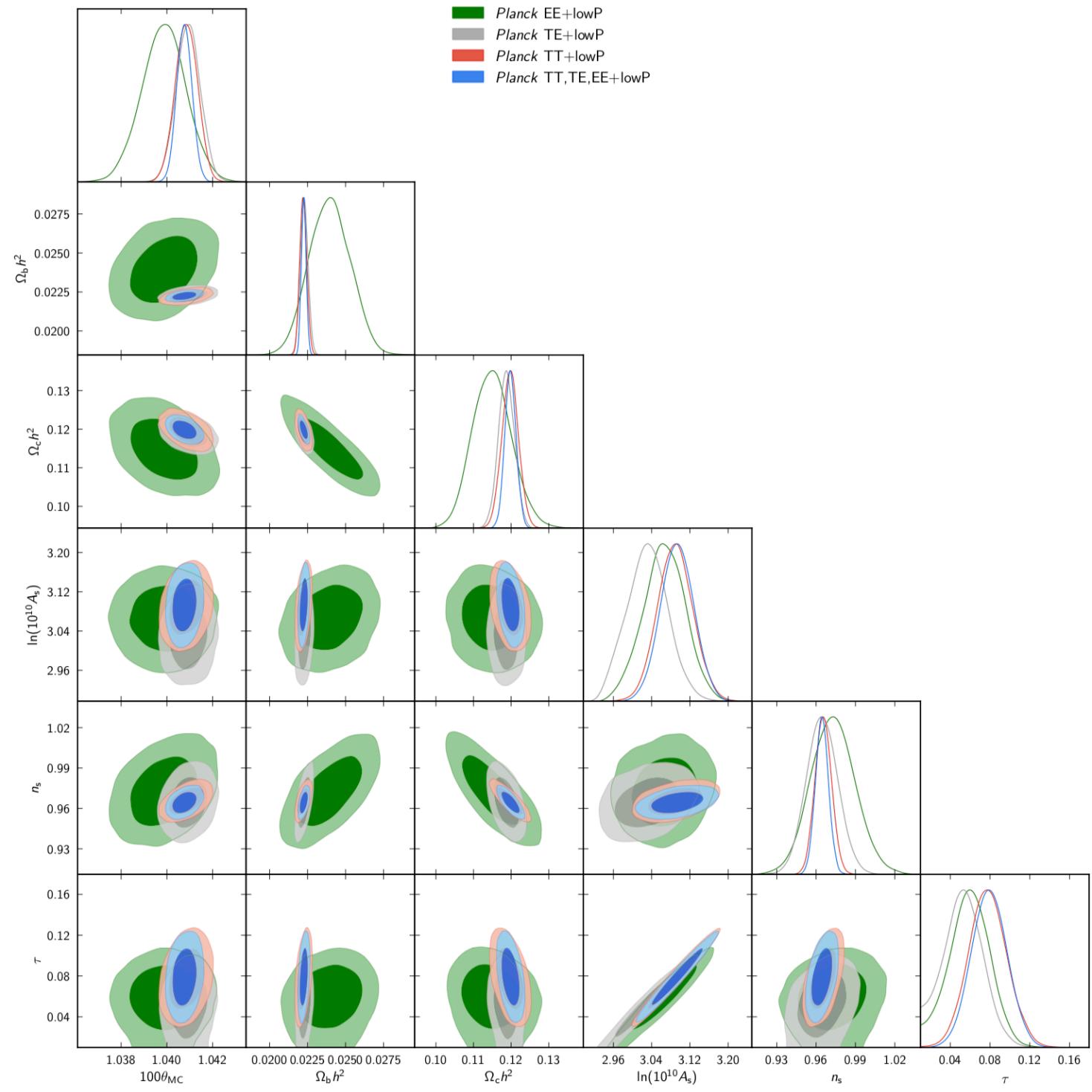
Parameters

$\theta$



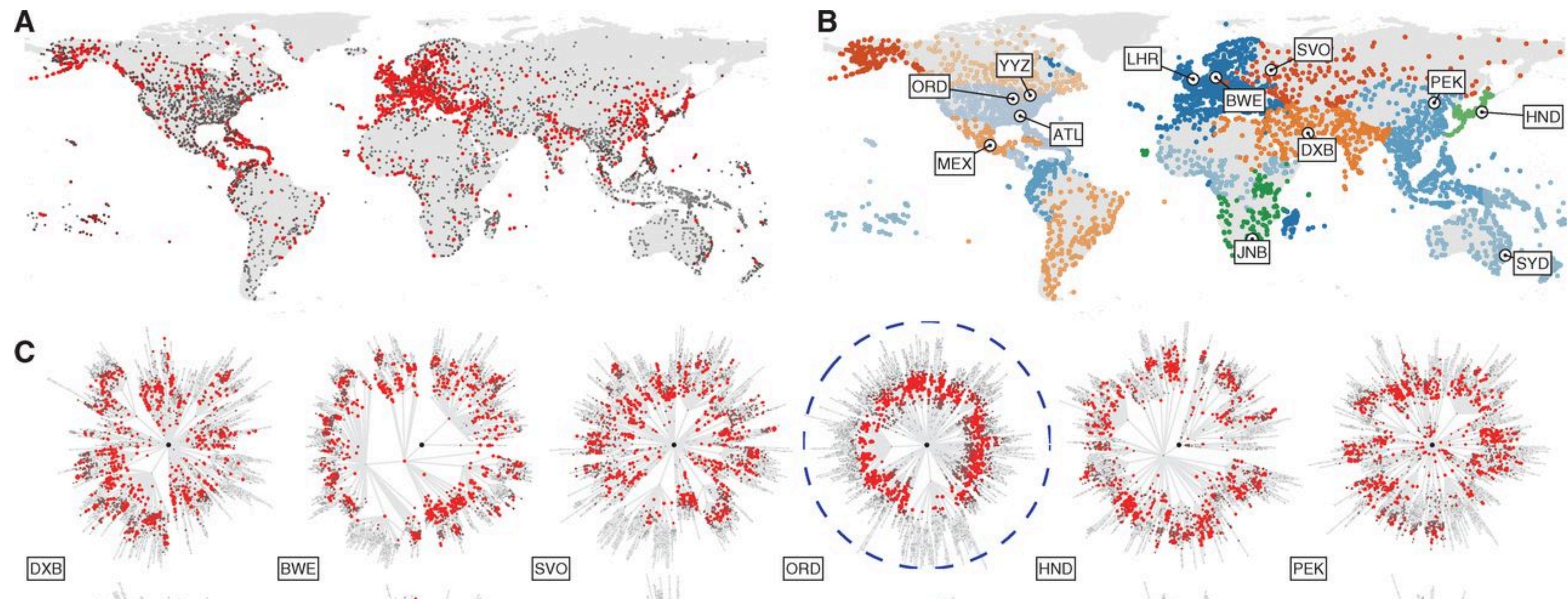
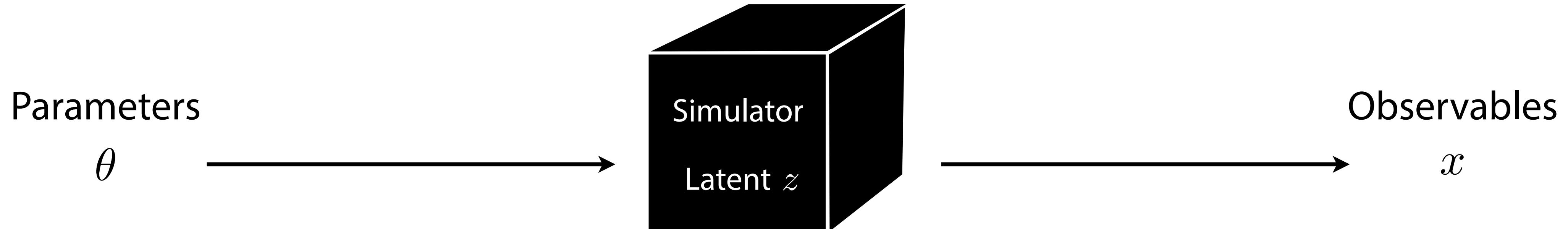
Observables

$x$



[Illustris 1405.2921]

# Epidemiology



[D. Brockmann, D. Helbing 2013]

# Particle physics

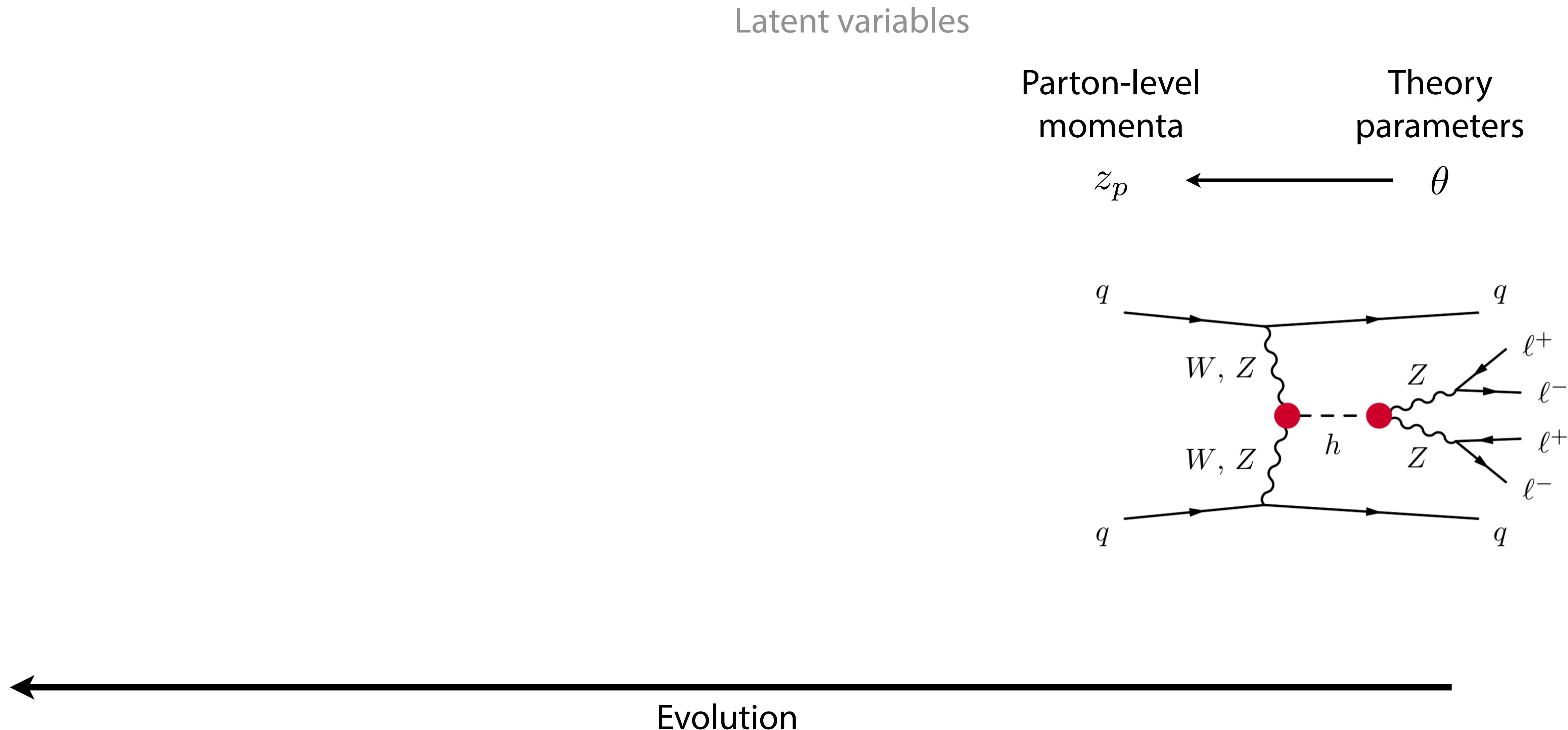
Theory  
parameters

$$\theta$$

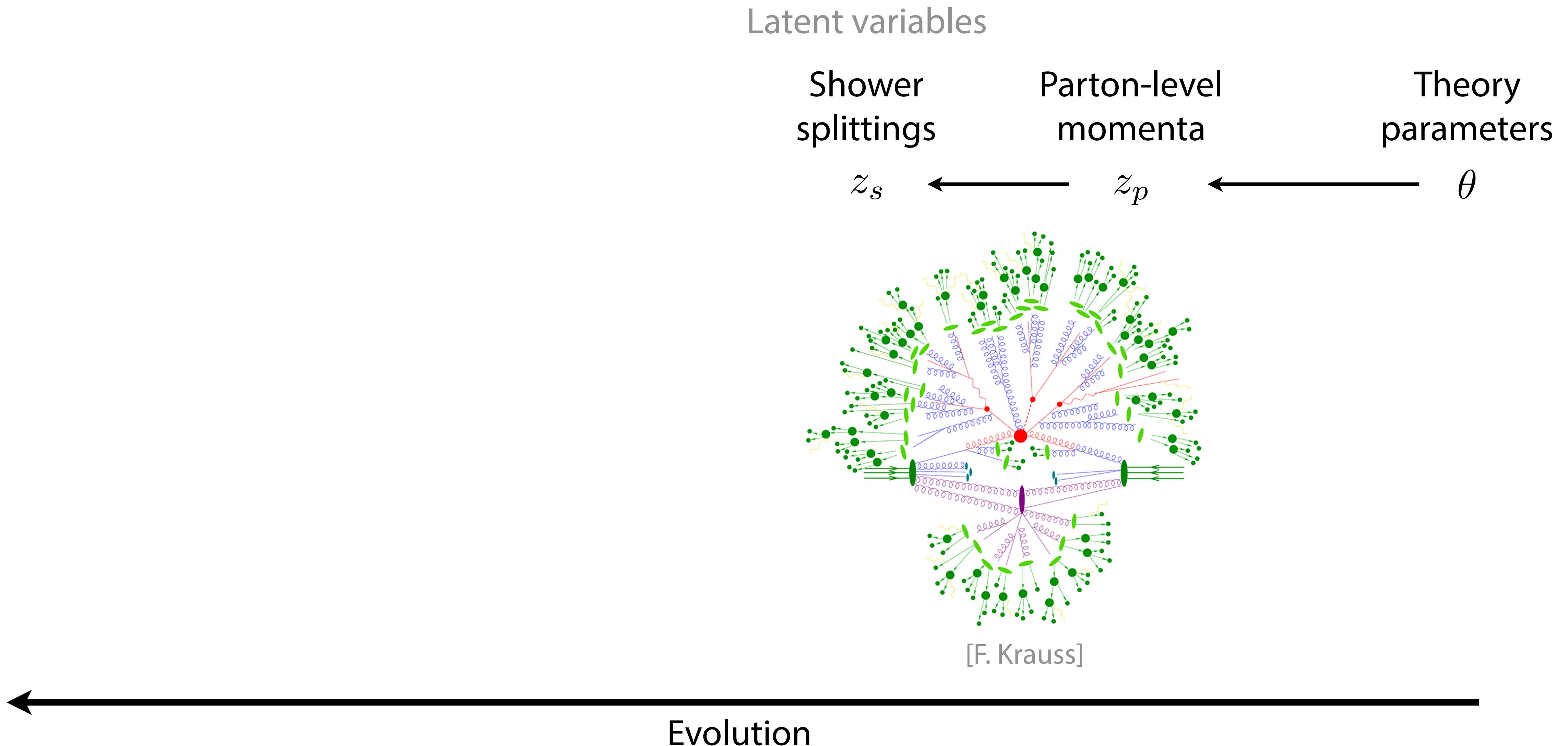


Evolution

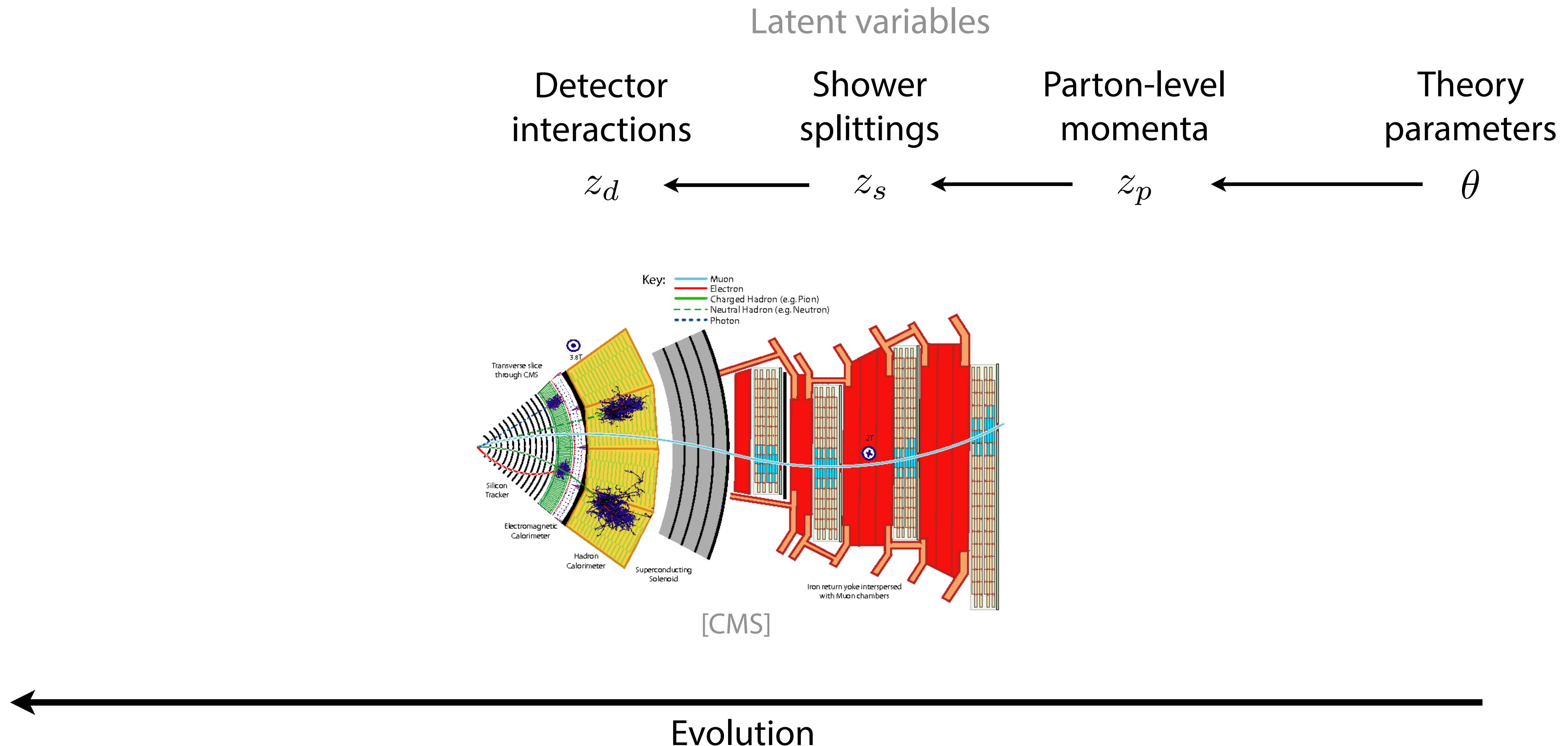
# Particle physics



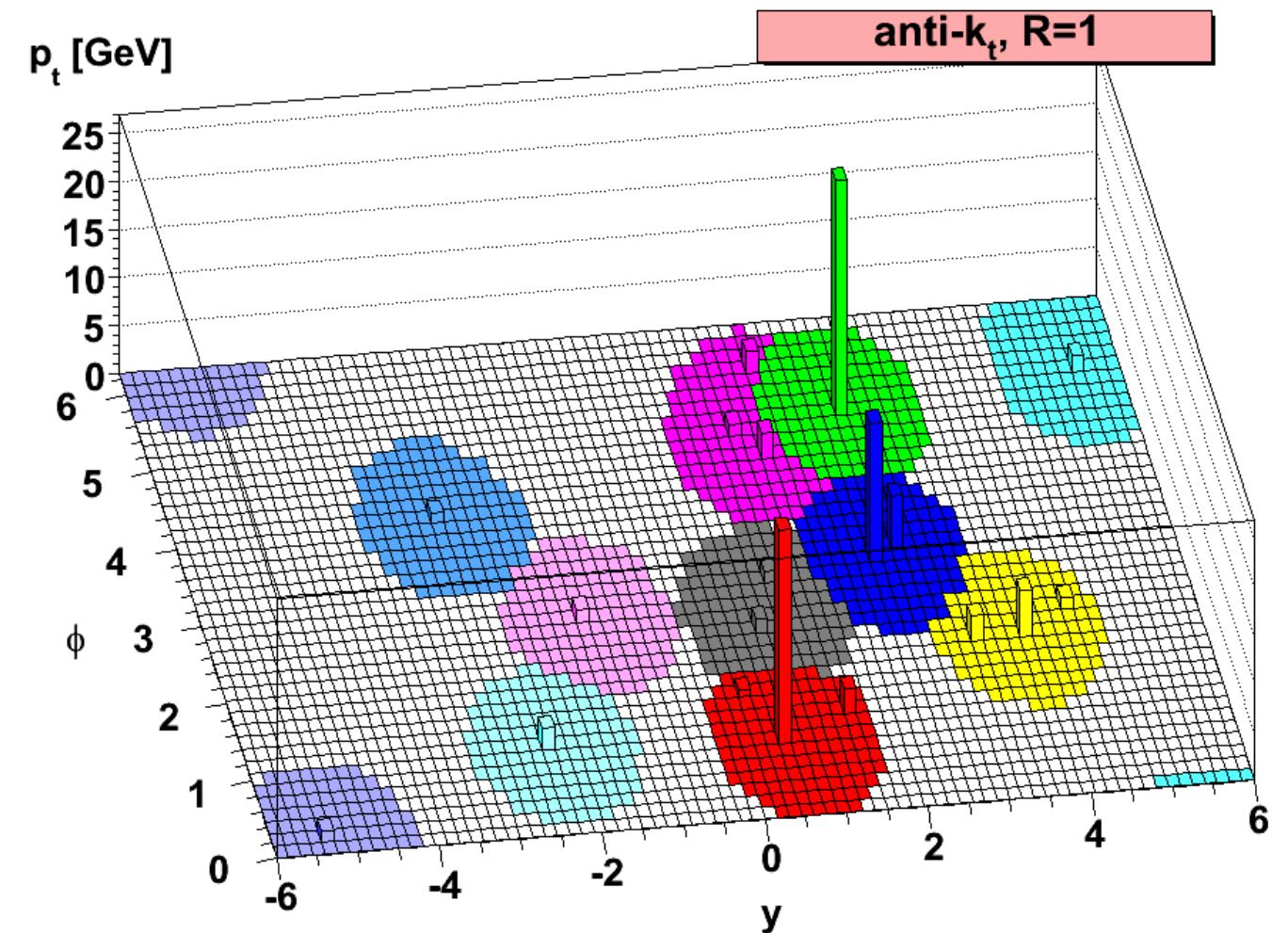
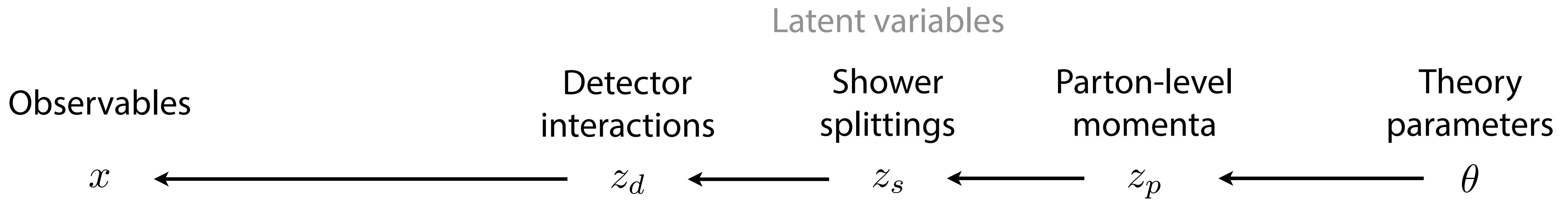
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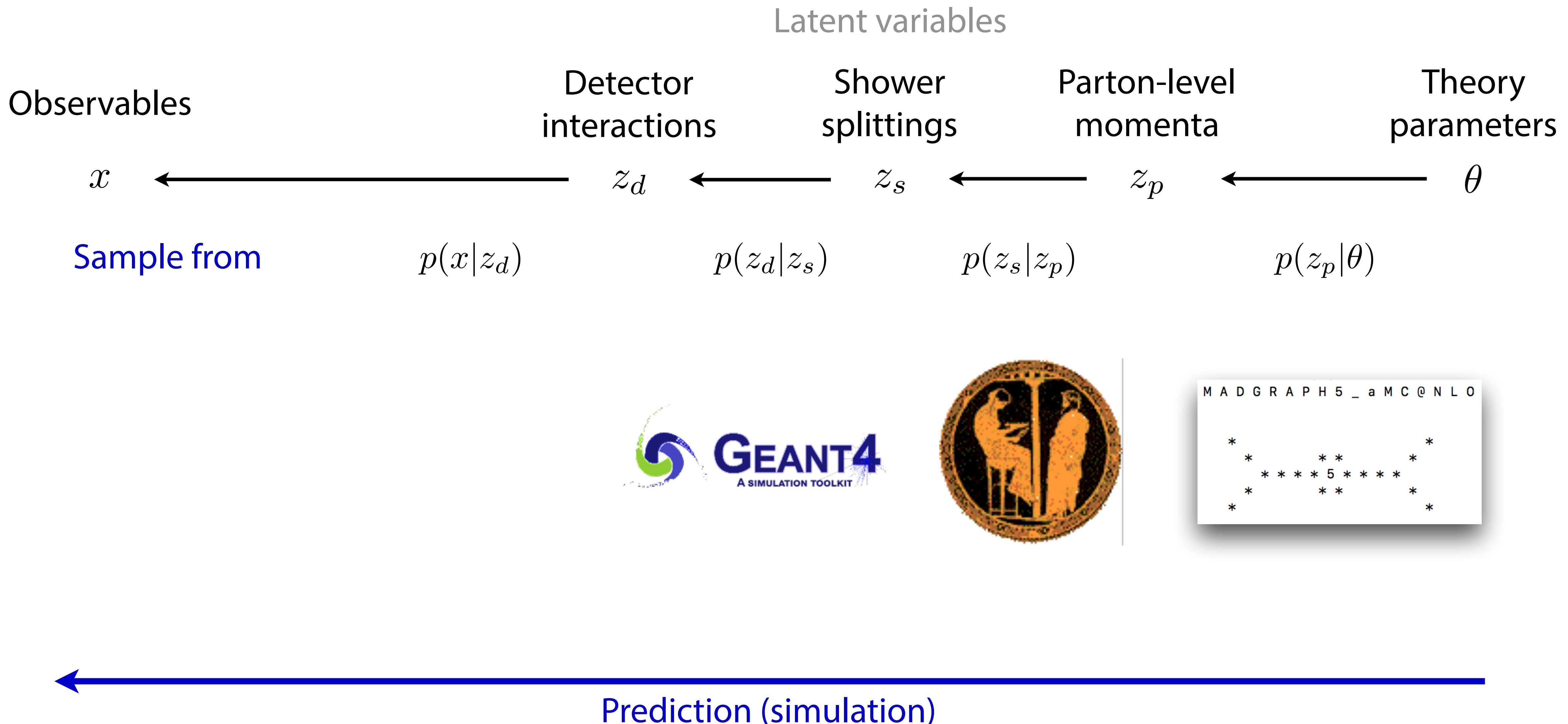


[M. Cacciari, G. Salam, G. Soyez 0802.1189]

