

Constraining effective field theories with machine learning

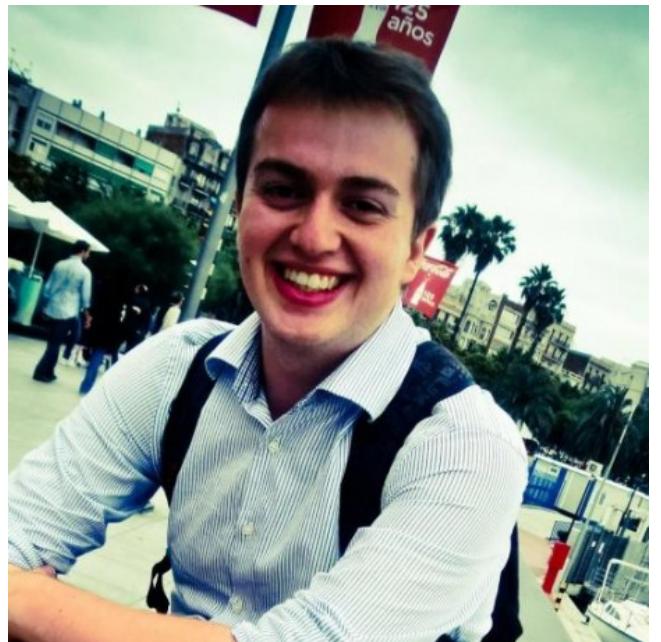
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HEFT 2019, Louvain-la-Neuve



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Gilles Louppe



Juan Pavez



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Irina Espejo



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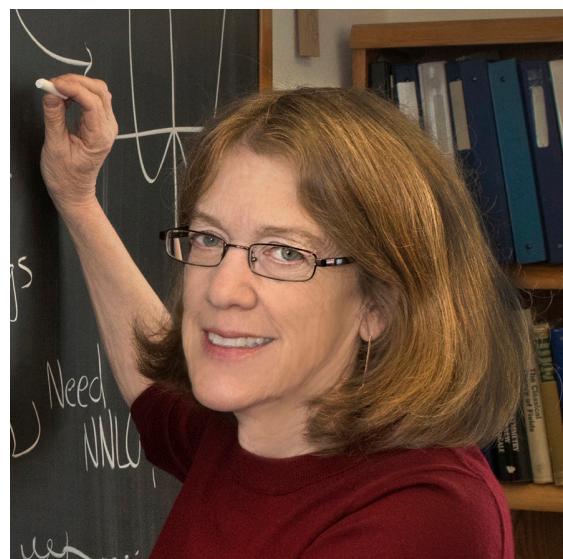
Sid Mishra-Sharma



Joeri Hermans



Tilman Plehn



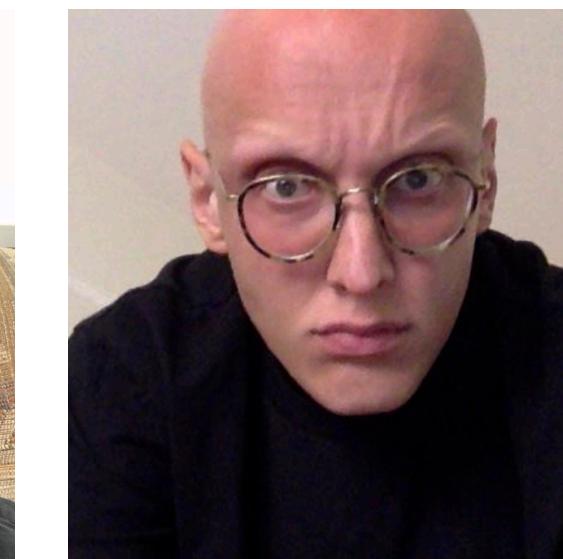
Sally Dawson



Sam Homiller



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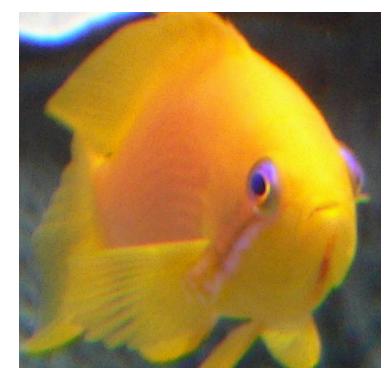


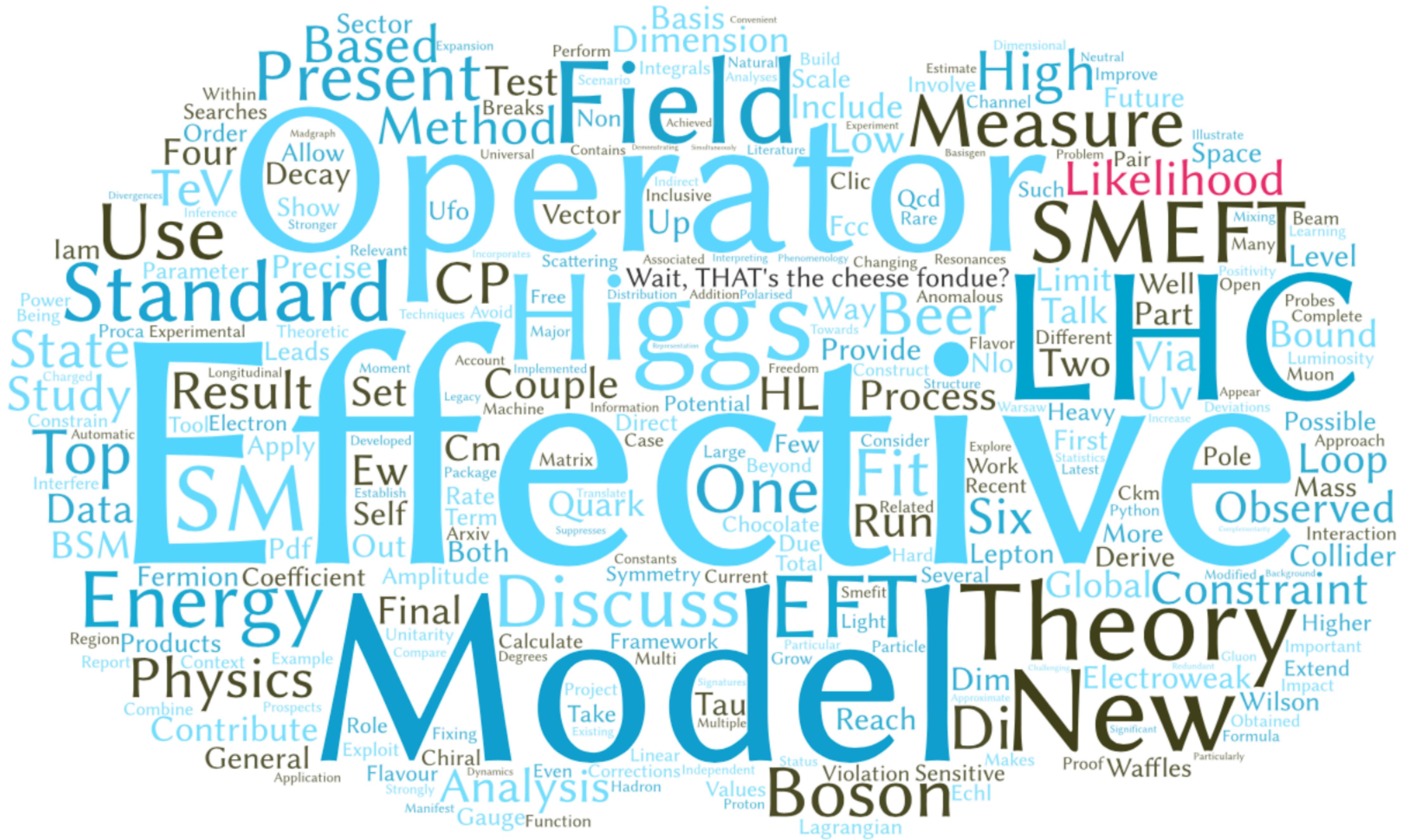
Marco Farina

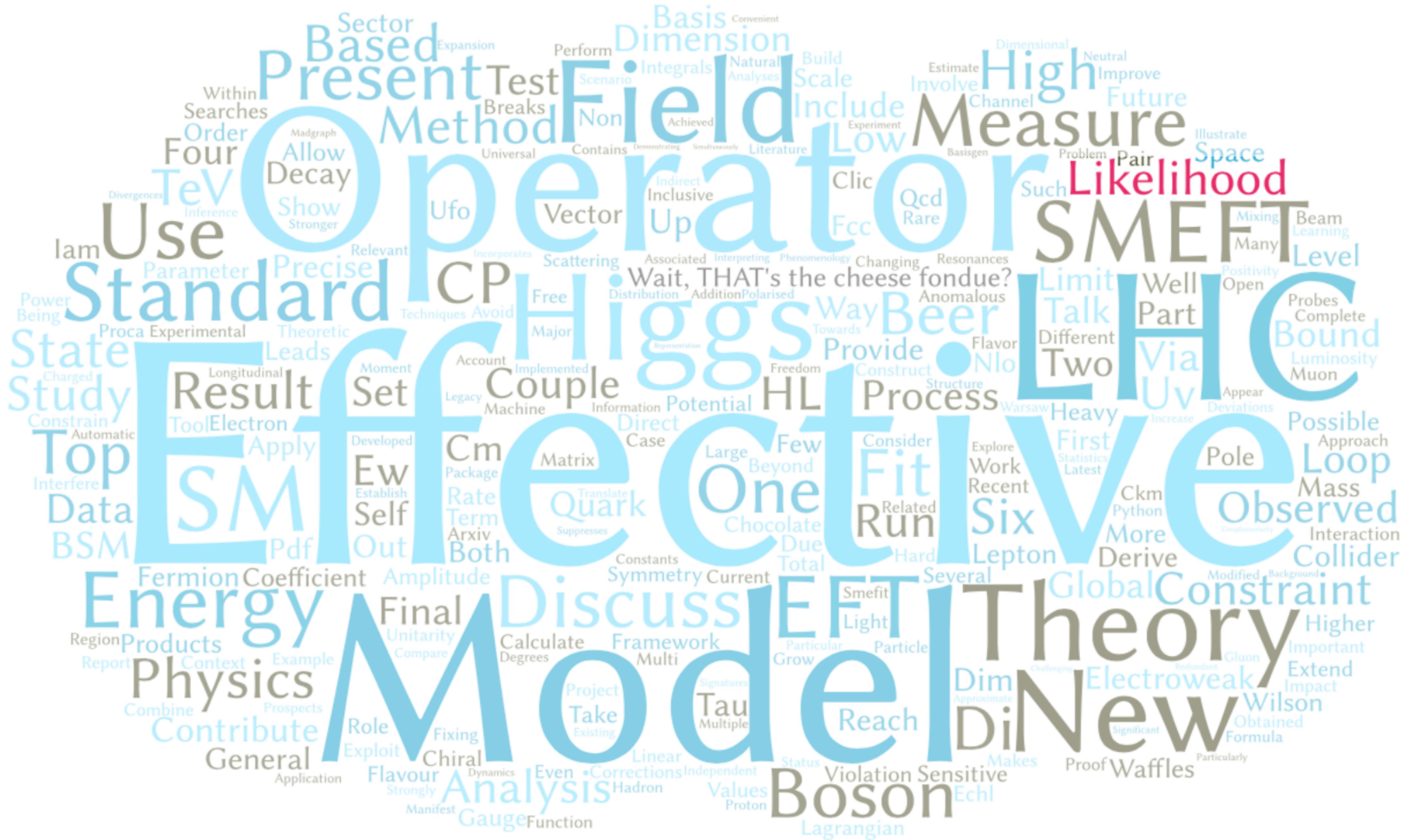
Thanks to Kyle, Gilles, Felix, Irina, and Sam for material and inspiration for slides!

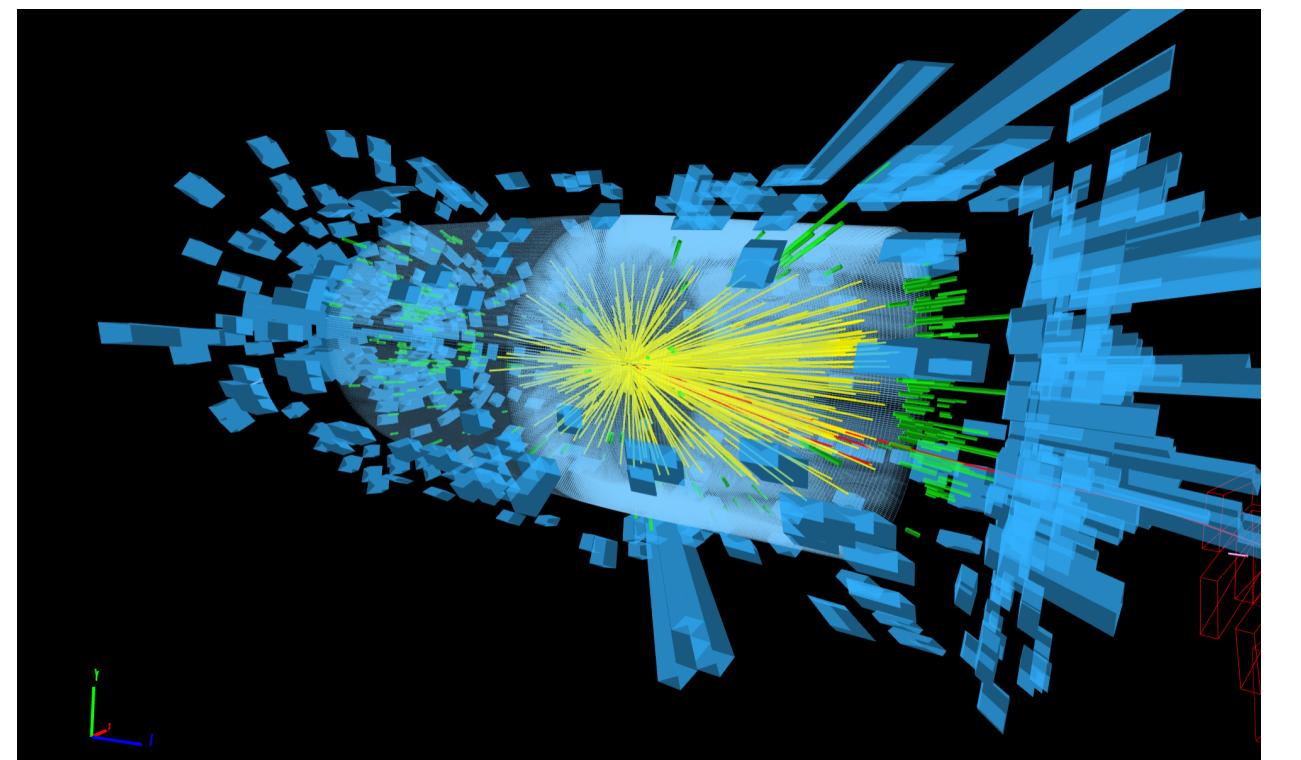


The SCAILFIN Project
scailfin.github.io

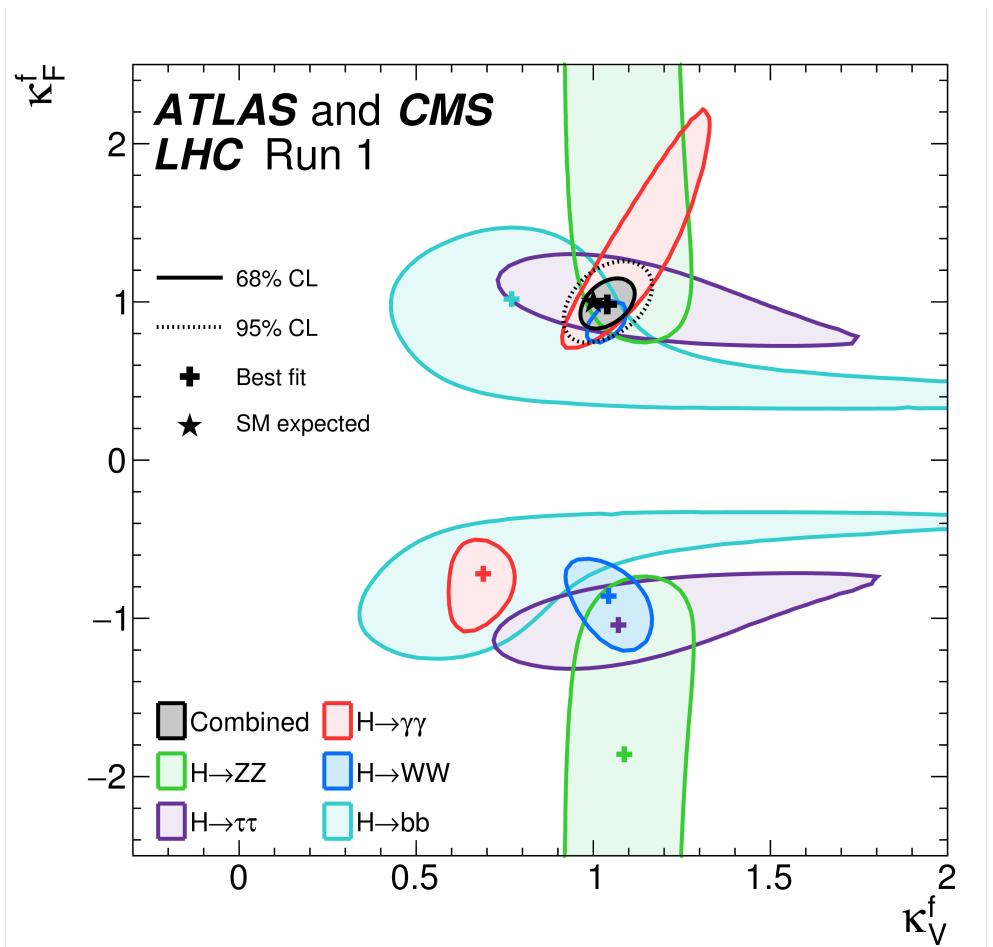




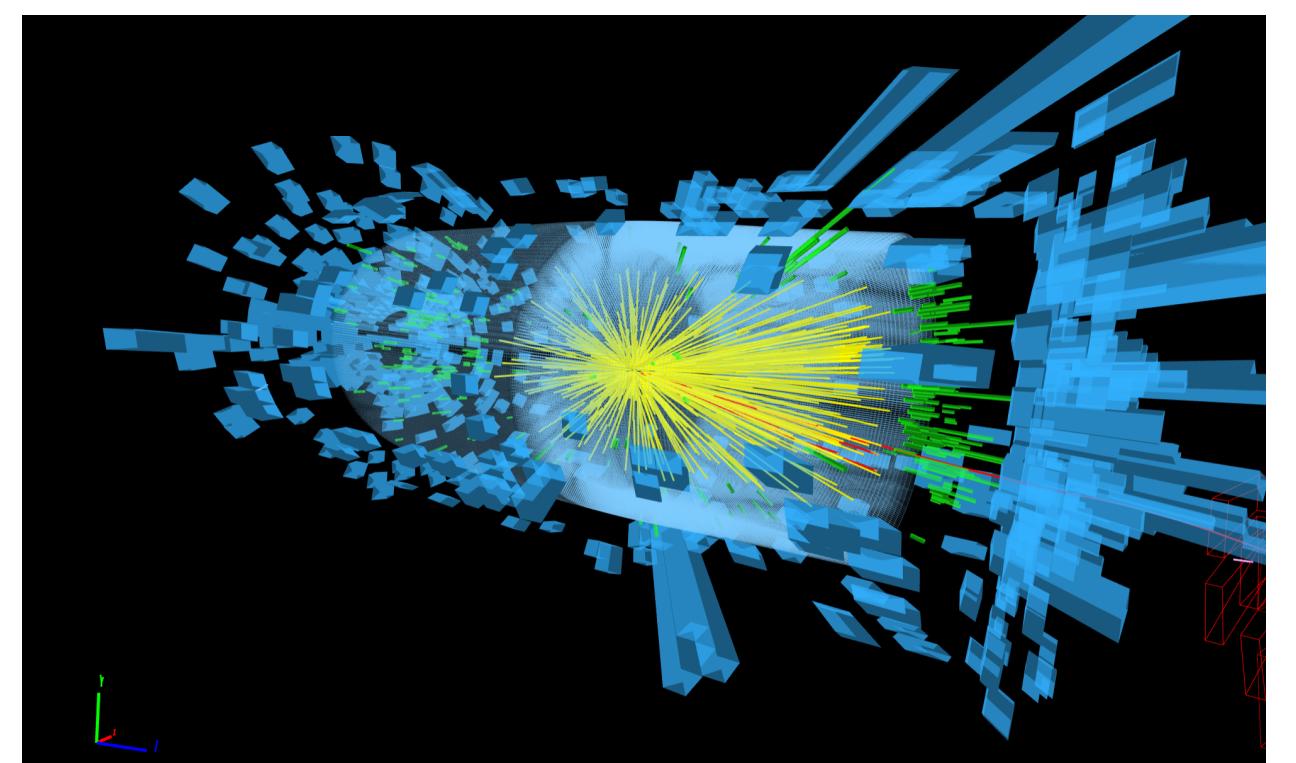




High-dimensional
event data x



Constraints on
parameters θ

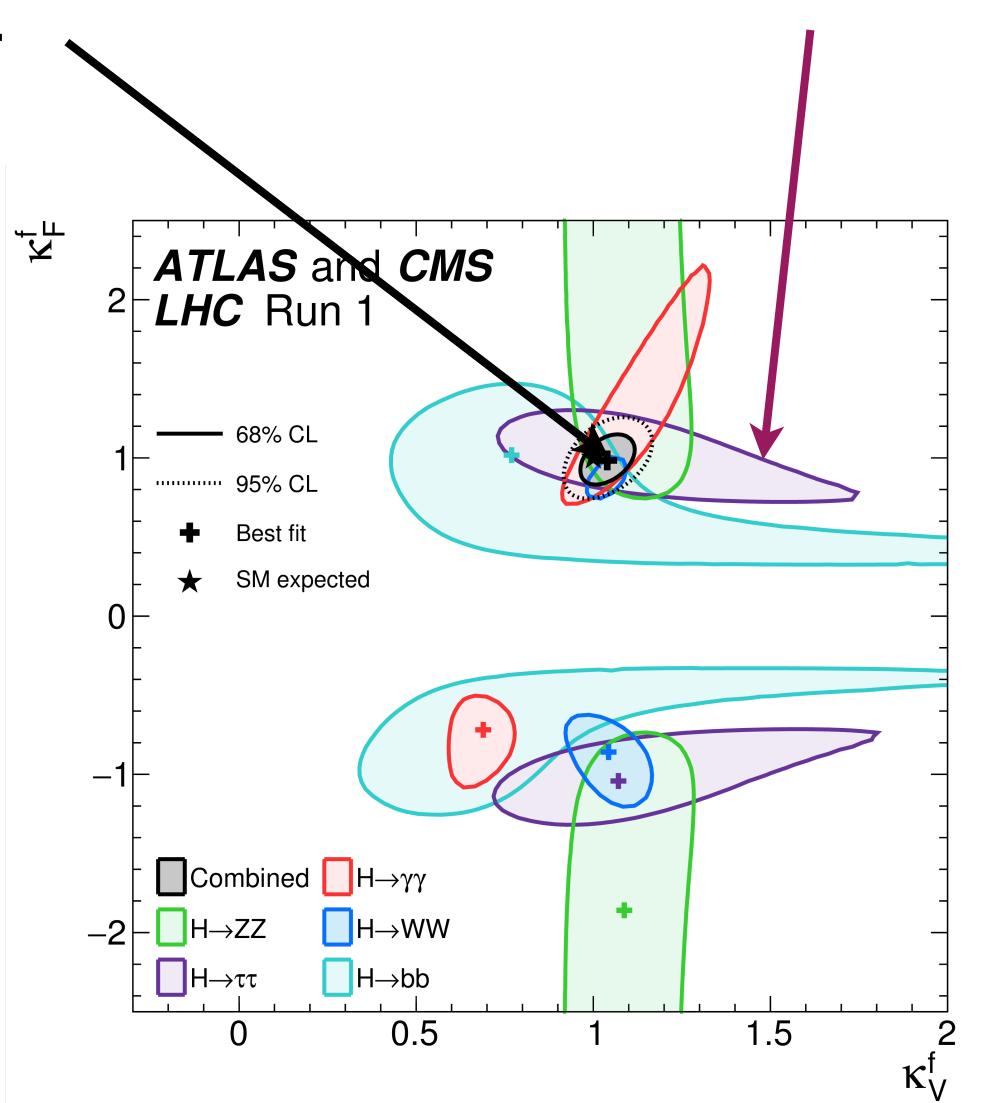


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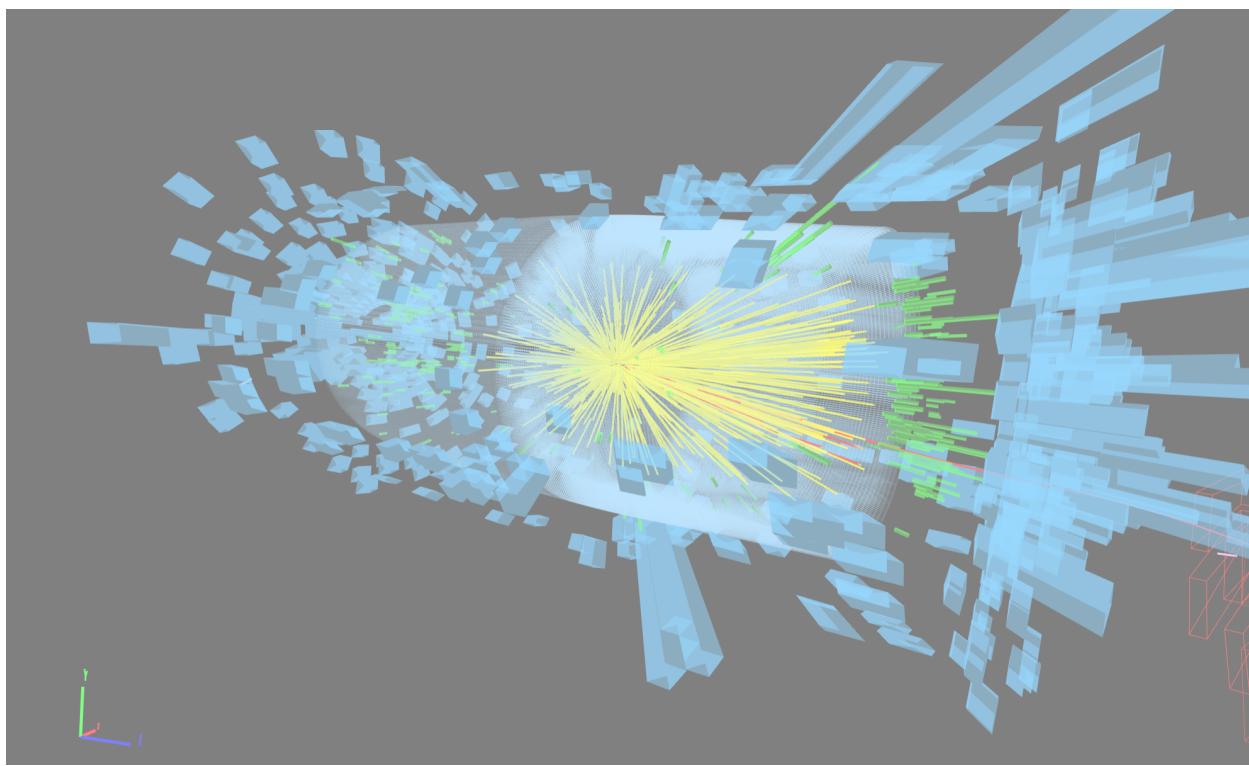


Likelihood function
 $p(x|\theta)$

Maximum-likelihood
estimator



Constraints on
parameters θ

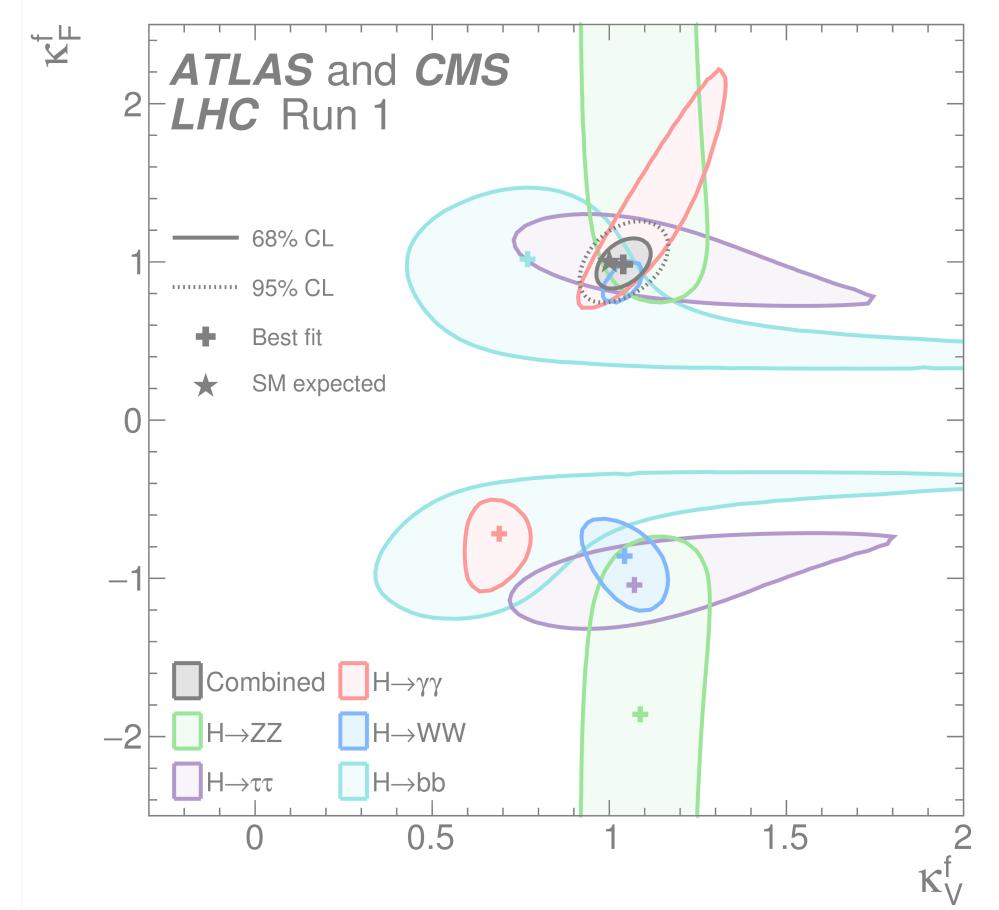


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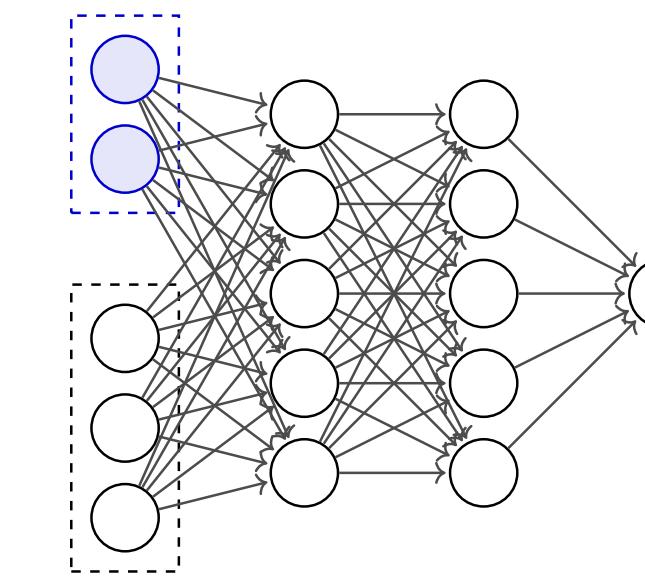
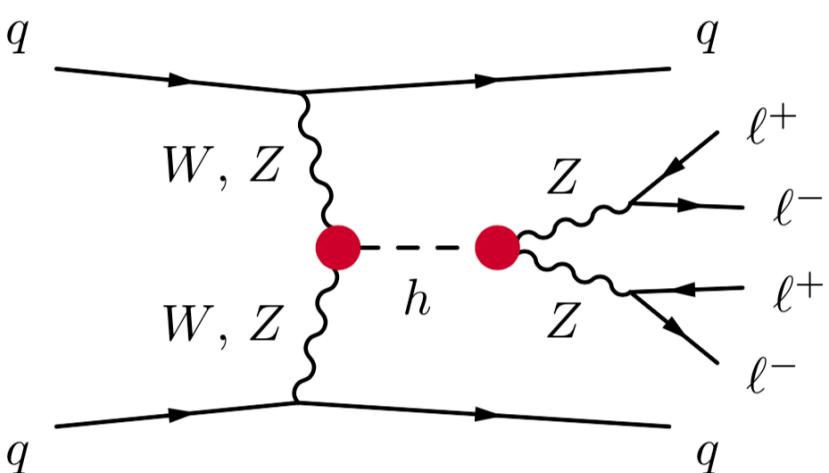
Surprisingly, when we want to use high-dimensional data and have to deal with the detector response, we do not have a good way to calculate the likelihood.



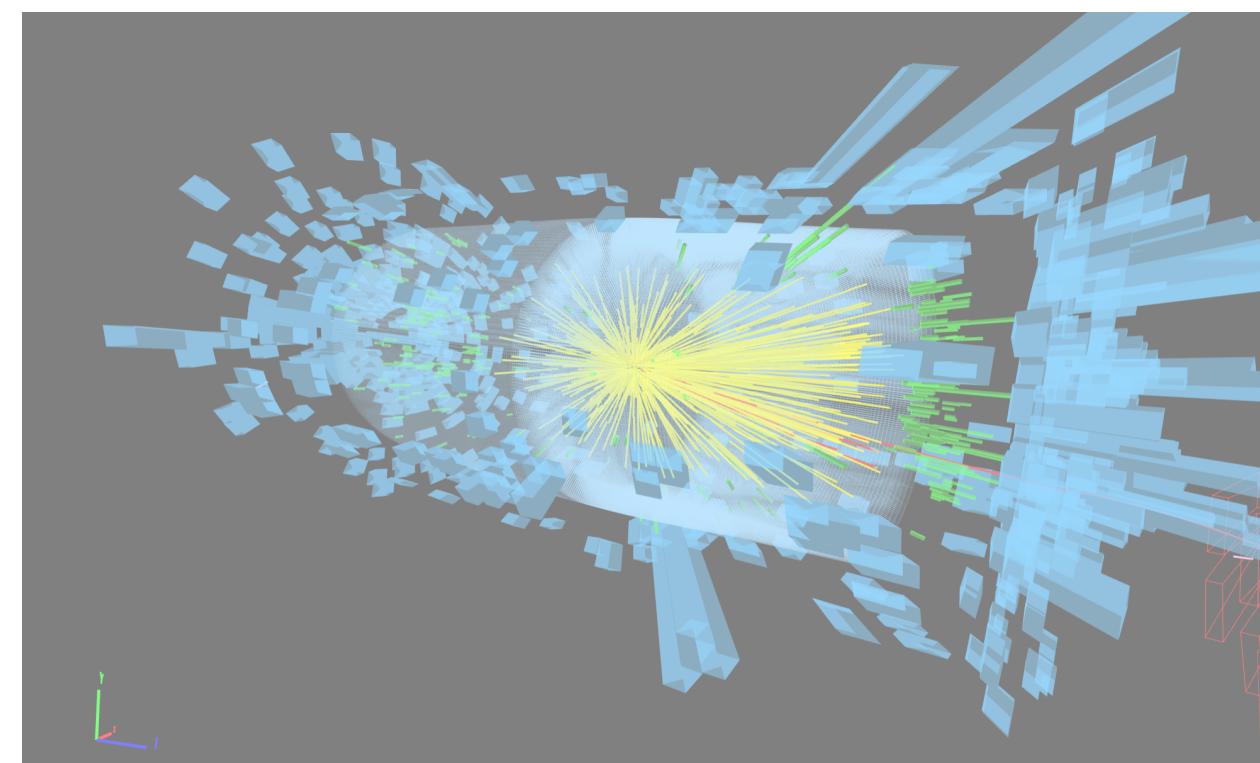
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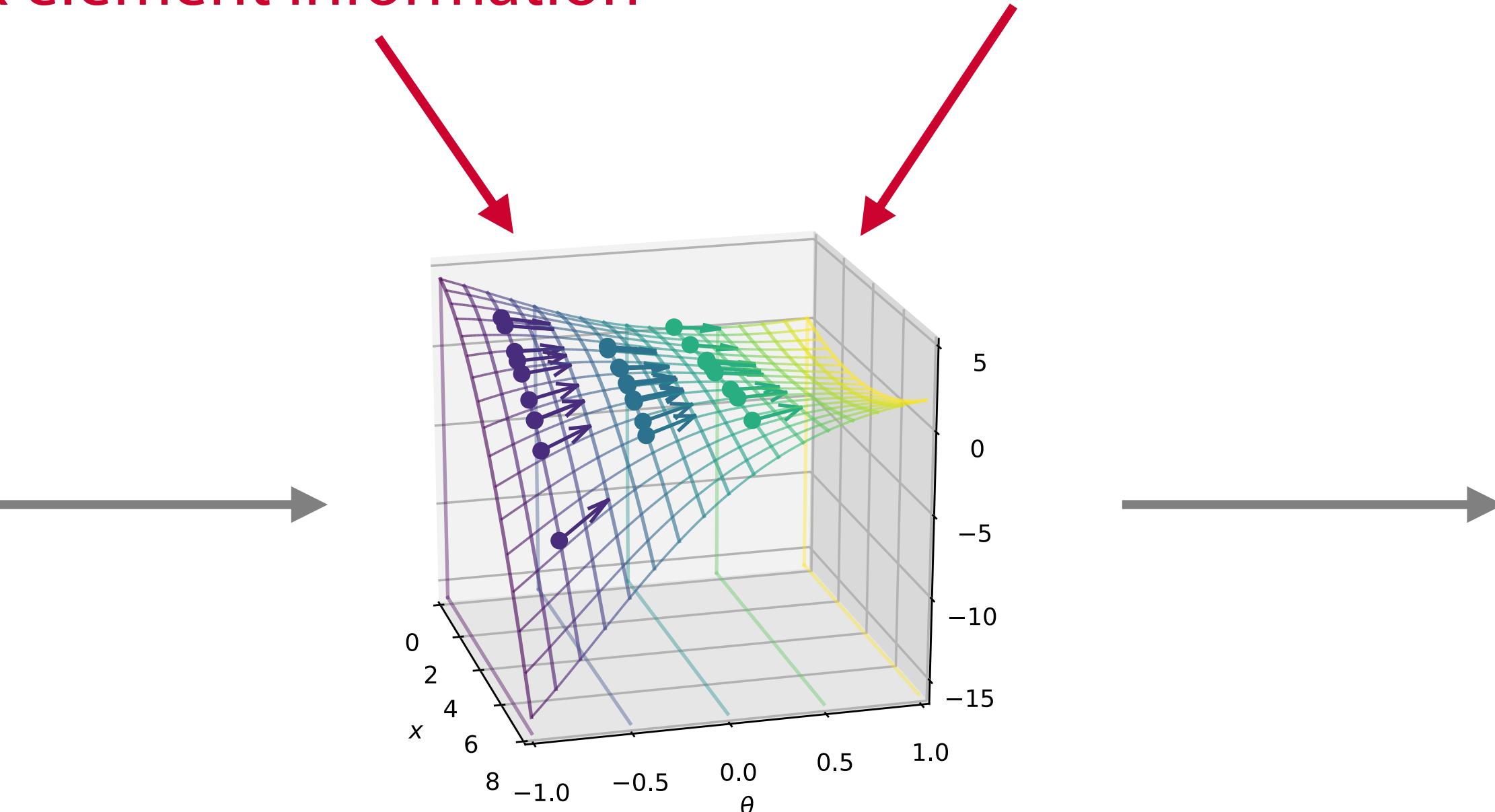
Constraints on
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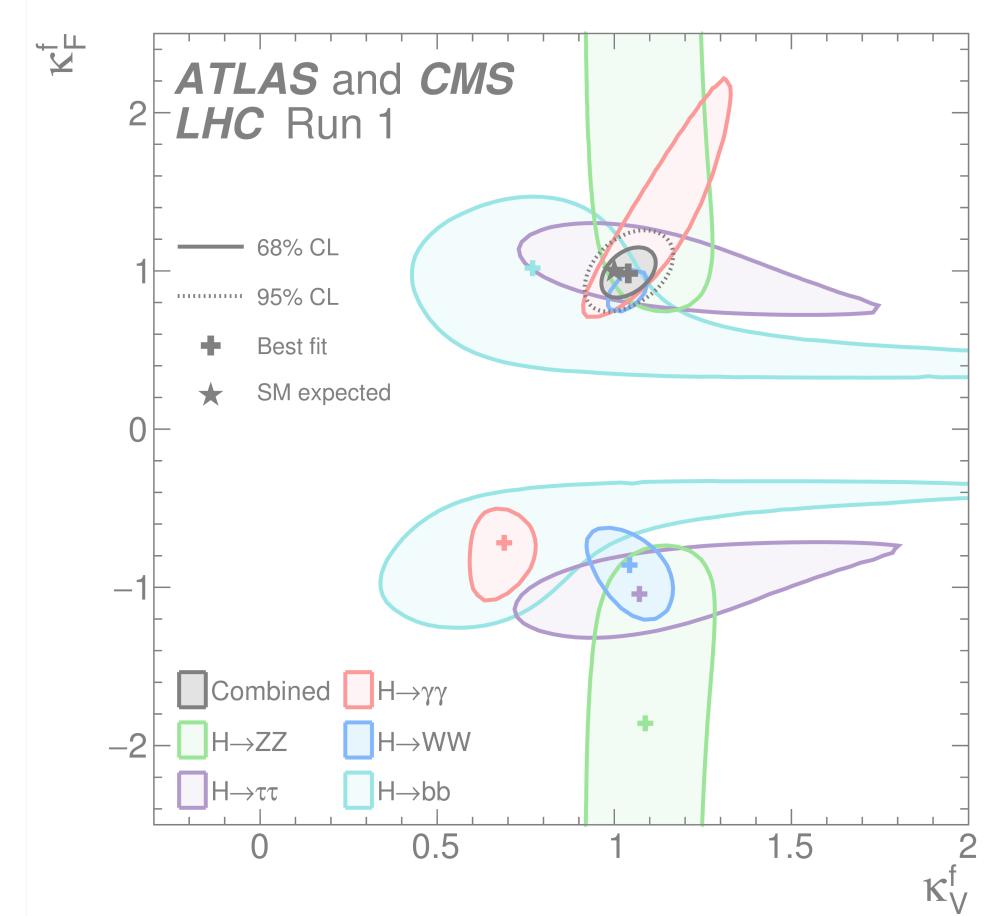
**Physics insight:
matrix element information**