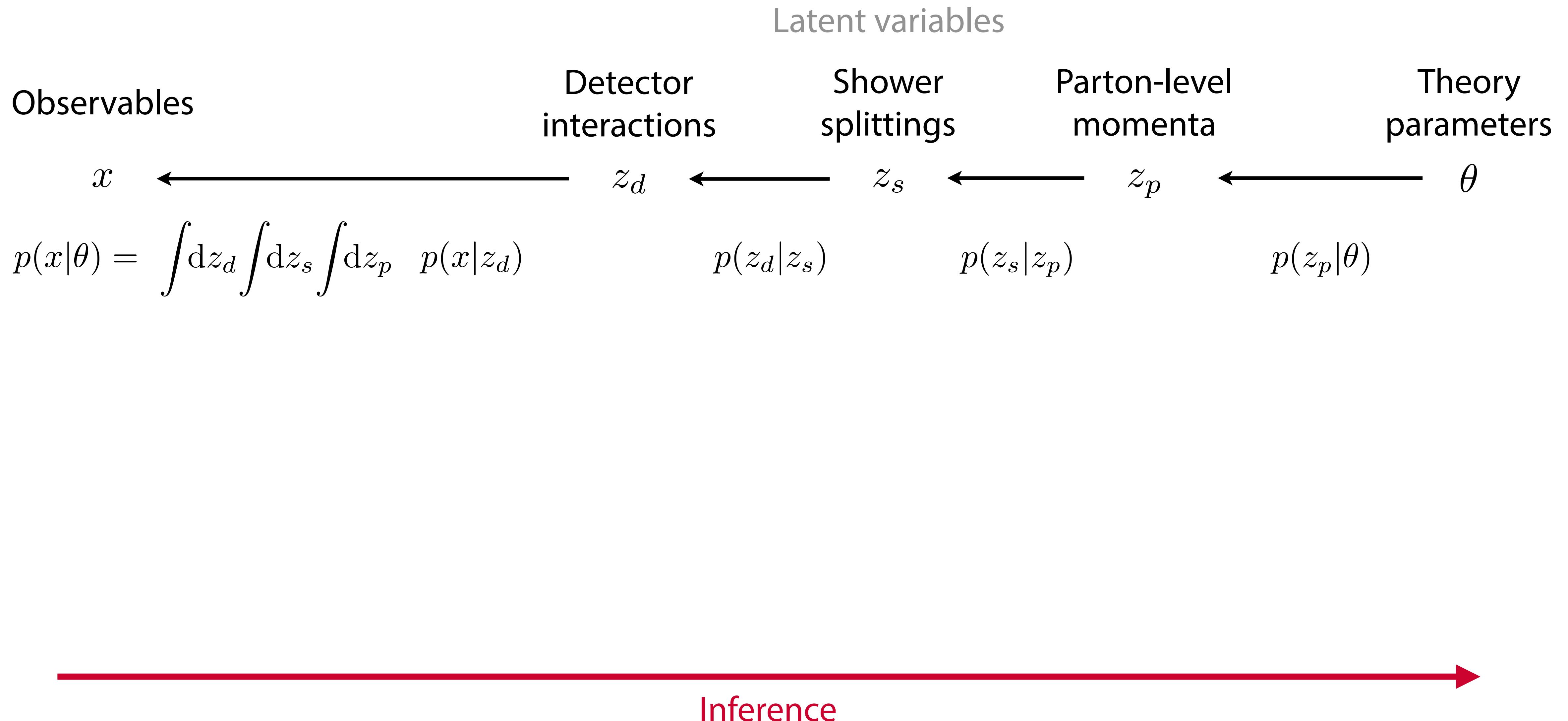


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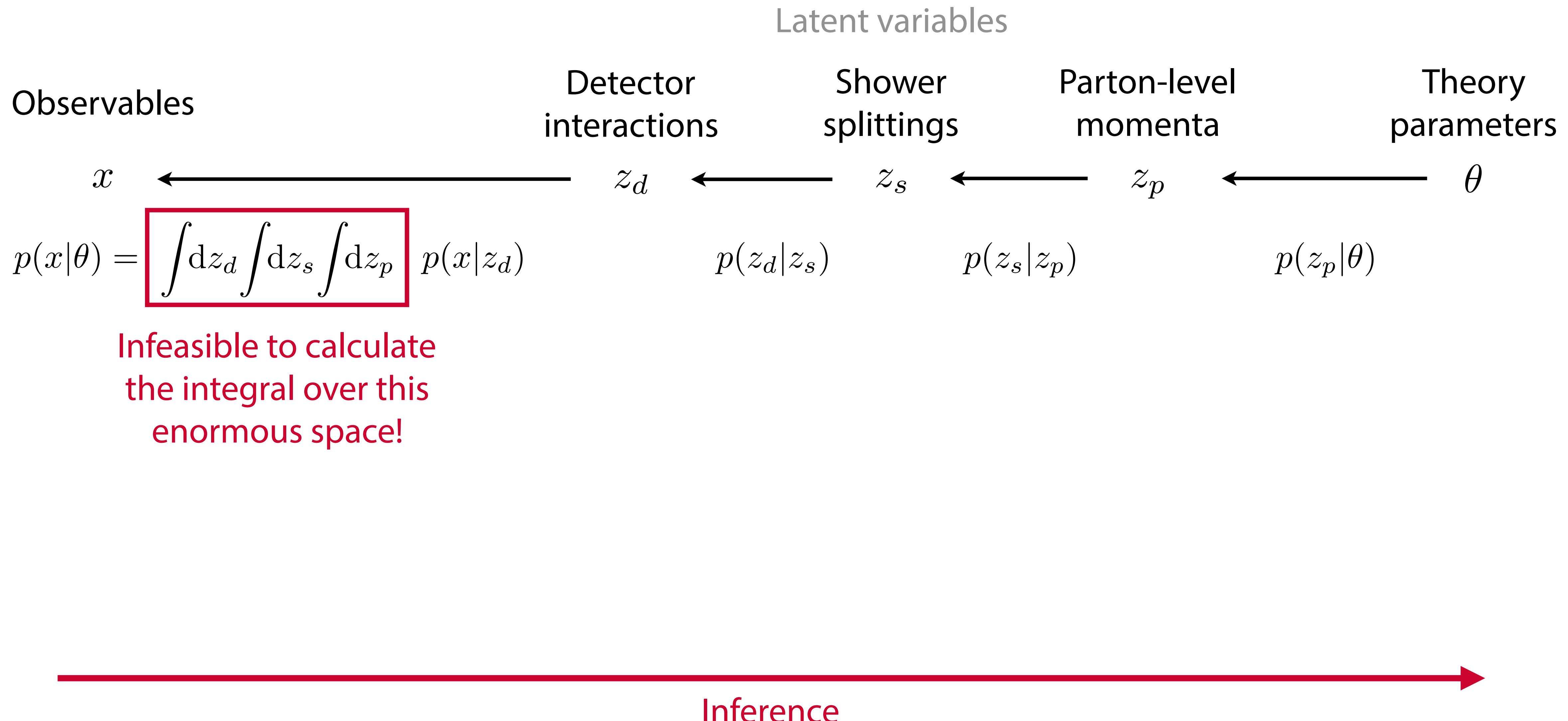
# Particle physics



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**Why has that not stopped us so far?**

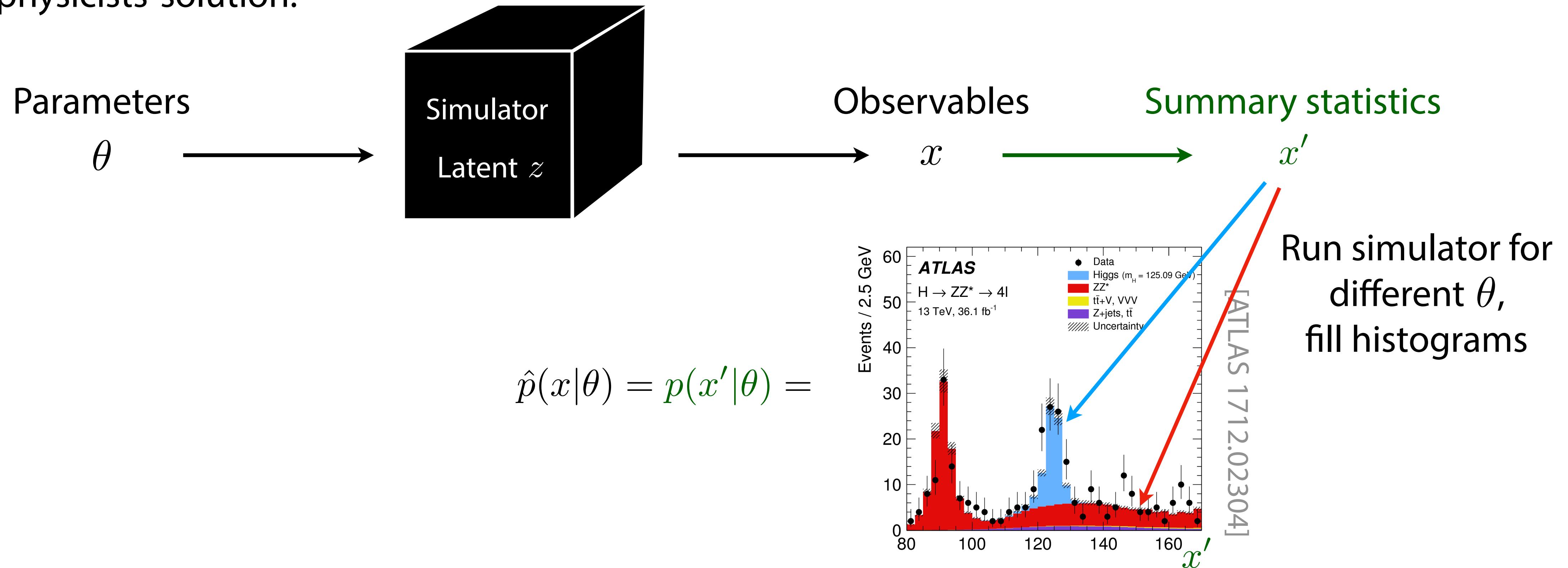
# Solve it by histogramming summary statistics

- Most physicists' solution:



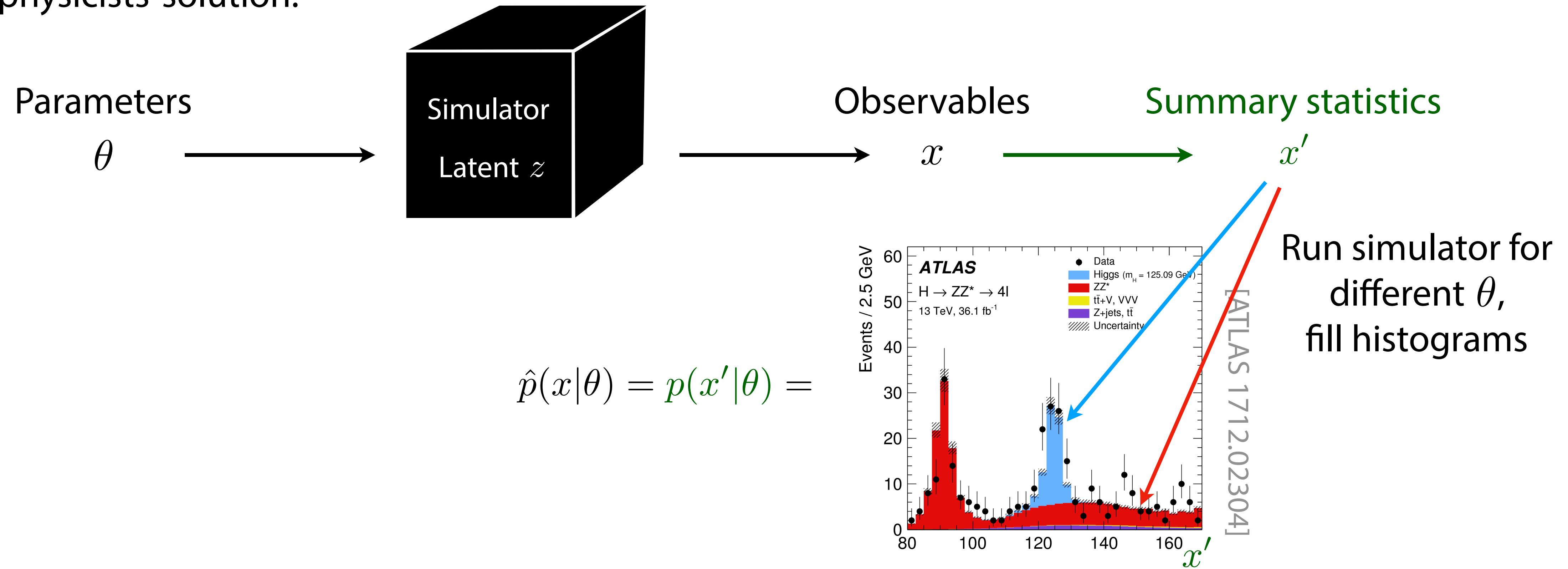
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# Solve it by histogramming summary statistics

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- How to choose  $x'$ ? Standard variables often lose information

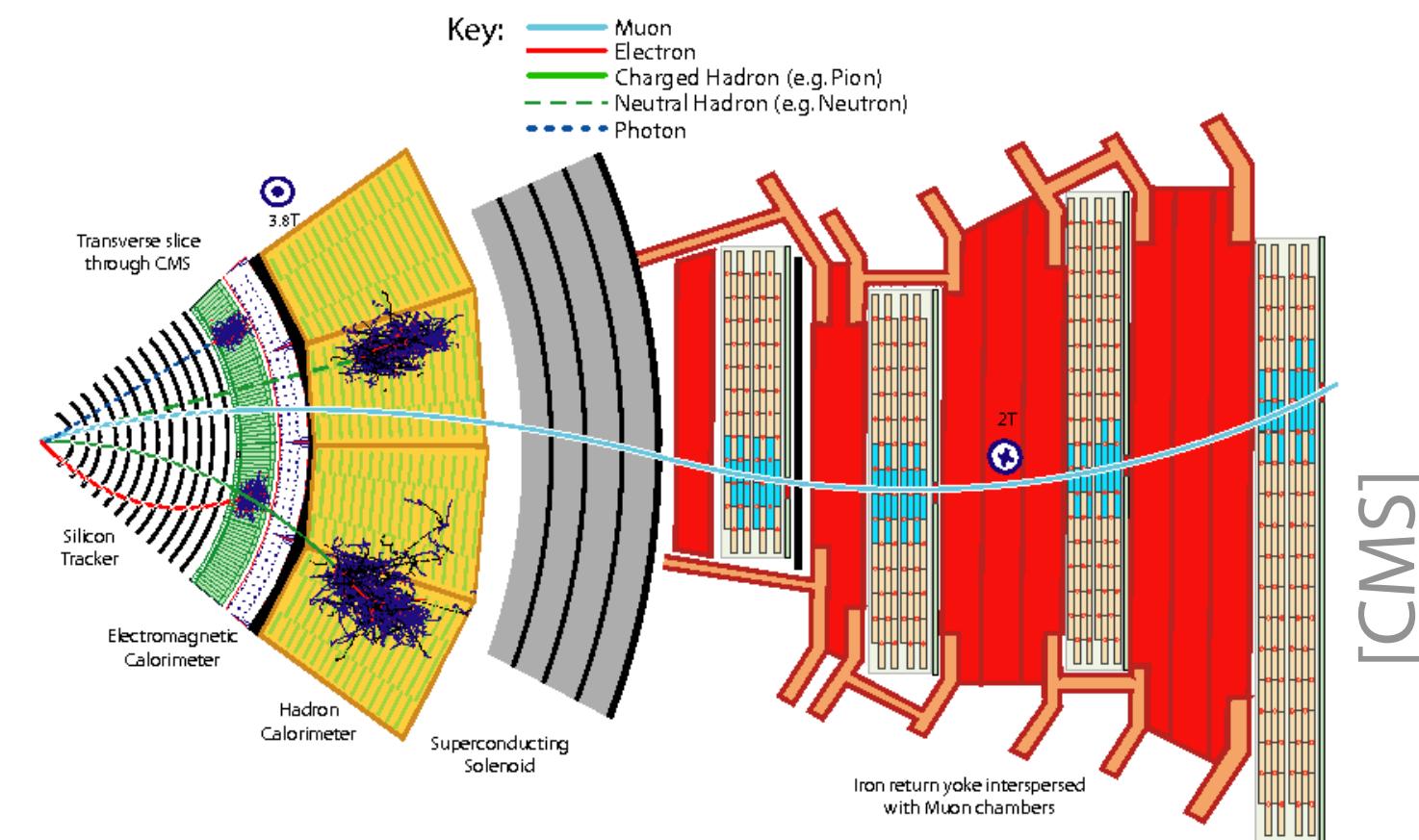
[JB, K. Cranmer, F. Kling, T. Plehn 1612.05261; JB, F. Kling, T. Plehn, T. Tait 1712.02350]

- “Curse of dimensionality”: Histograms don't scale to high-dimensional  $x$

# Solve it by approximating the integral

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

$$p(x|\theta) = \int dz_d \int dz_s \int dz_p p(x|z_d) p(z_d|z_s) p(z_s|z_p) p(z_p|\theta)$$



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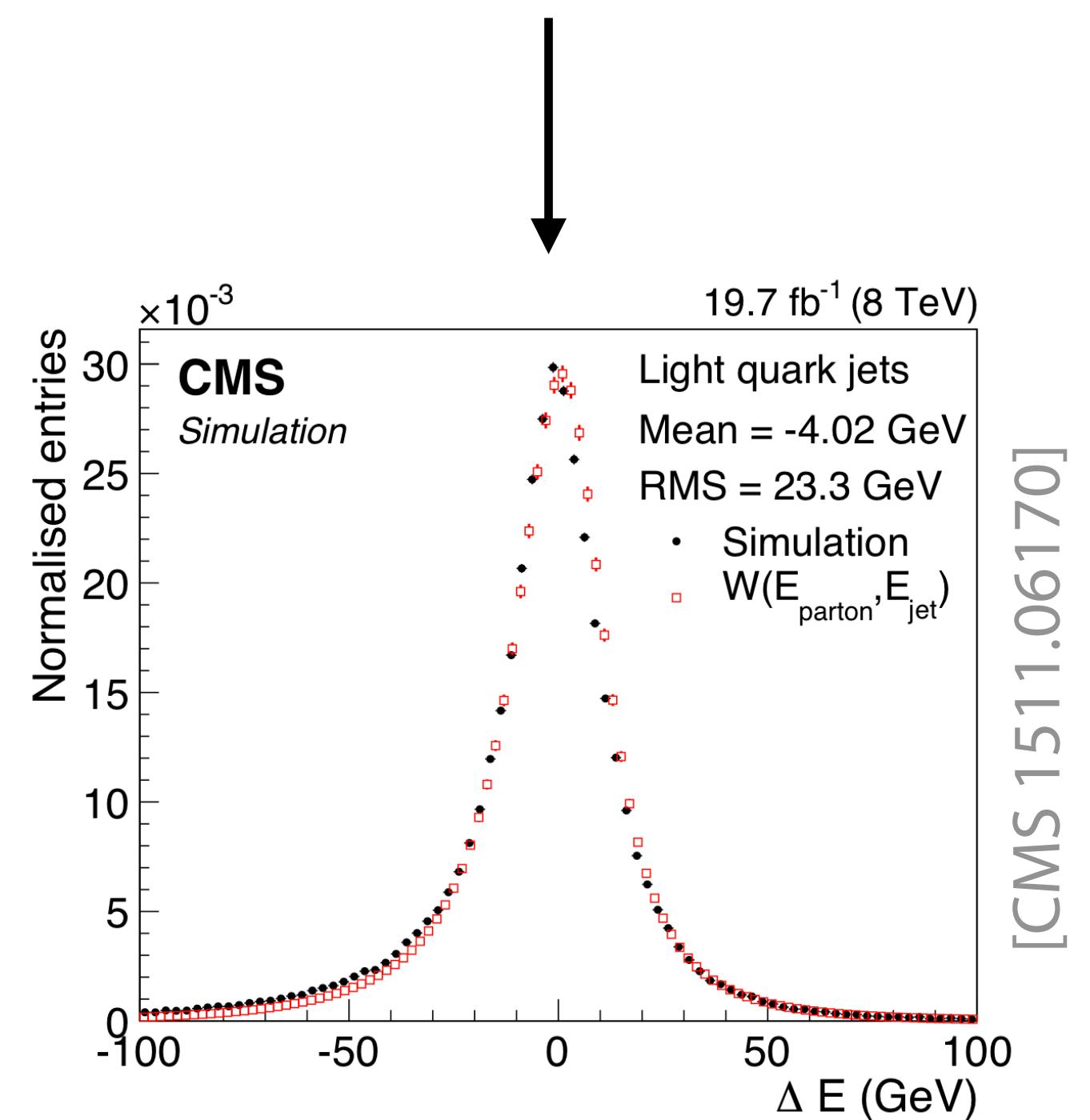
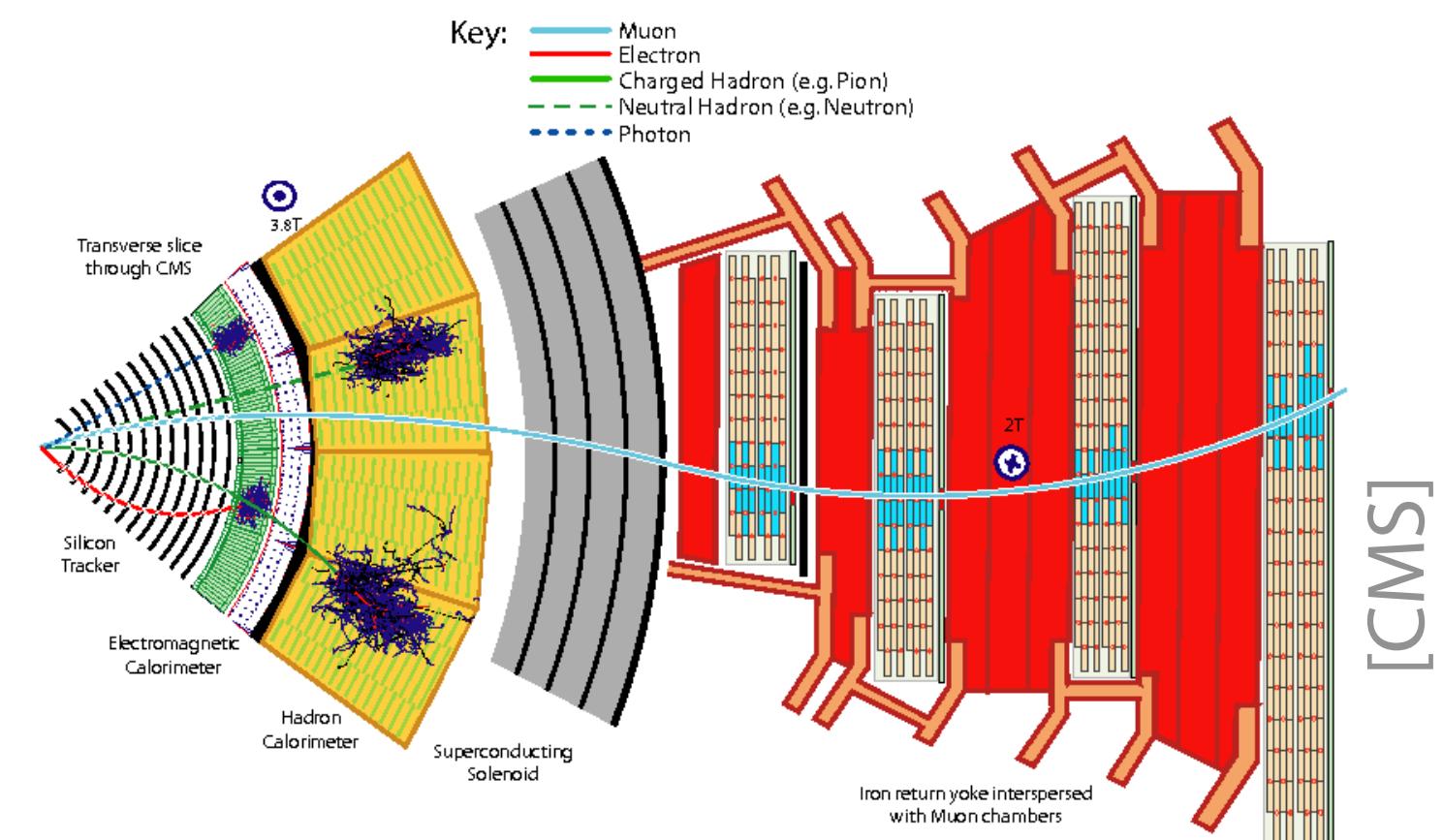
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- Matrix Element Method: [K. Kondo 1988]

- approximate **shower + detector effects** into **transfer function**  $\hat{p}(x|z_p)$
- explicitly calculate remaining integral

$$\hat{p}(x|\theta) = \int dz_p \hat{p}(x|z_p) p(z_p|\theta)$$

- Shower / Event Deconstruction [D. E. Soper, M. Spannowsky 1102.3480]  
extend explicit calculation to the shower



# Solve it by approximating the integral

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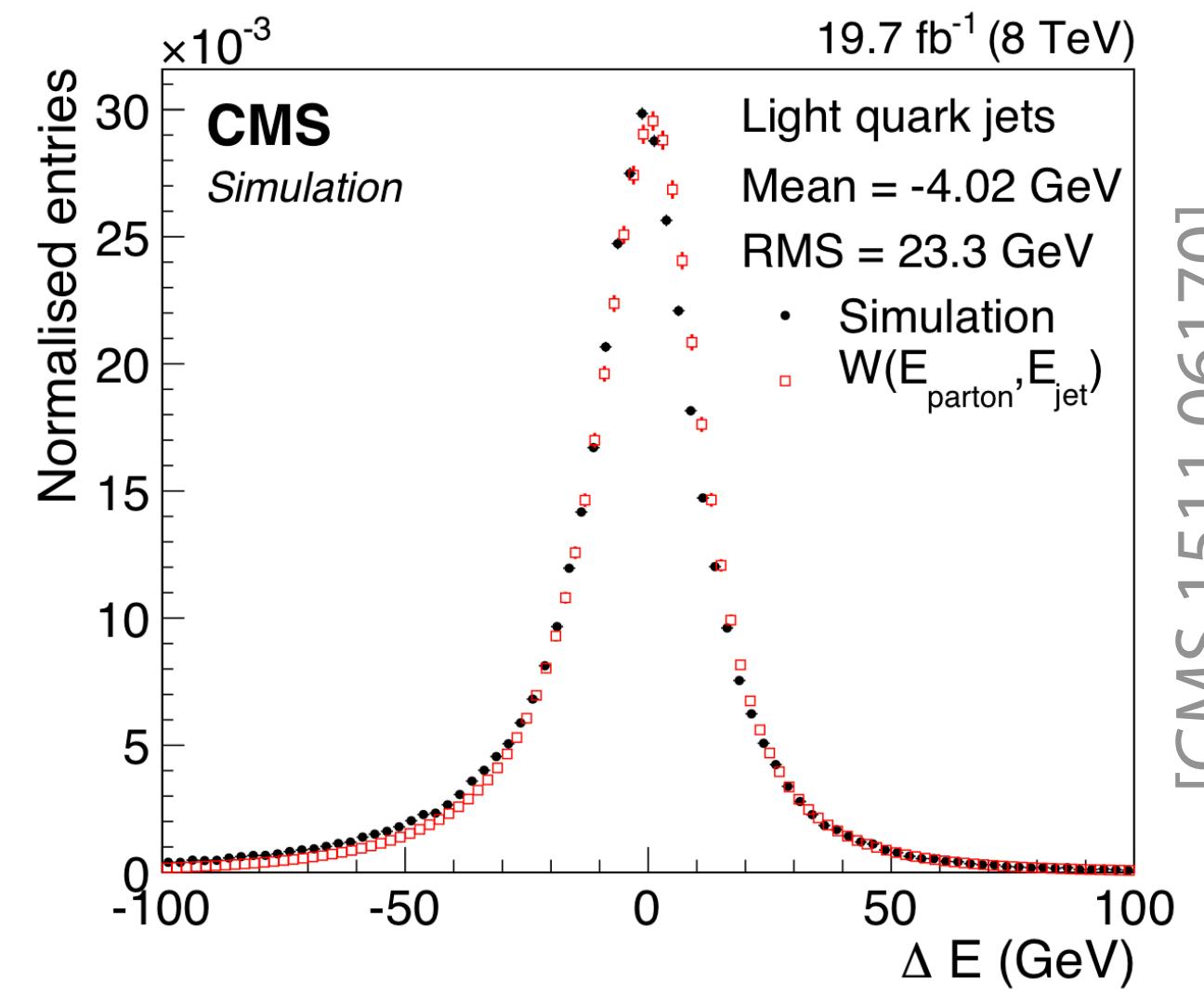
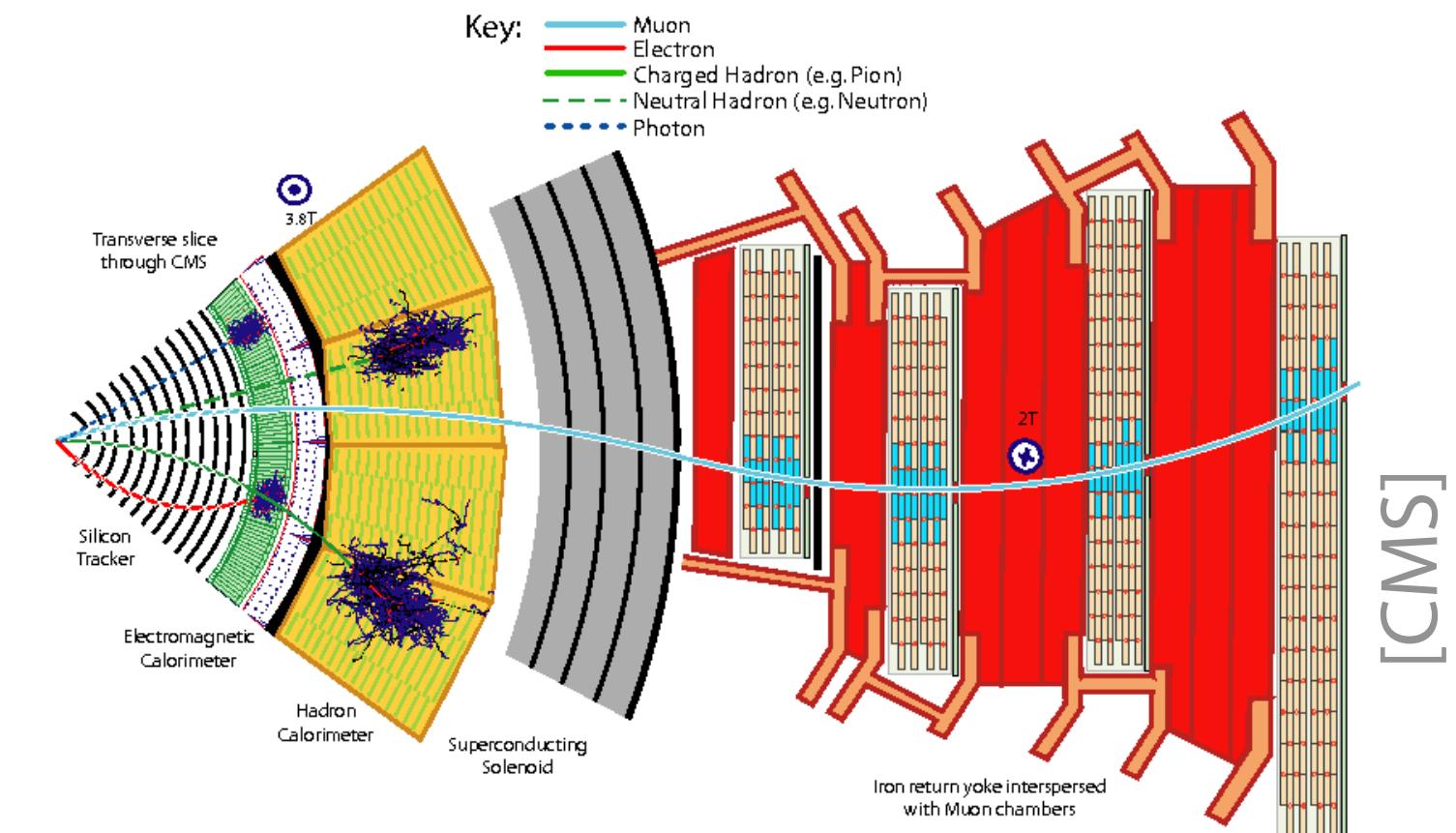
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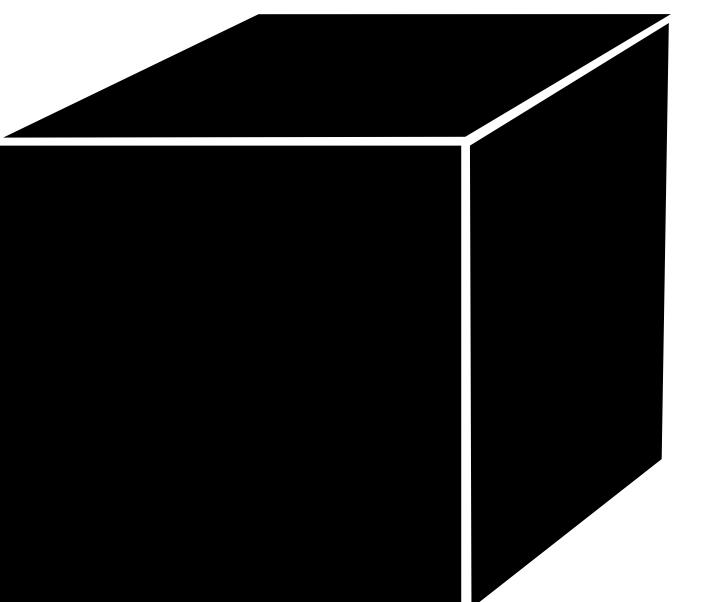
- Uses matrix-element information, no summary statistics necessary, but:
  - ad-hoc transfer functions
  - evaluation still requires calculating an expensive integral



# Likelihood-free inference methods

Treat simulator as black box:

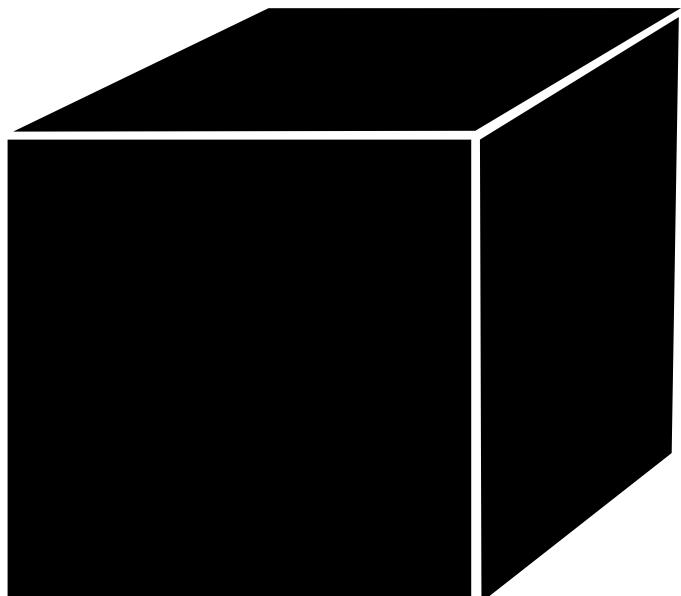
- Histograms of observables,  
Approximate Bayesian Computation  
Rely on summary statistics
- Machine learning techniques  
Density networks, CARL, autoregressive models,  
normalizing flows, ...