High-dimensional
event data x



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



Constraints on
parameters θ

LHC measurements as a likelihood-free inference problem

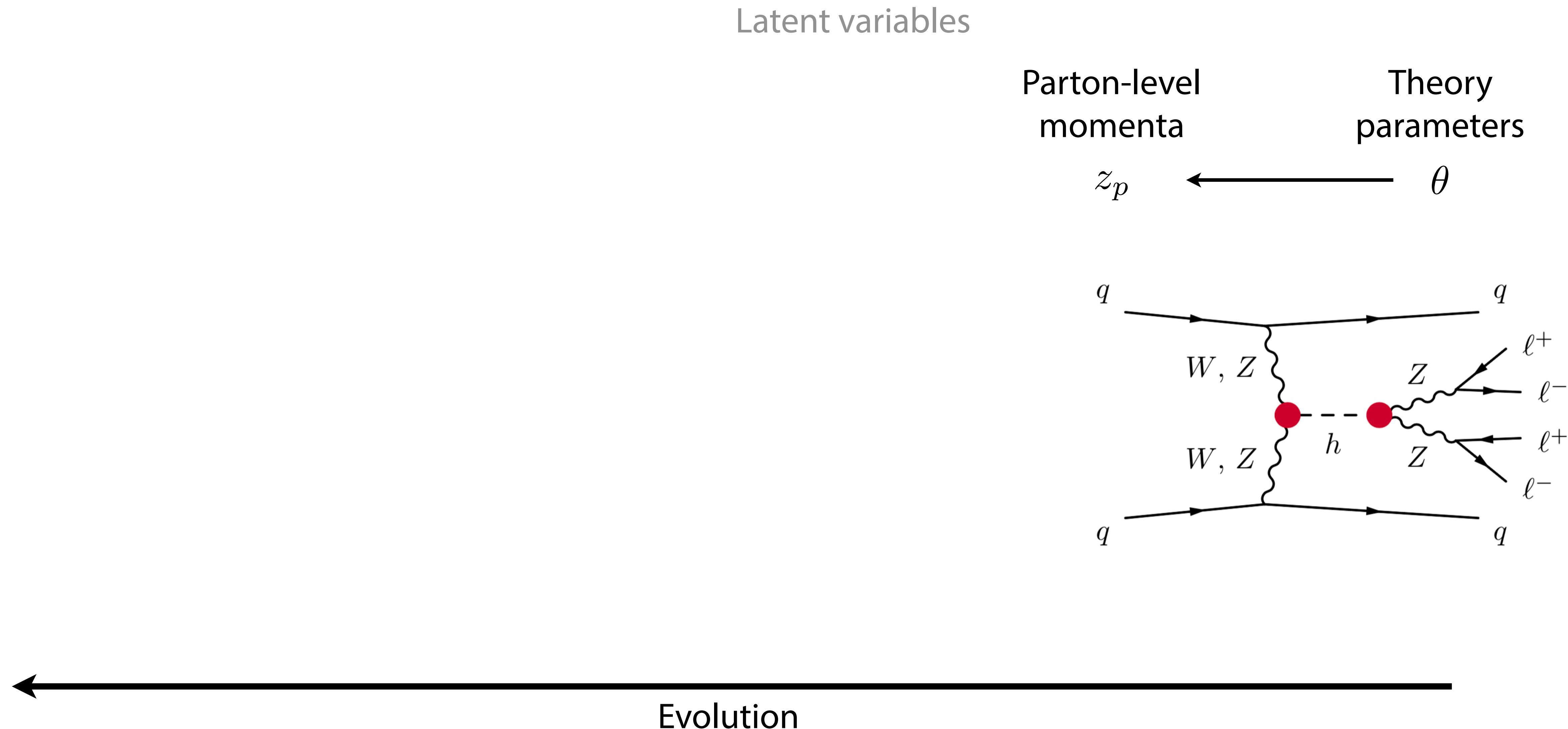
Modelling particle physics processes

Theory
parameters
 θ

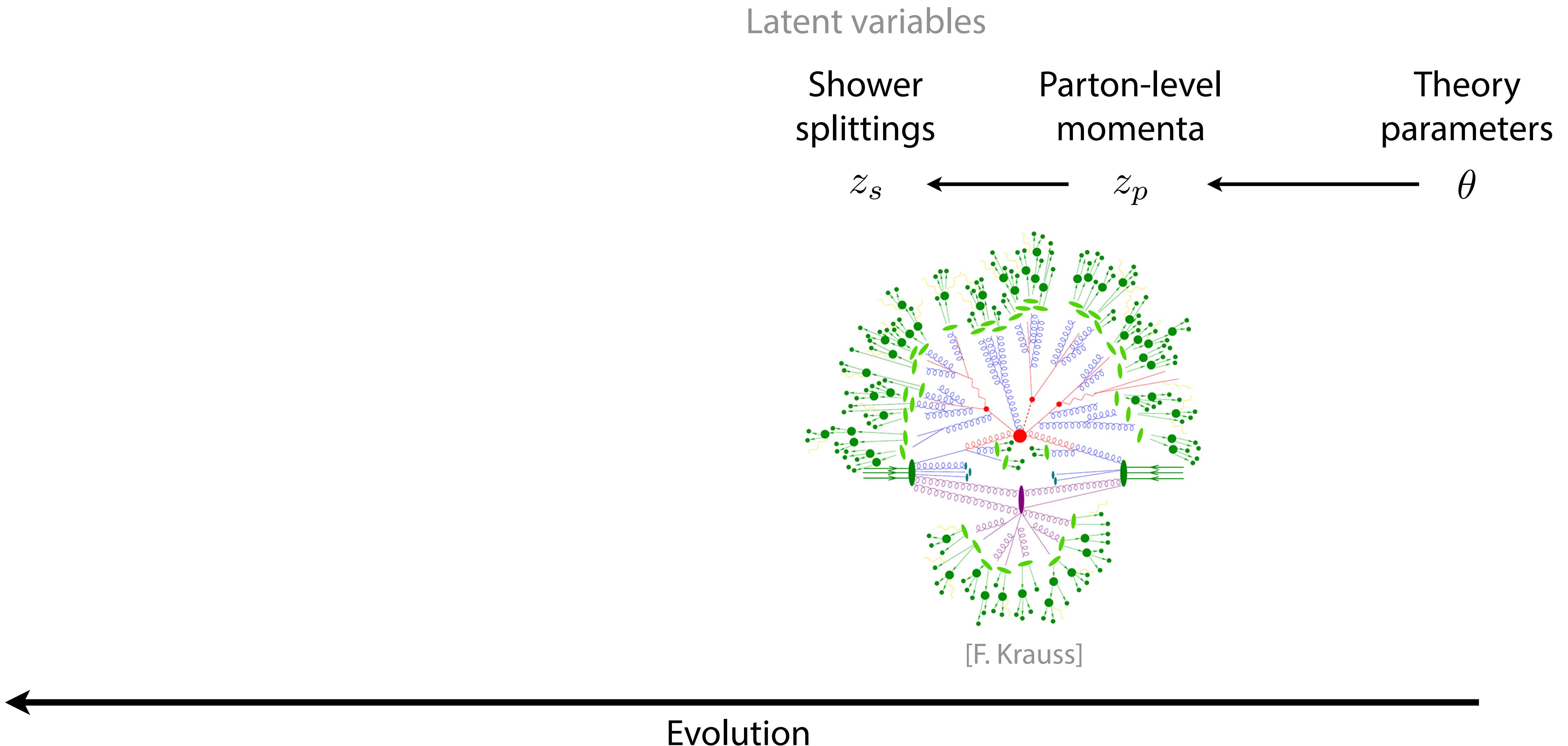


Evolution

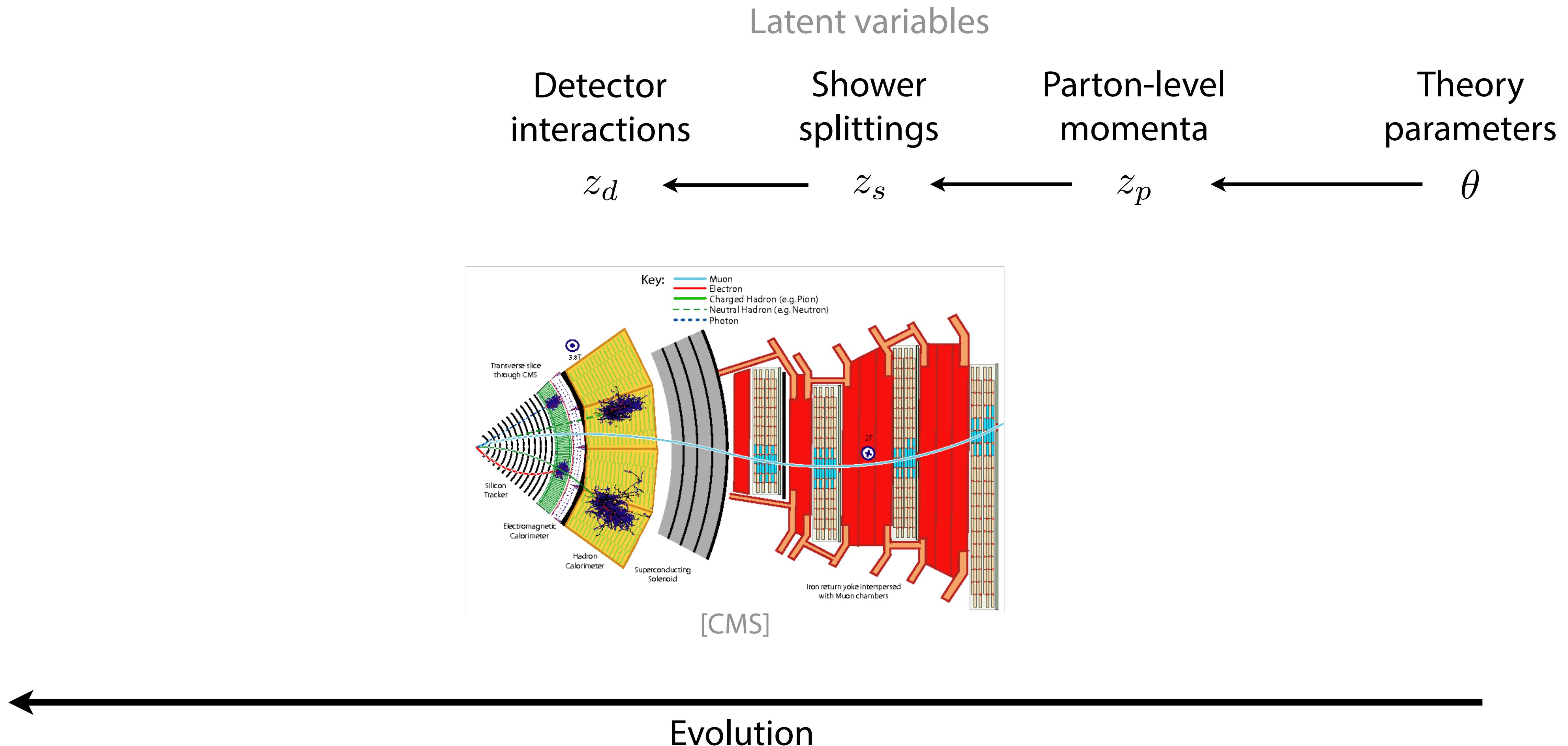
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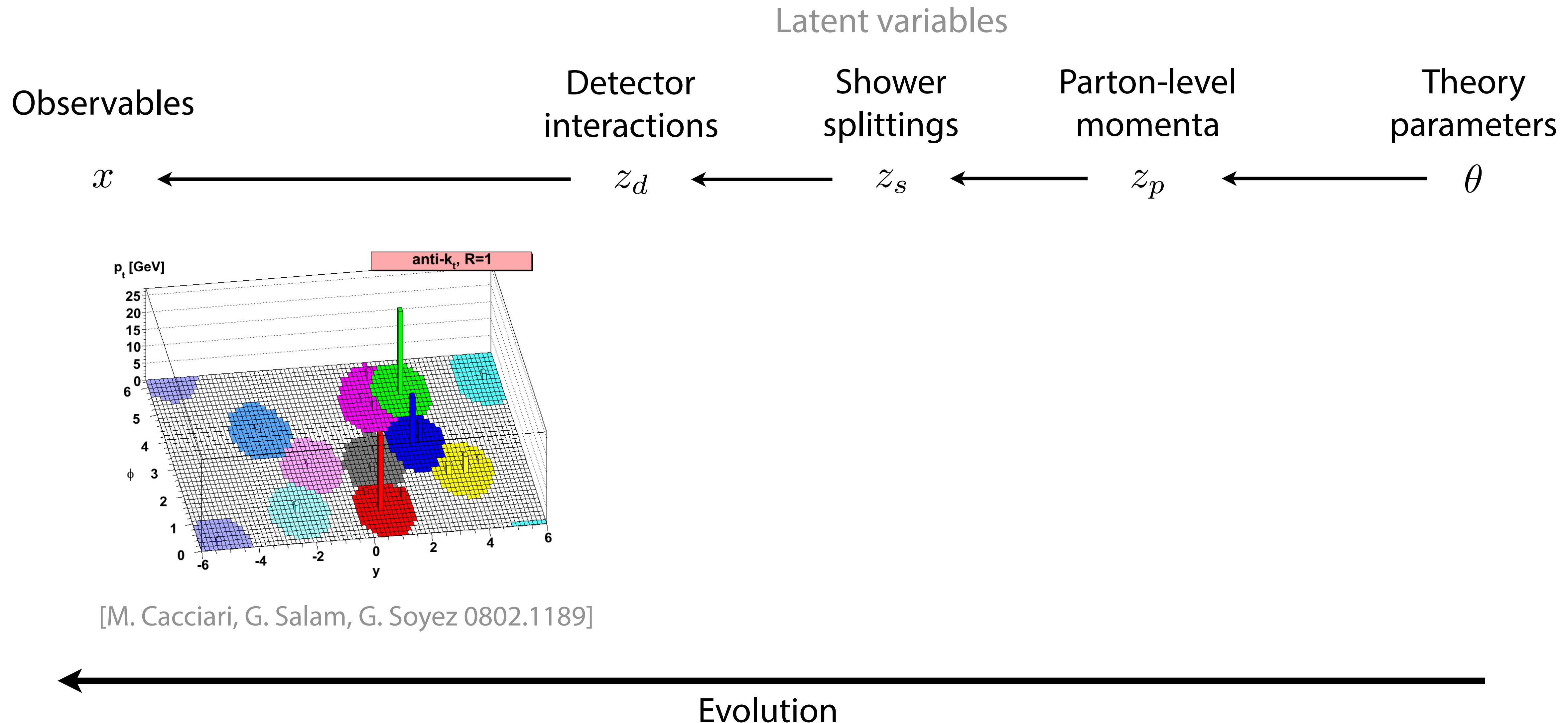
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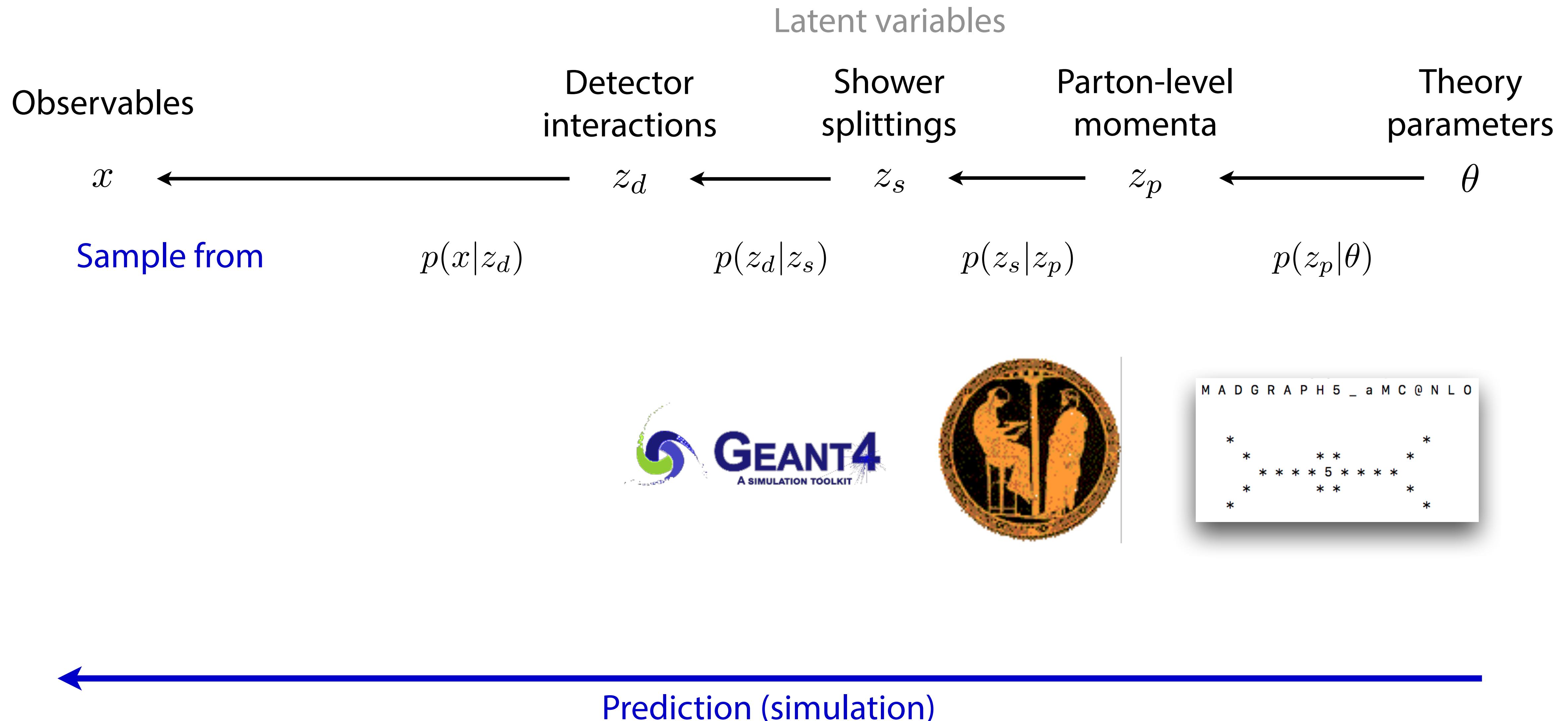
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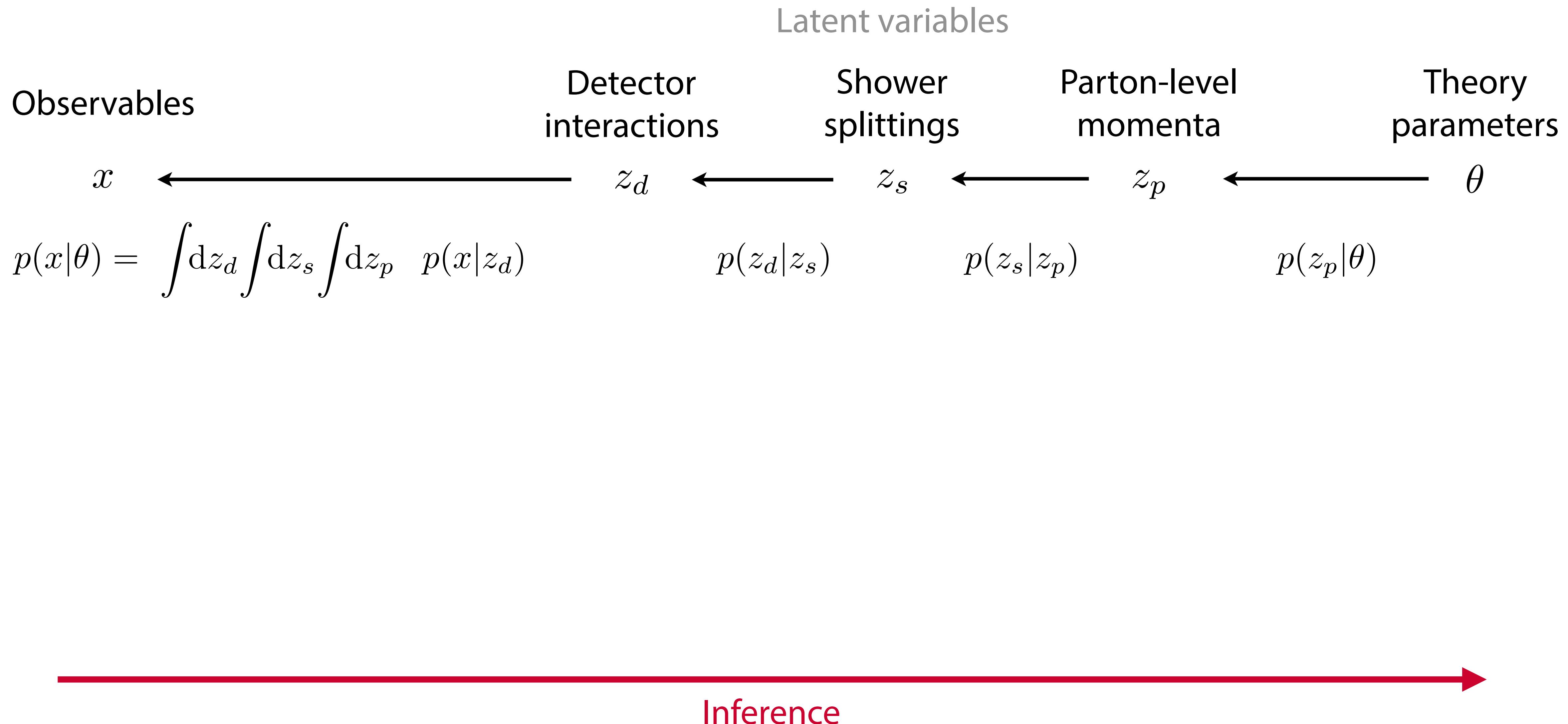
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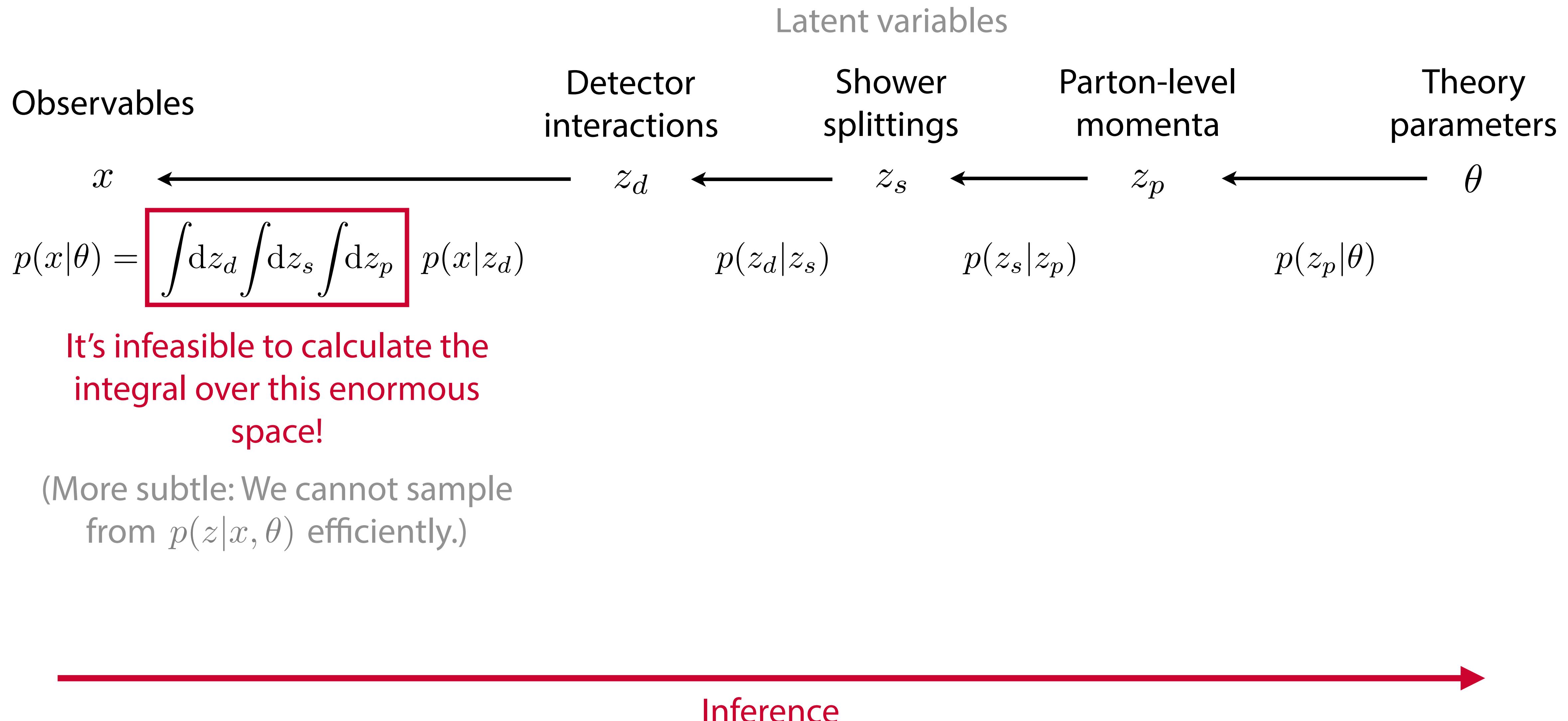
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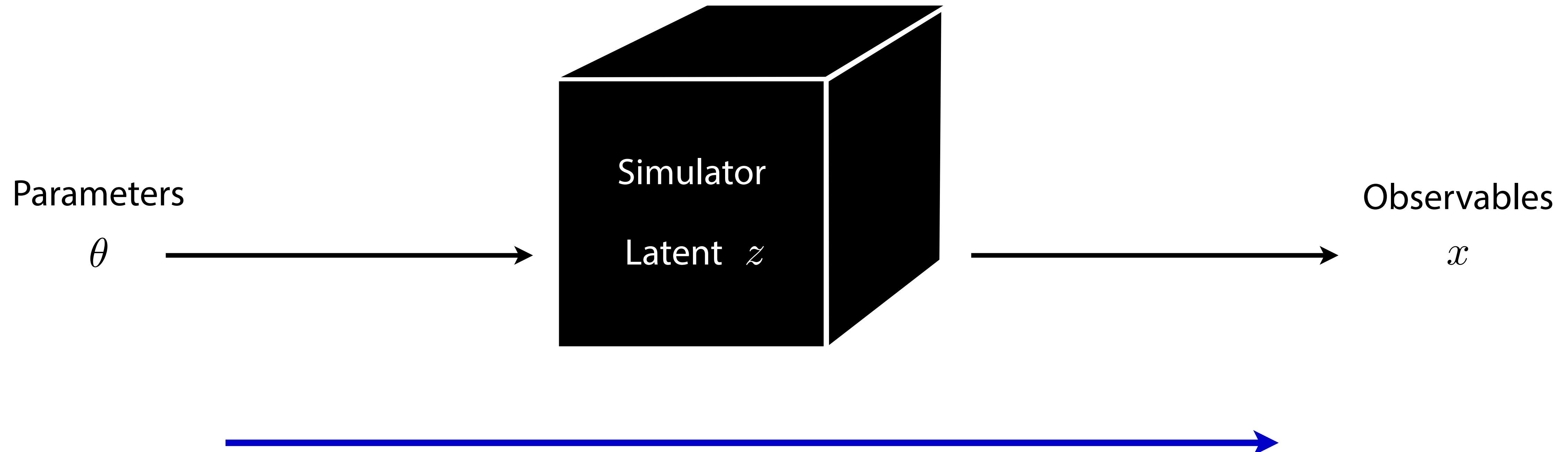
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Modelling particle physics processes



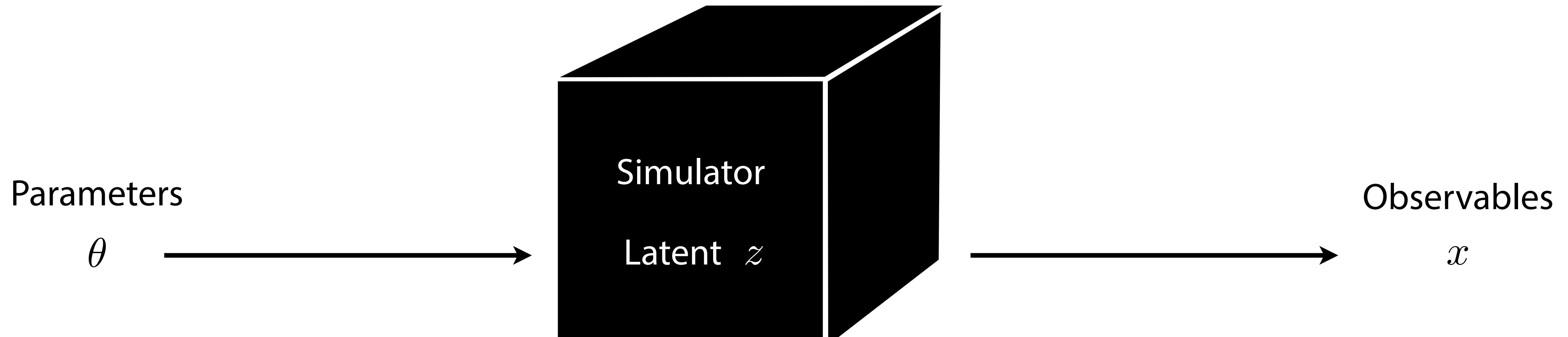
Likelihood-free inference / implicit models



Prediction:

- Well-understood mechanistic model
- Simulator can generate samples

Likelihood-free inference / implicit models



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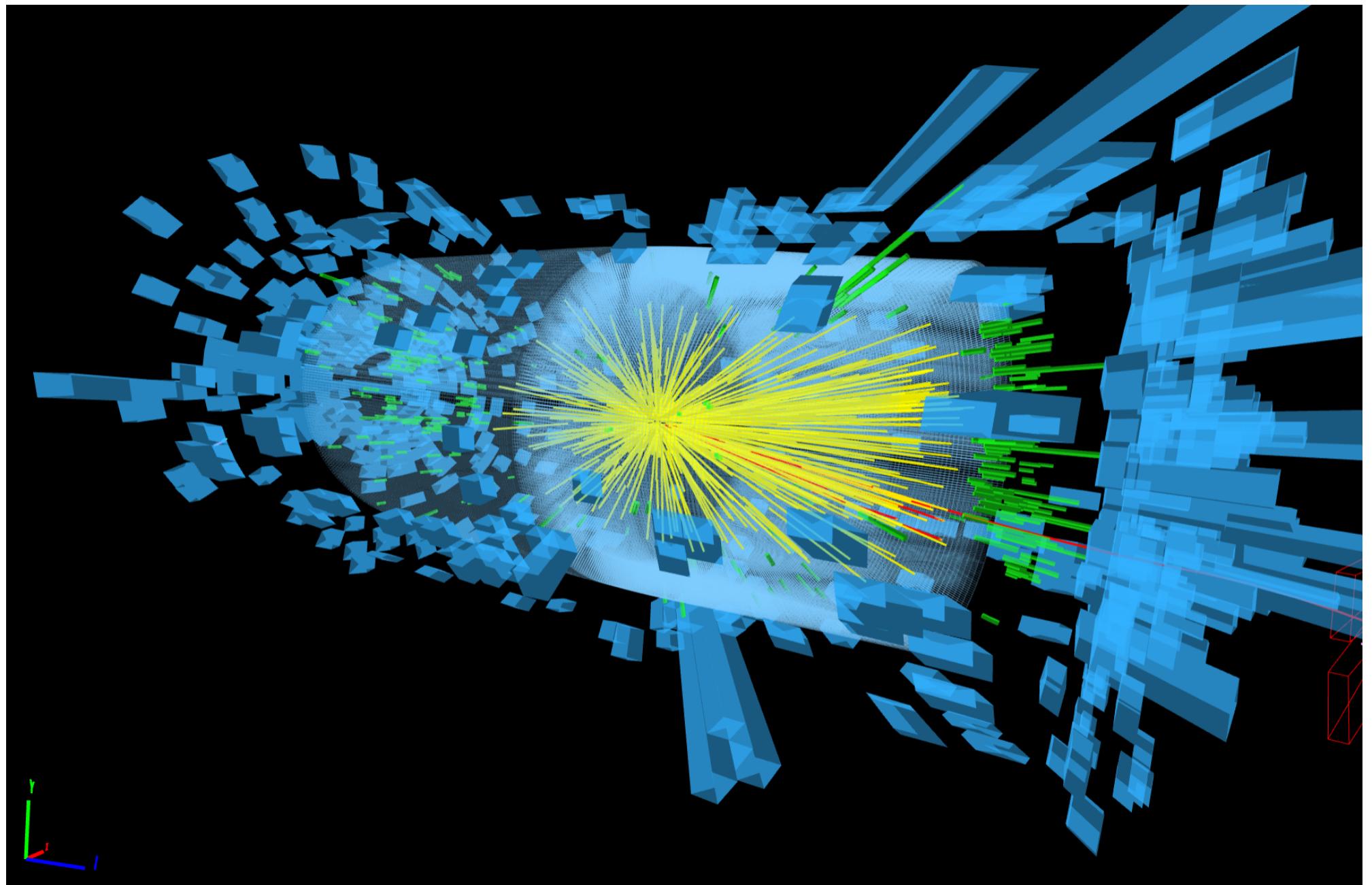
- Well-understood mechanistic model
- Simulator can generate samples

Inference:

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

Why has that not stopped us before?

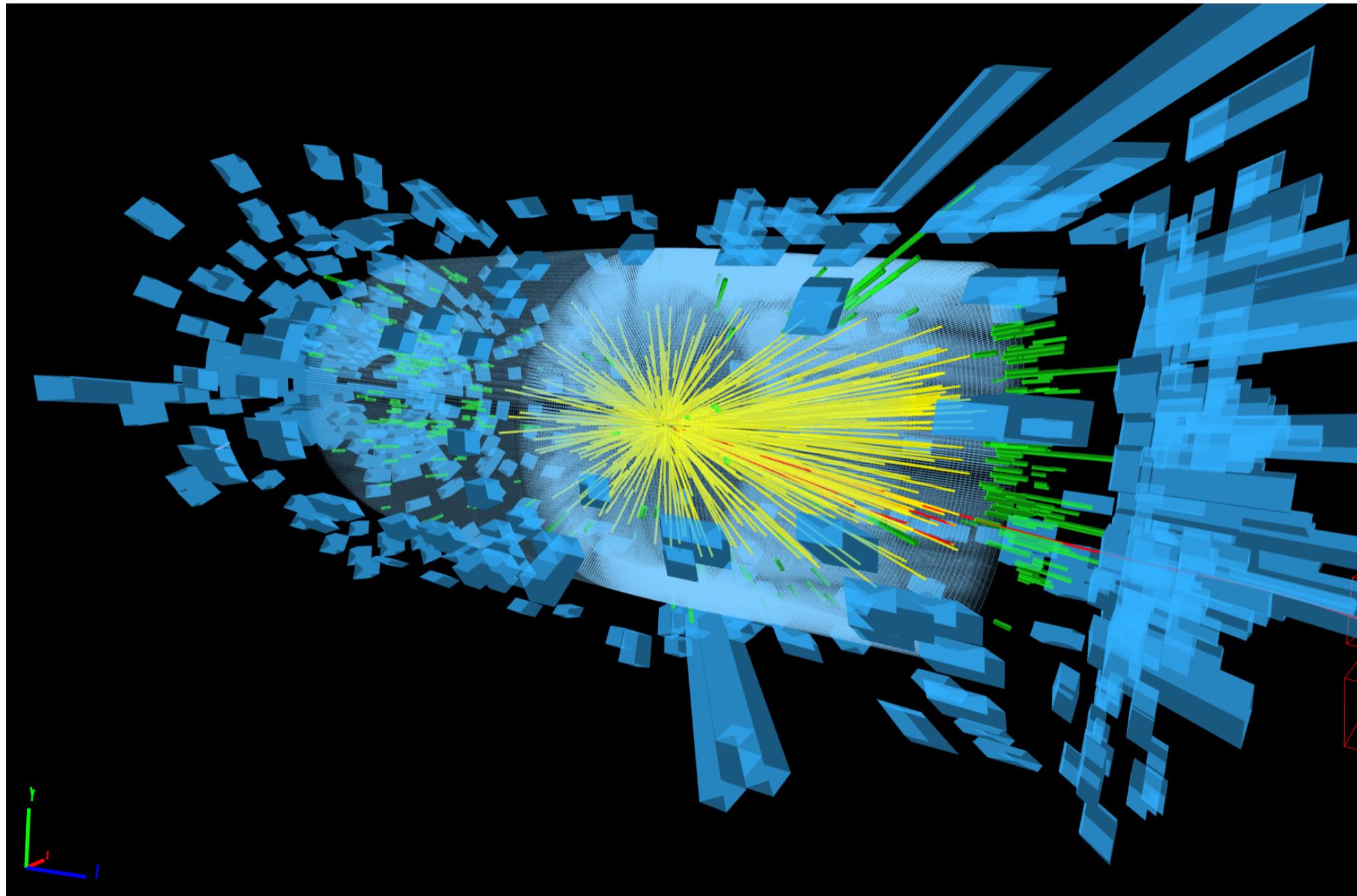
Solve it with summary statistics



High-dimensional event data x

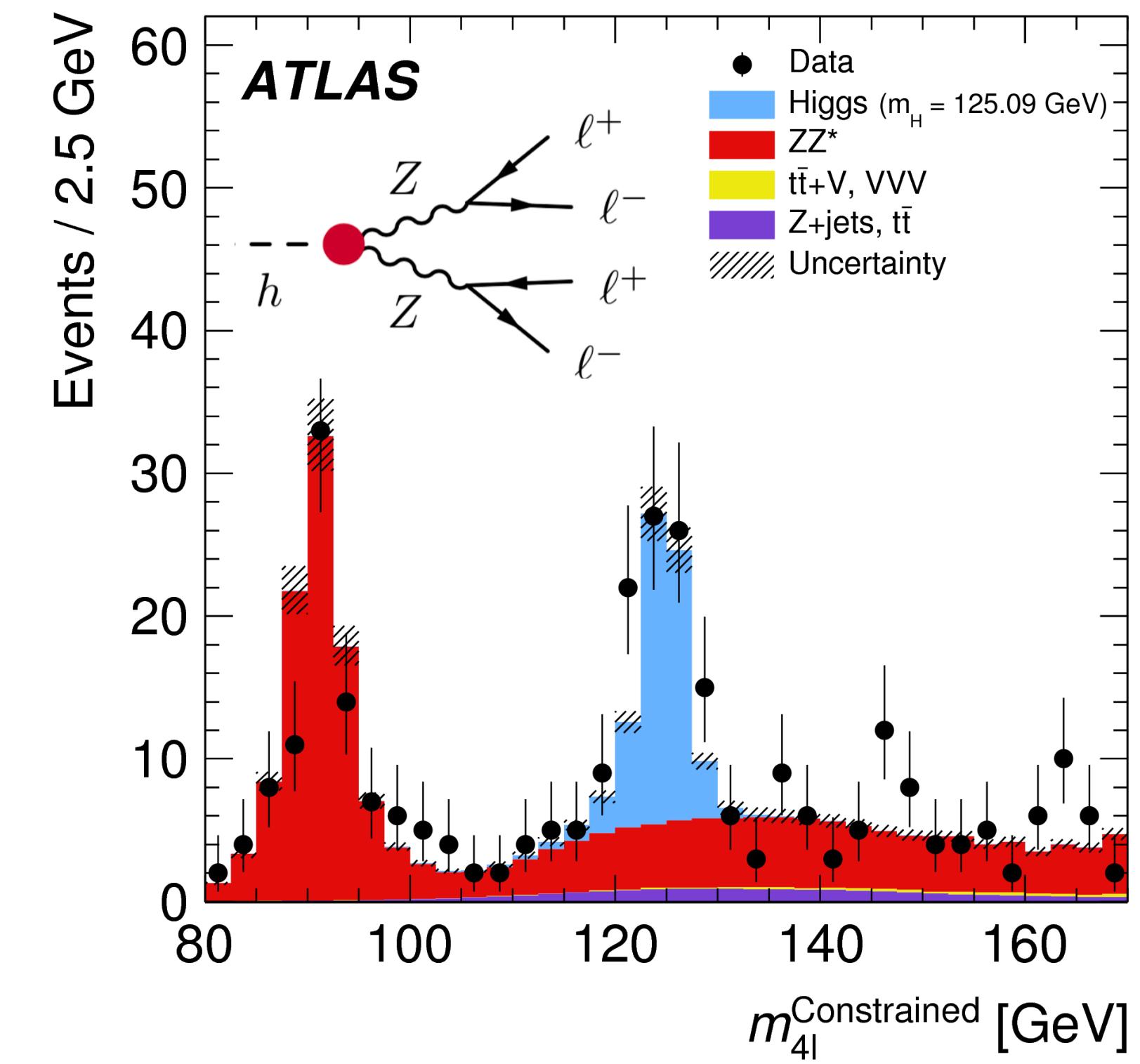
$p(x|\theta)$ cannot be calculated

Solve it with summary statistics



High-dimensional event data x

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



One or two summary statistics x'

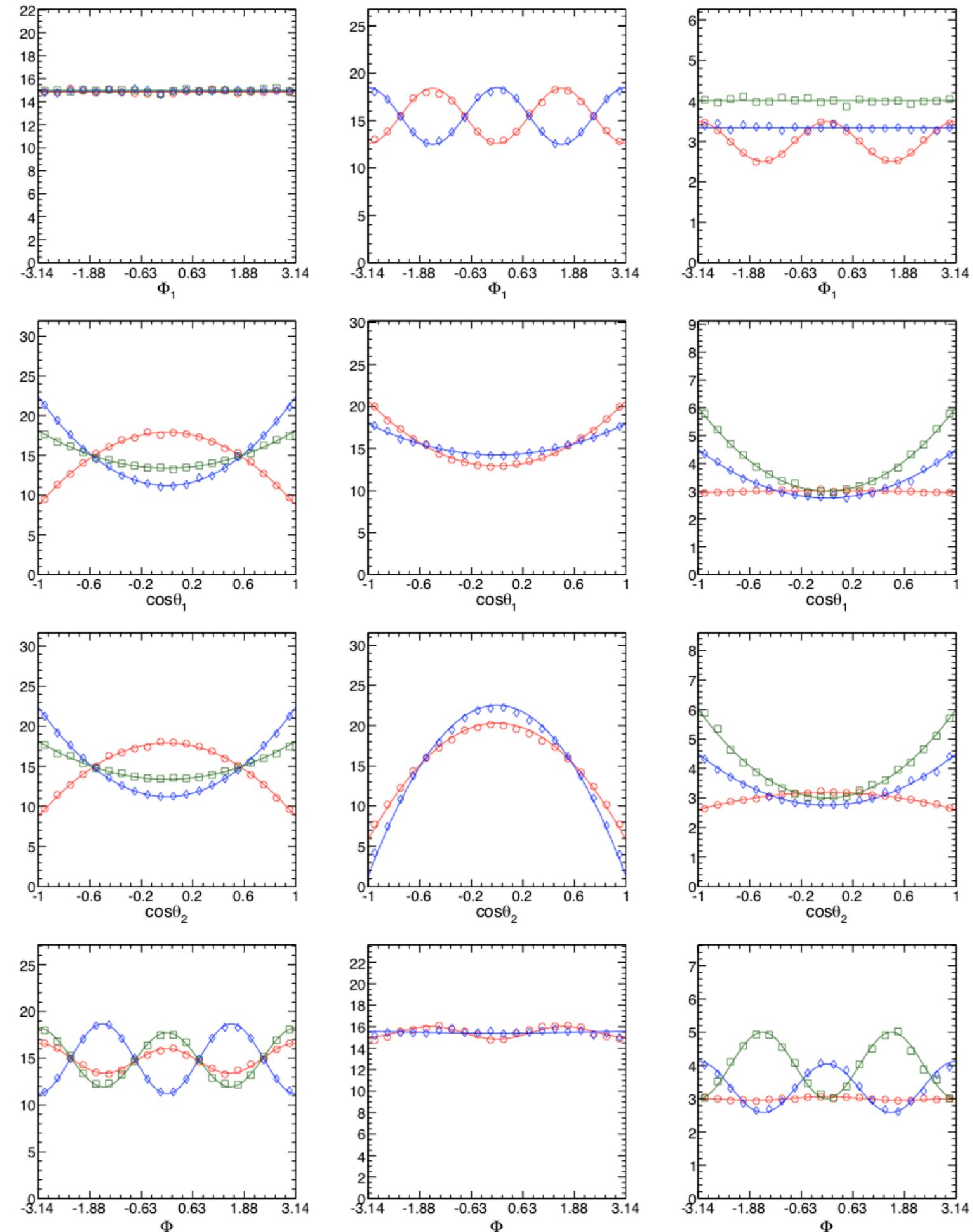
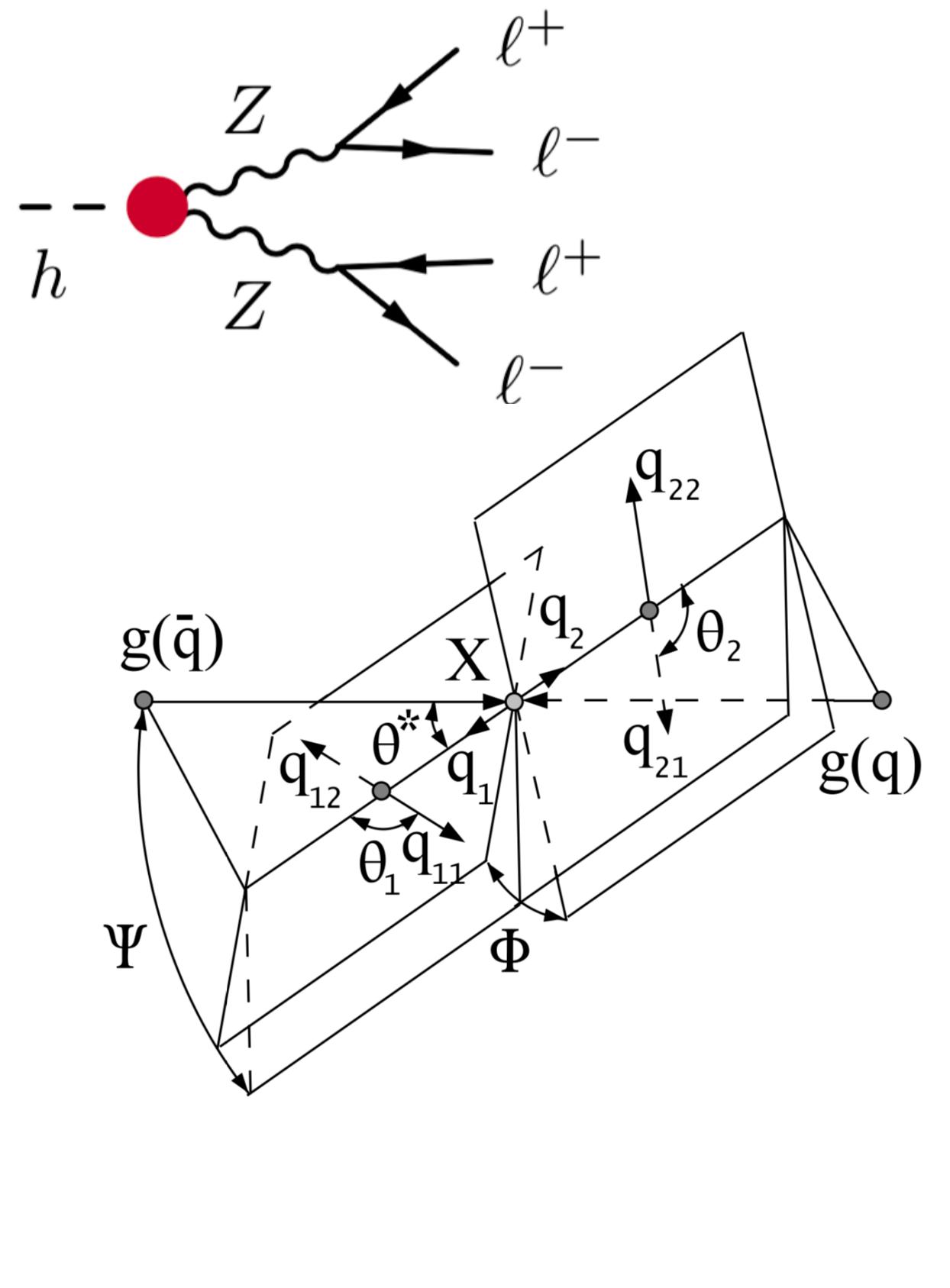
$p(x'|\theta)$ can be estimated
with histograms, KDE, ...

Summary statistics for EFT measurements?

- Choosing summary statistics x' is difficult and problem-dependent
- Often there is no single good standard variable — 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 high-dimensional x including all correlations (“fully differential cross section”)

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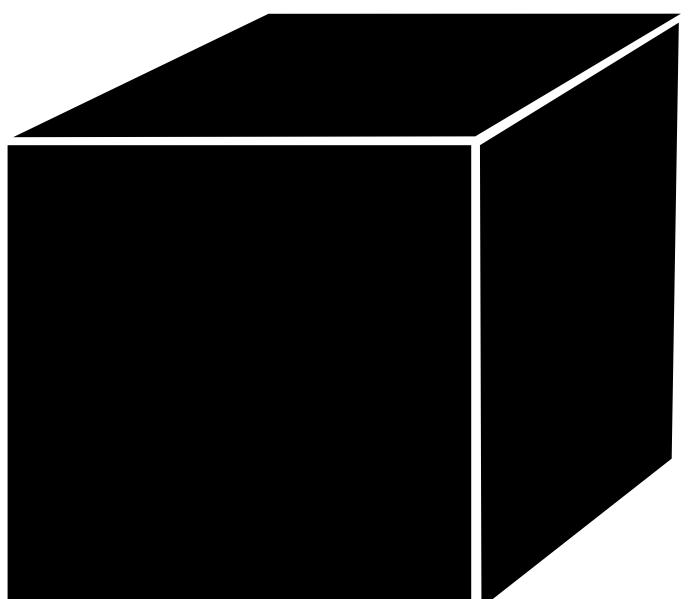


[Bolognesi et al. 1208.4018]

An incomplete list of likelihood-free inference methods

Treat simulator as black box:

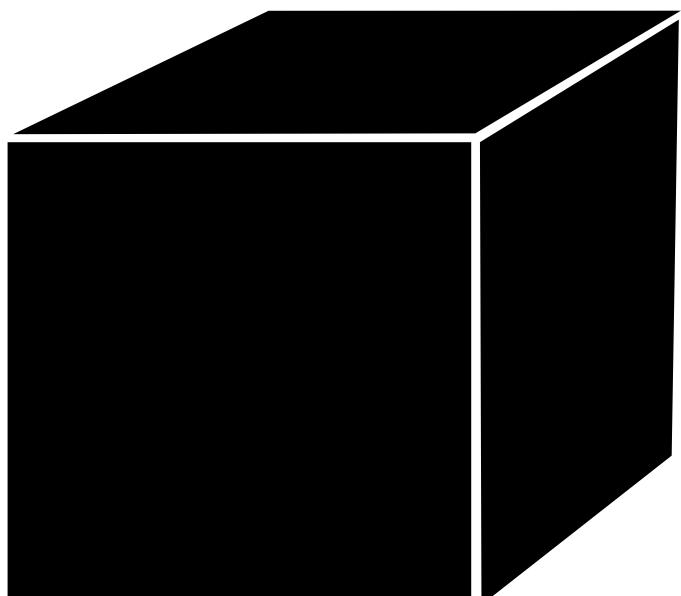
- Histograms of observables,
Approximate Bayesian Computation
Rely on summary statistics
- Machine learning techniques
Density networks, CARL, autoregressive models,
normalizing flows, ...



An incomplete list of likelihood-free inference methods

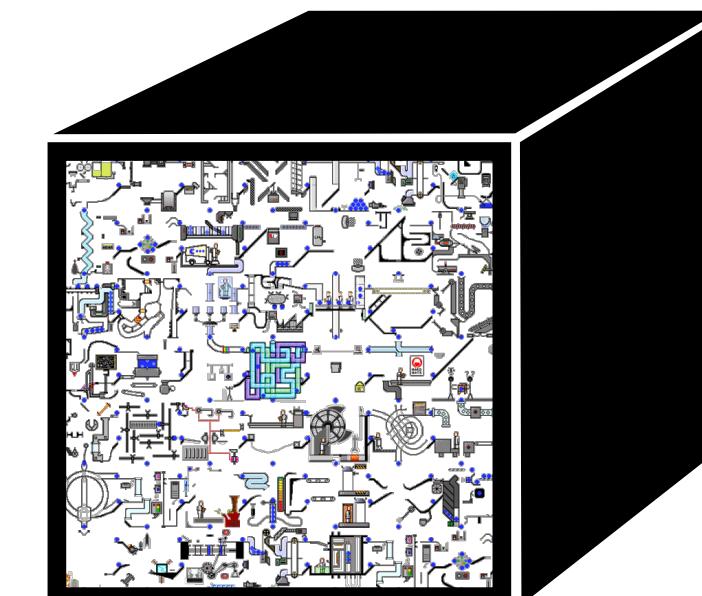
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Use physics insights:

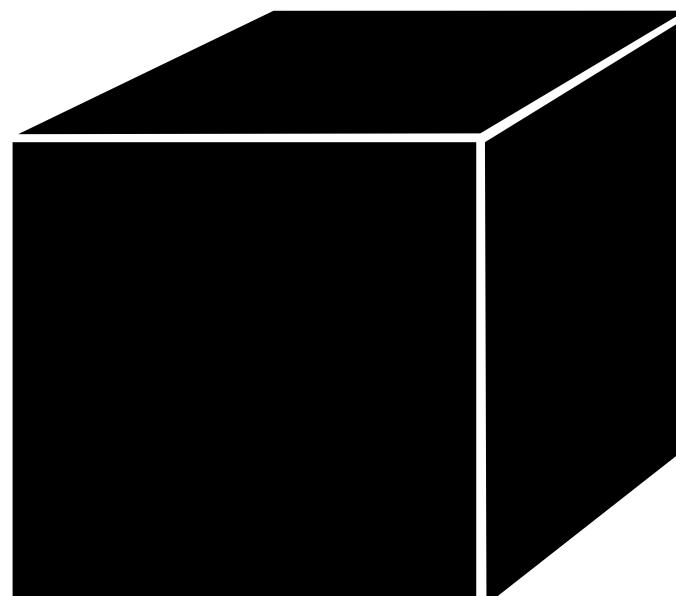
- Matrix Element Method, Optimal Observables,
Shower Deconstruction, Event Deconstruction
Neglect or approximate shower + detector,
explicitly calculate z integral



An incomplete list of likelihood-free inference methods

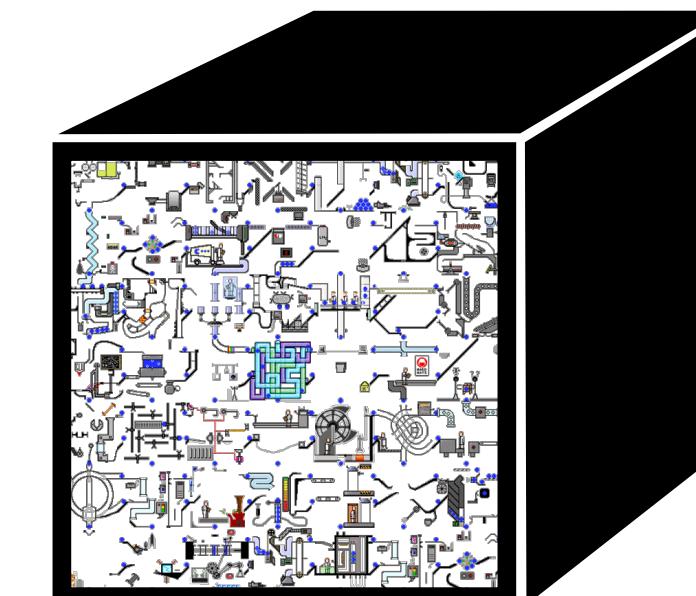
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Use physics insights:

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



New!