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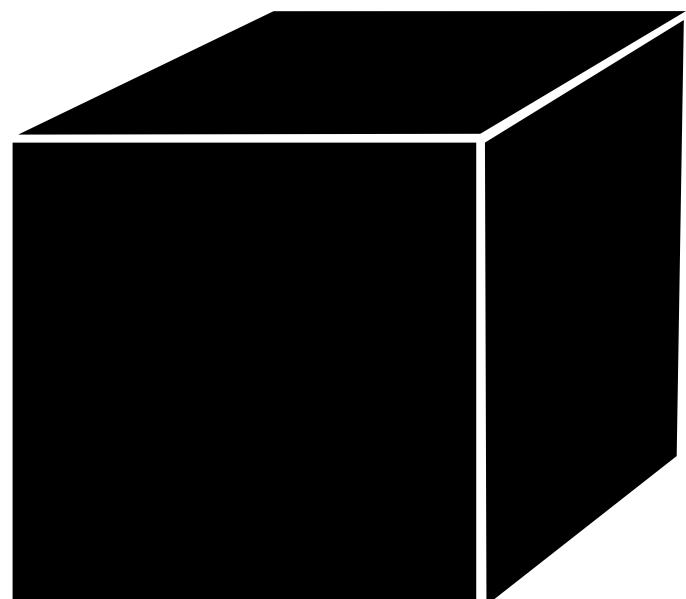
Use latent structure:

- Matrix Element Method, Optimal Observables,  
Shower Deconstruction, Event Deconstruction  
Neglect or approximate shower + detector, explicitly calculate  
 $\mathcal{Z}$  integral

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Use latent structure:

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Shower Deconstruction, Event Deconstruction  
Neglect or approximate shower + detector, explicitly calculate  
 $\mathcal{Z}$  integral
- Mining gold from the simulator  
Leverage matrix-element information + machine learning

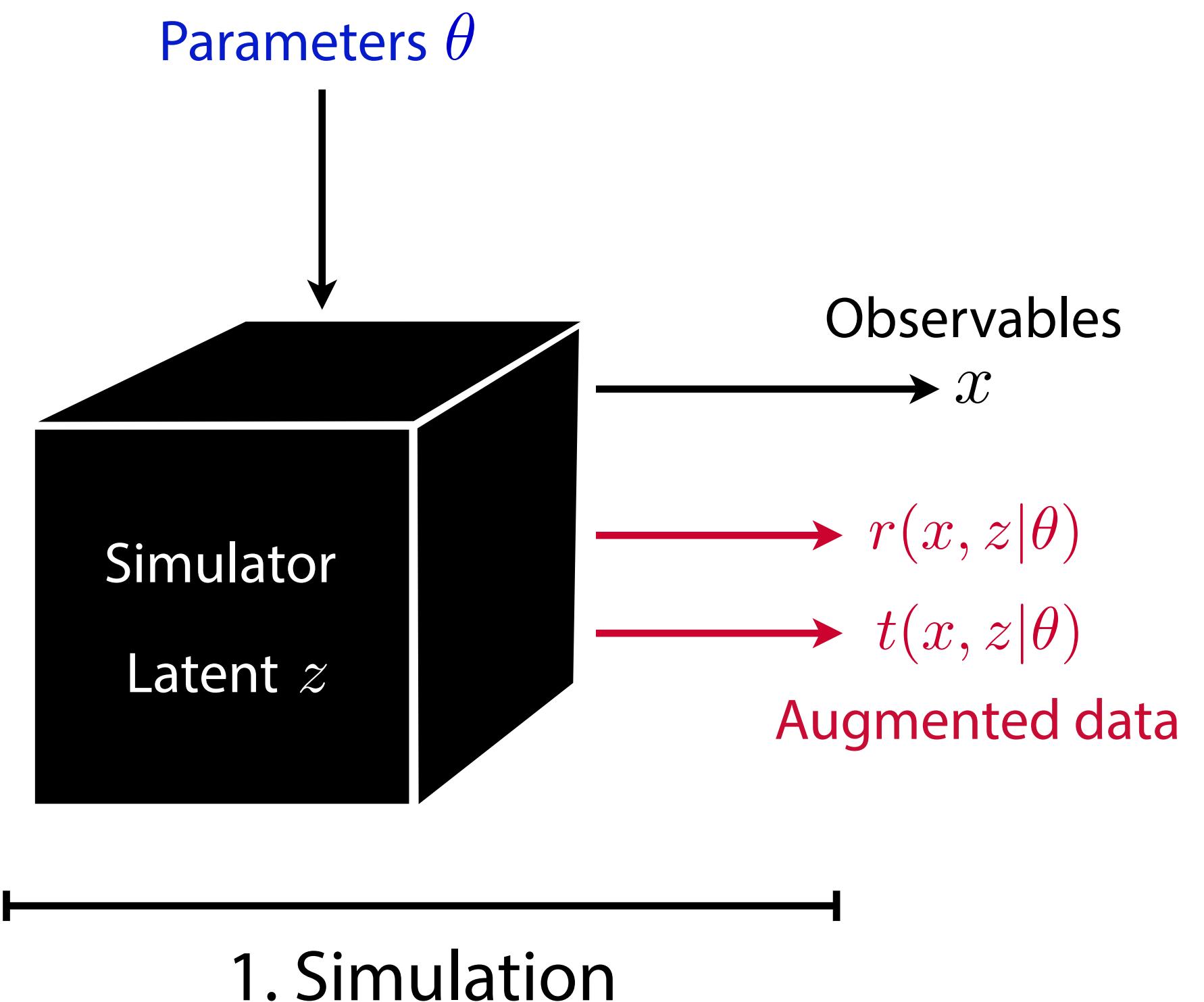
New!



# A new approach: Mining gold from the simulator

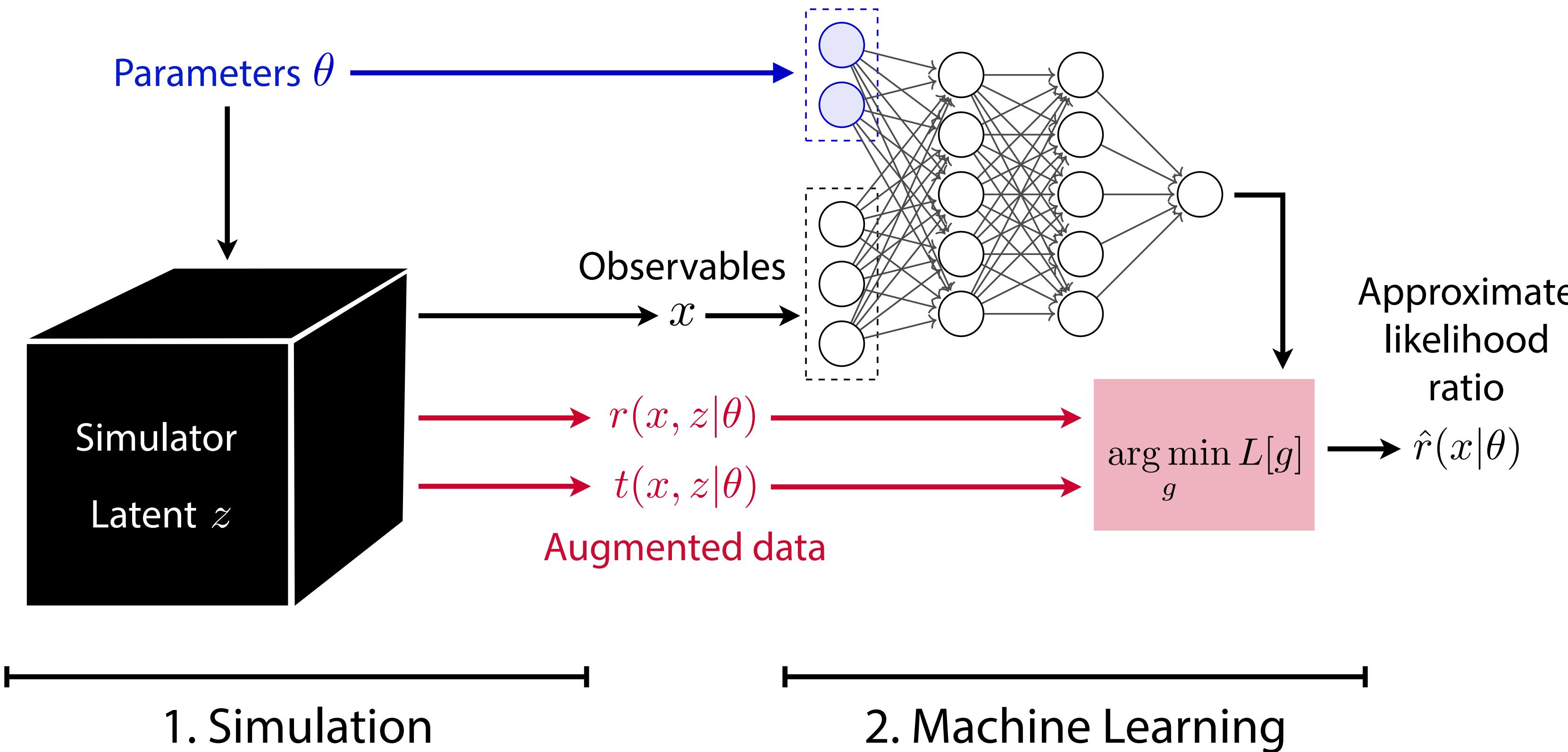
[JB, K. Cranmer, G. Louppe, J. Pavez 1805.00013, 1805.00020, 1805.12244;  
with M. Stoye 1808.00973; with F. Kling in progress]

# Bird's-eye view



“Mining gold”: Extract additional information from simulator

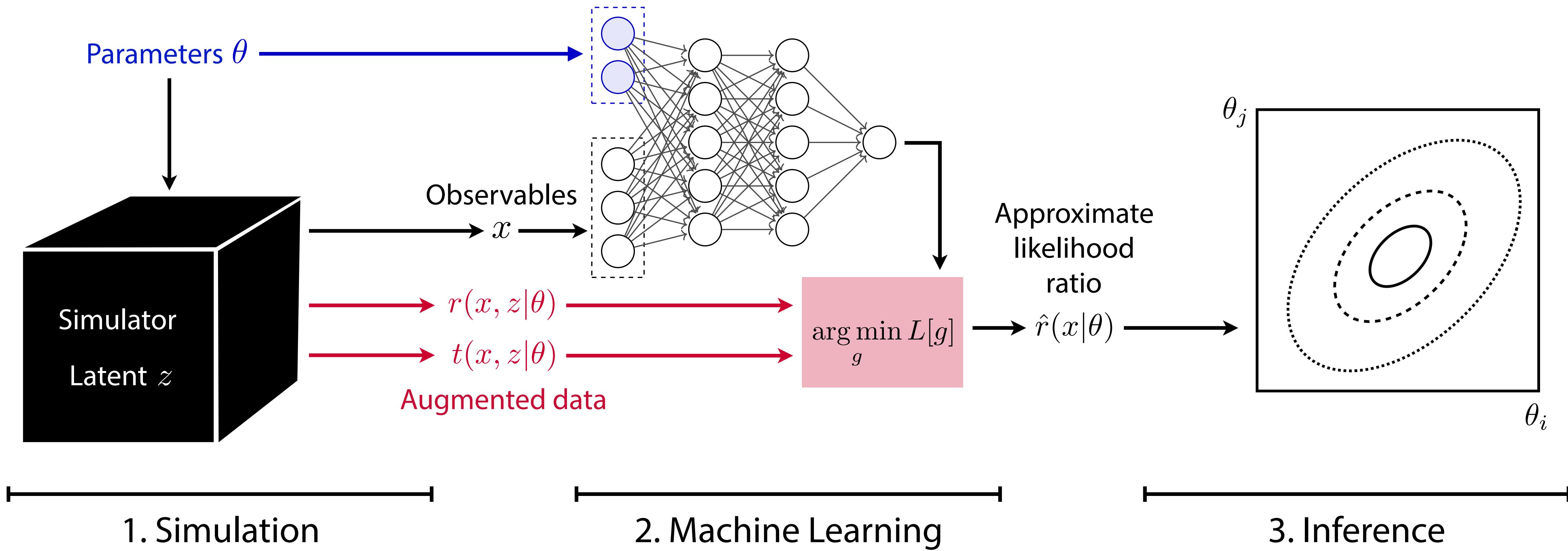
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“Mining gold”: Extract additional information from simulator

Use this information to train estimator for likelihood ratio

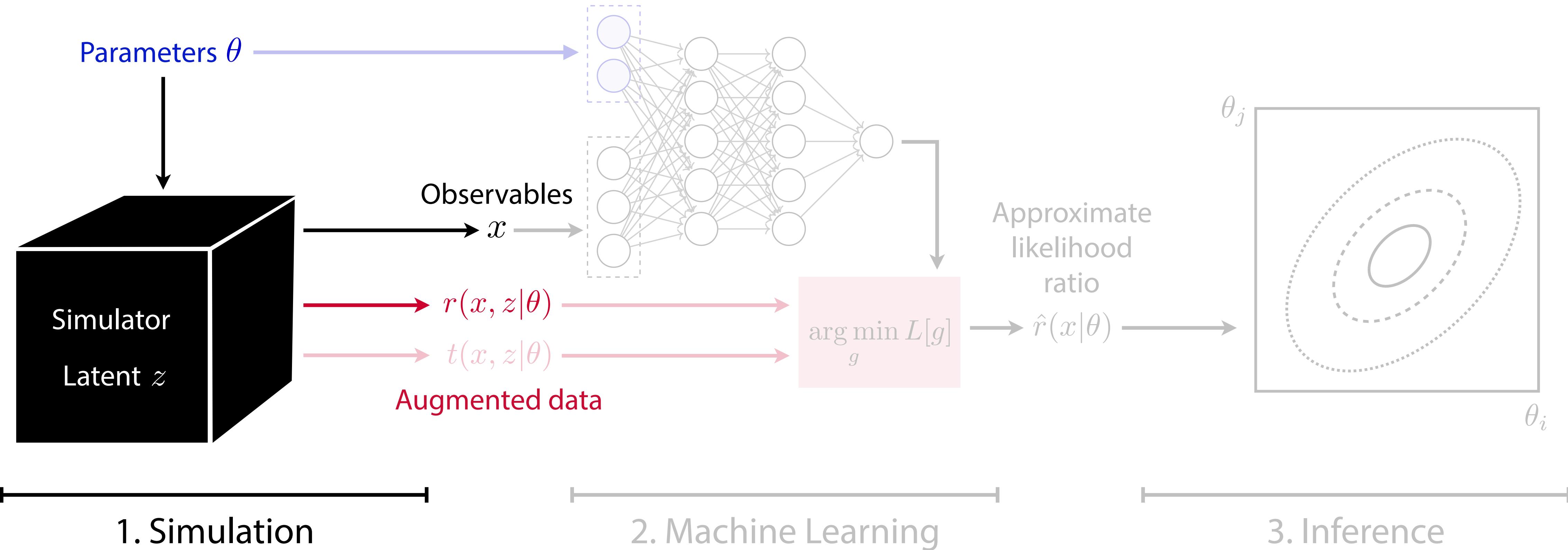
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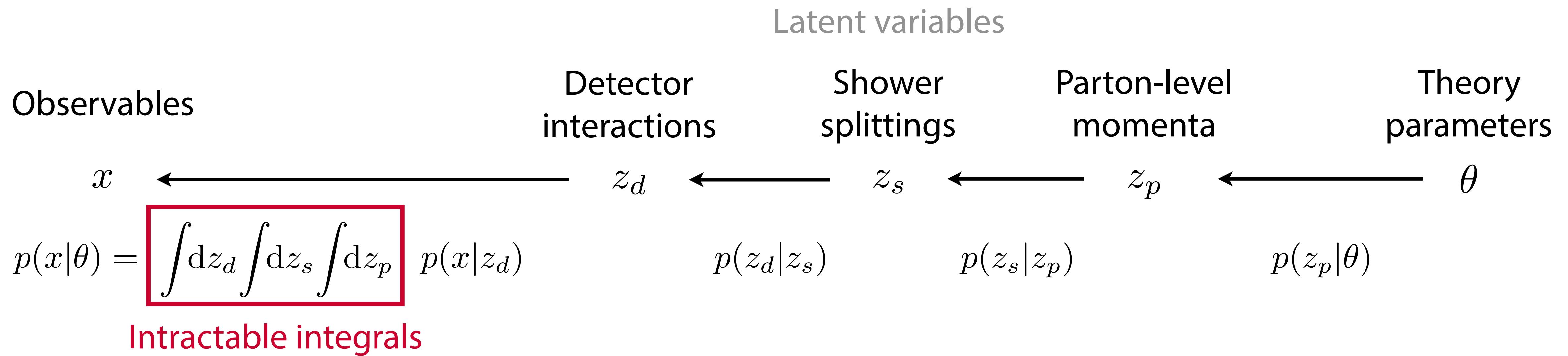
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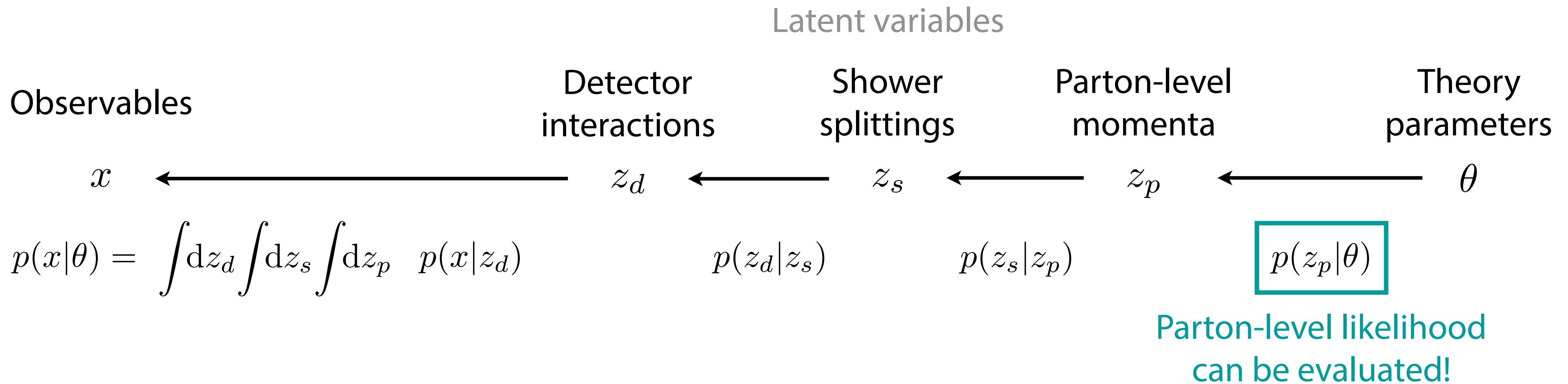
Limit setting with standard hypothesis tests



# Mining gold from the simulator



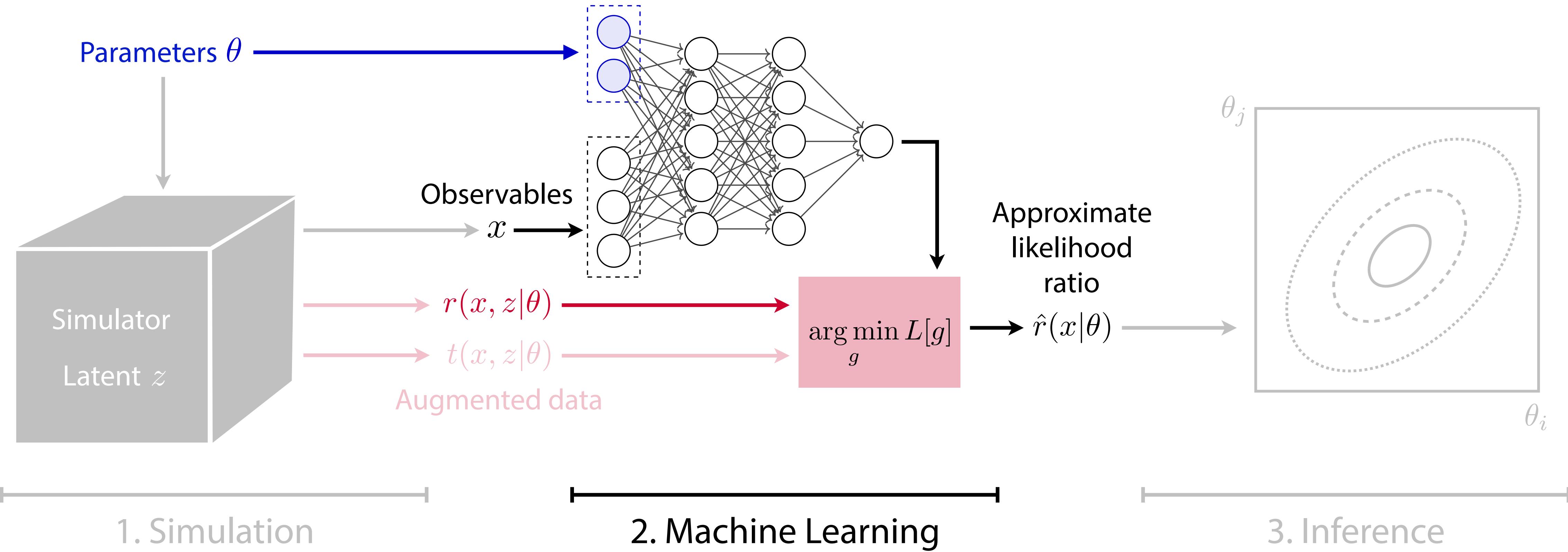
# Mining gold from the simulator



⇒ For each generated event, we can calculate the **joint likelihood ratio** conditional on its specific evolution:

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

$$\frac{p(z_p|\theta_0)}{p(z_p|\theta_1)}$$



# The value of gold

We can calculate the joint likelihood ratio

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We want the likelihood ratio function

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# The value of gold

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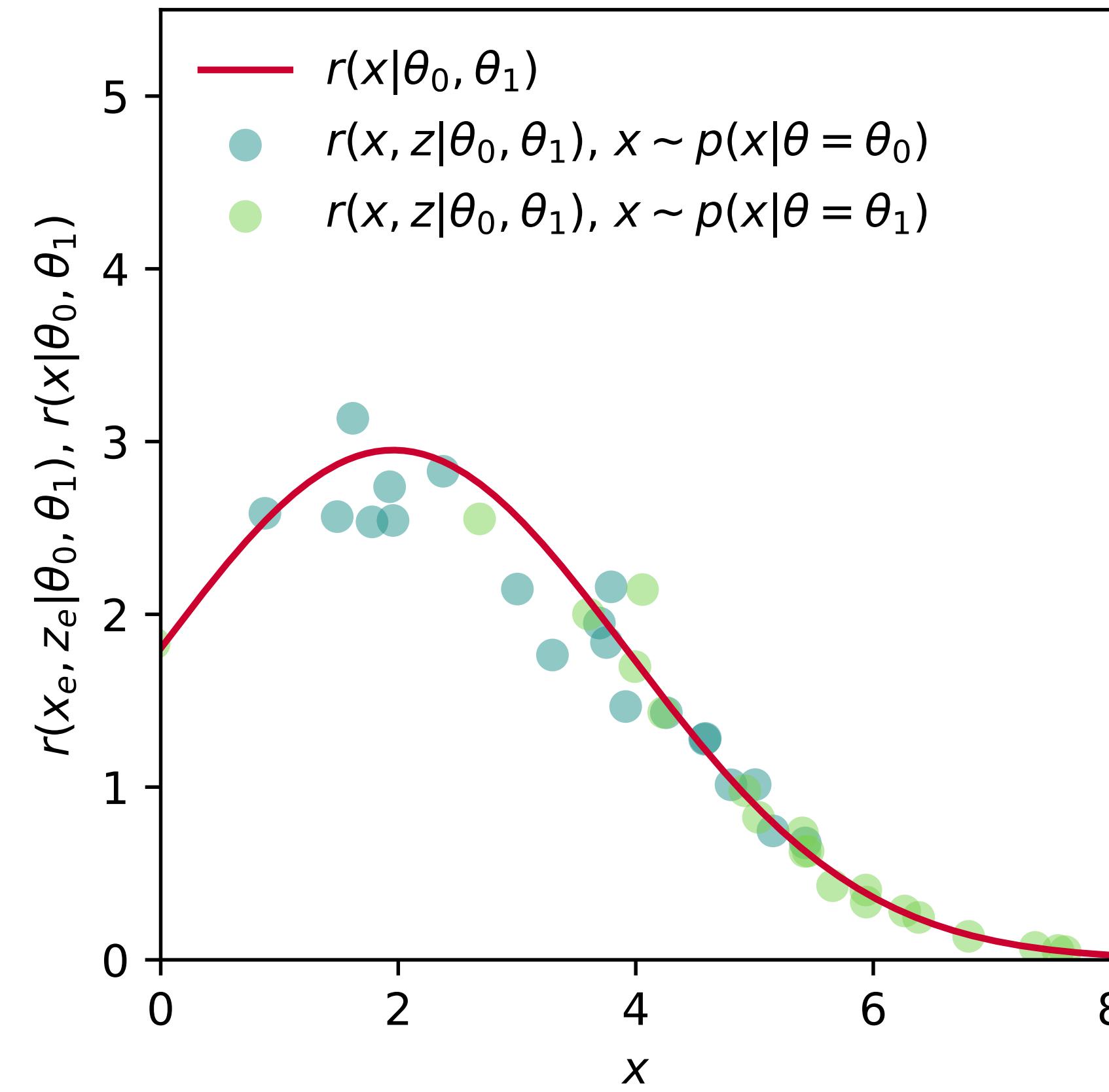
$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$



$r(x, z|\theta_0, \theta_1)$  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 the functional

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

One can show it is minimized by

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

We want the likelihood ratio function

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

# Machine learning = applied calculus of variations

We can get a precise estimator of the likelihood ratio by numerically minimizing a functional:

$$\hat{r}(x|\theta_0, \theta_1) = \underbrace{\arg \min_{\hat{r}(x|\theta_0, \theta_1)} \int dx \int dz p(x, z|\theta_1) \left[ \hat{r}(x|\theta_0, \theta_1) - r(x, z|\theta_0, \theta_1) \right]^2}_{L_r[\hat{r}(x|\theta_0, \theta_1)]}$$

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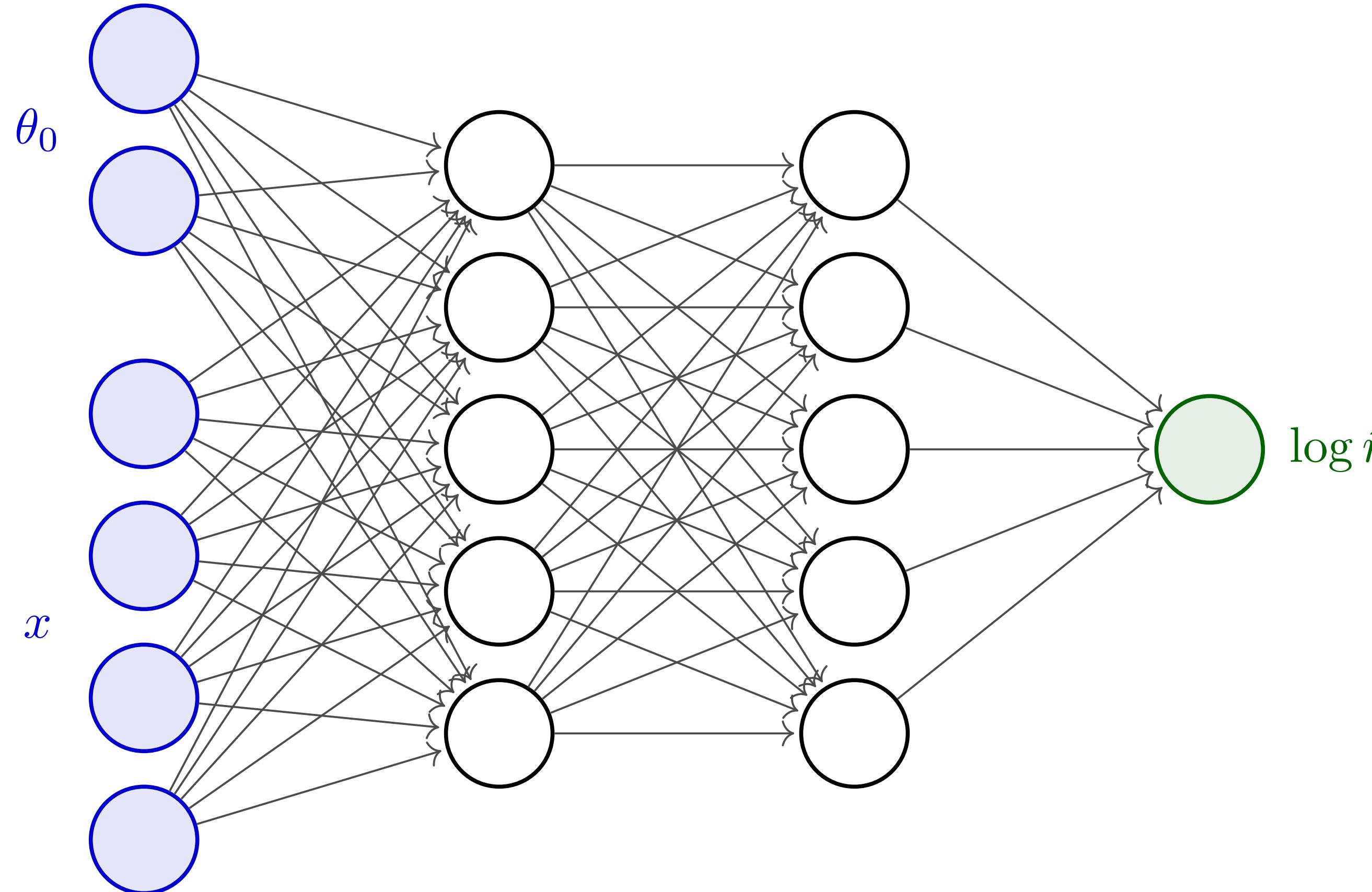
We do this through machine learning:

- Functional  $L_r$  → Loss function

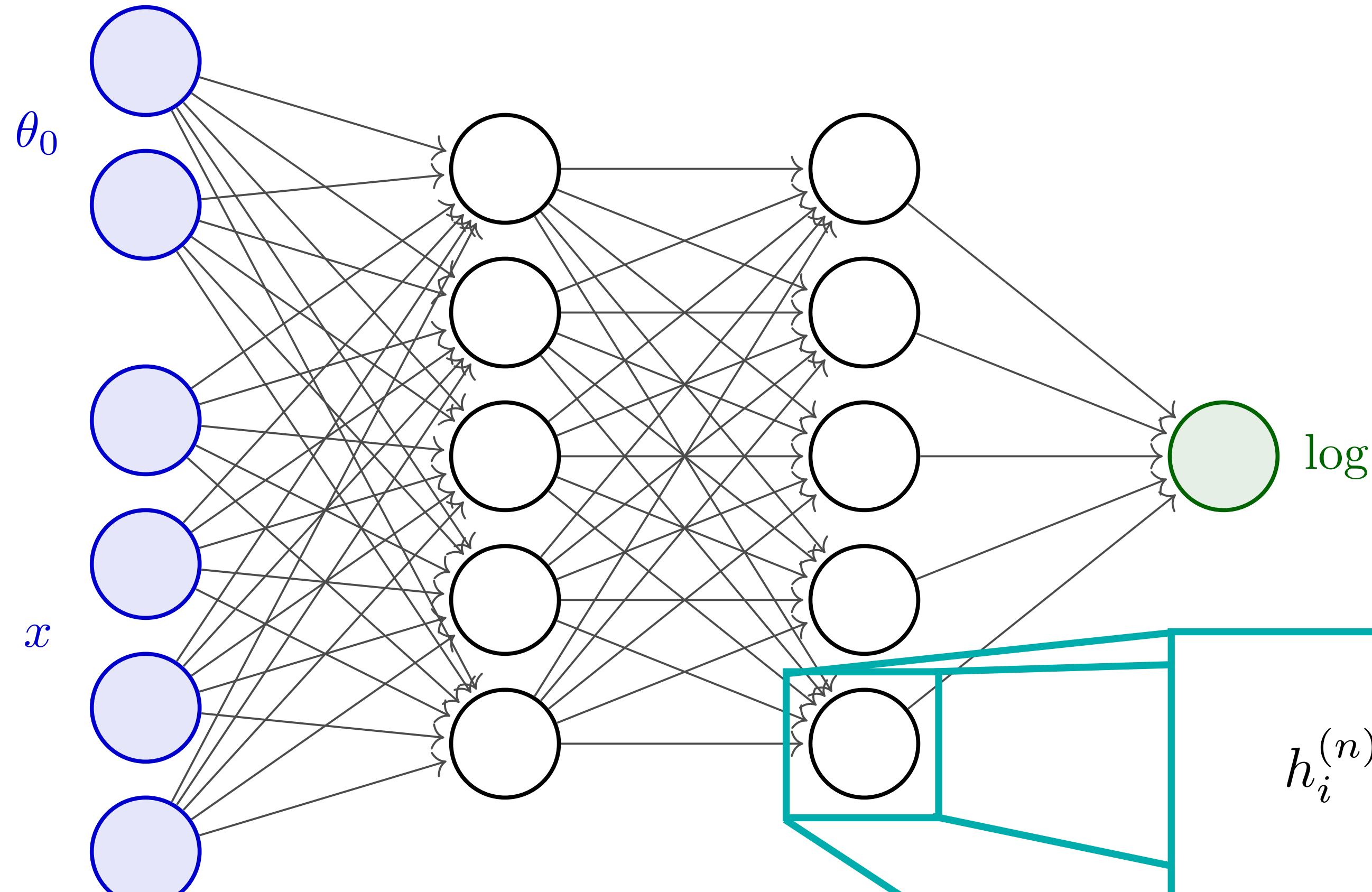
$$\hat{L}_r[\hat{r}(x|\theta_0, \theta_1)] = \frac{1}{N} \sum_{(x_i, z_i) \sim p(x, z|\theta_1)} \left[ \hat{r}(x_i|\theta_0, \theta_1) - r(x_i, z_i|\theta_0, \theta_1) \right]^2$$

- Variational family  $\hat{r}(x|\theta_0, \theta_1)$  → Flexible parametric function (e.g. neural network)
- Exact minimization → Numerical optimization algorithm (e.g. stochastic gradient descent)

# Neural networks = universal function approximators

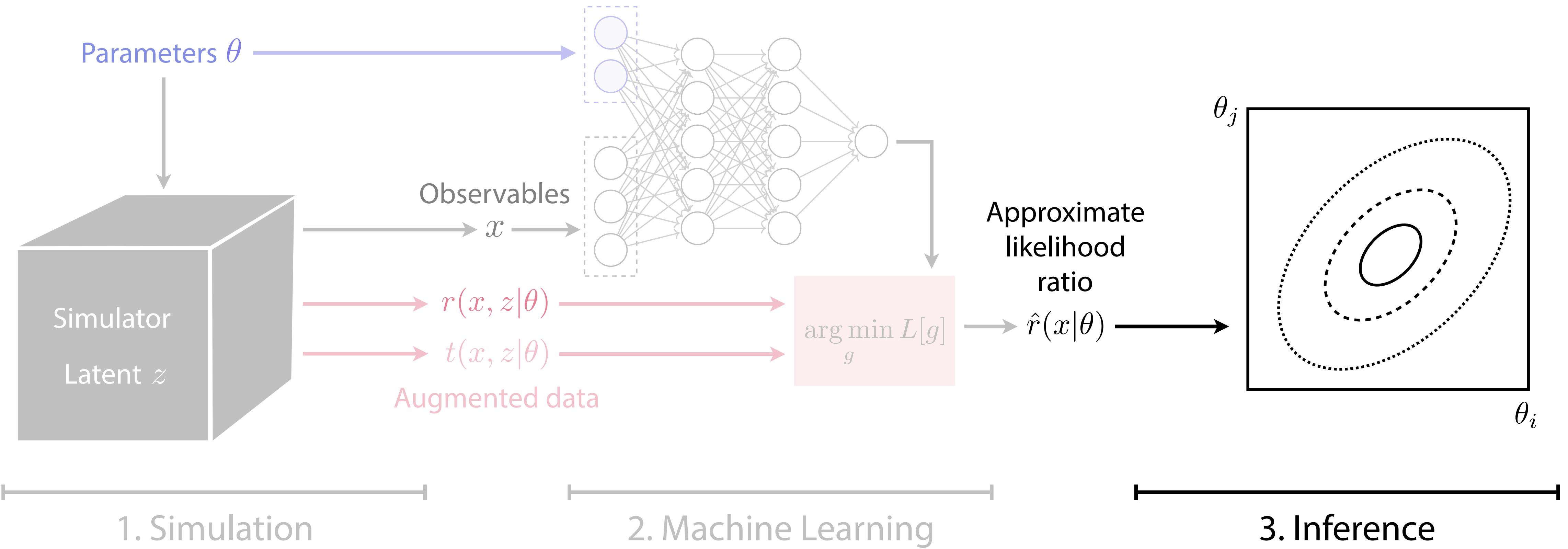


# Neural networks = universal function approximators



$$h_i^{(n)} = f \left( \sum_k w_{ik}^{(n)} h_k^{(n-1)} + b_i^{(n)} \right)$$

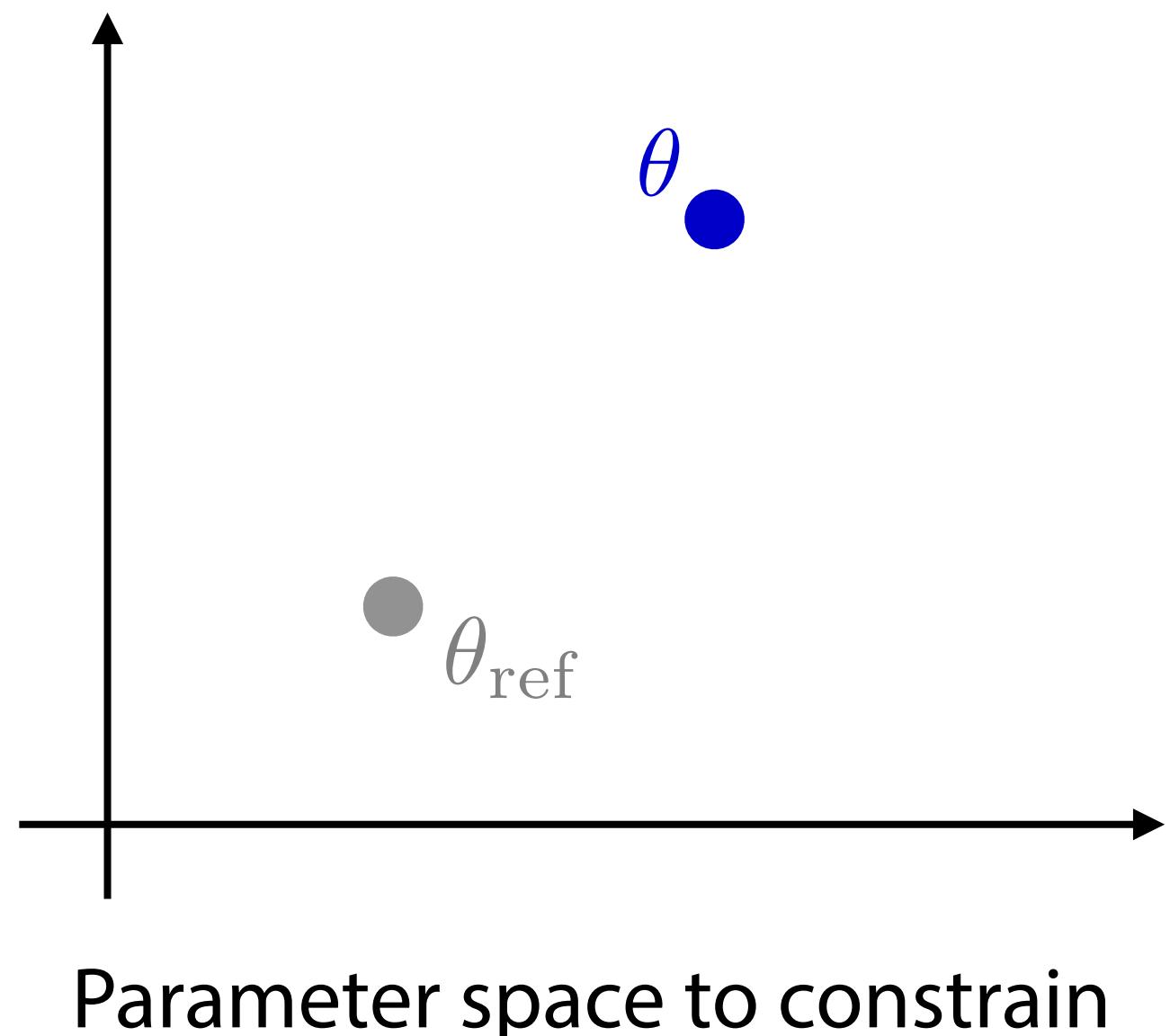
where the weights  $w_{ik}^{(n)}, b_i^{(n)}$  are parameters “trained” by the optimizer



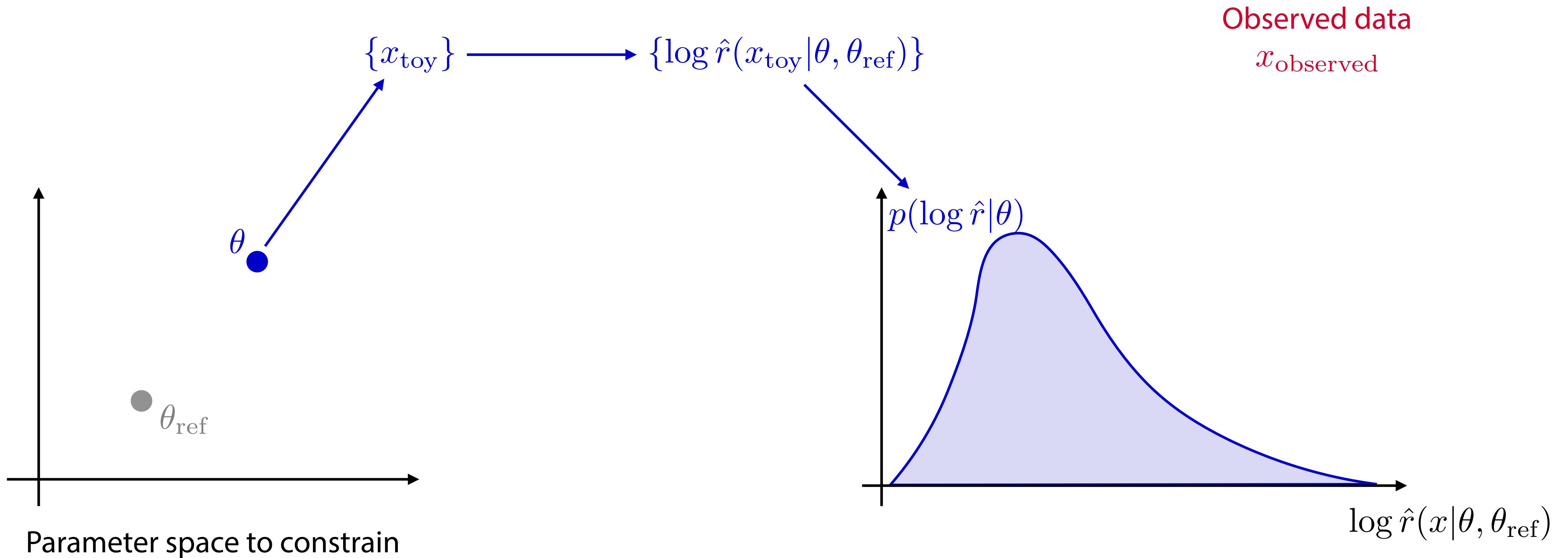
# Limit setting (most LHC physicists are frequentists)

Observed data

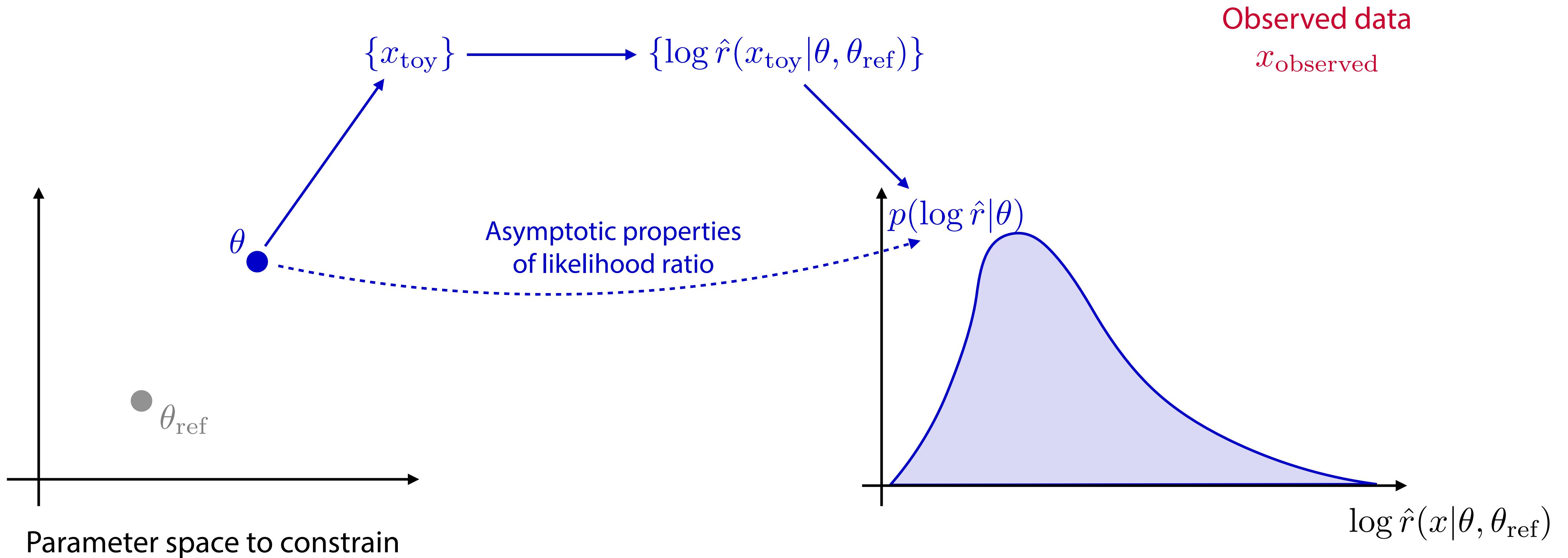
$x_{\text{observed}}$



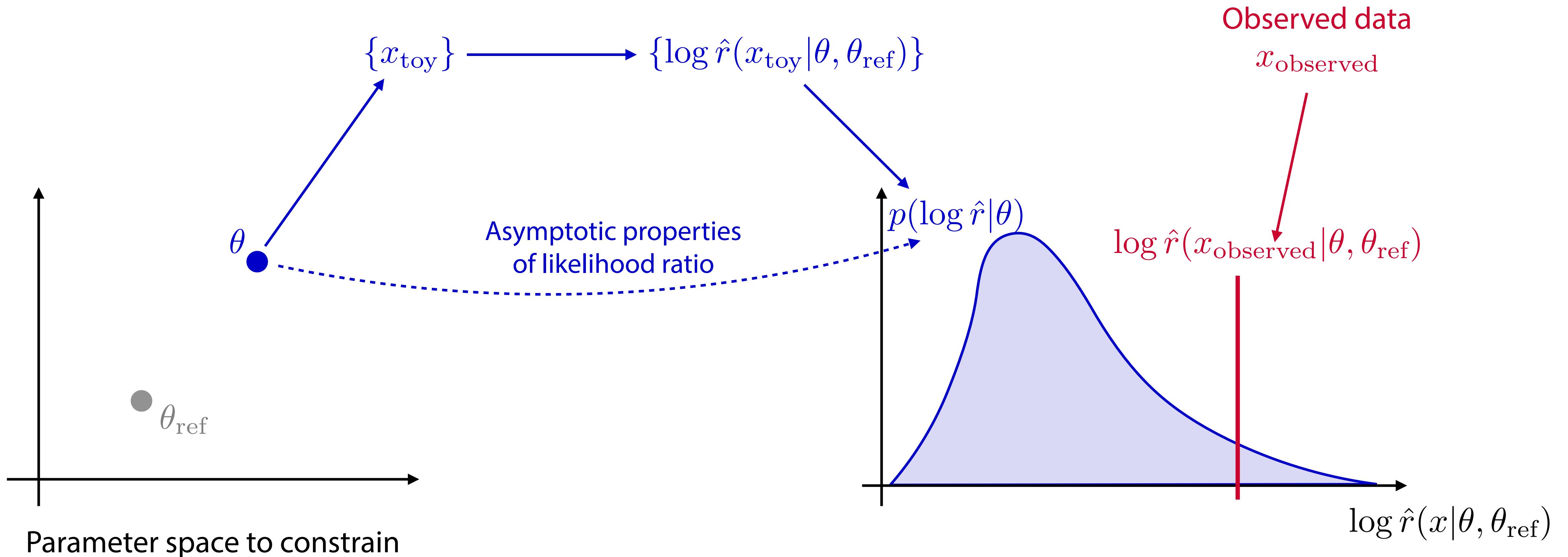
# Limit setting (most LHC physicists are frequentists)



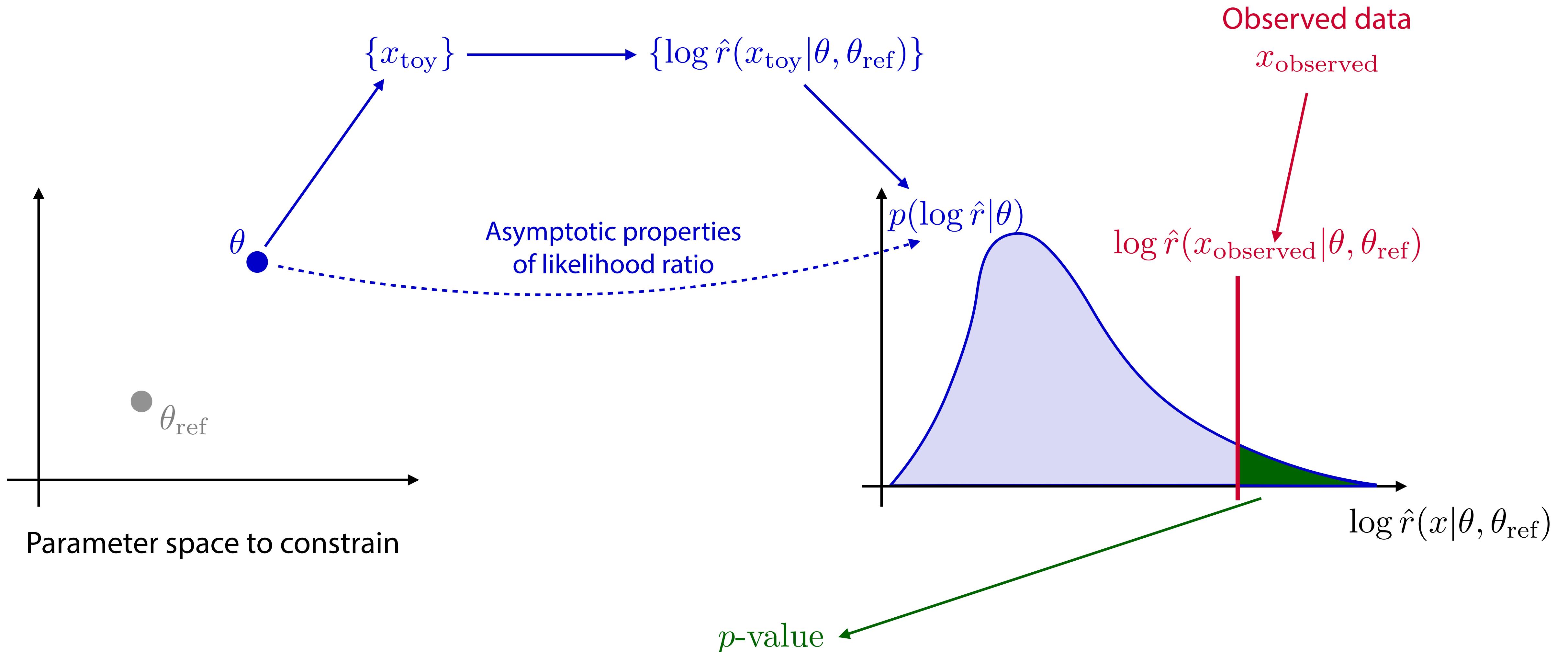
# Limit setting (most LHC physicists are frequentists)



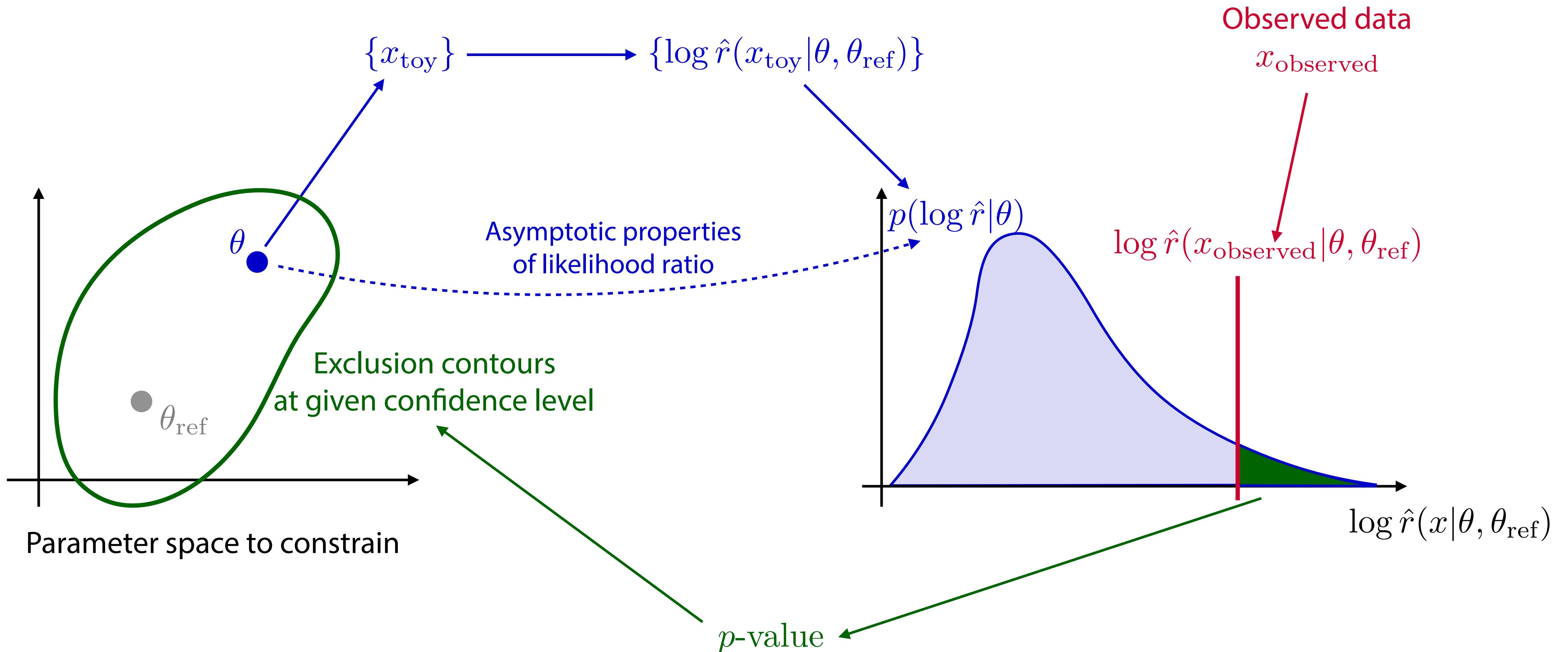
# Limit setting (most LHC physicists are frequentists)



# Limit setting (most LHC physicists are frequentists)



# Limit setting (most LHC physicists are frequentists)



# The likelihood ratio is the most powerful test statistic

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

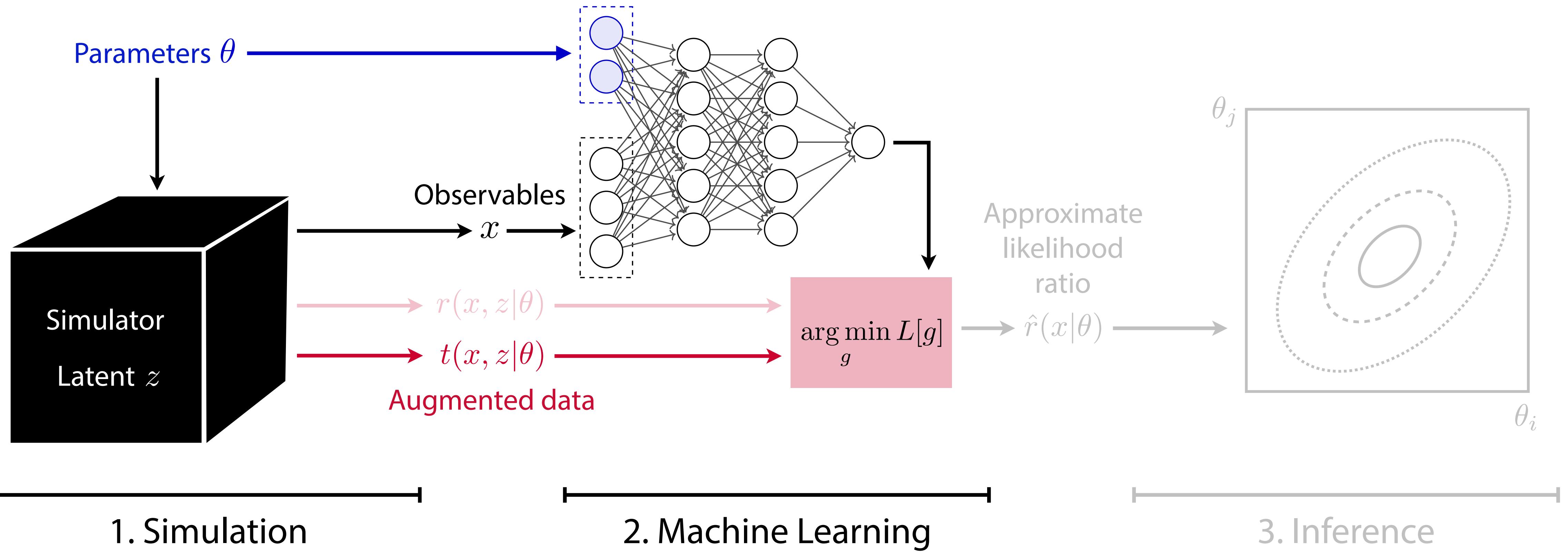
*By J. NEYMAN, Nencki Institute, Soc. Sci. Lit. Varsoviensis, and Lecturer at the Central College of Agriculture, Warsaw, and E. S. PEARSON, Department of Applied Statistics, University College, London.*

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

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

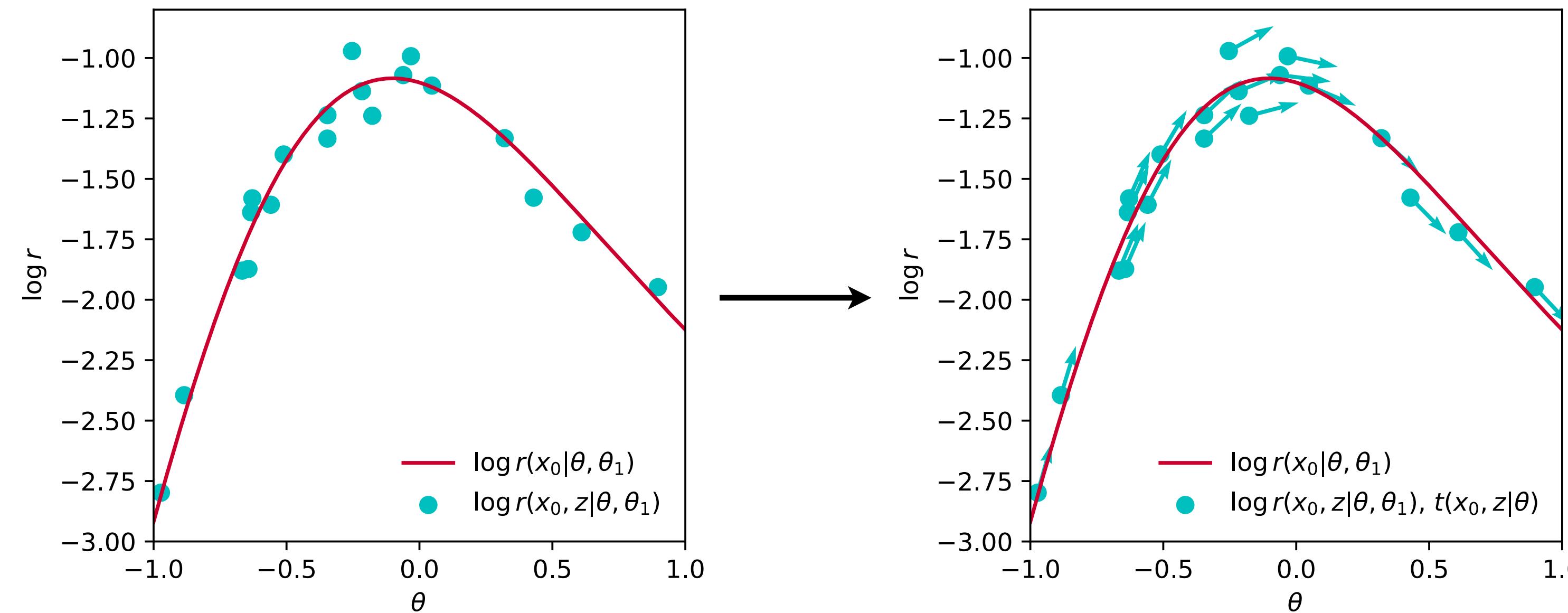
### CONTENTS.