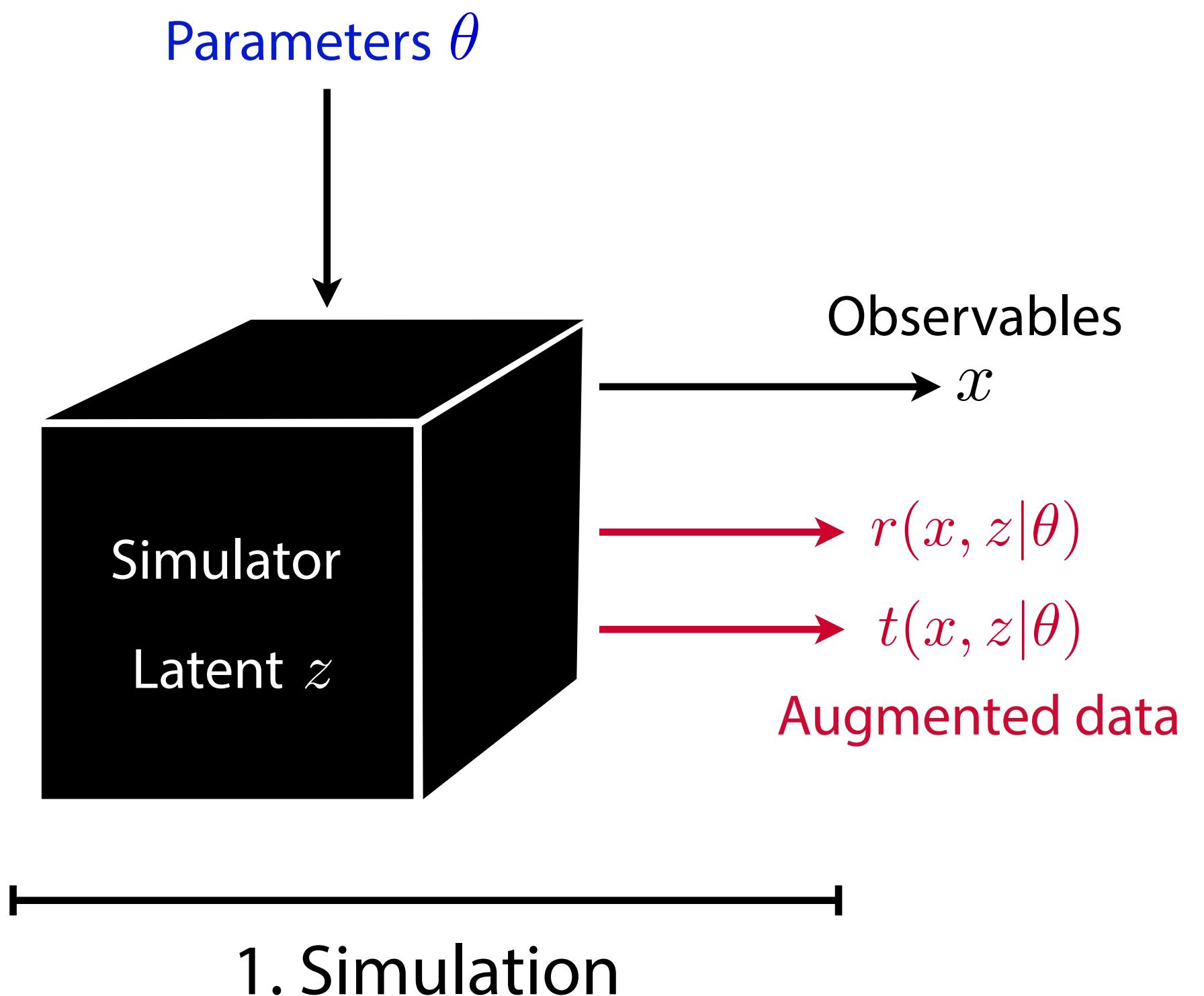
A new approach: “Mining gold” from the simulator

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

What if we could estimate the likelihood...

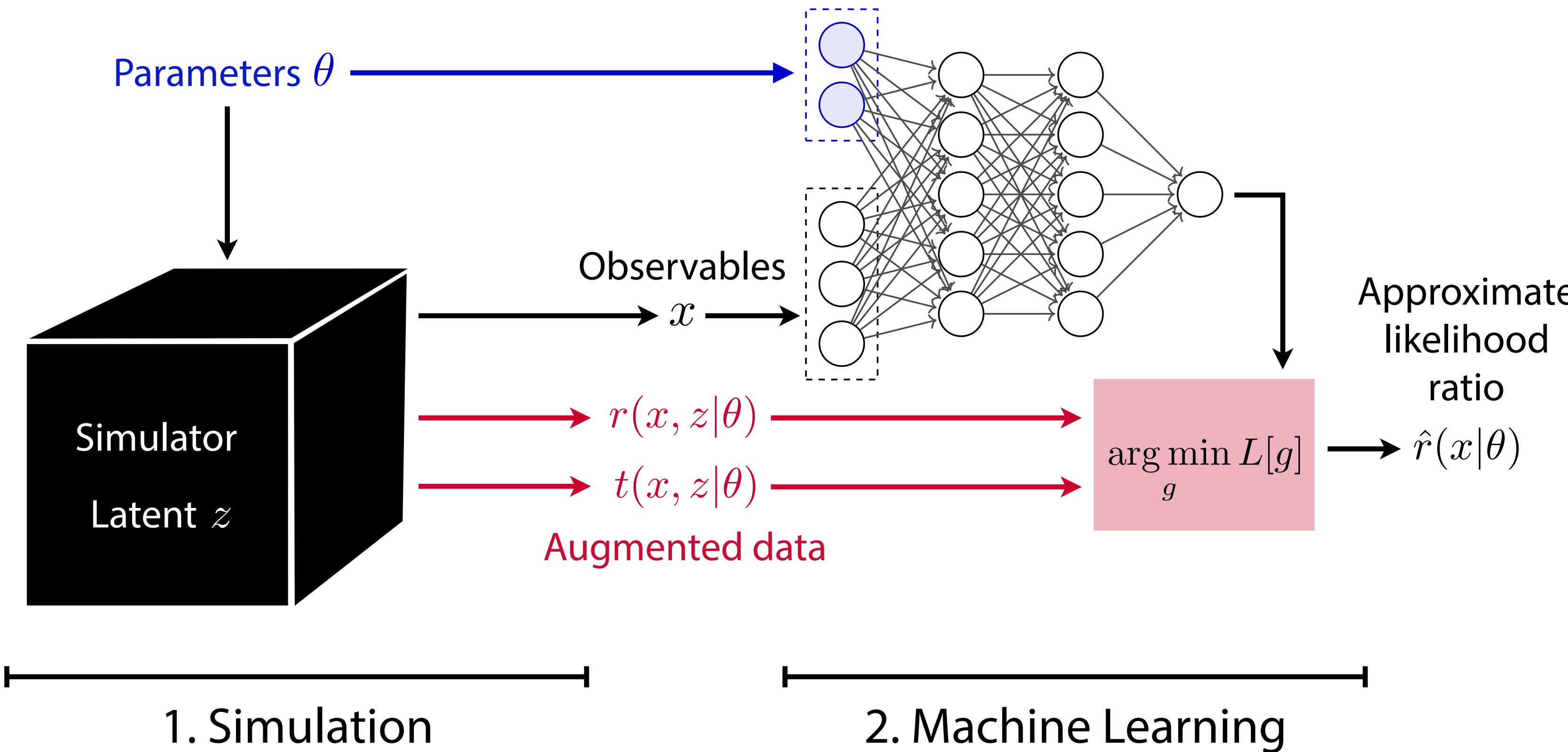
- for high-dimensional observables, including correlations?
like MEM: no need to pick summary statistics
- including state-of-the-art shower and detector models?
allowing for extra radiation, no need for transfer functions
- in microseconds?
amortized inference: train once, then always evaluate fast
- requiring less training examples than established machine learning methods?
using matrix element information: “ML version of MEM”

Bird's-eye view



“Mining gold”: Extract additional information from simulator

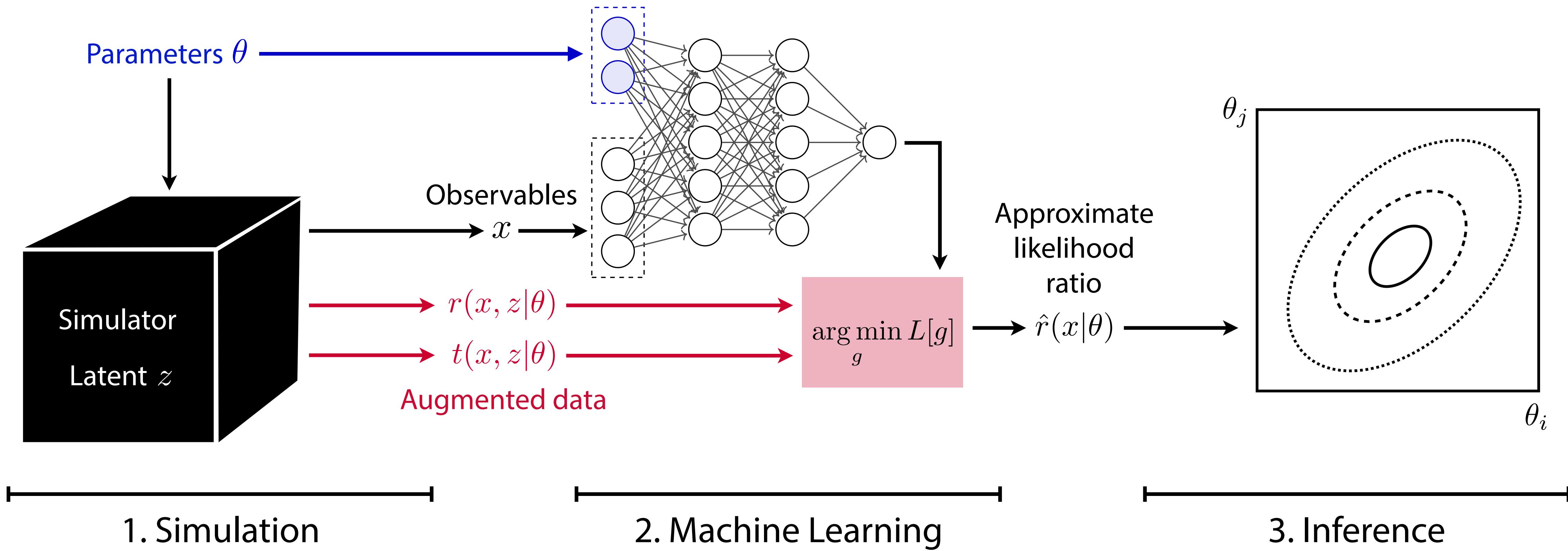
Bird's-eye view



“Mining gold”: Extract additional information from simulator

Use this information to train estimator for likelihood ratio

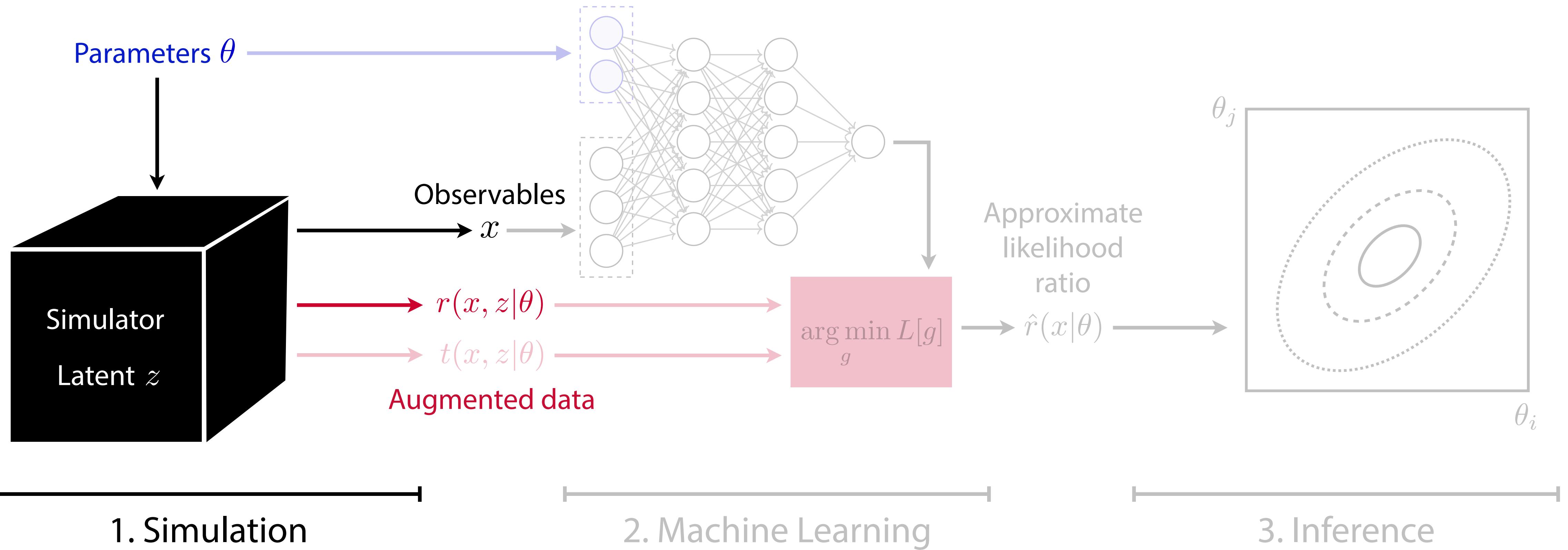
Bird's-eye view



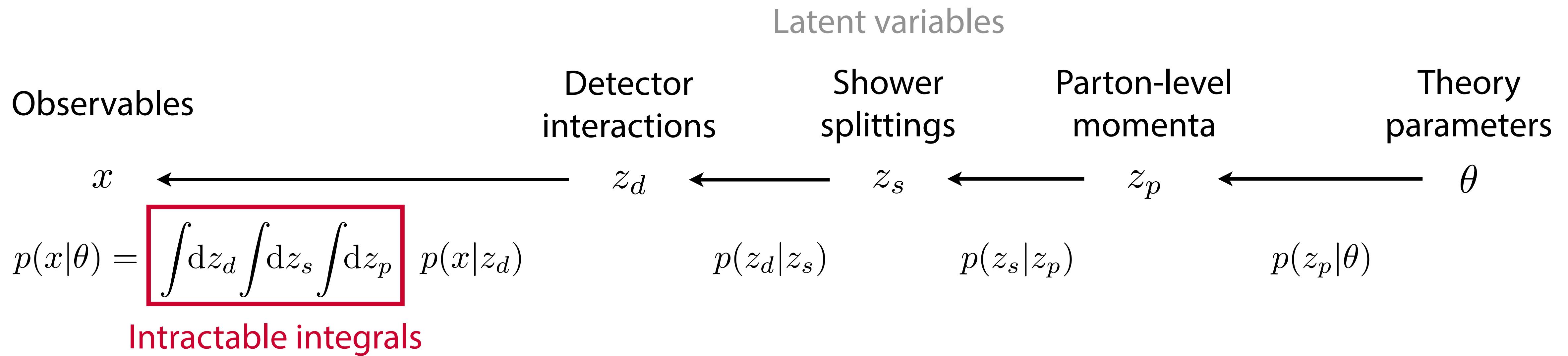
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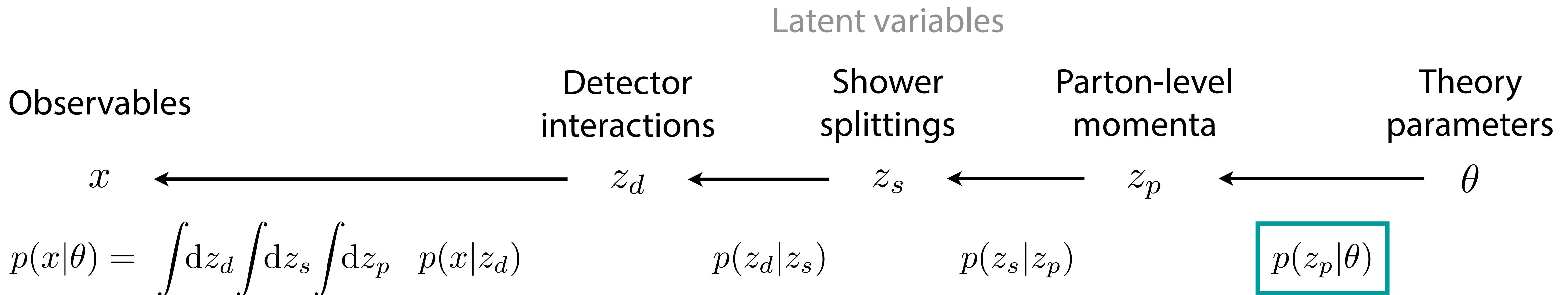
Limit setting with standard hypothesis tests



Mining gold from the simulator



Mining gold from the simulator

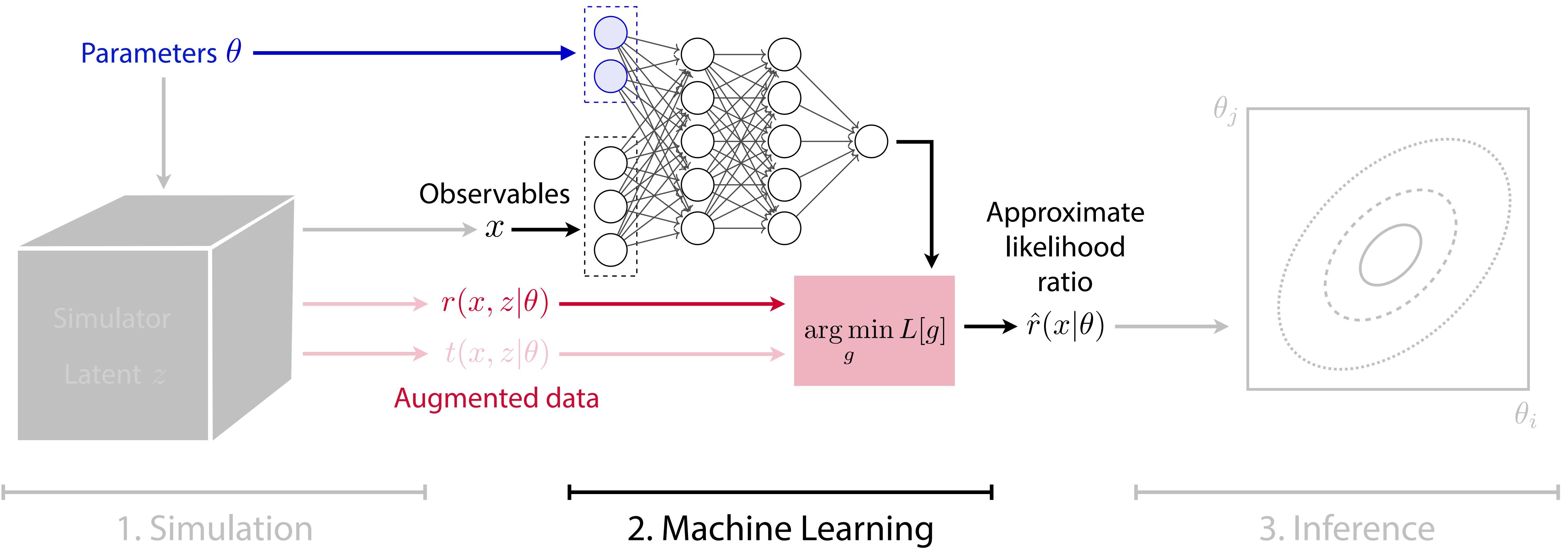


Parton-level likelihood
is given by matrix element
and can be evaluated!

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

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

$$\frac{p(z_p|\theta_0)}{p(z_p|\theta_1)} \sim \frac{|\mathcal{M}(z_p|\theta_0)|^2}{|\mathcal{M}(z_p|\theta_1)|^2}$$



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 ?)

We want the **likelihood ratio function**

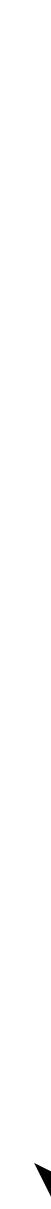
$$r(x | \theta_0, \theta_1) \equiv \frac{p(x | \theta_0)}{p(x | \theta_1)}$$

("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

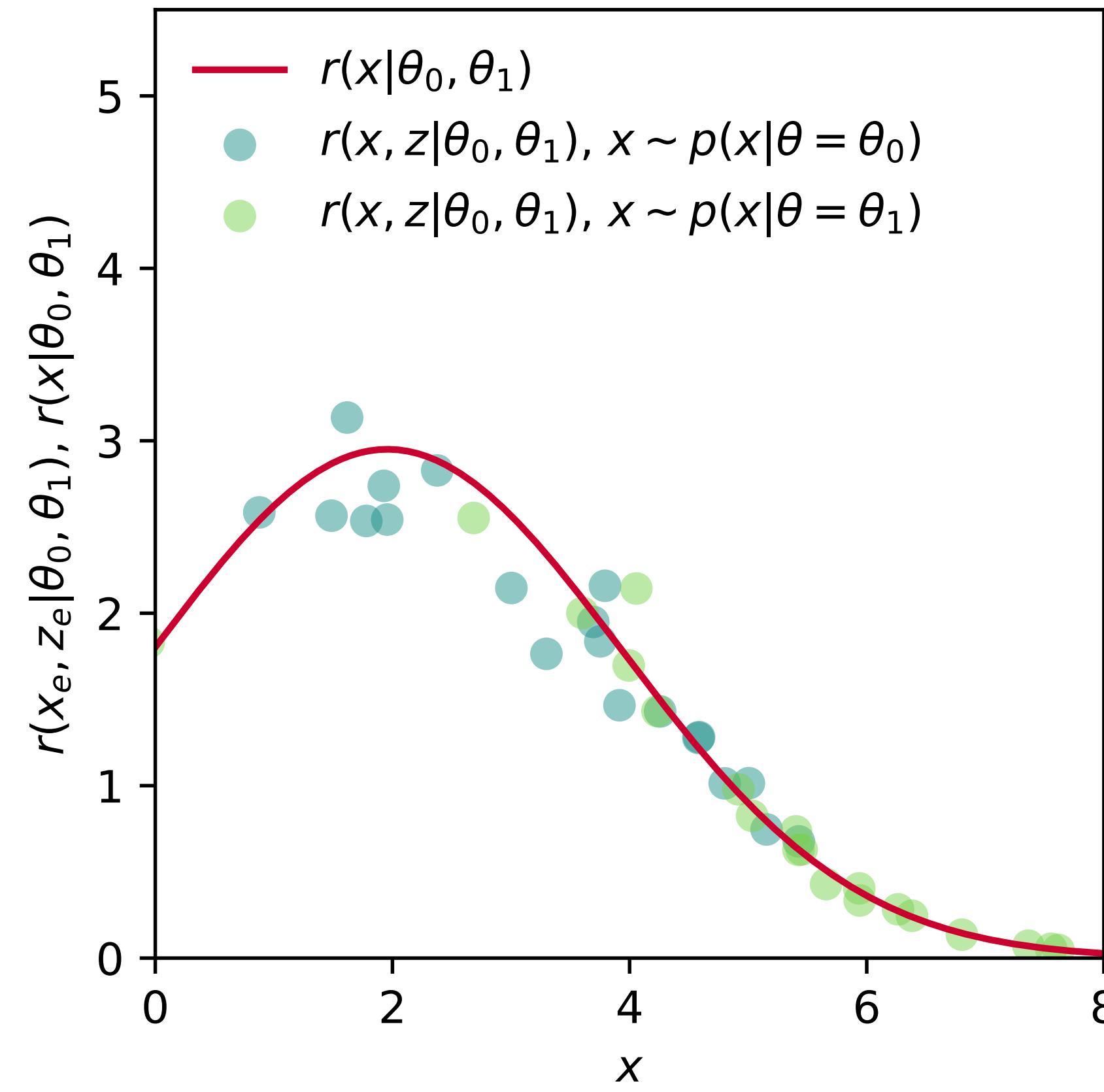
$$r(x, z | \theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p | \theta_0)}{p(x, z_d, z_s, z_p | \theta_1)}$$