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



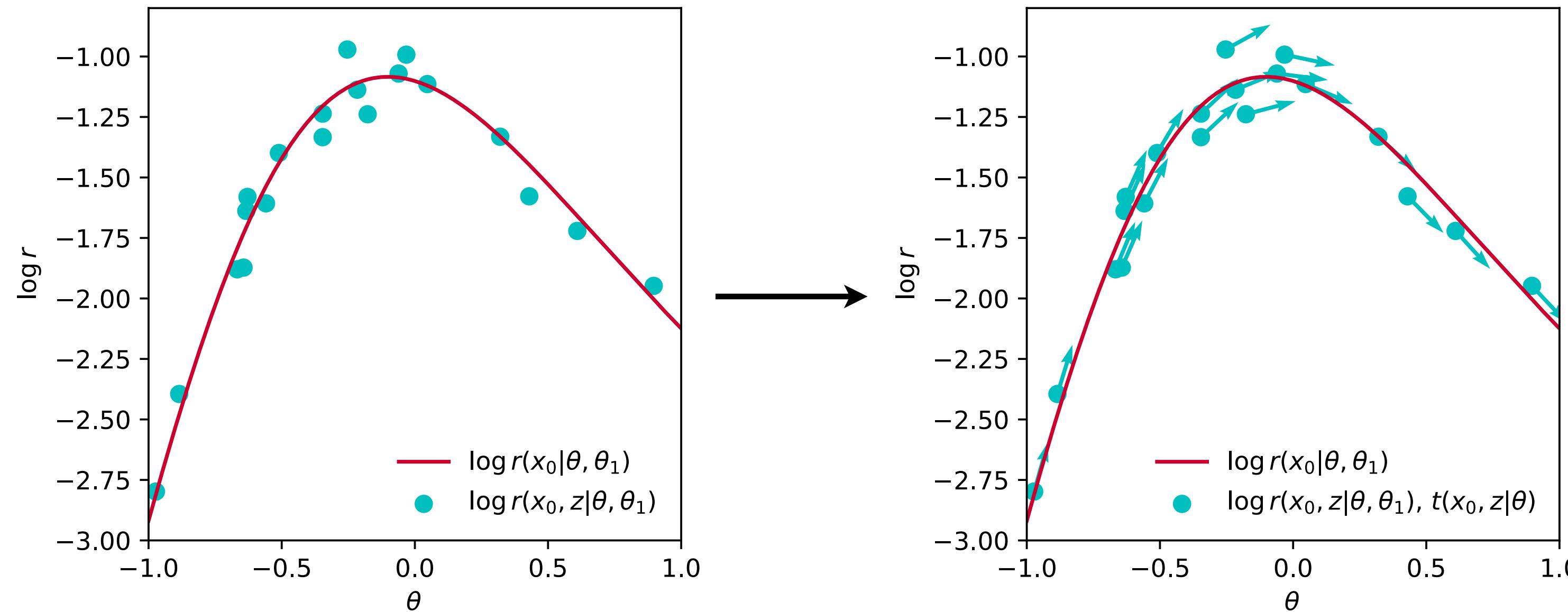
# One more piece: the score

- Knowing derivative often helps fitting:



# One more piece: the score

- Knowing derivative often helps fitting:



- In our case, the relevant quantity is the **score**  $t(x|\theta_0) \equiv \nabla_{\theta} \log p(x|\theta) \Big|_{\theta_0}$ .
- The score fully characterizes the likelihood function in the neighborhood of  $\theta_0$
- The score itself is intractable. But...

# Learning the score

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

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



We want the **score**

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

# Learning the score

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

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We want the **score**

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

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

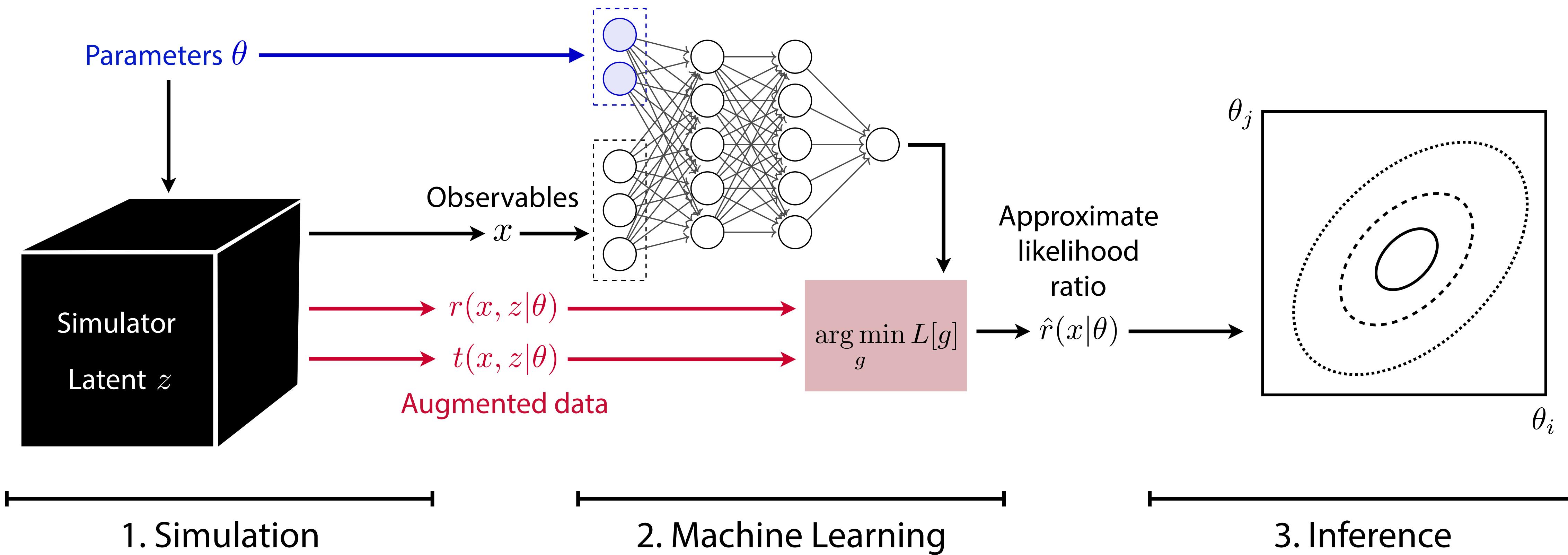
$$L_t[\hat{t}(x|\theta_0)] = \int dx \int dz \ p(x, z|\theta_0) \left[ (\hat{t}(x|\theta_0) - t(x, z|\theta_0))^2 \right].$$

One can show it is minimized by

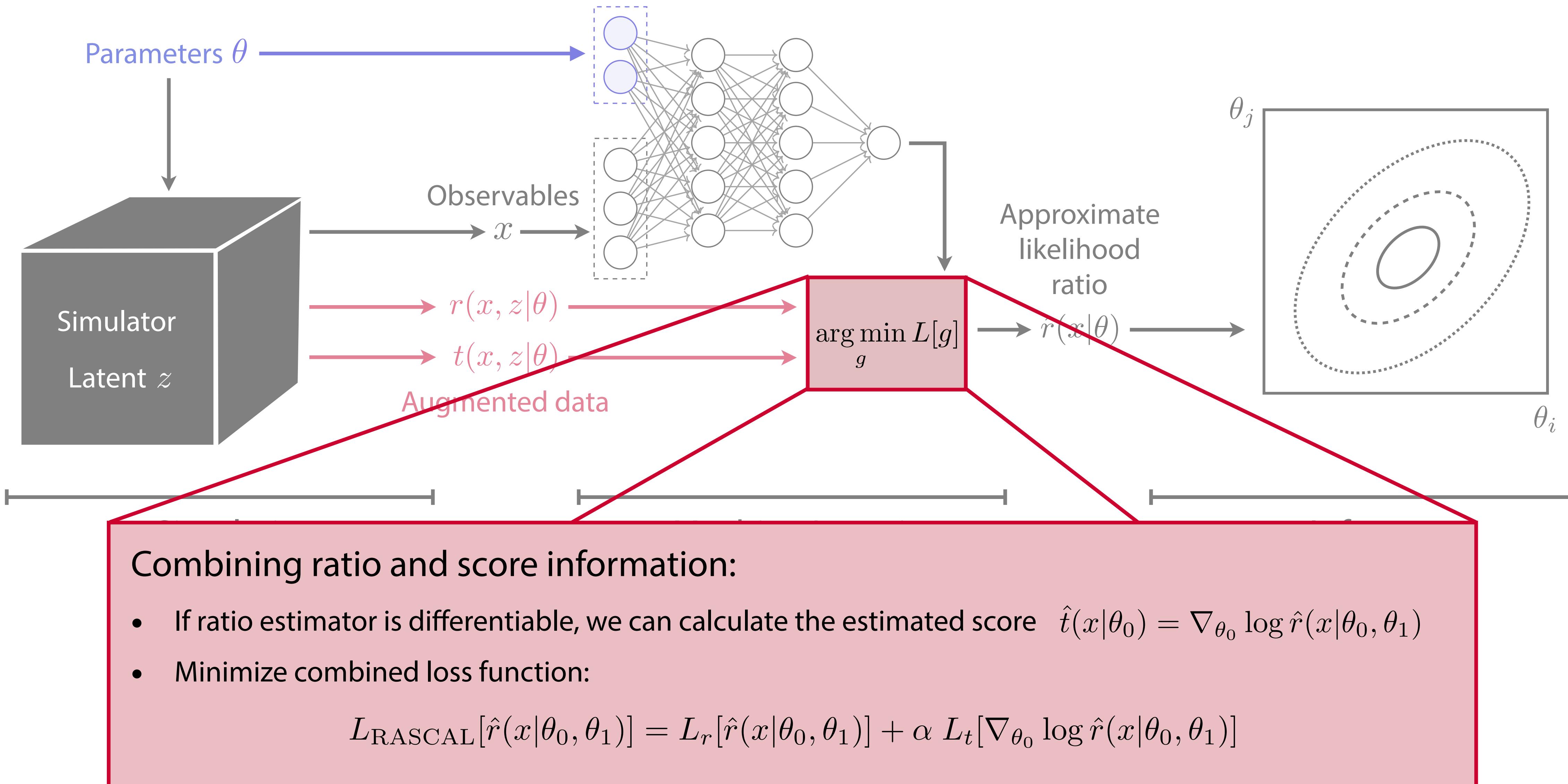
$$t(x|\theta_0) = \arg \min_{\hat{t}(x|\theta_0)} L_t[\hat{t}(x|\theta_0)] !$$

Again, we implement this minimization  
through machine learning

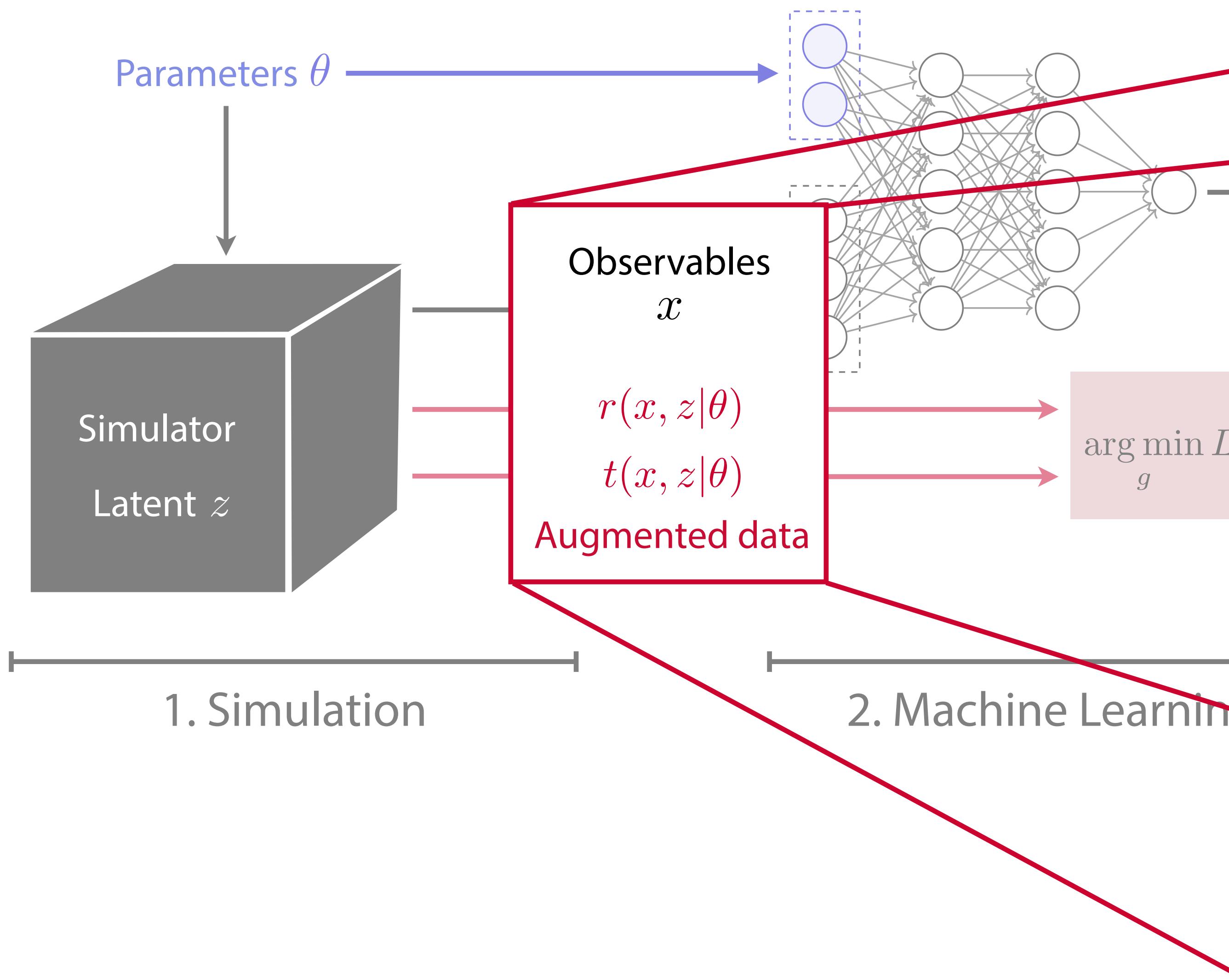
# Putting the pieces together: RASCAL (Ratio and score approximate likelihood ratio)



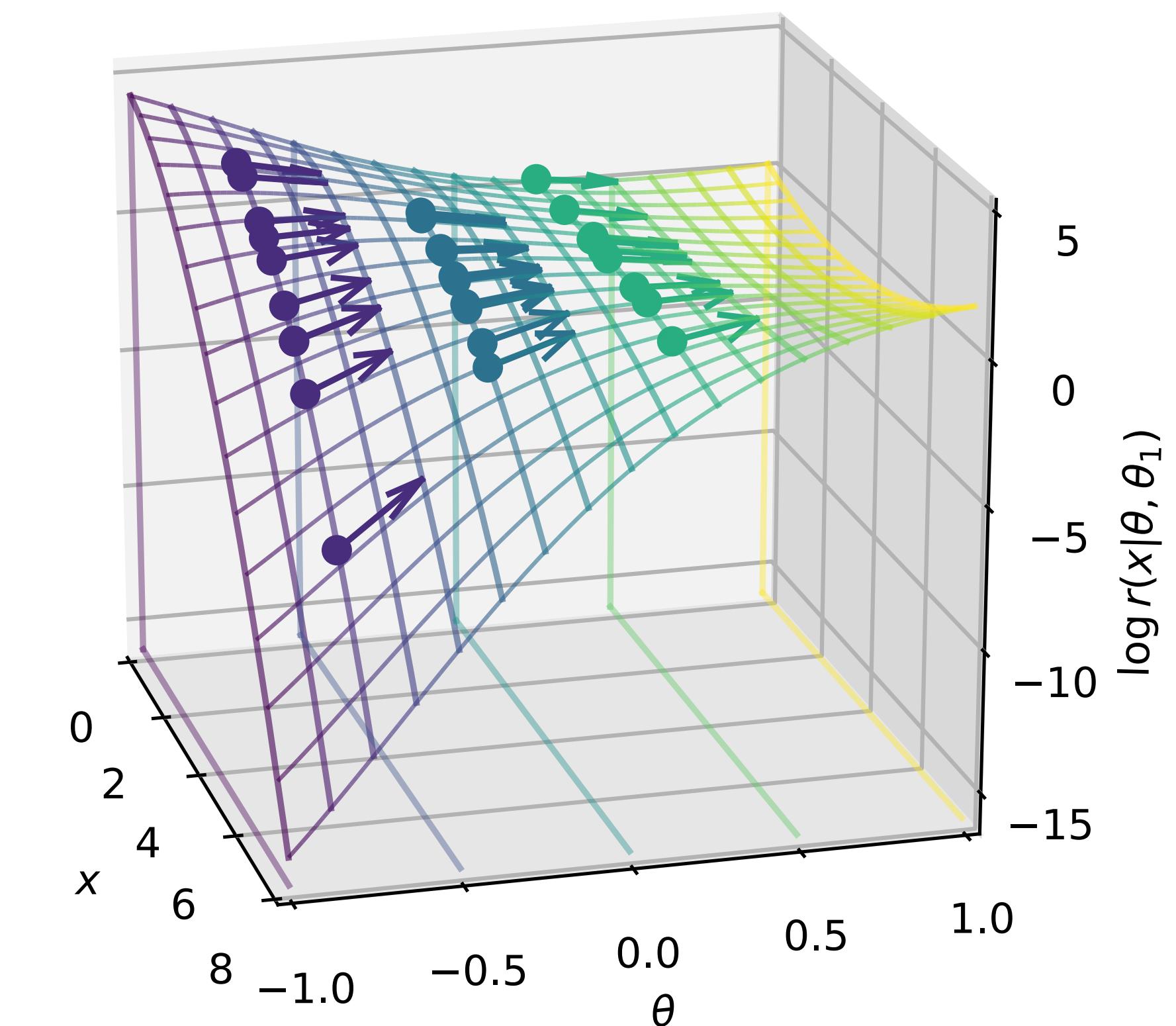
# Putting the pieces together: RASCAL (Ratio and score approximate likelihood ratio)



# Putting the pieces together: RASCAL (Ratio and score approximate likelihood ratio)

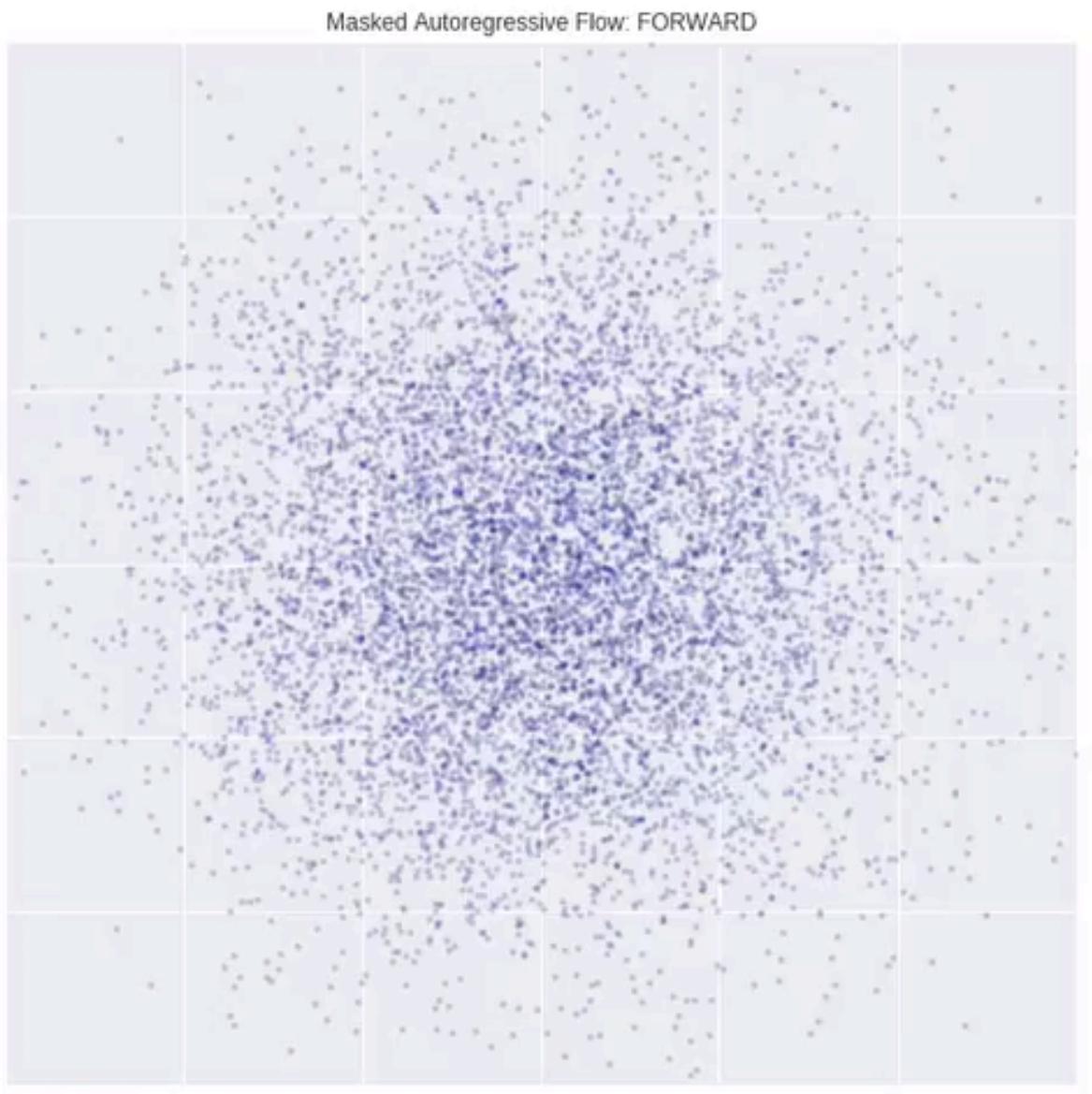


RASCAL combines three orthogonal pieces of information



# Alternatives and extensions

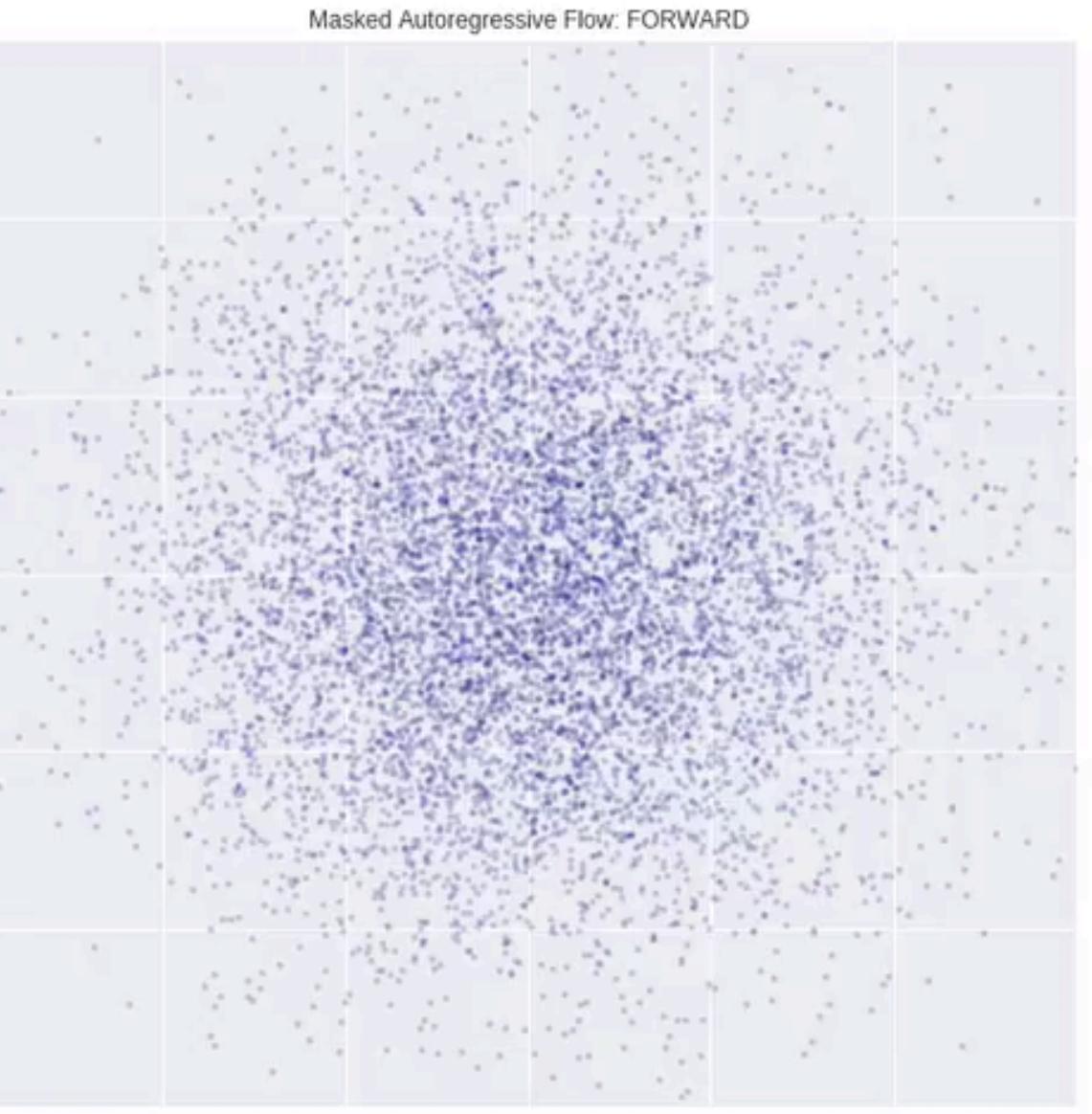
- More than one way to the likelihood (ratio)!
  - ALICE: use cross entropy instead of squared error loss
  - SCANDAL: combine with neural density estimators,  
e.g. Masked Autoregressive Flows  
[G. Papamakarios, T. Pavlakou, I. Murray 1705.07057]
  - SALLY / SALLINO: use estimated score as “optimal observable”



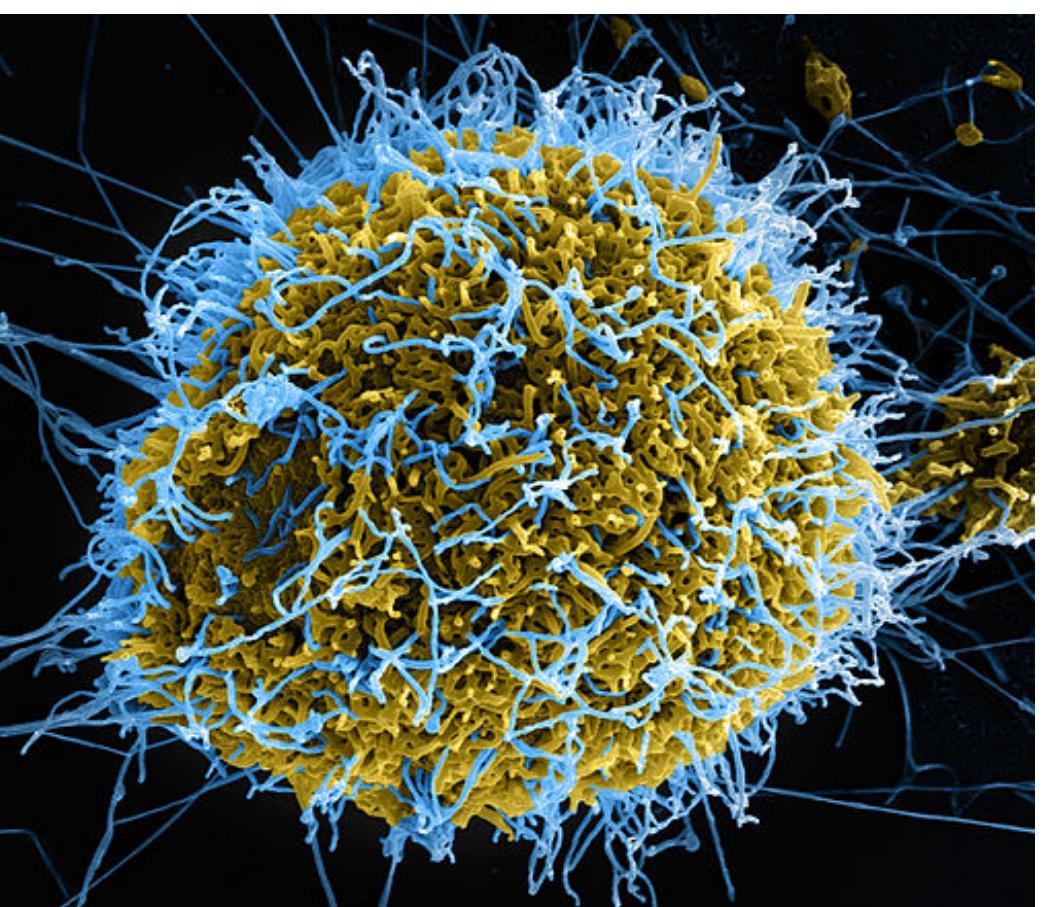
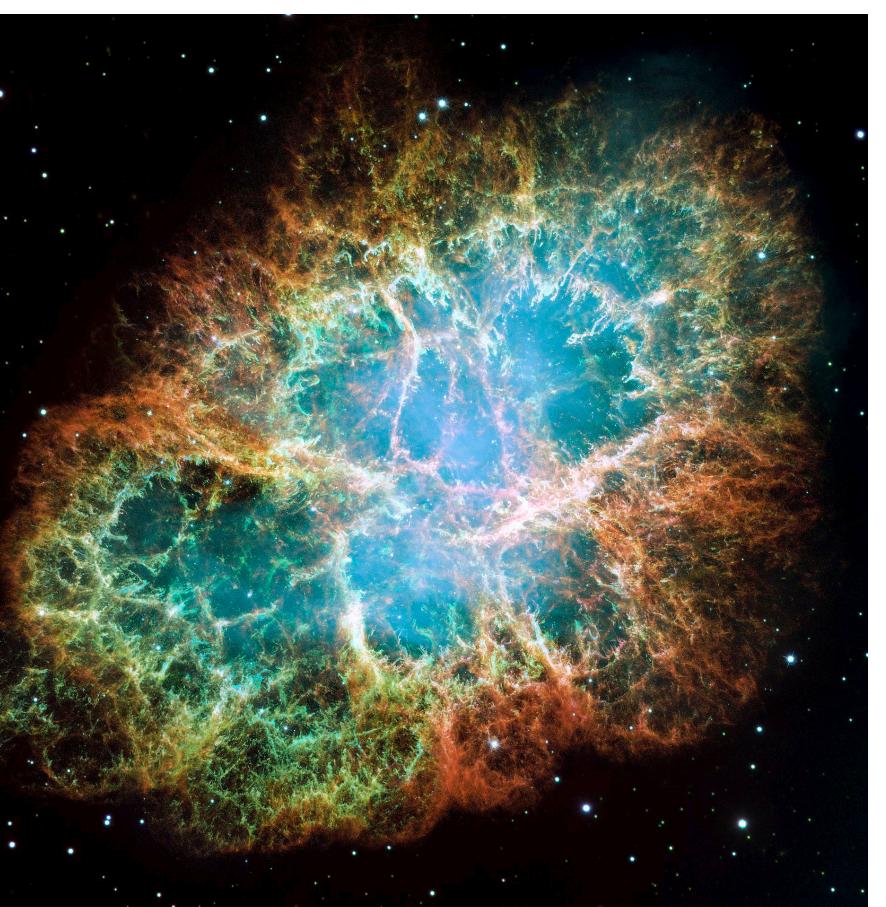
[Alex Mordvintsev]

# Alternatives and extensions

- More than one way to the likelihood (ratio)!
  - ALICE: use cross entropy instead of squared error loss
  - SCANDAL: combine with neural density estimators, e.g. Masked Autoregressive Flows  
[G. Papamakarios, T. Pavlakou, I. Murray 1705.07057]
  - SALLY / SALLINO: use estimated score as “optimal observable”



- What if we don't fully trust the simulator?
  - Nuisance parameters to model systematic uncertainties
  - Learn robustness with adversarial training  
[G. Louppe, M. Kagan, K. Cranmer 1611.01046]
- More general than particle physics
  - Currently being adapted to cosmology and epidemiology



[Alex Mordvintsev] [NASA, NIAID]

- 

Treat simulator as black box:

- Histograms of observables,  
Approximate Bayesian Computation  
Rely on summary statistics
- Machine learning techniques  
Density networks, CARL, autoregressive models,  
normalizing flows, ...