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

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

It is minimized by

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

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

We want the likelihood ratio function

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

Machine learning = applied calculus of variations

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

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

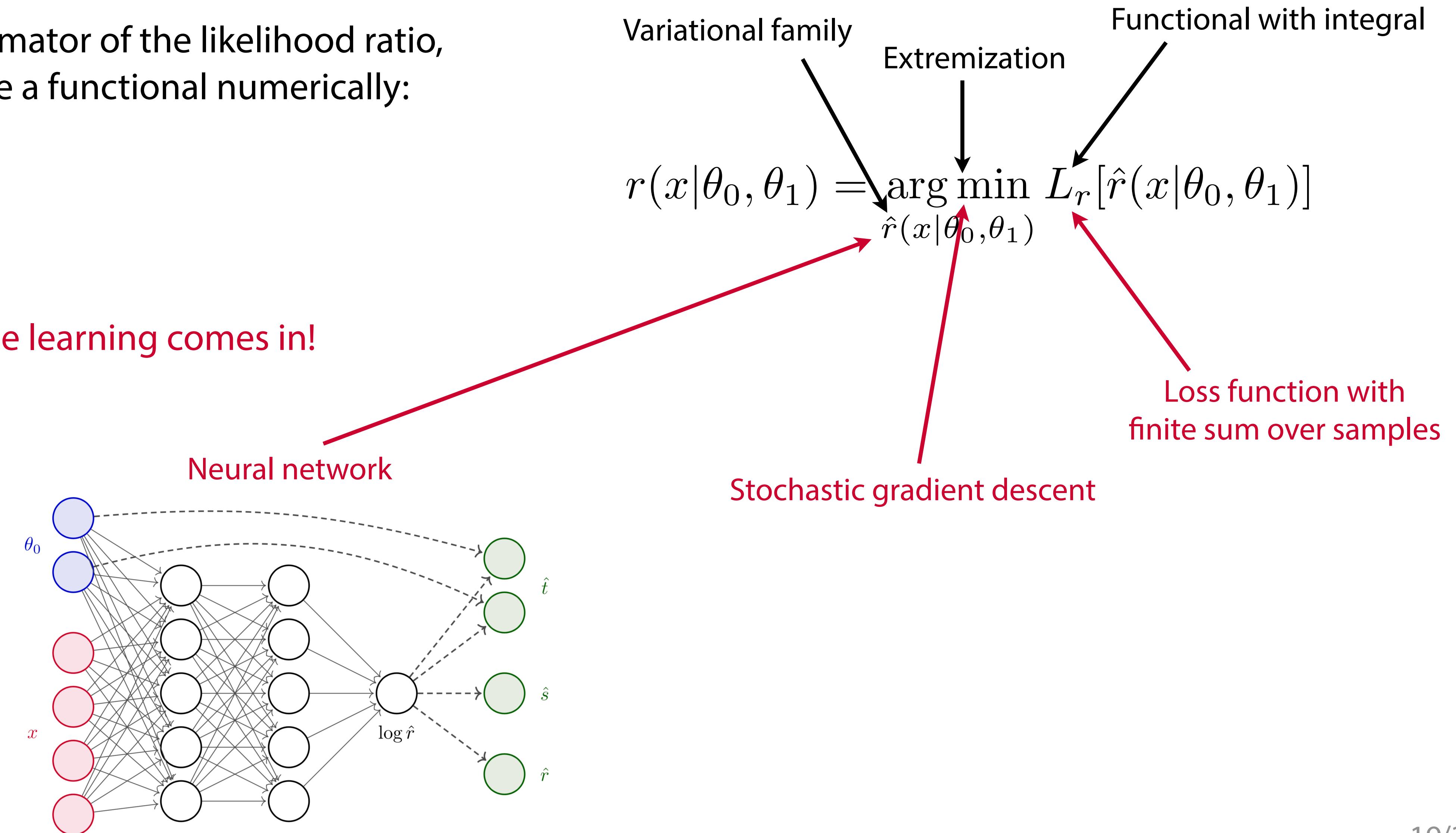
Variational family Extremization Functional with integral

```
graph TD; A[Variational family] --> B[Extremization]; B --> C[Functional with integral];
```

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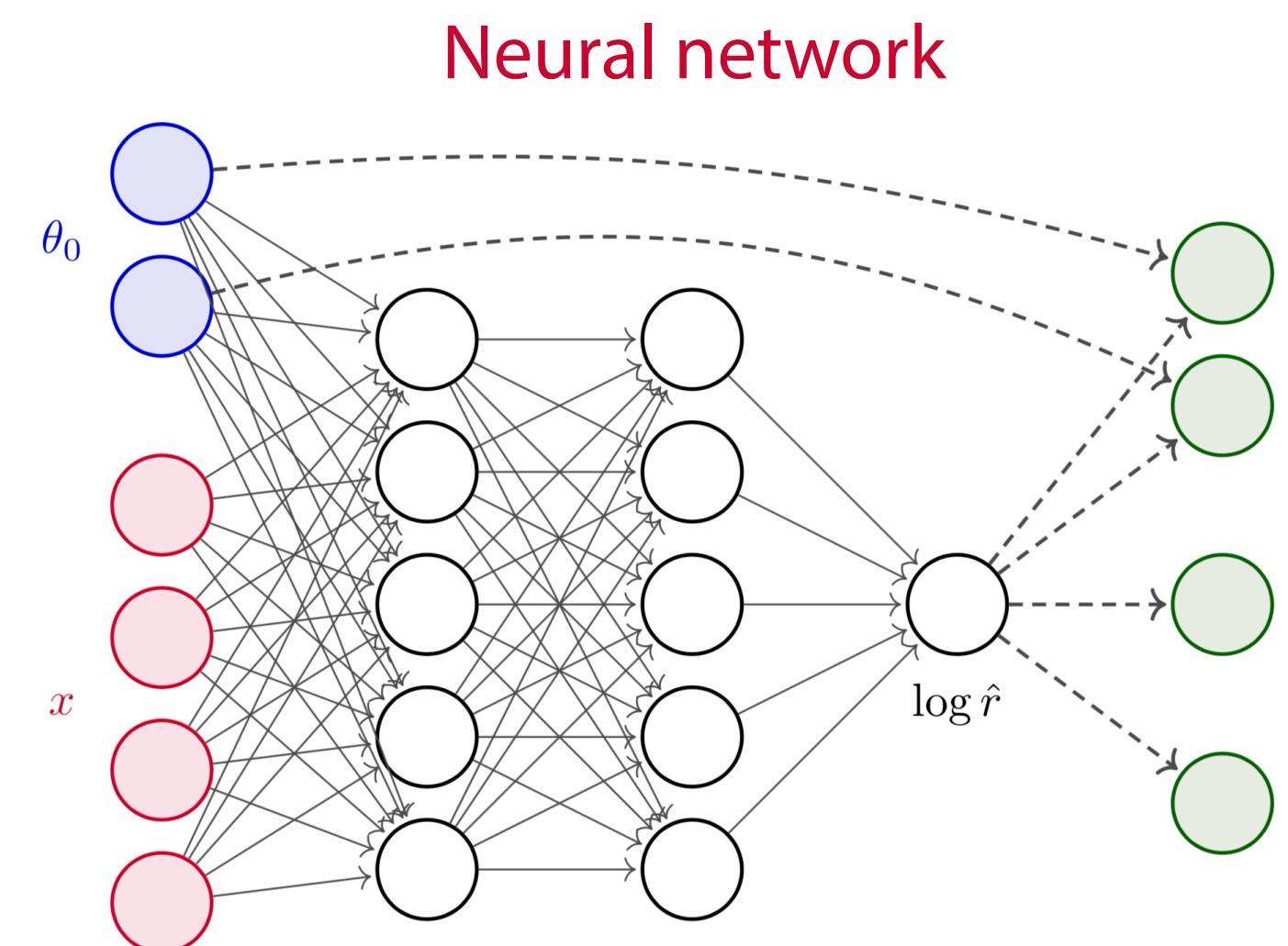
This is where machine learning comes in!



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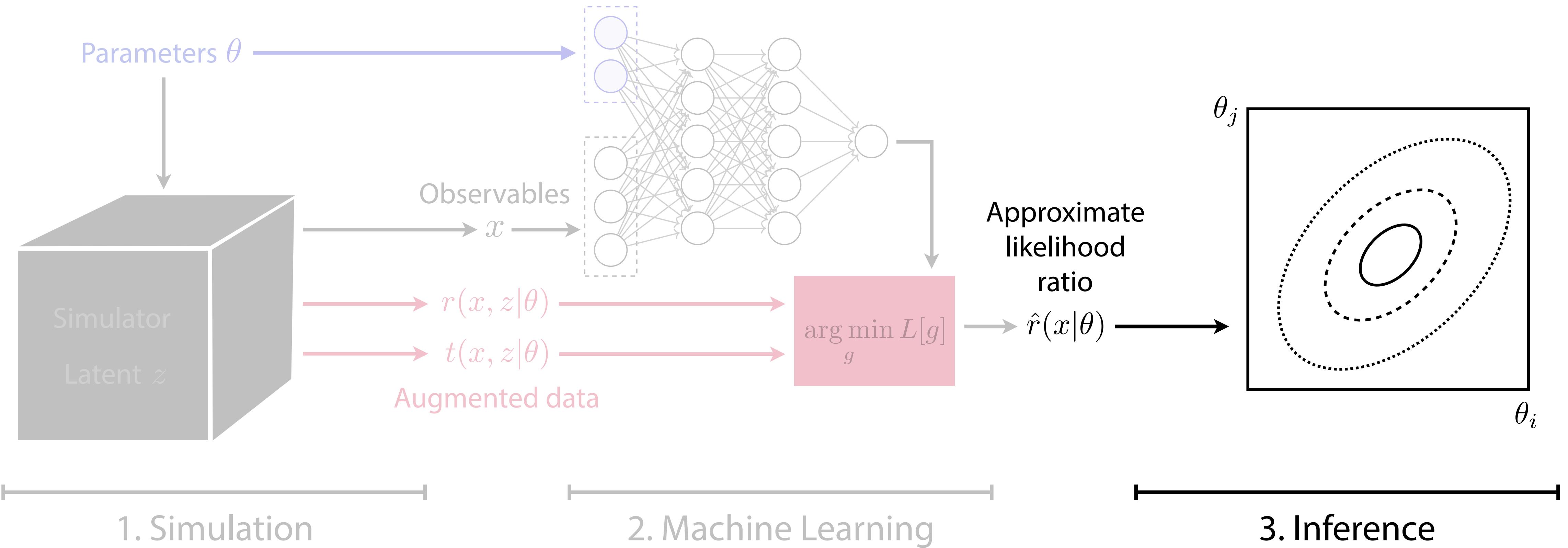
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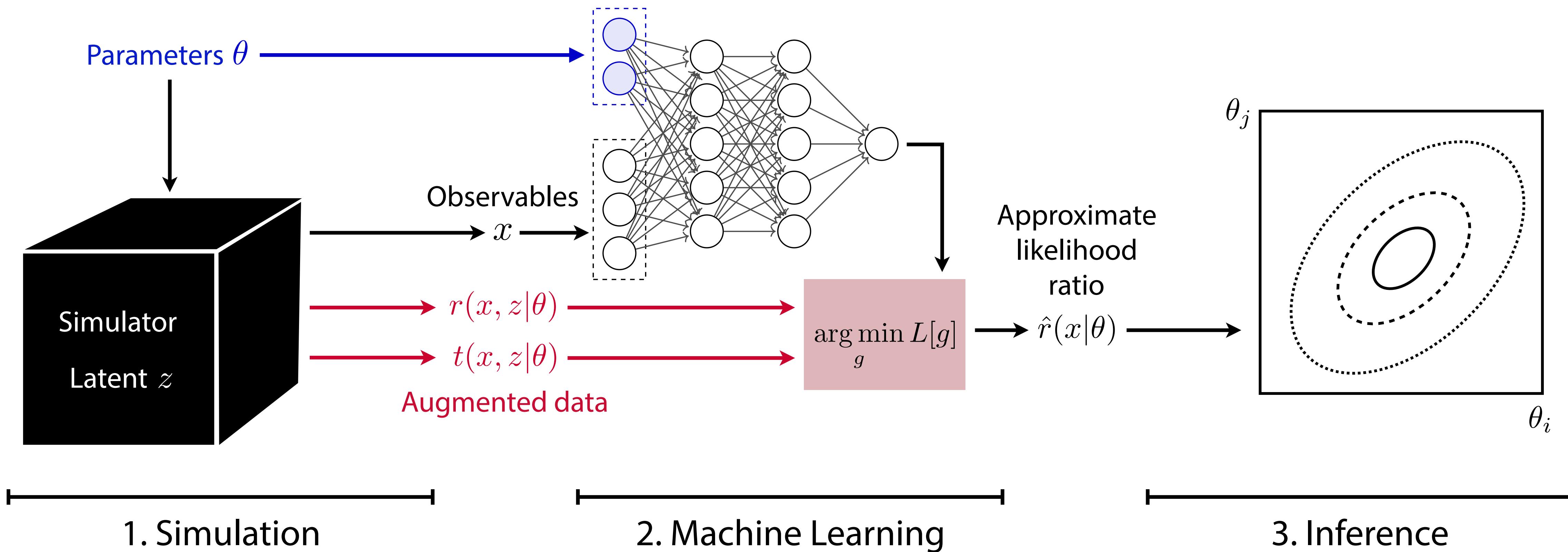
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Variational family
Extremization
Functional with integral
Loss function with finite sum over samples
Stochastic gradient descent

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



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



“The machine learning version of the Matrix Element Method”

Learning optimal observables

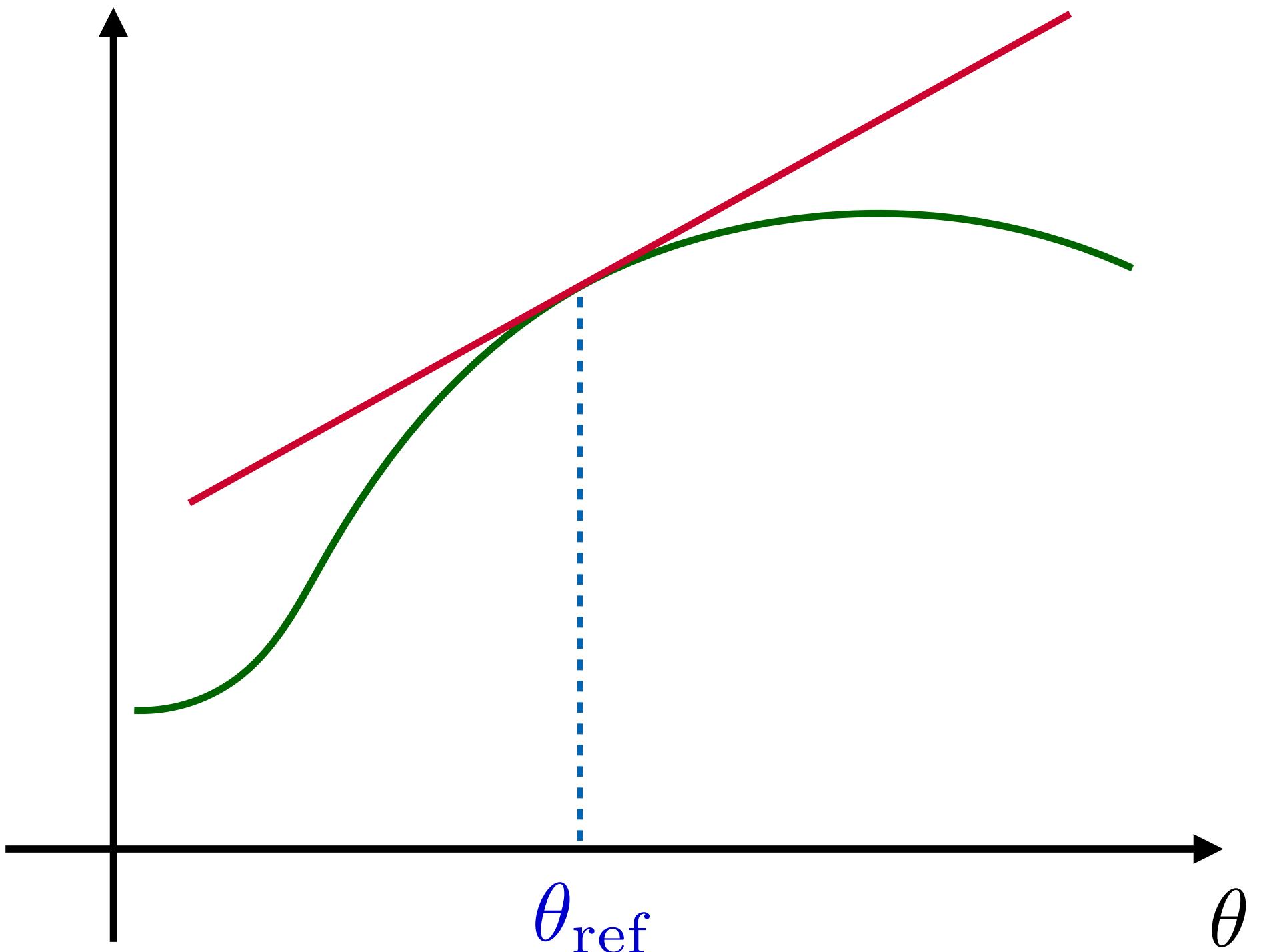
[JB, K. Cranmer, G. Louppe, J. Pavez 1805.00013, 1805.00020, 1805.12244]

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} :

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



The local model

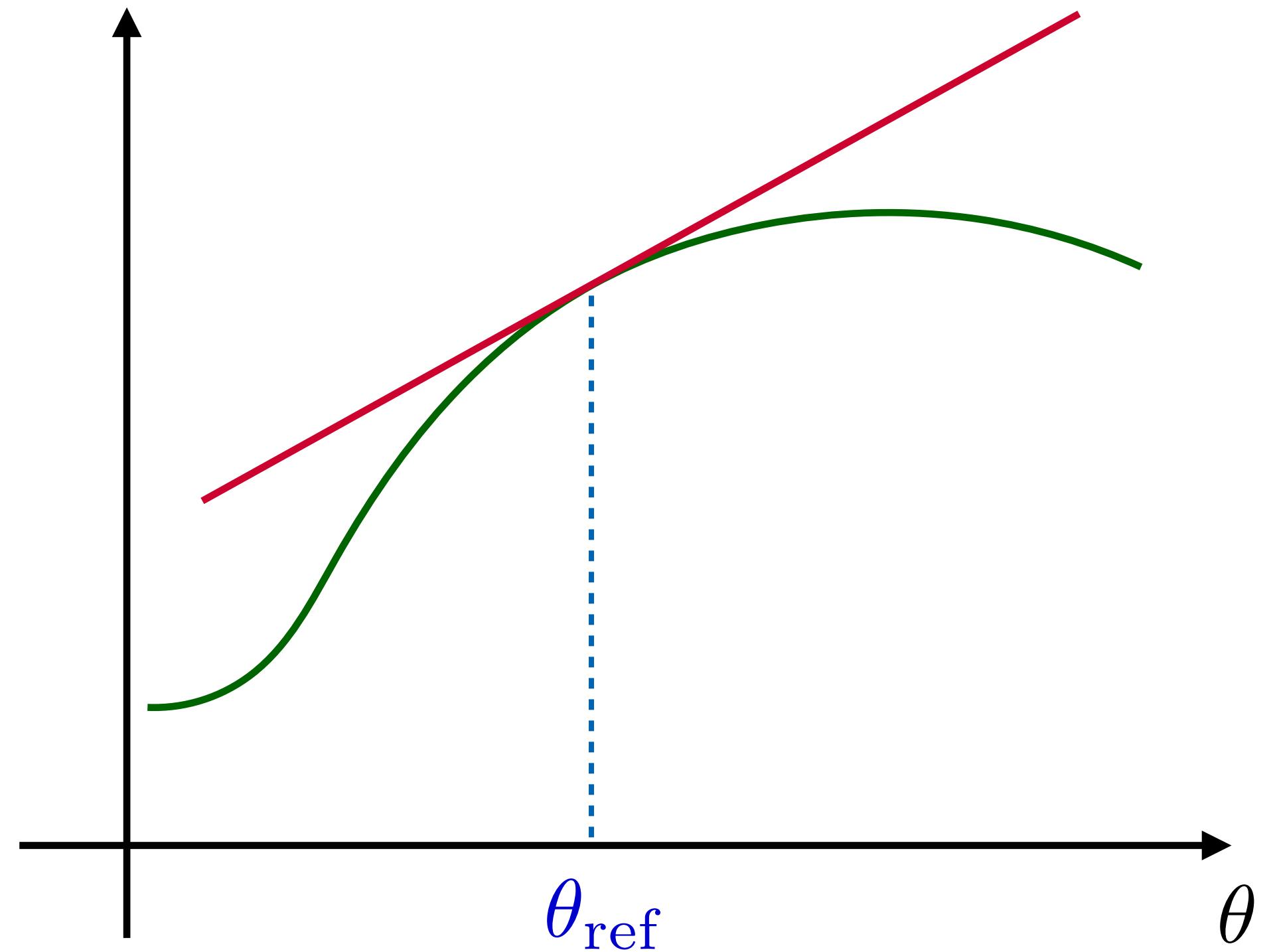
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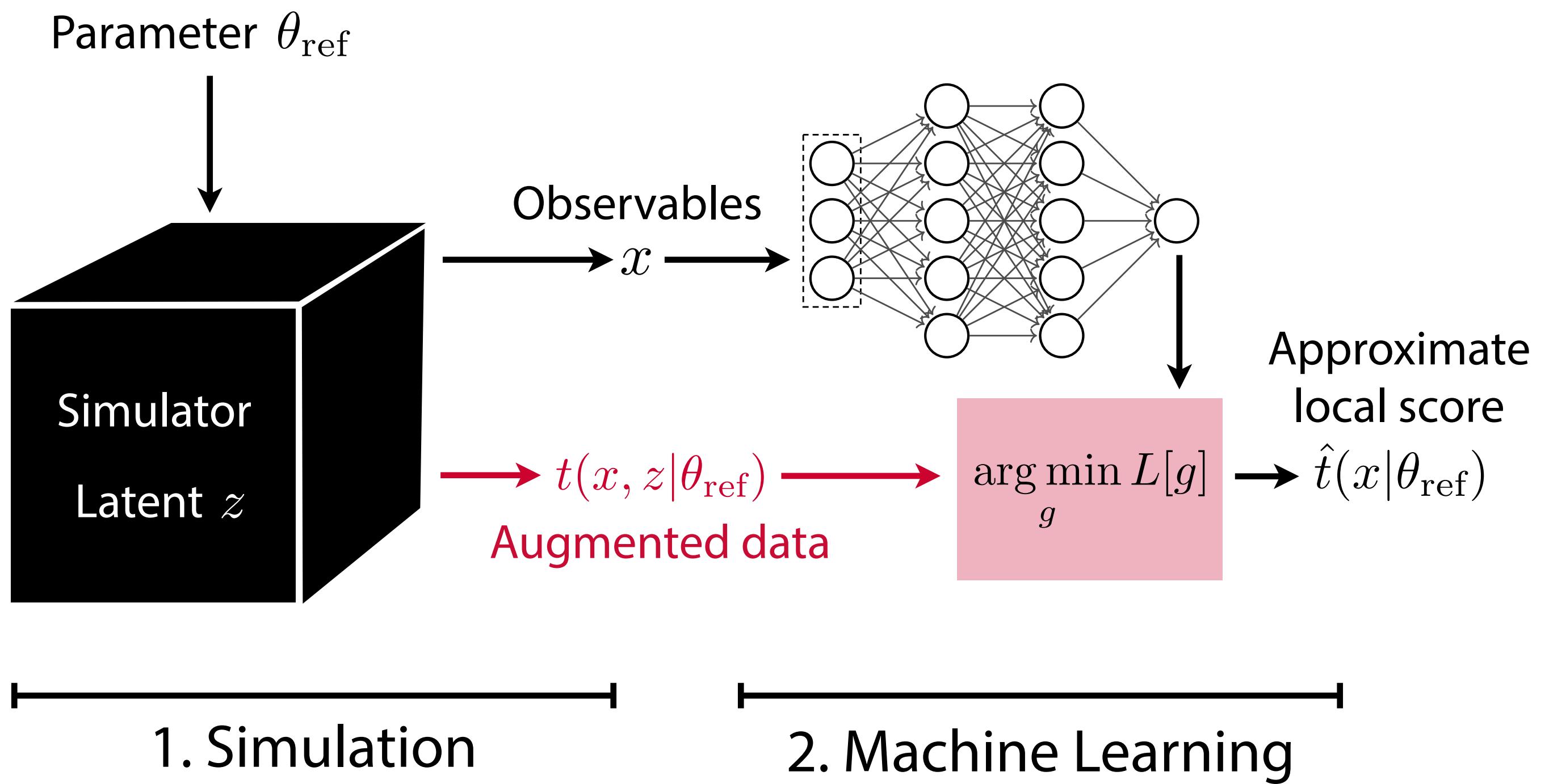
In the neighborhood of θ_{ref} (e.g. close to the SM):

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

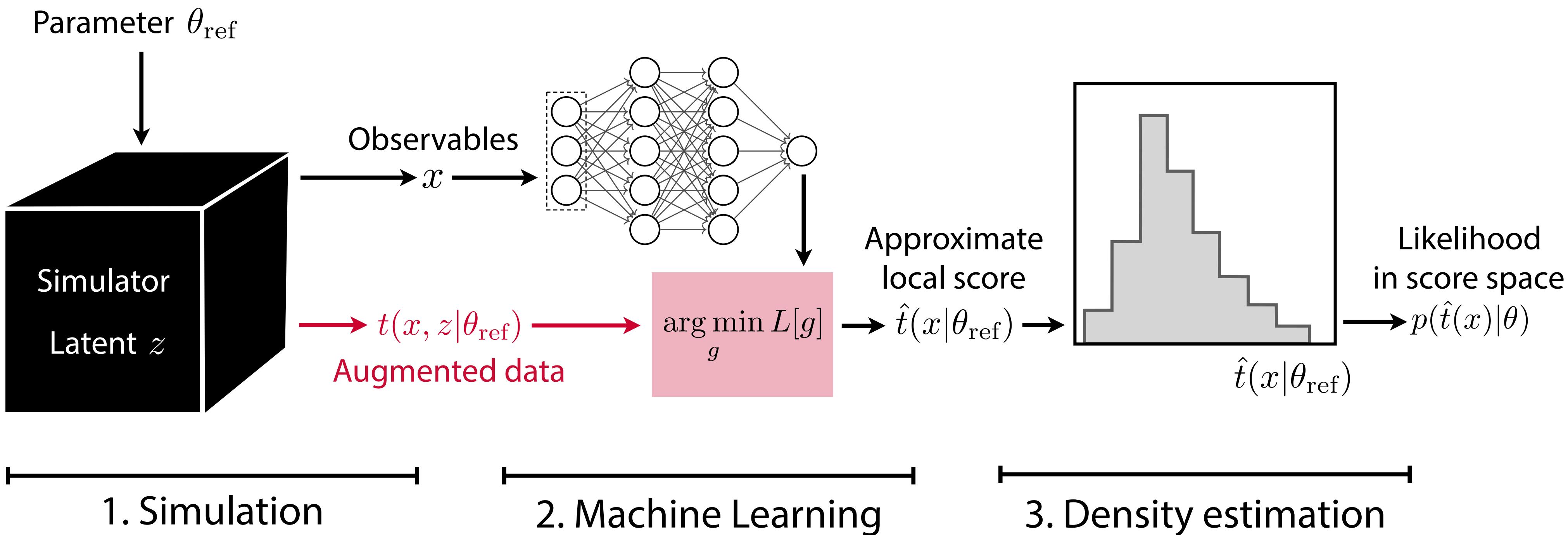


The score itself is intractable. But we can use the same trick as for the likelihood ratio!