Use latent structure:

- Matrix Element Method, Optimal Observables,  
Shower Deconstruction  
Neglect or approximate shower + detector, explicitly calculate  
 $z$  integral
- Mining gold from the simulator  
Leverage matrix-element information + machine learning

New!

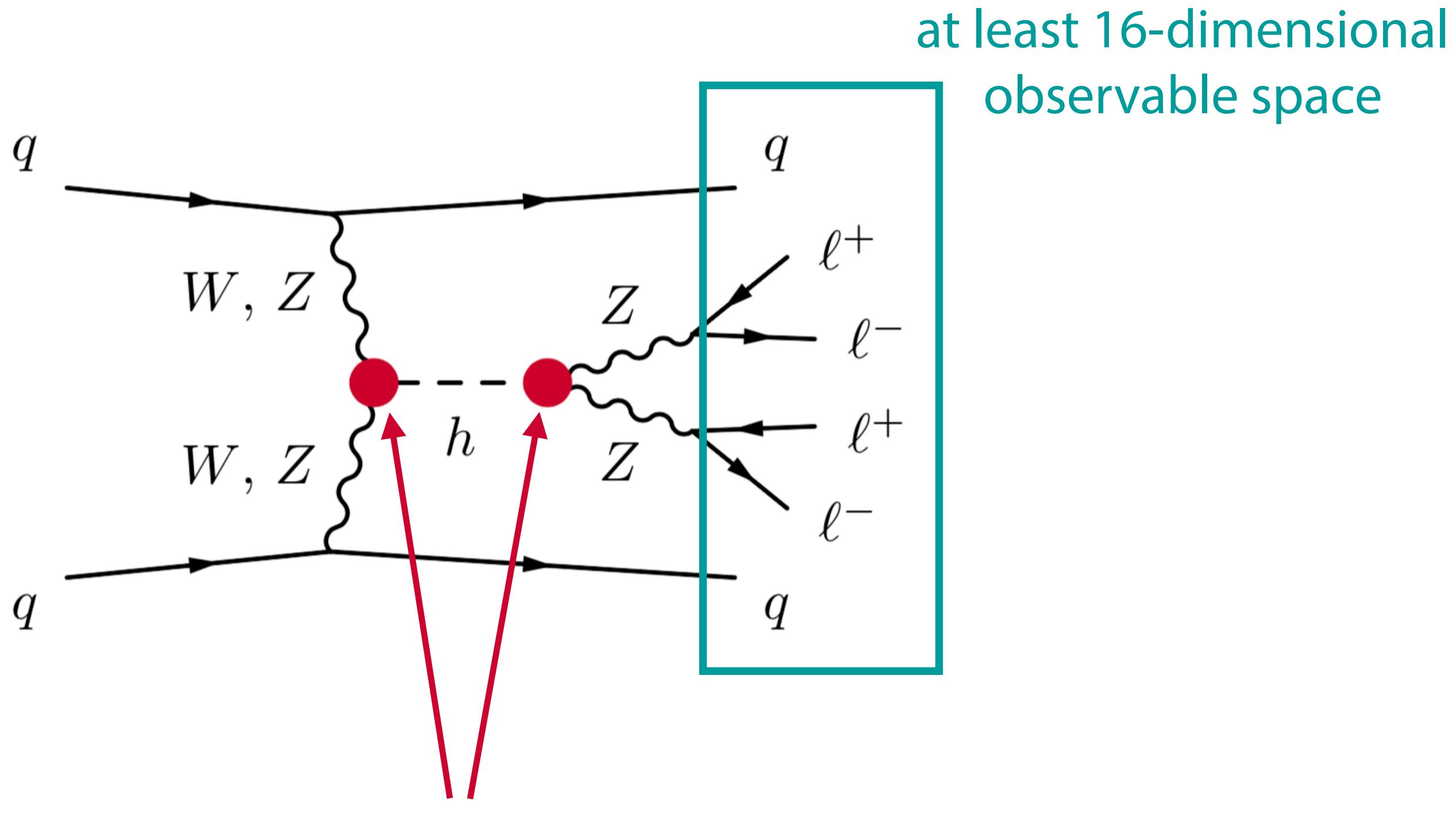
	Histograms, ABC	Neural density est.	Matrix-Element Method	RASCAL etc
High-dimensional observables		✓	✓	✓
Realistic shower, detector sim.	✓	✓	transfer fns.	✓
Uses matrix element information			✓	✓
Evaluation	fast	fast	expensive	fast

# EFT example

[JB, K. Cranmer, G. Louppe, J. Pavez 1805.00013, 1805.00020, 1805.12244;  
with M. Stoye 1808.00973]

# Proof of concept

Higgs production in weak boson fusion:

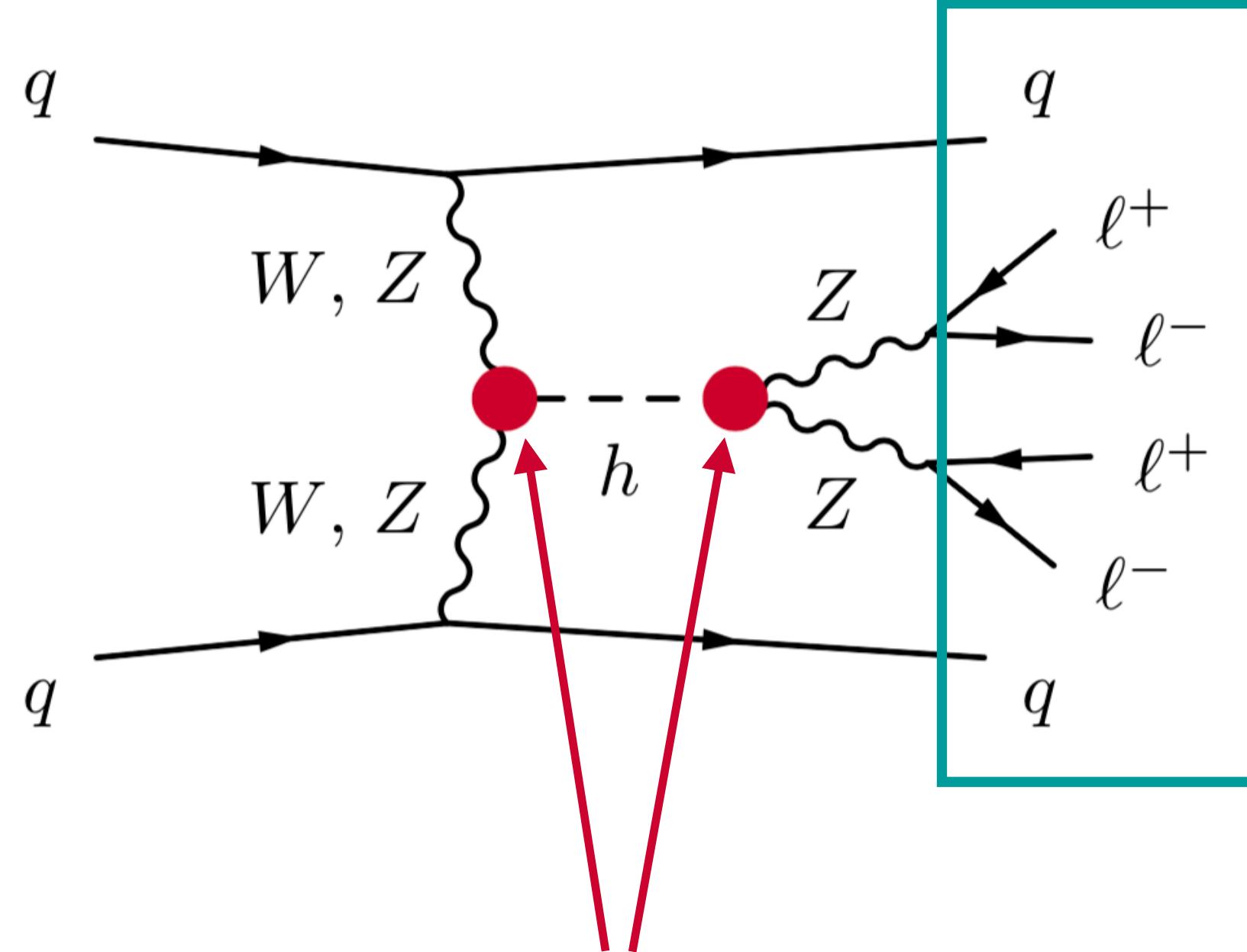


Exciting new physics might hide here!  
We parameterize it with two EFT coefficients:

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

# Proof of concept

Higgs production in weak boson fusion:



at least 16-dimensional  
observable space

Exciting new physics might hide here!

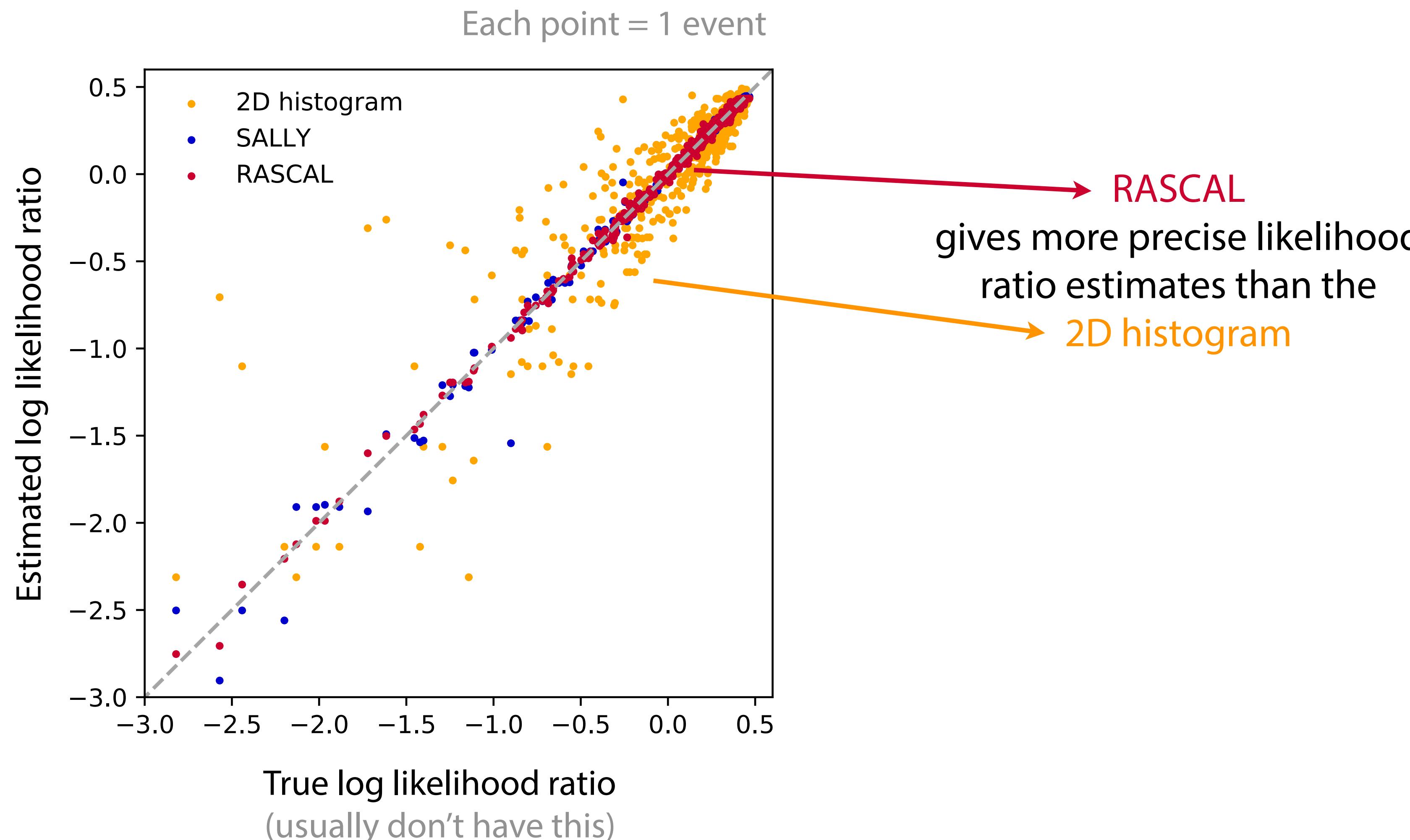
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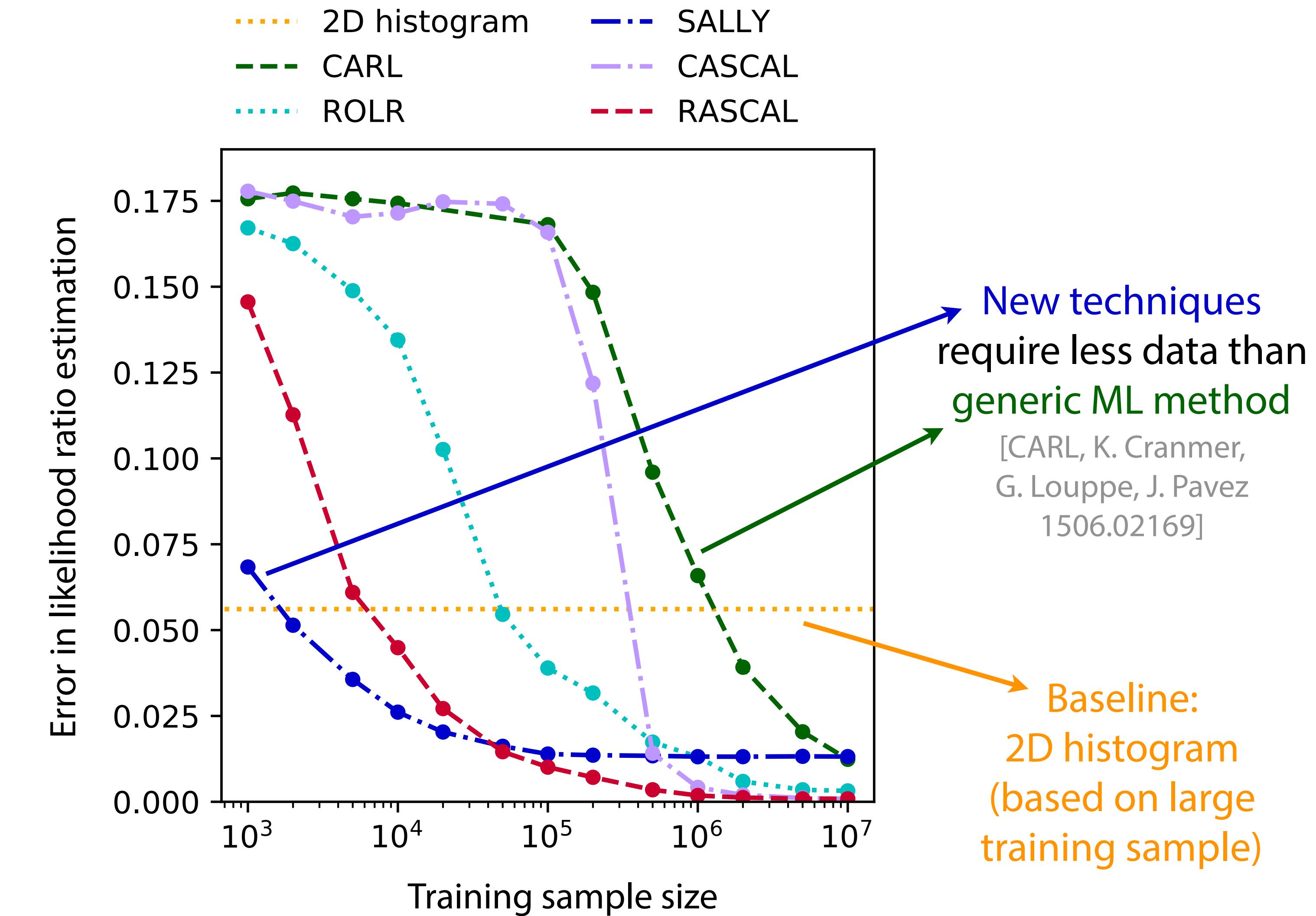
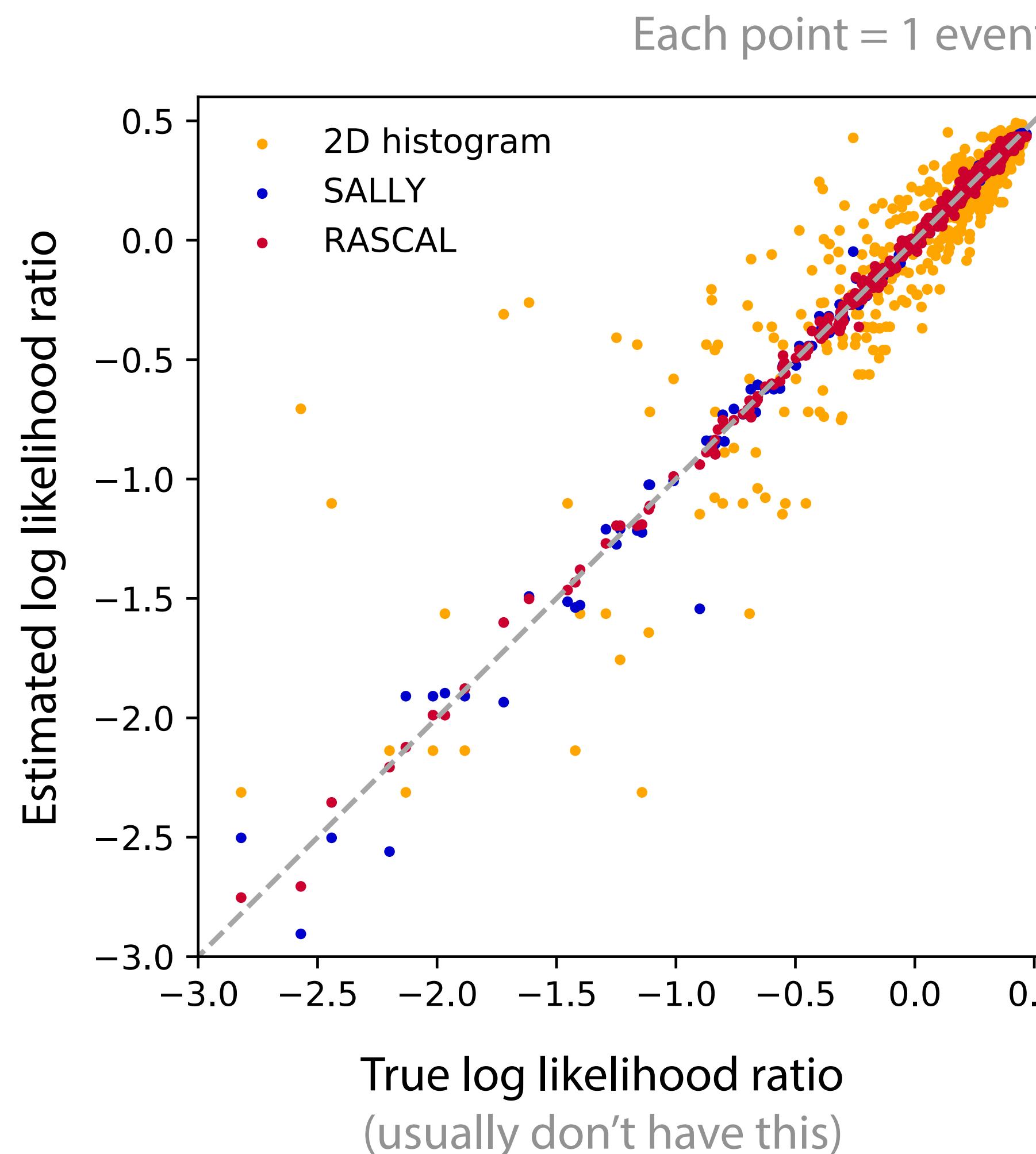
- Goal: constrain the **two EFT parameters**
  - new inference methods
  - baseline: 2d histogram analysis of **jet momenta & angular correlations**
- Two scenarios:
  - Simplified setup in which we can compare to true likelihood
  - “Realistic” simulation with approximate detector effects
- Simulation:  
MadGraph + MadMax

[J. Alwall et al. 1405.0301; K. Cranmer, T. Plehn  
hep-ph/0605268; T. Plehn, P. Schichtel, D.  
Wiegand 1311.2591]

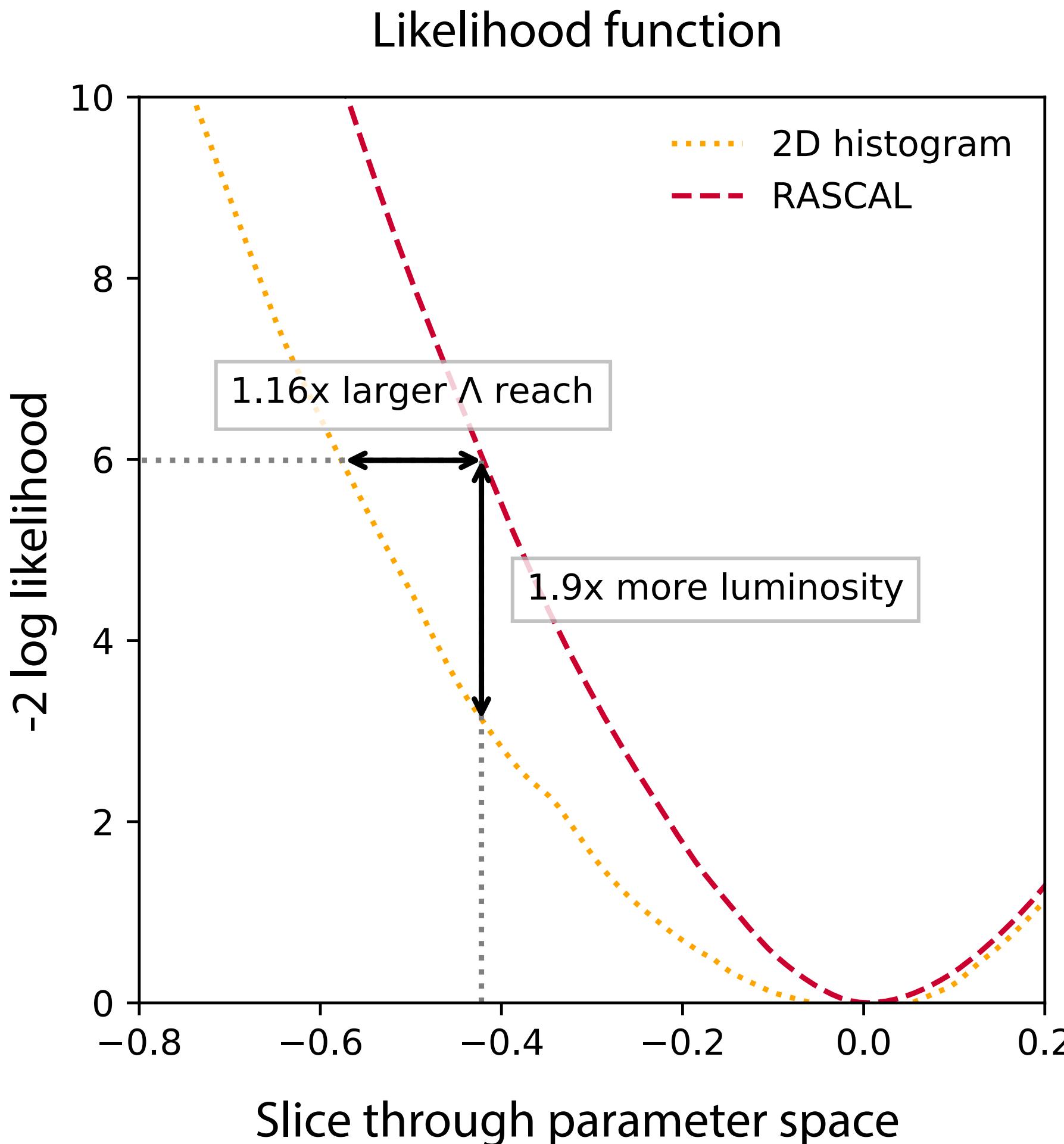
# More precise likelihood ratio estimates with less training data



# More precise likelihood ratio estimates with less training data

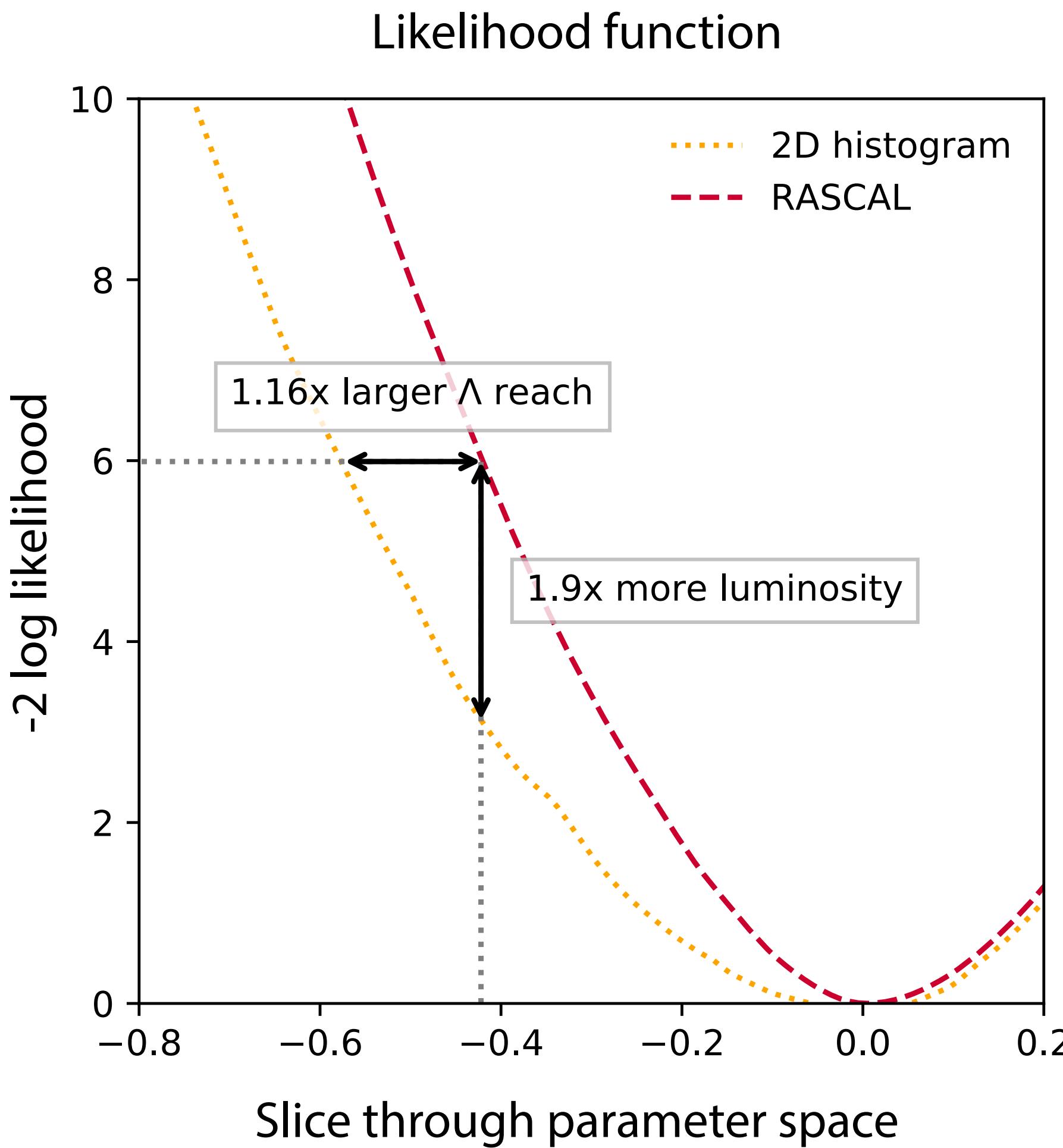


# Better sensitivity to new physics

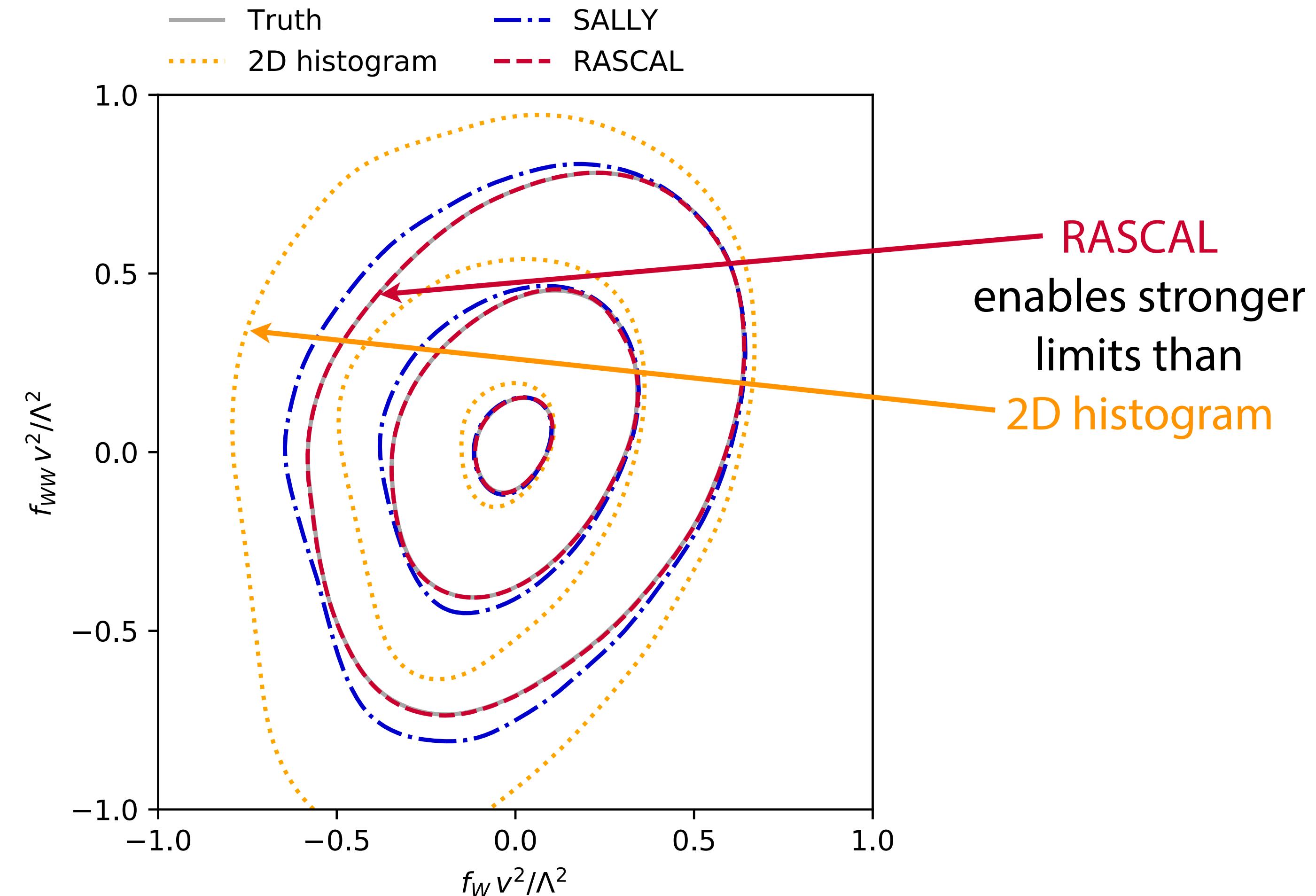


Results are based on 36 observed events, assuming SM

# Better sensitivity to new physics

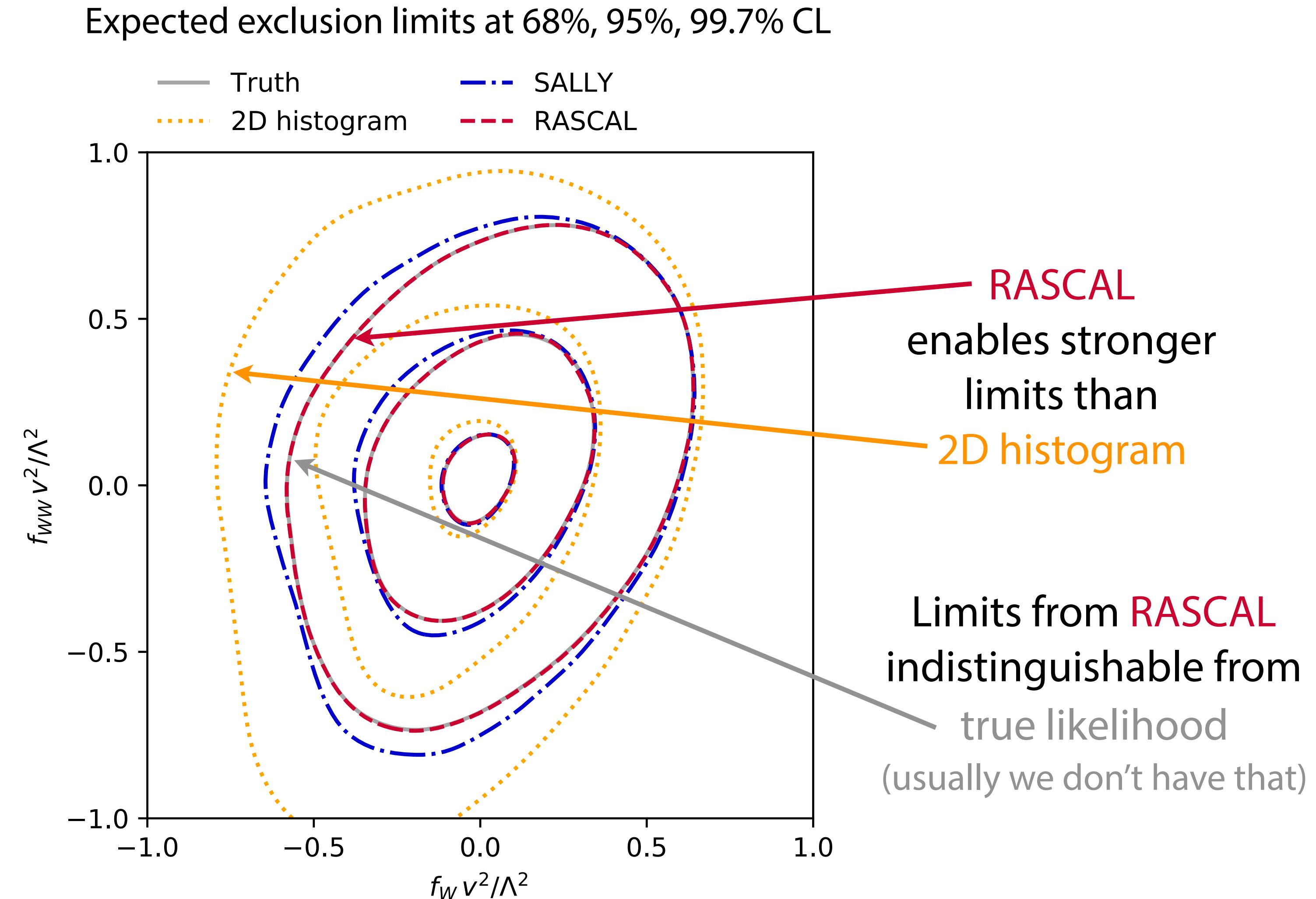
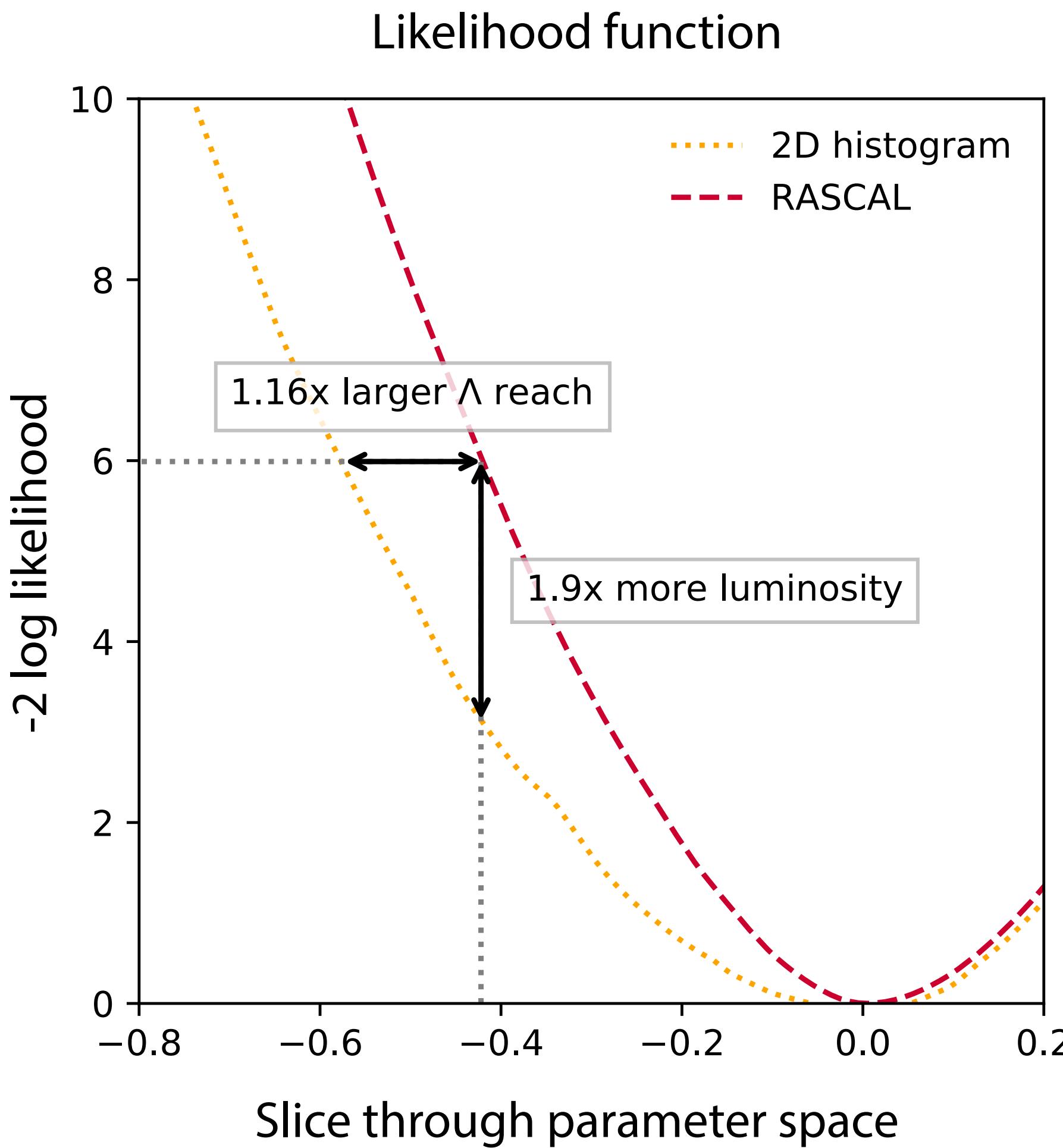


Expected exclusion limits at 68%, 95%, 99.7% CL



Results are based on 36 observed events, assuming SM

# Better sensitivity to new physics



Results are based on 36 observed events, assuming SM

# MadMiner

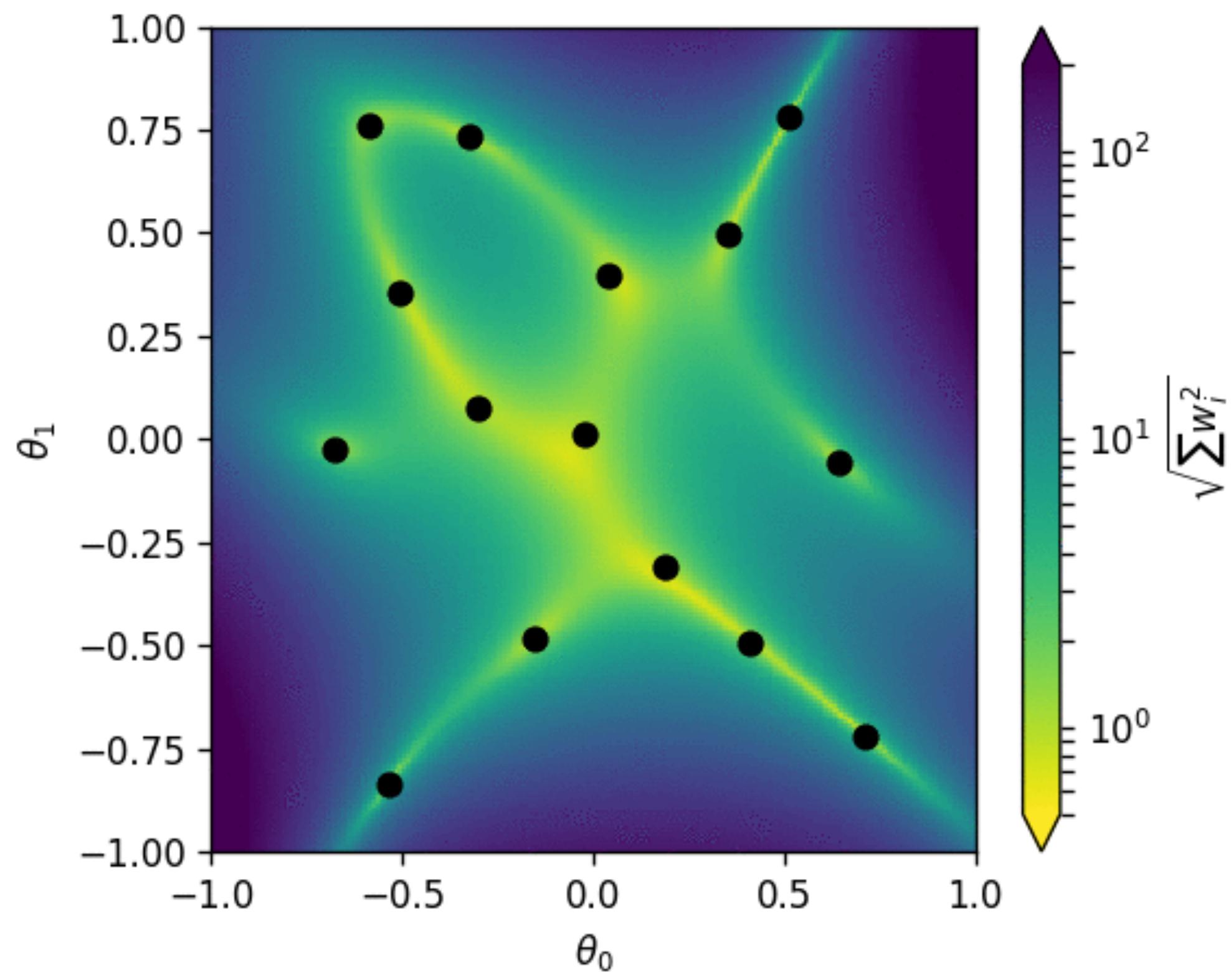
[JB, K. Cranmer, F. Kling in progress]

# Can I use any of this?

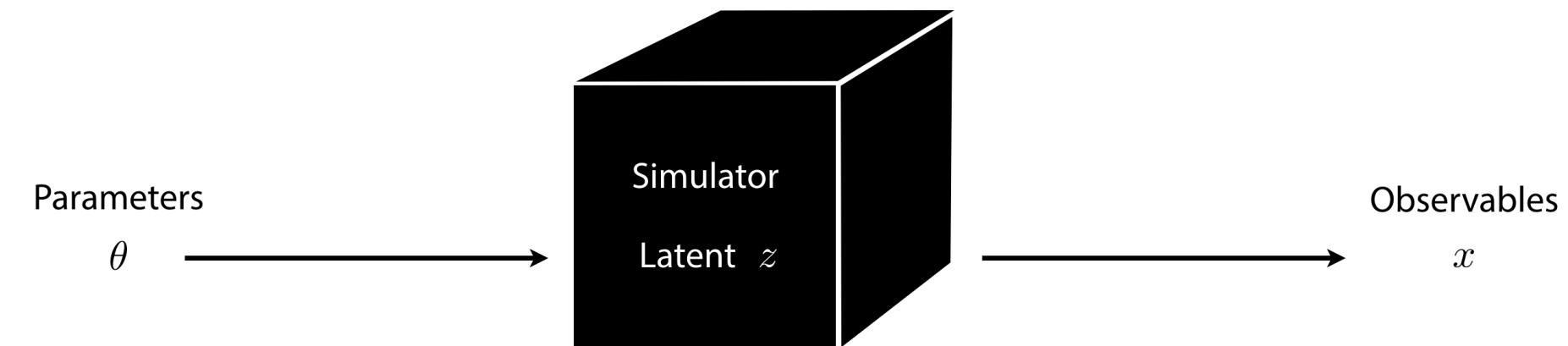
Yes! To make that as painless as possible, we're working on the python package **MadMiner**:

- “Mining gold” from MadGraph + Pythia + detector simulation
- Morphing: reconstruct full dependence on model parameters from few MC runs
- Likelihood ratio estimation with RASCAL and friends
- Calculate Fisher information (truth or reco level)

Come visit us soon at [github.com/johannbrehmer/madminer!](https://github.com/johannbrehmer/madminer)!

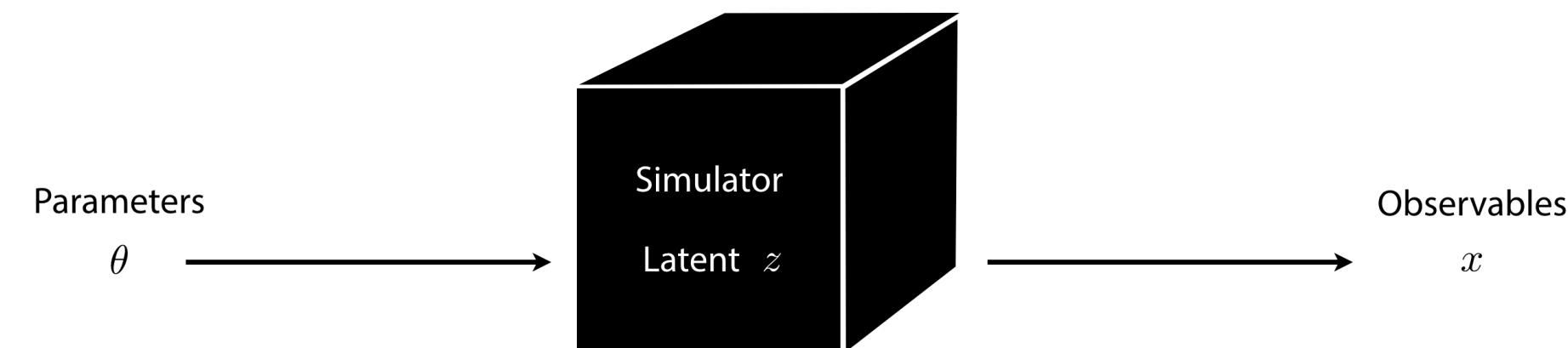


# A new approach to simulator-based inference

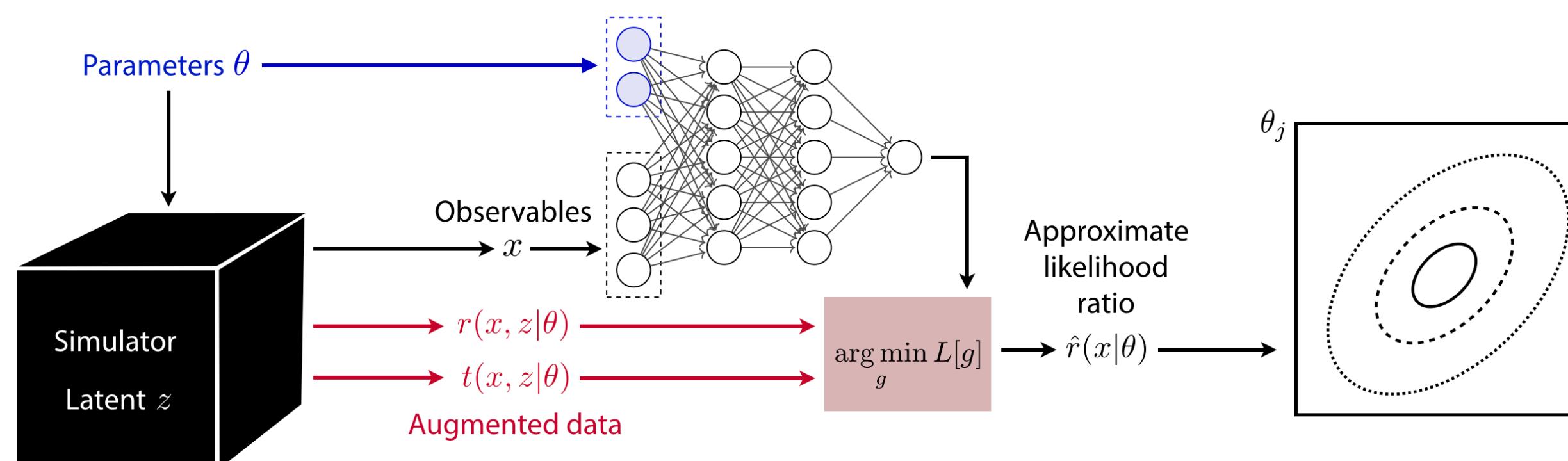


- Many LHC analyses (and much of modern science) are based on simulations, “likelihood-free”

# A new approach to simulator-based inference

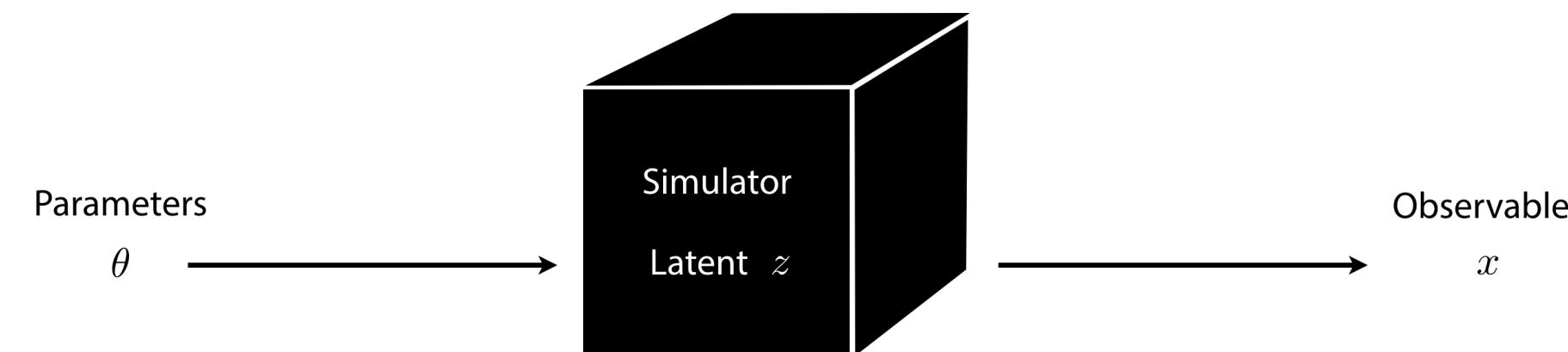


- Many LHC analyses (and much of modern science) are based on simulations, “likelihood-free”

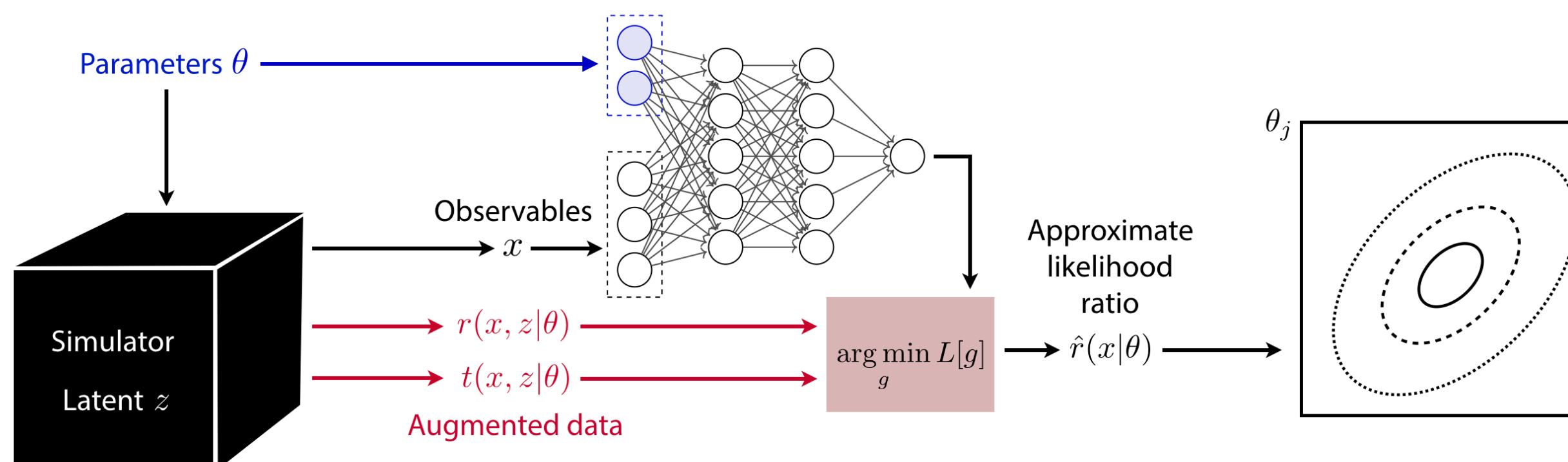


- New multivariate inference techniques: Leverage more information from simulator + power of machine learning

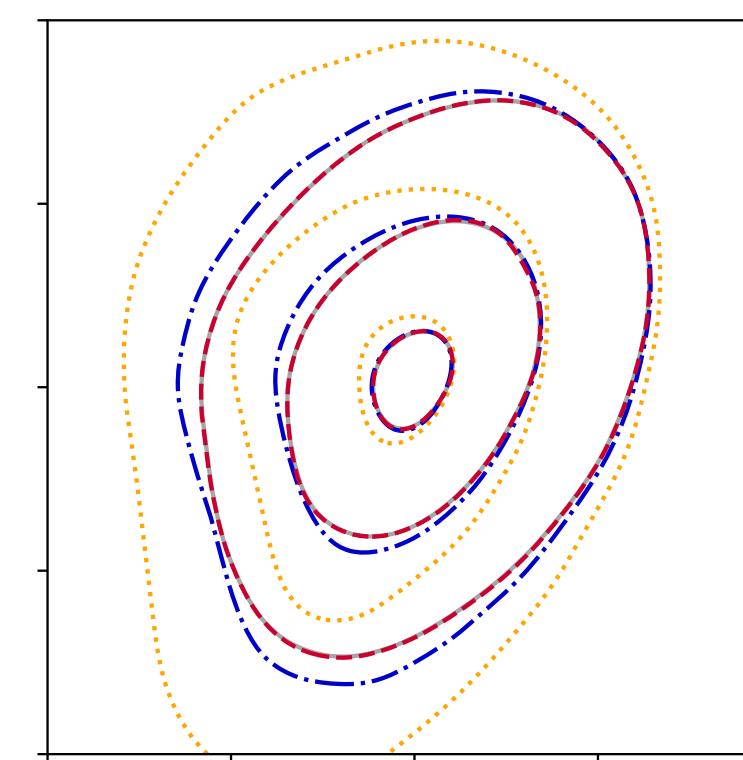
# A new approach to simulator-based inference



- Many LHC analyses (and much of modern science) are based on simulations, “likelihood-free”



- New multivariate inference techniques:  
Leverage more information from simulator + power of machine learning
- First application to LHC physics:  
Stronger EFT constraints with less simulations



# References



Kyle Cranmer



Gilles Louppe



Juan Pavez



Markus Stoye



Felix Kling



Tilman Plehn



Tim Tait

KC, GL, JP:

Approximating Likelihood Ratios with Calibrated Discriminative Classifiers

[1506.02169]

JB, KC, FK, TP:

Better Higgs Measurements Through Information Geometry

[1612.05261]

JB, FK, TP, TT:

Better Higgs-CP Measurements Through Information Geometry

[1712.02350]

JB, KC, GL, JP:

**Constraining Effective Field Theories with Machine Learning**

[1805.00013]

JB, KC, GL, JP:

**A Guide to Constraining Effective Field Theories with Machine Learning**

[1805.00020]

JB, GL, JP, KC:

Mining gold from implicit models to improve likelihood-free inference

[1805.12244]

MS, JB, GL, JP, KC:

Likelihood-free inference with an improved cross-entropy estimator

[1808.00973]

JB, KC, FK:

MadMiner

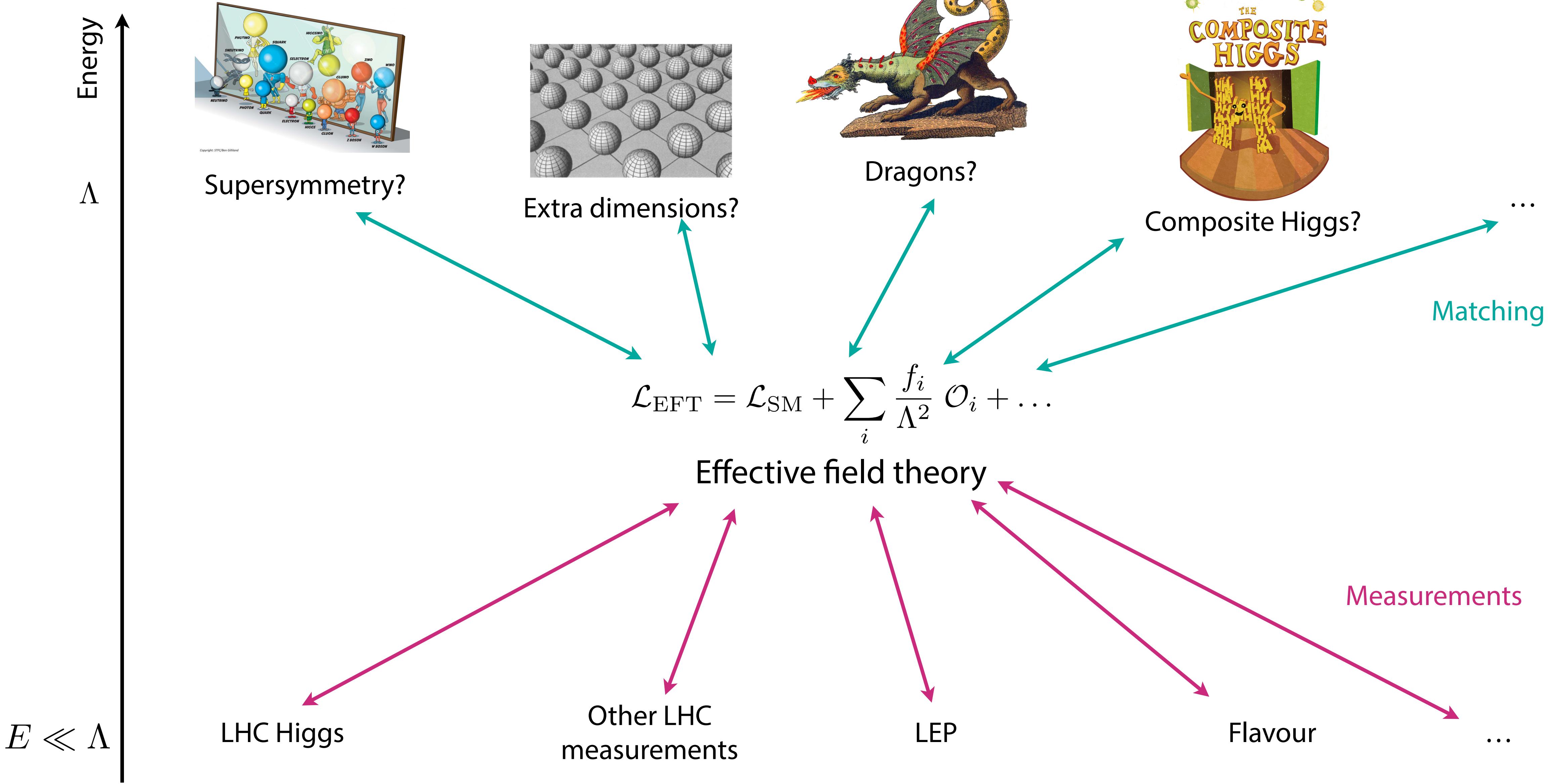
In preparation

+ new projects with Sally Dawson, Irina Espejo, Sam Homiller, Marvin Meng, Duccio Pappadopulo, Josh Rudermann...