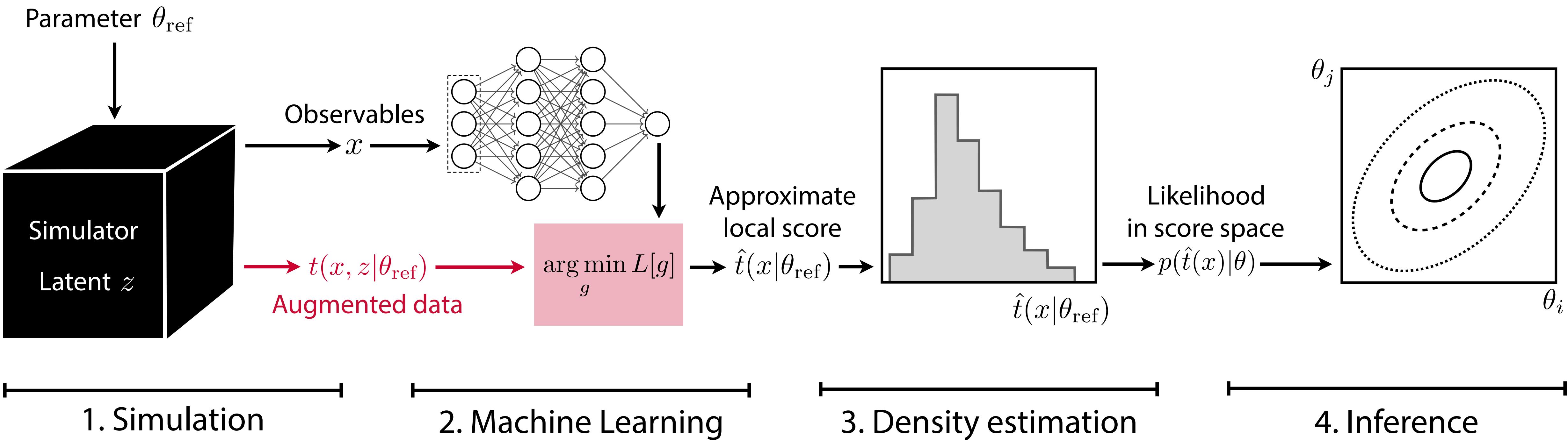
SALLY (Score approximates likelihood locally)



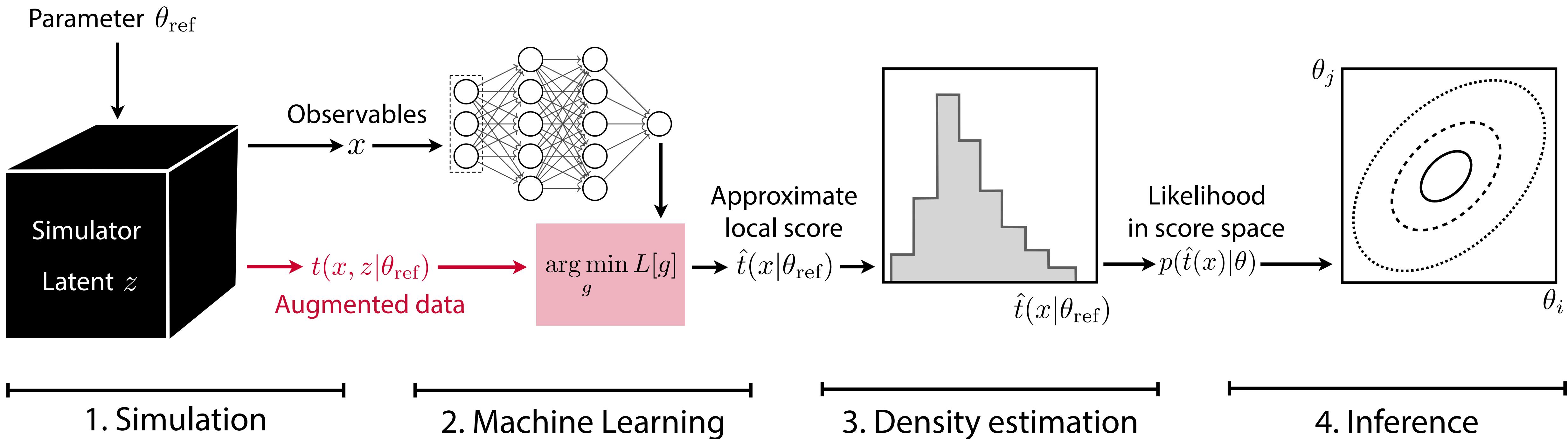
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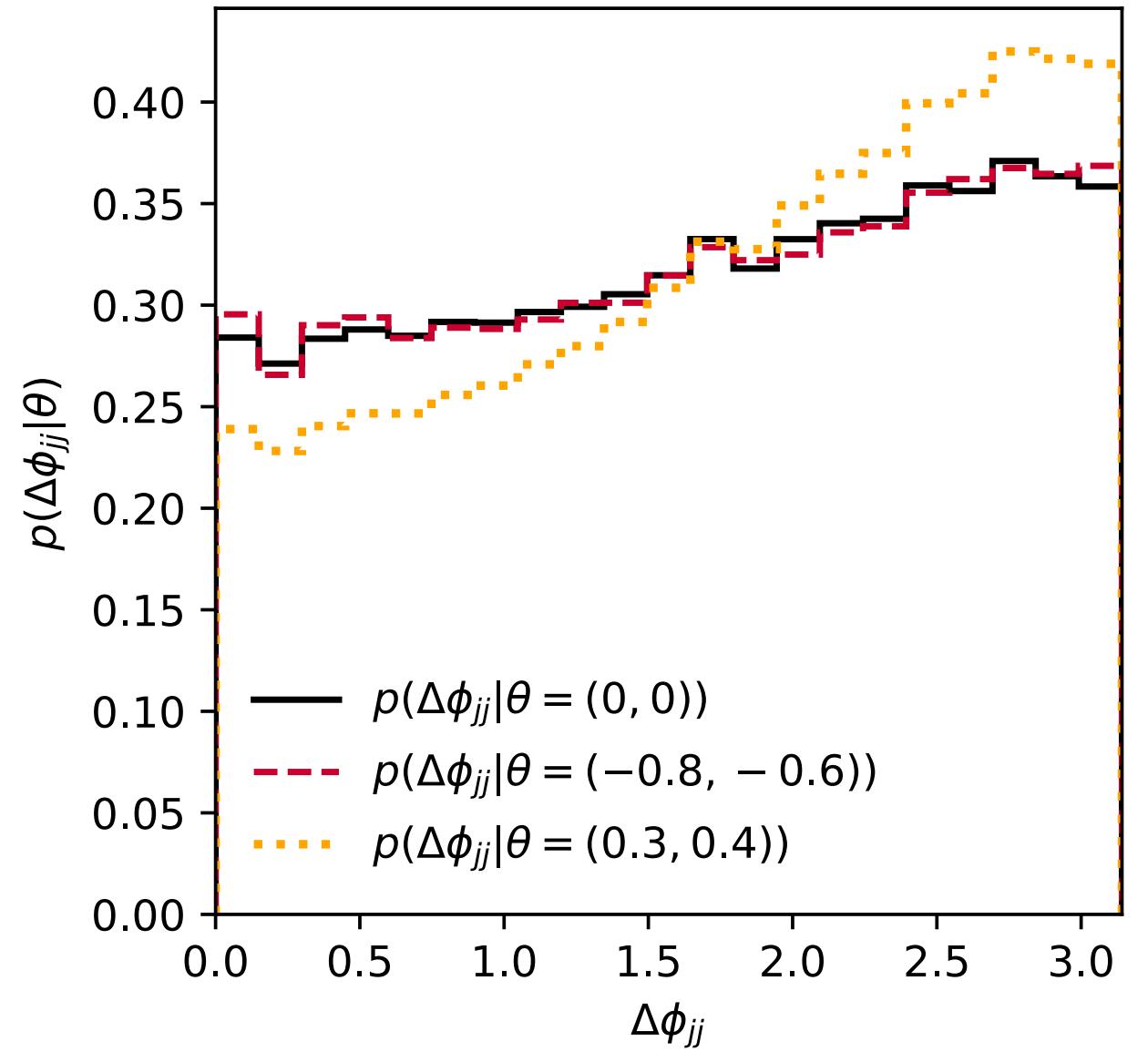
SALLY (Score approximates likelihood locally)



“The machine learning version of Optimal Observables”:

- Simpler & more robust than RASCAL
- Just as powerful close to θ_{ref} , but can lead to suboptimal limits further away

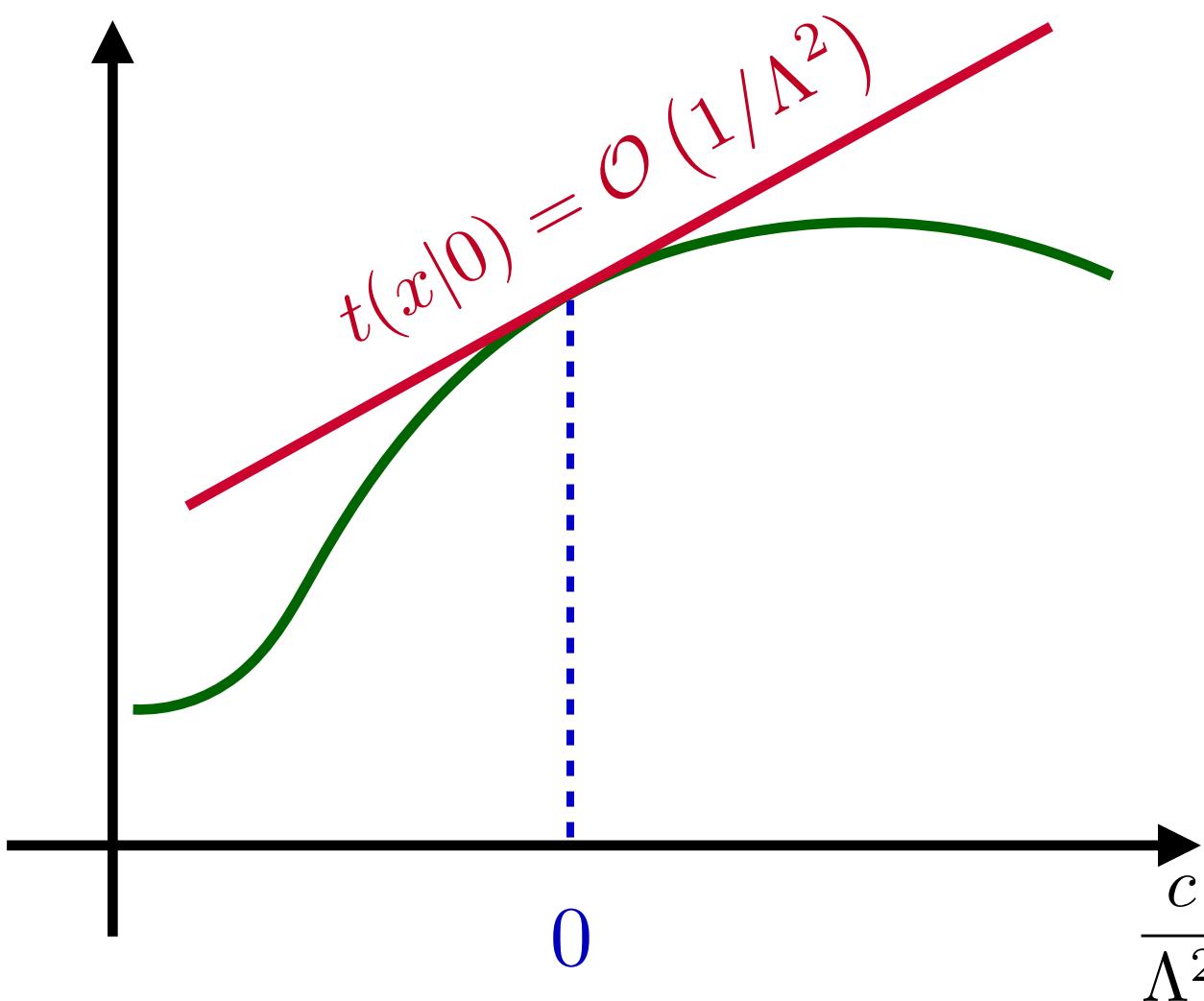
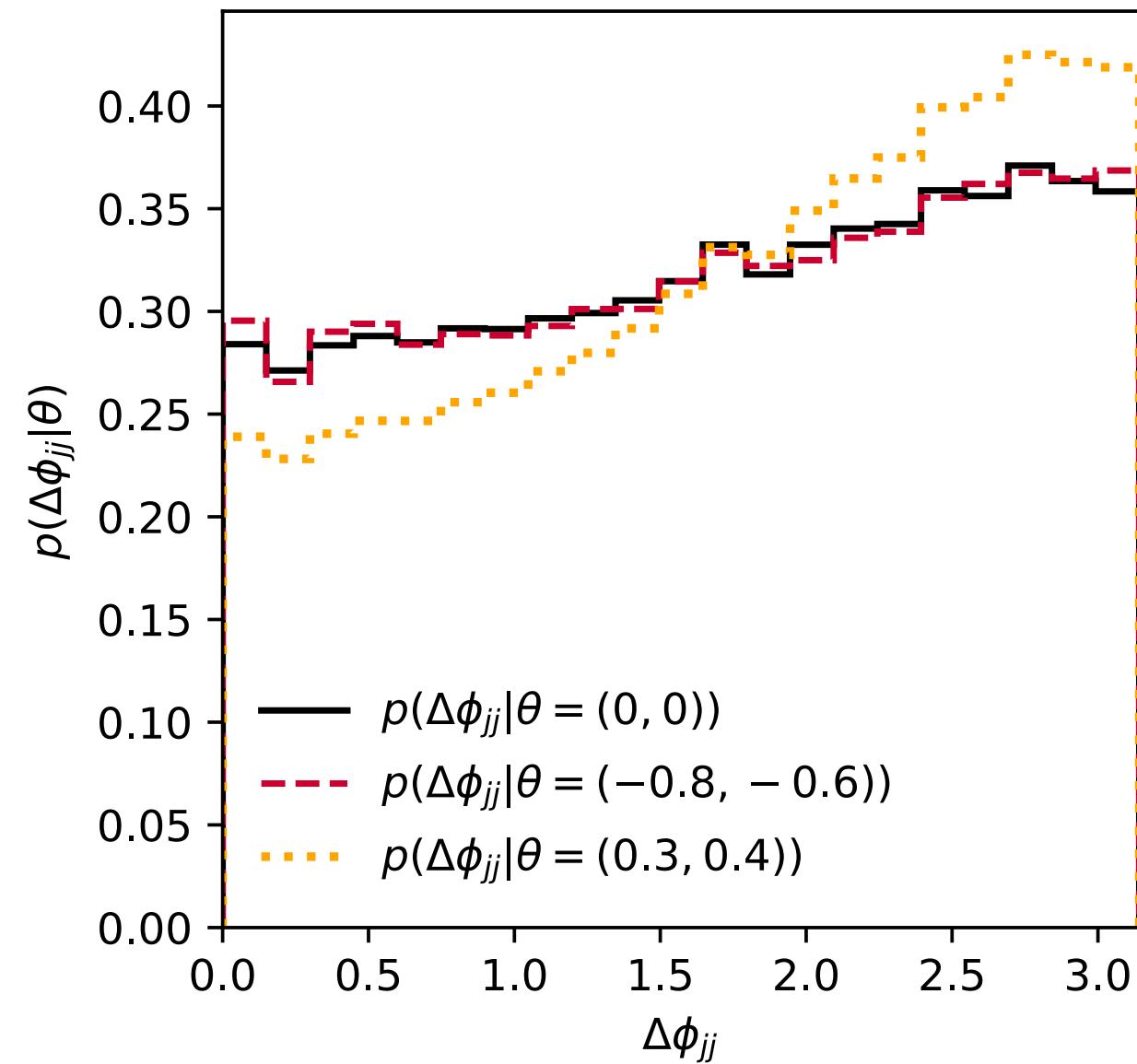
Perfect match for EFT measurements



- Good for subtle kinematic effects

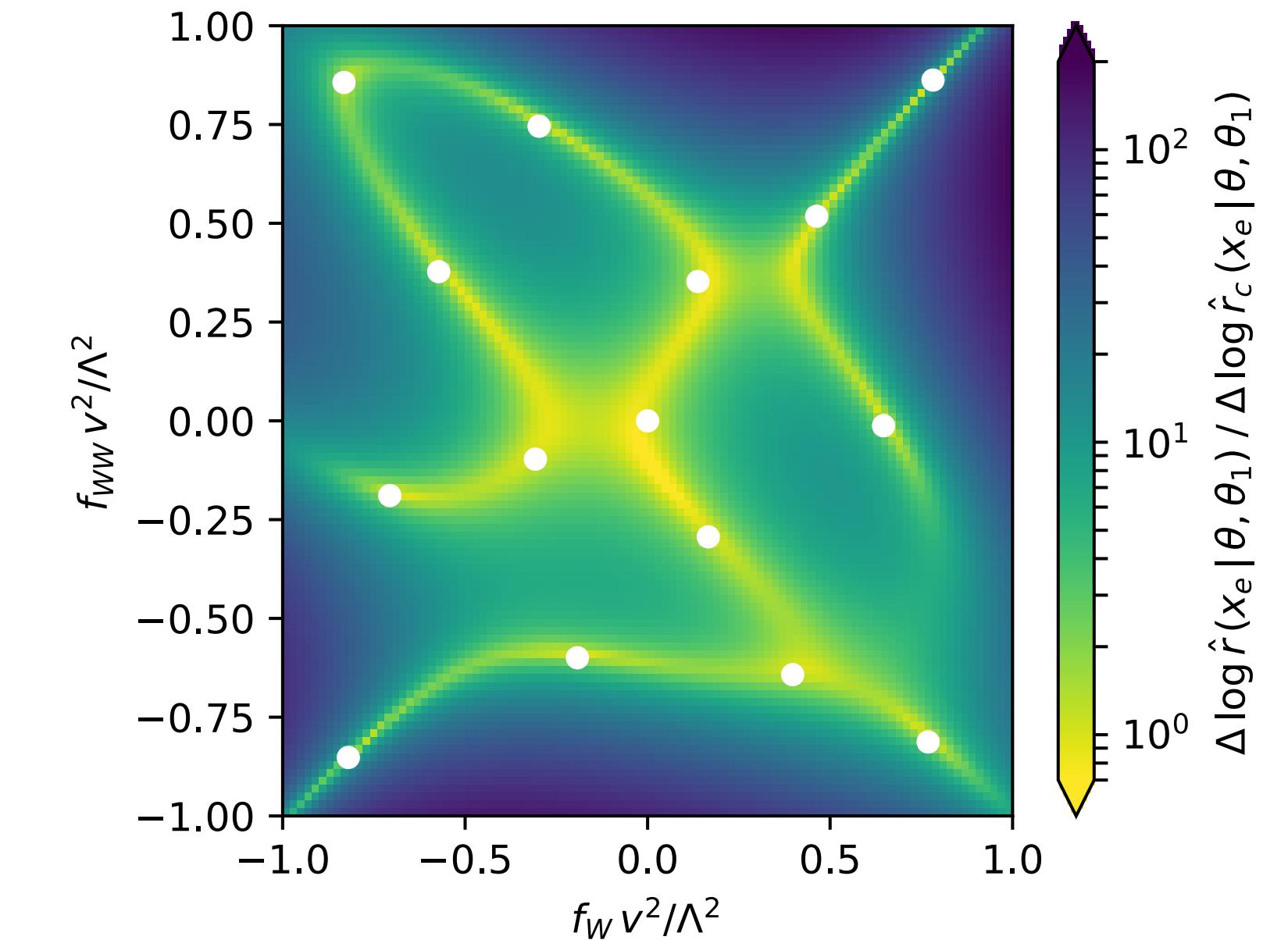
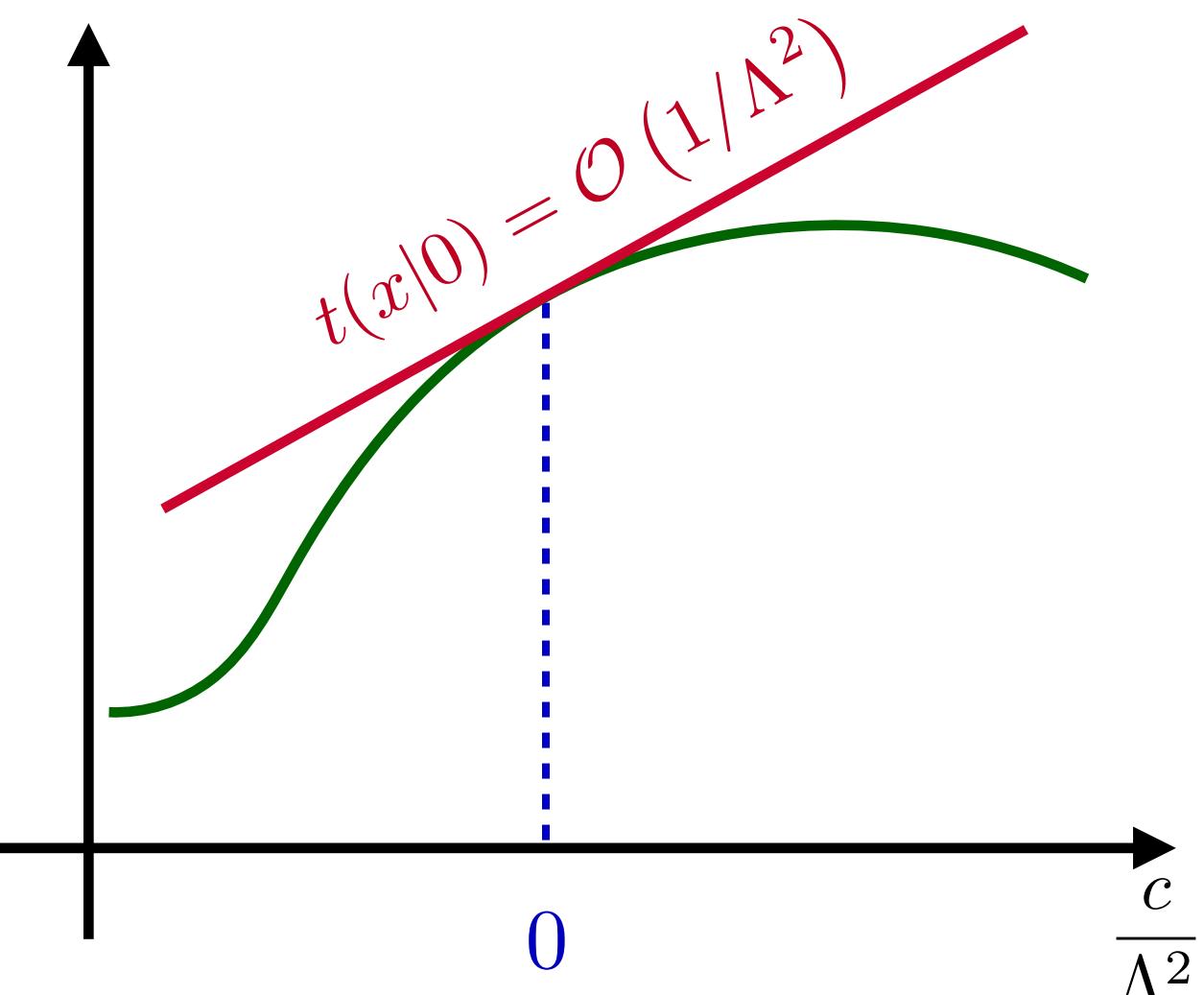
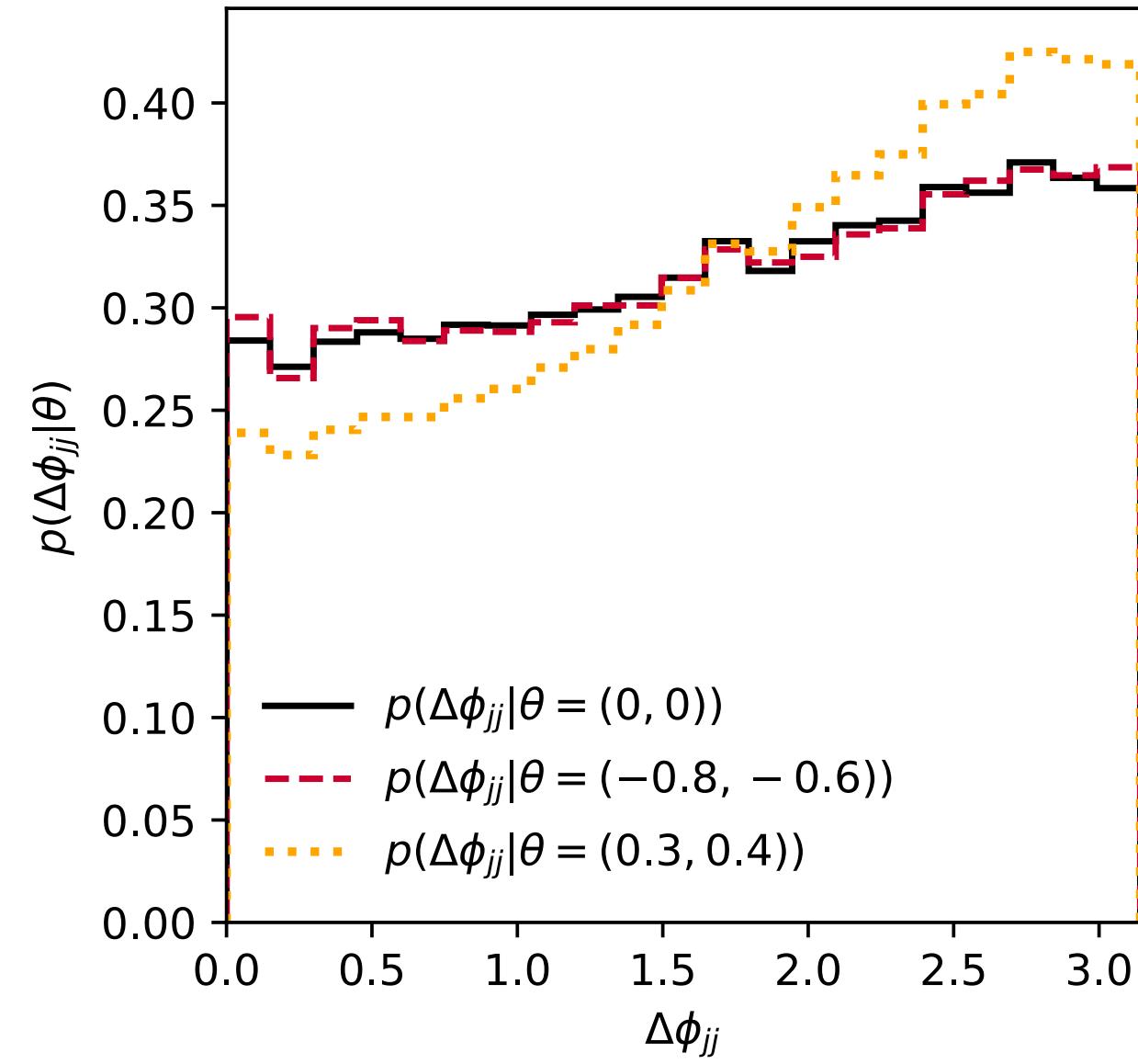
(Subtle point: Large overlap of kinematic distributions reduces variance of joint likelihood ratio / joint score)