Thanks to Kyle and Gilles for inspiring many slides!

# Bonus material

# Effective field theory



# Variational calculus

$$\begin{aligned} L[\hat{g}(x)] &= \int dx dz \textcolor{red}{p}(x, z|\theta) |g(x, z) - \hat{g}(x)|^2 \\ &= \underbrace{\int dx \left[ \hat{g}^2(x) \int dz \textcolor{red}{p}(x, z|\theta) - 2\hat{g}(x) \int dz \textcolor{red}{p}(x, z|\theta) g(x, z) + \int dz \textcolor{red}{p}(x, z|\theta) g^2(x, z) \right]}_{F(x)} \end{aligned}$$

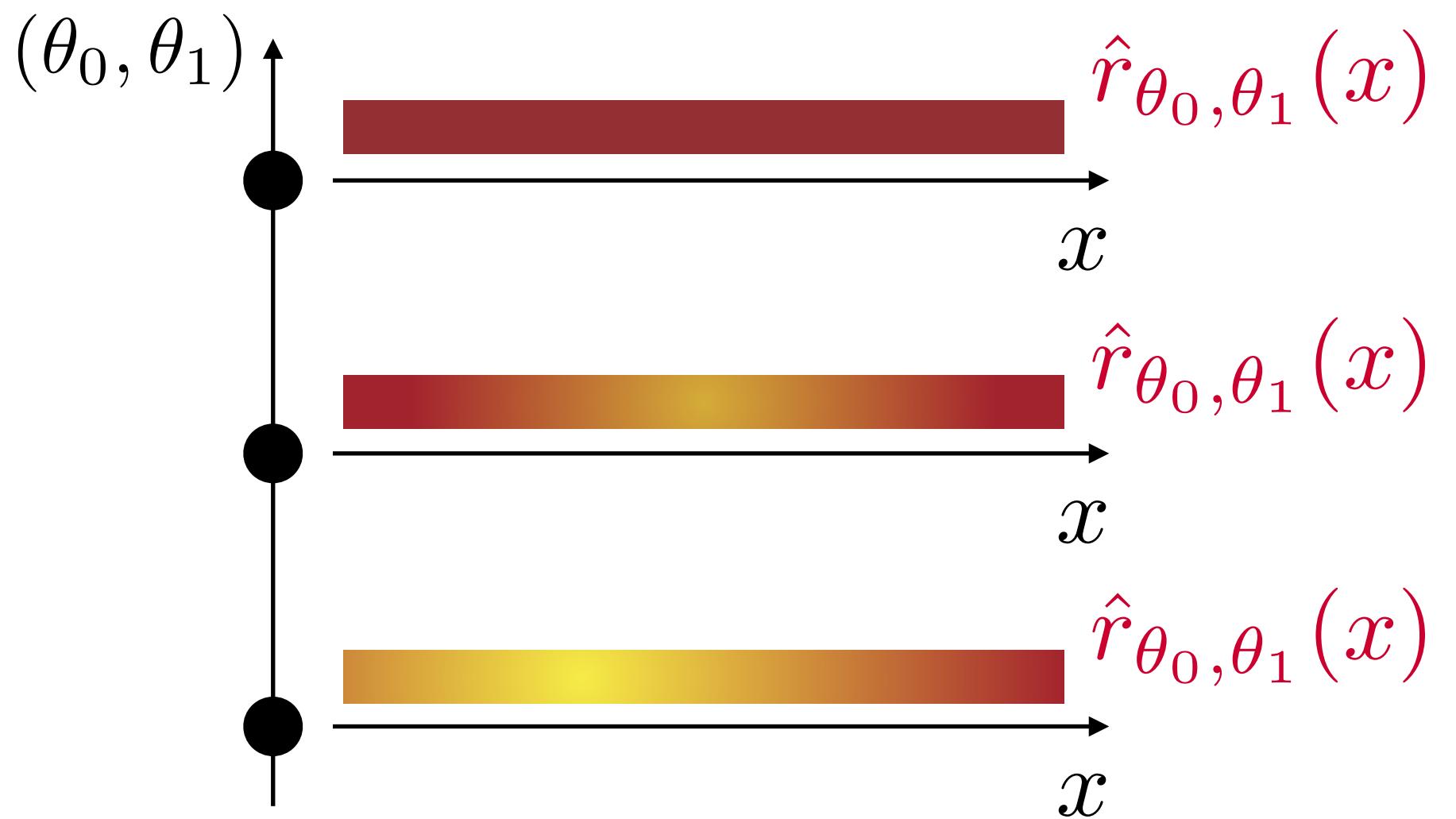
$$0 = \frac{\delta F}{\delta \hat{g}} \Big|_{g^*} = 2\hat{g} \underbrace{\int dz \textcolor{red}{p}(x, z|\theta)}_{=\textcolor{red}{p}(x|\theta)} - 2 \int dz \textcolor{red}{p}(x, z|\theta) g(x, z)$$

$$g^*(x) = \frac{1}{\textcolor{red}{p}(x|\theta)} \int dz \textcolor{red}{p}(x, z|\theta) g(x, z)$$

# Two types of likelihood ratio estimators

A) Point by point:

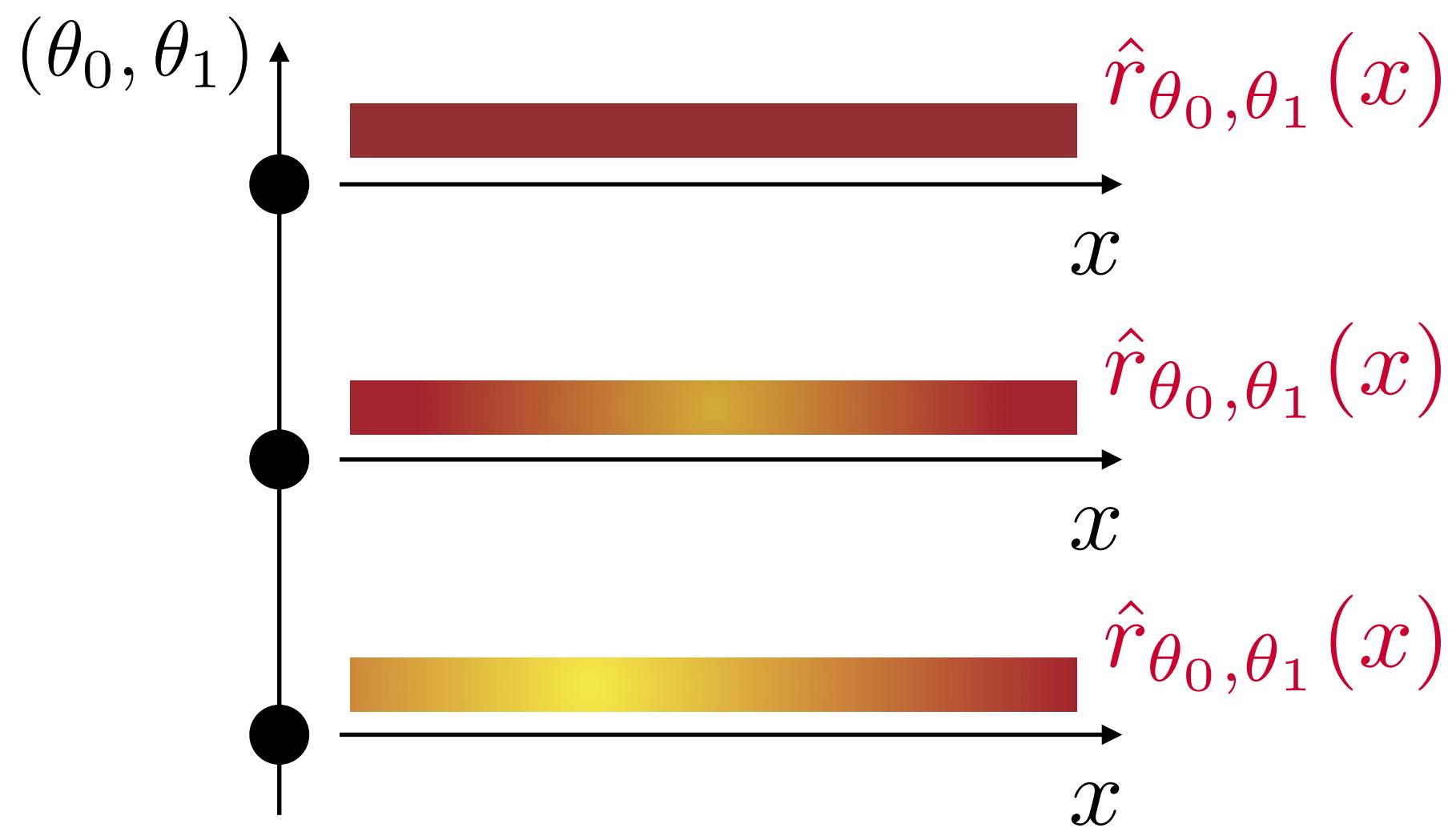
- first, define grid of parameter points  $\{(\theta_0, \theta_1)\}$
- for each combination  $(\theta_0, \theta_1)$ ,  
create separate estimator  $\hat{r}_{\theta_0, \theta_1}(x)$
- final results can be interpolated between grid points



# Two types of likelihood ratio estimators

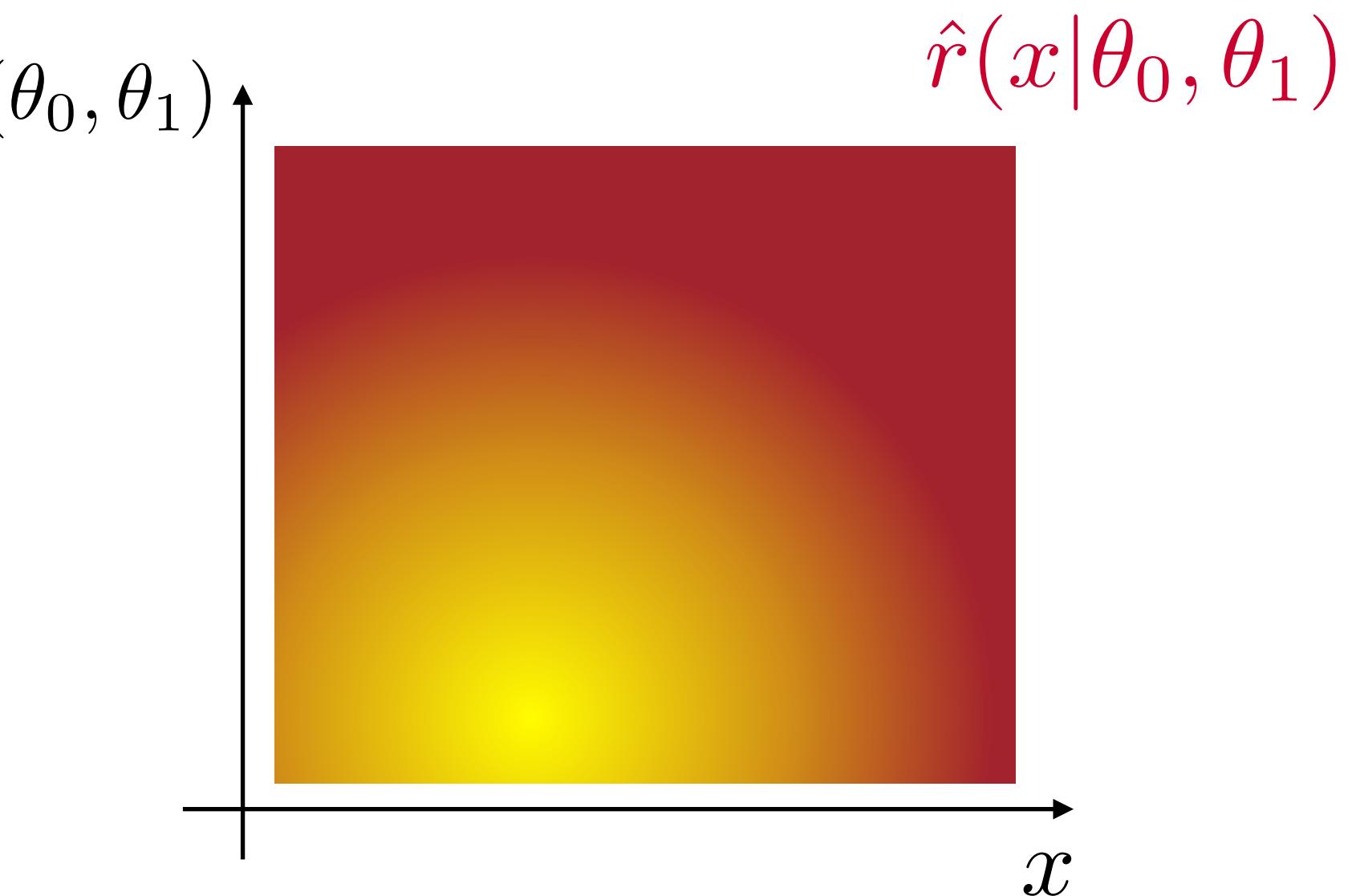
## A) Point by point:

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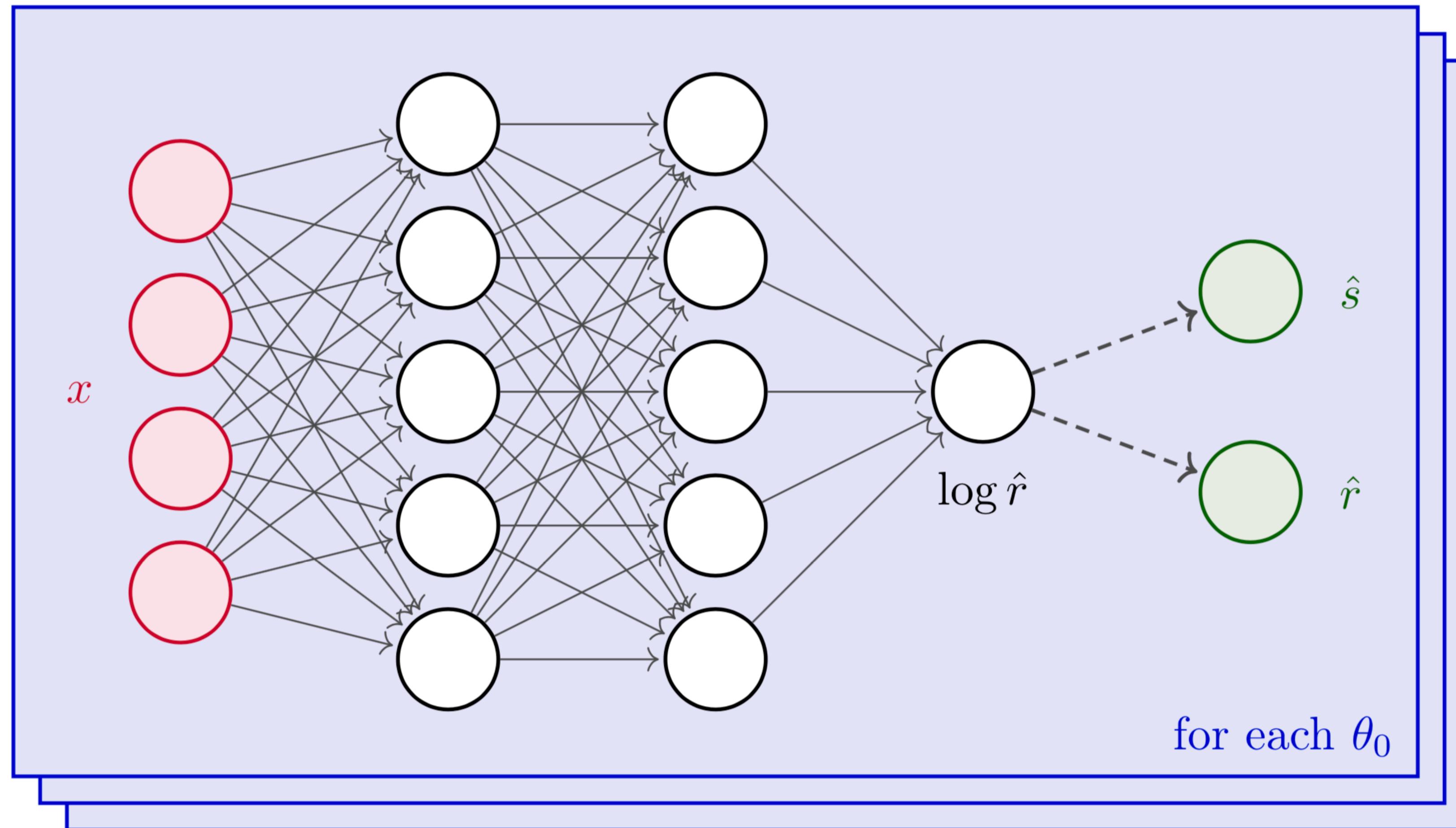


## B) Parameterized:

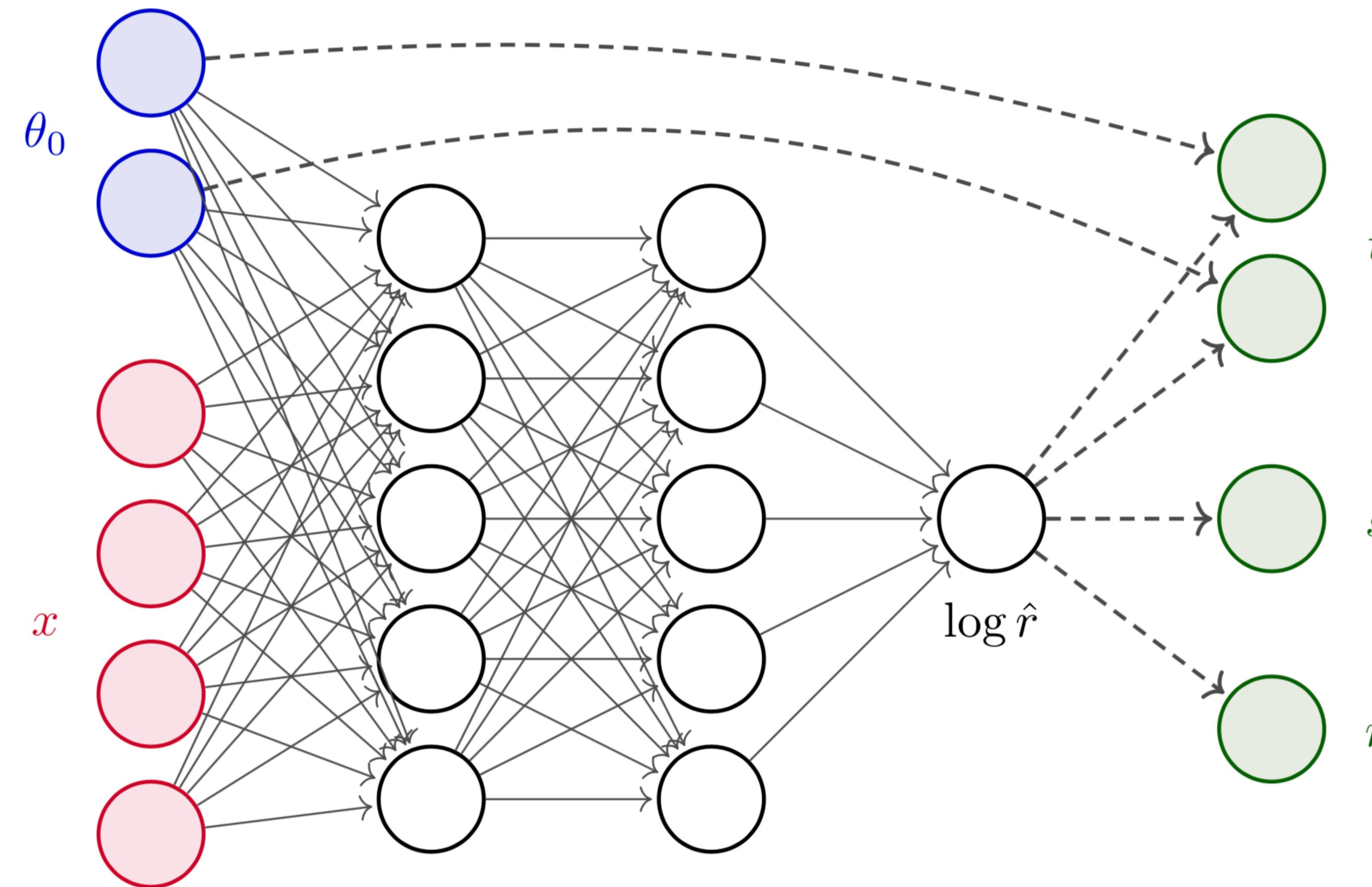
- [P. Baldi et al. 1506.02169]
- create one estimator  $\hat{r}(x|\theta_0, \theta_1)$  that is a function of  $\theta_0$  and  $\theta_1$
  - no further interpolation necessary
  - “borrows information” from close points



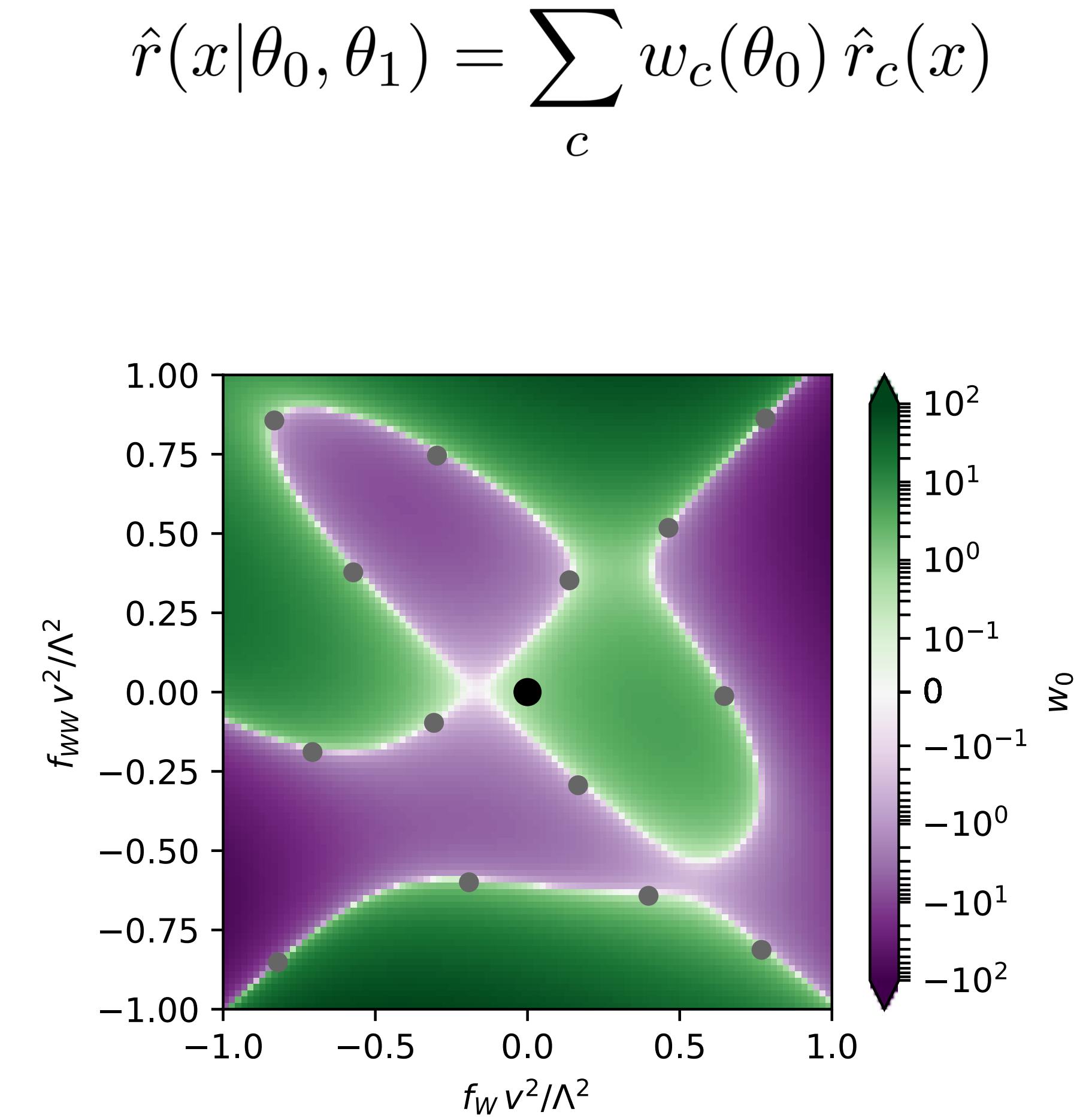
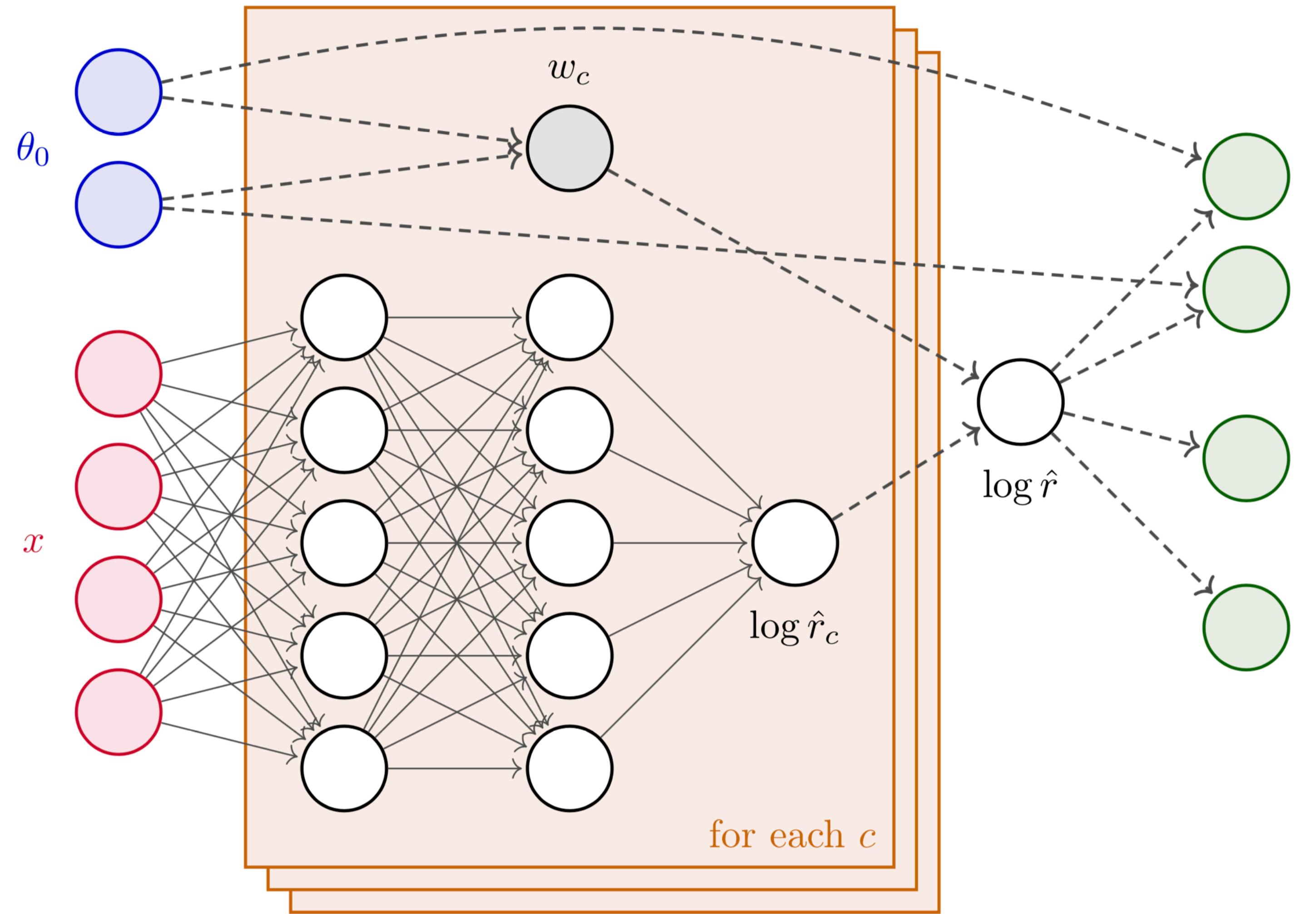
# Point by point



# (Agnostic) parameterized estimators



# Morphing-aware parameterized estimators



# Detector effects