Perfect match for EFT measurements



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- Interference effects can be isolated using SALLY at the SM (SMALLY?)

Perfect match for EFT measurements



- Good for subtle kinematic effects
(Subtle point: Large overlap of kinematic distributions reduces variance of joint likelihood ratio / joint score)

- Interference effects can be isolated using SALLY at the SM (SMALLY?)

- Morphing techniques allow fast reweighting to any parameter points
[e.g. ATL-PHYS-PUB-2015-047]

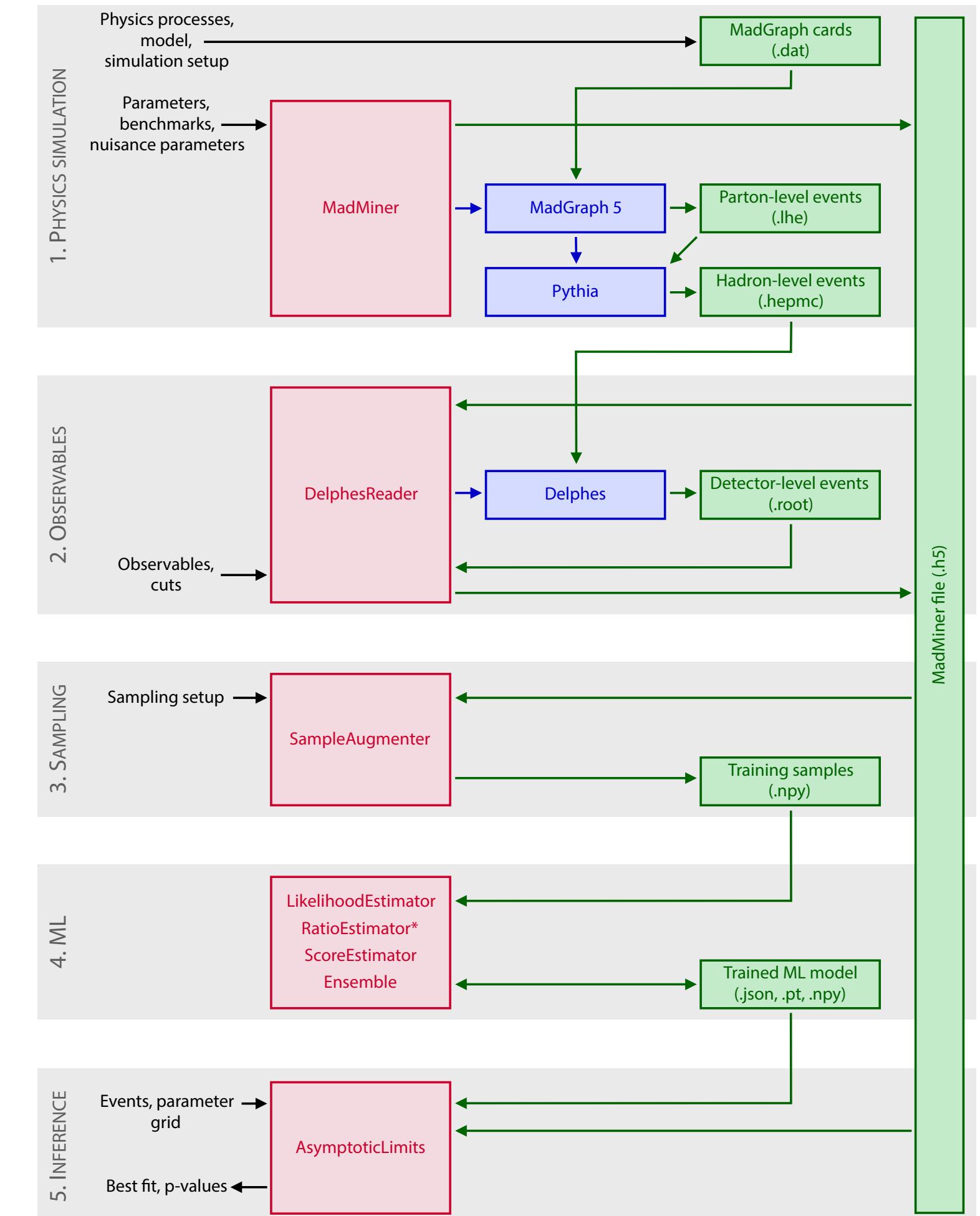
In practice

Automation

[JB, F. Kling, I. Espejo, K. Cranmer doi: 10.5281/zenodo.1489147]

We are developing **MadMiner**, which makes it straightforward to apply the new techniques to LHC problems

- Out of the box: Pheno-level analyses
 - MadGraph, Pythia, Delphes
 - Systematic uncertainties from PDF / scale variation
- Scalable to state-of-the-art experimental tools
 - Mostly requires bookkeeping of fully differential cross sections
- Modular interface
 - Extensive documentation
 - Embedded into Python / ML ecosystem



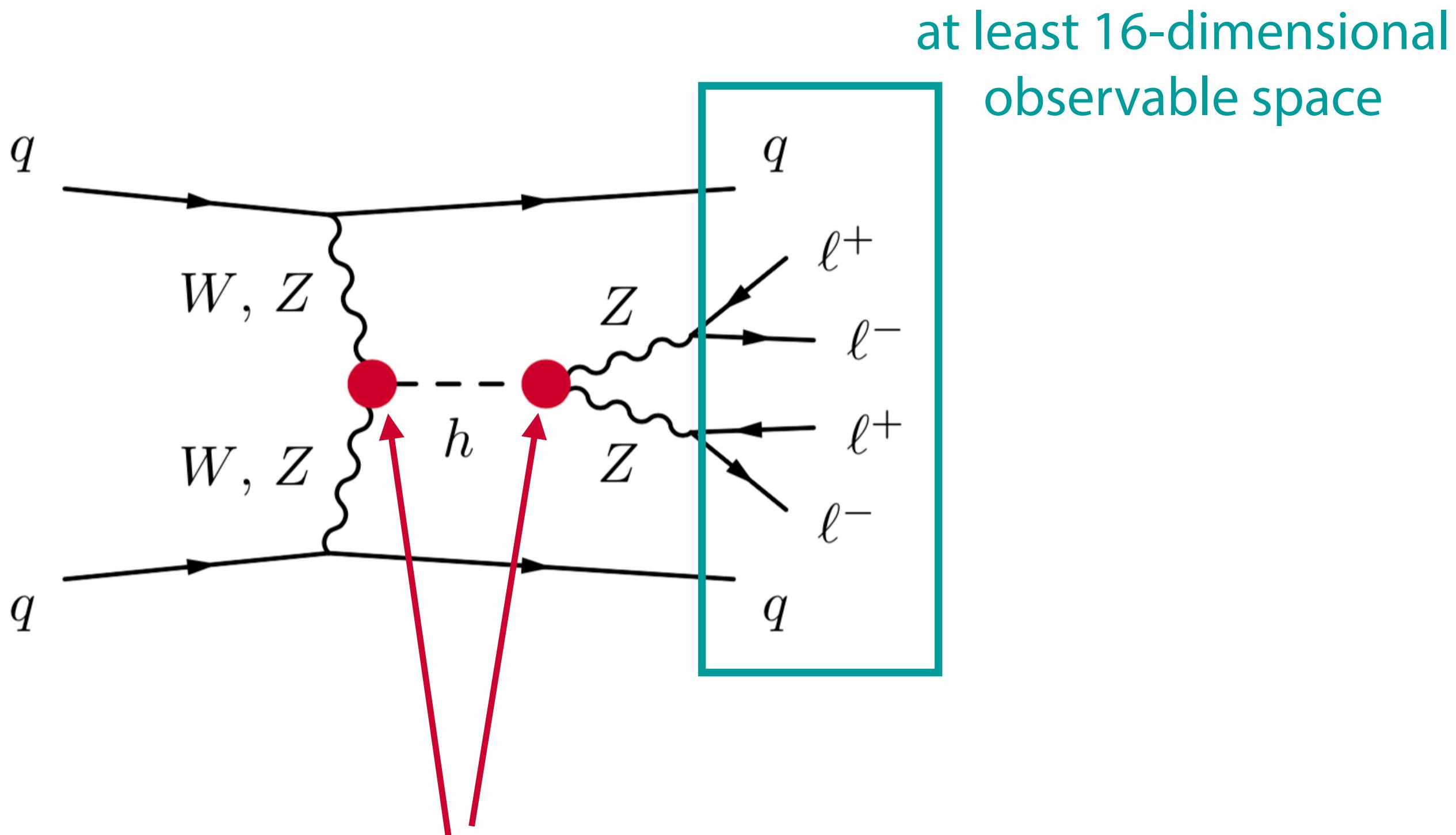
github.com/johannbrehmer/madminer

madminer.readthedocs.io

`pip install madminer`

Proof of concept: Higgs production in weak boson fusion

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



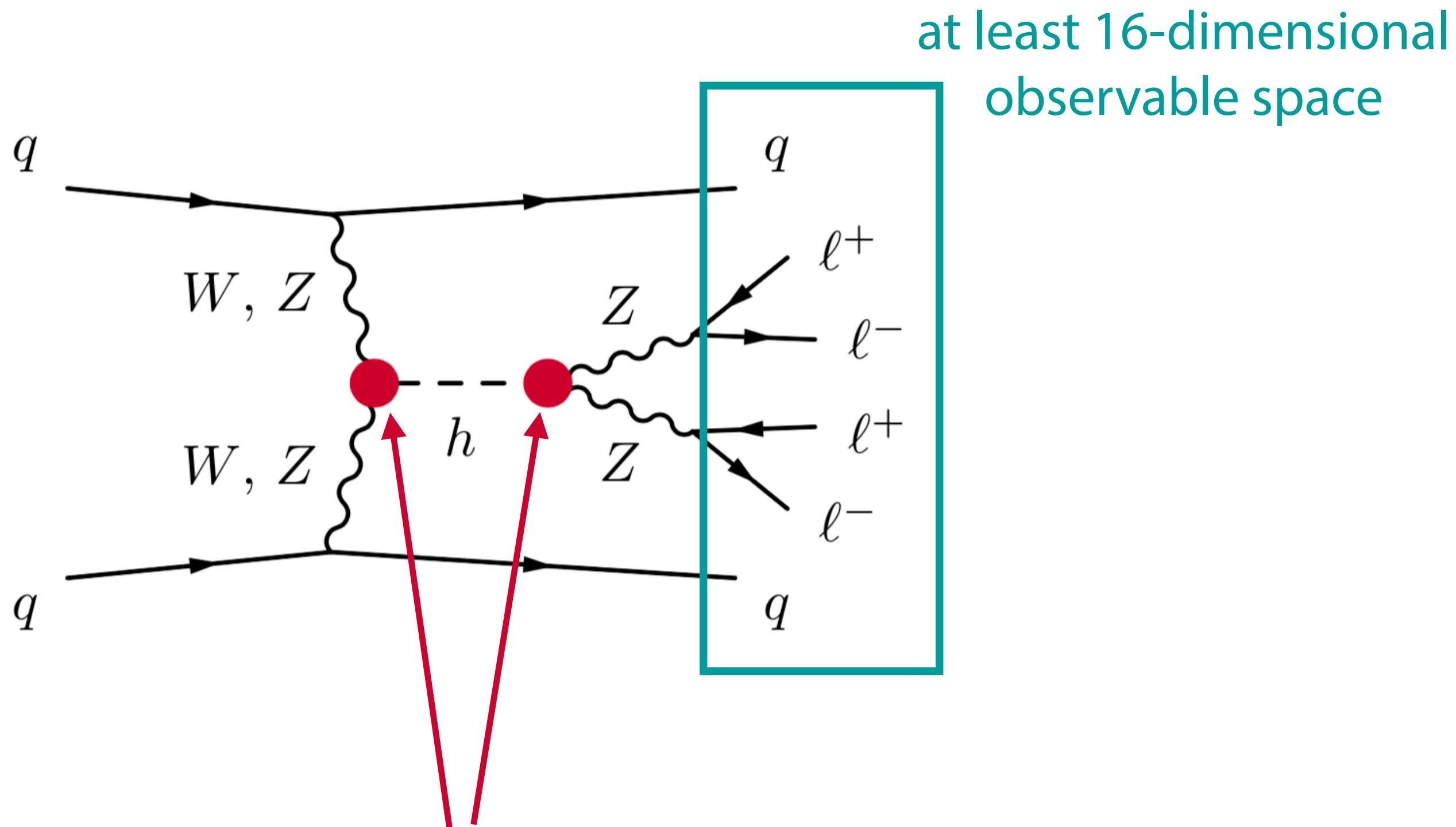
Exciting new physics might hide here!

We parameterize it with two EFT coefficients:

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

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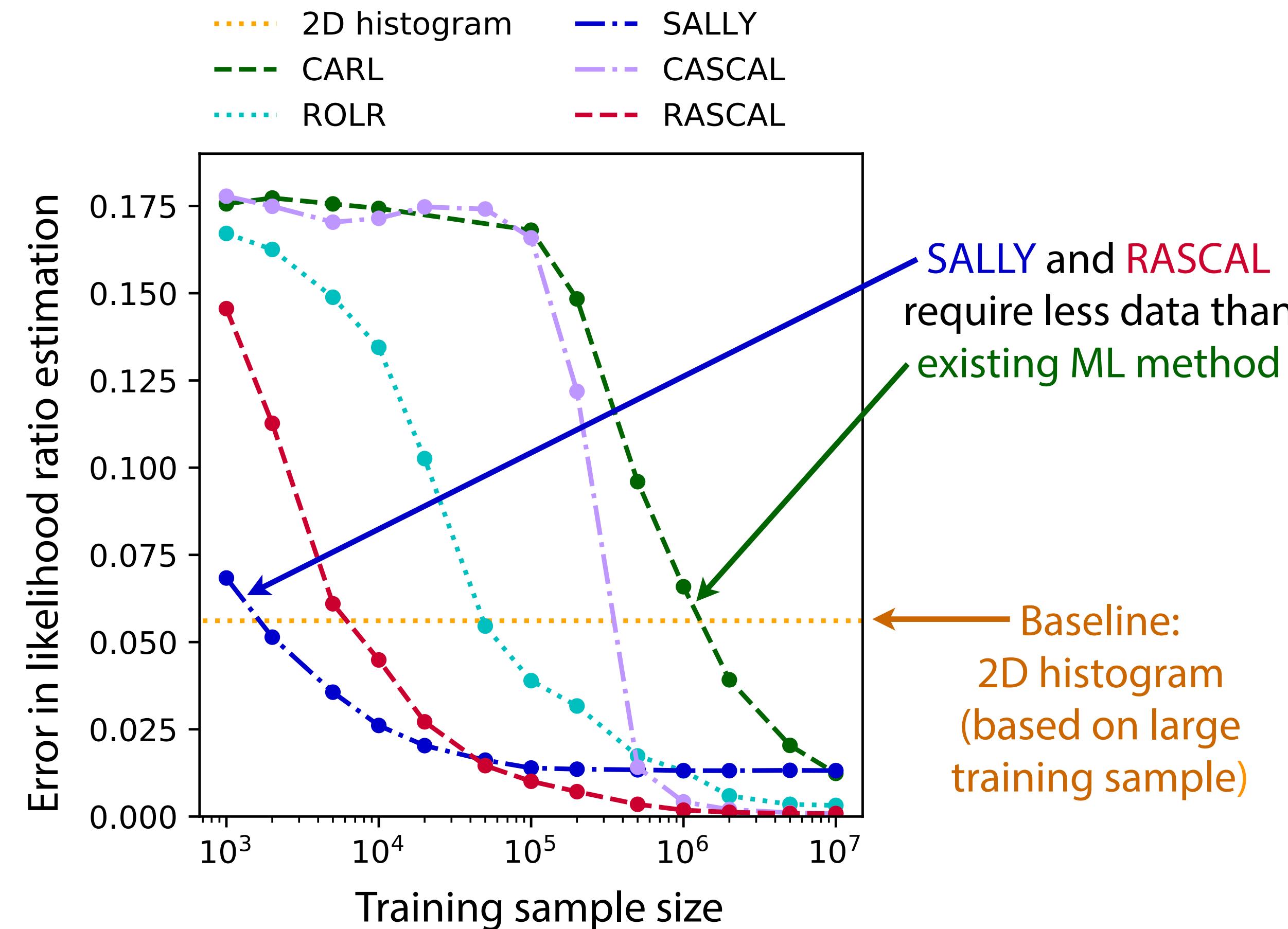
Goal: constrain the two EFT parameters

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

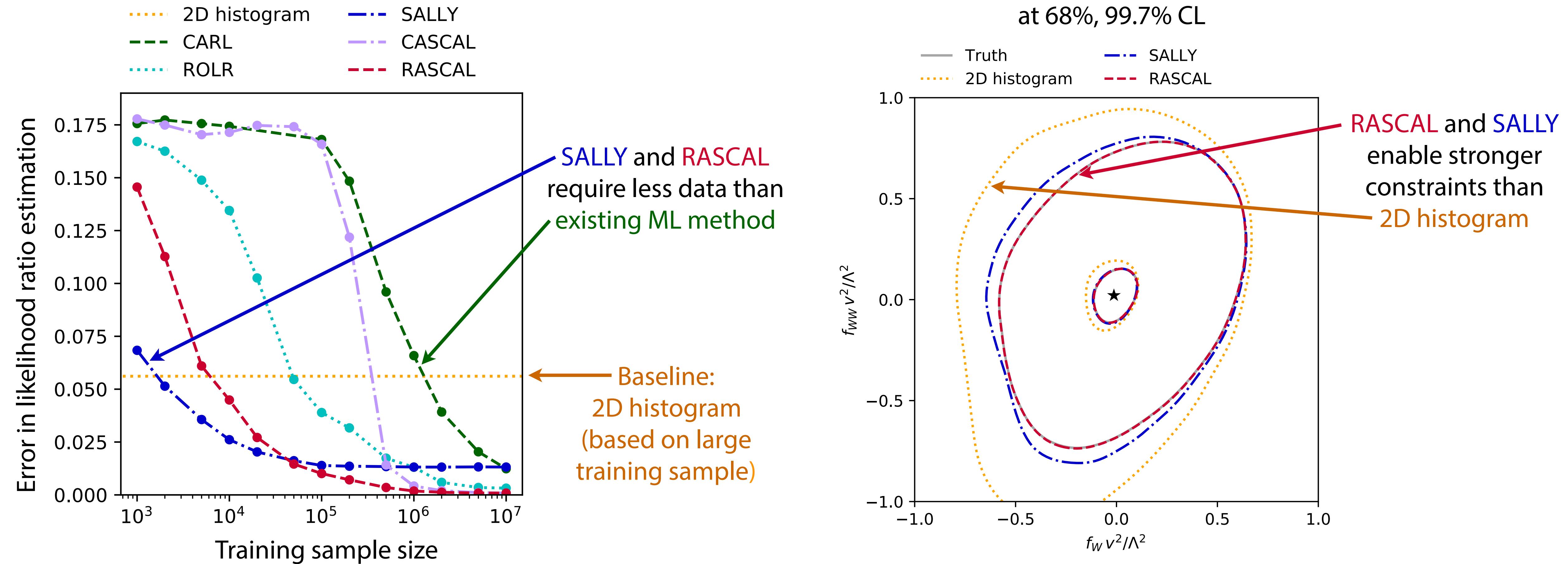
Two scenarios:

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

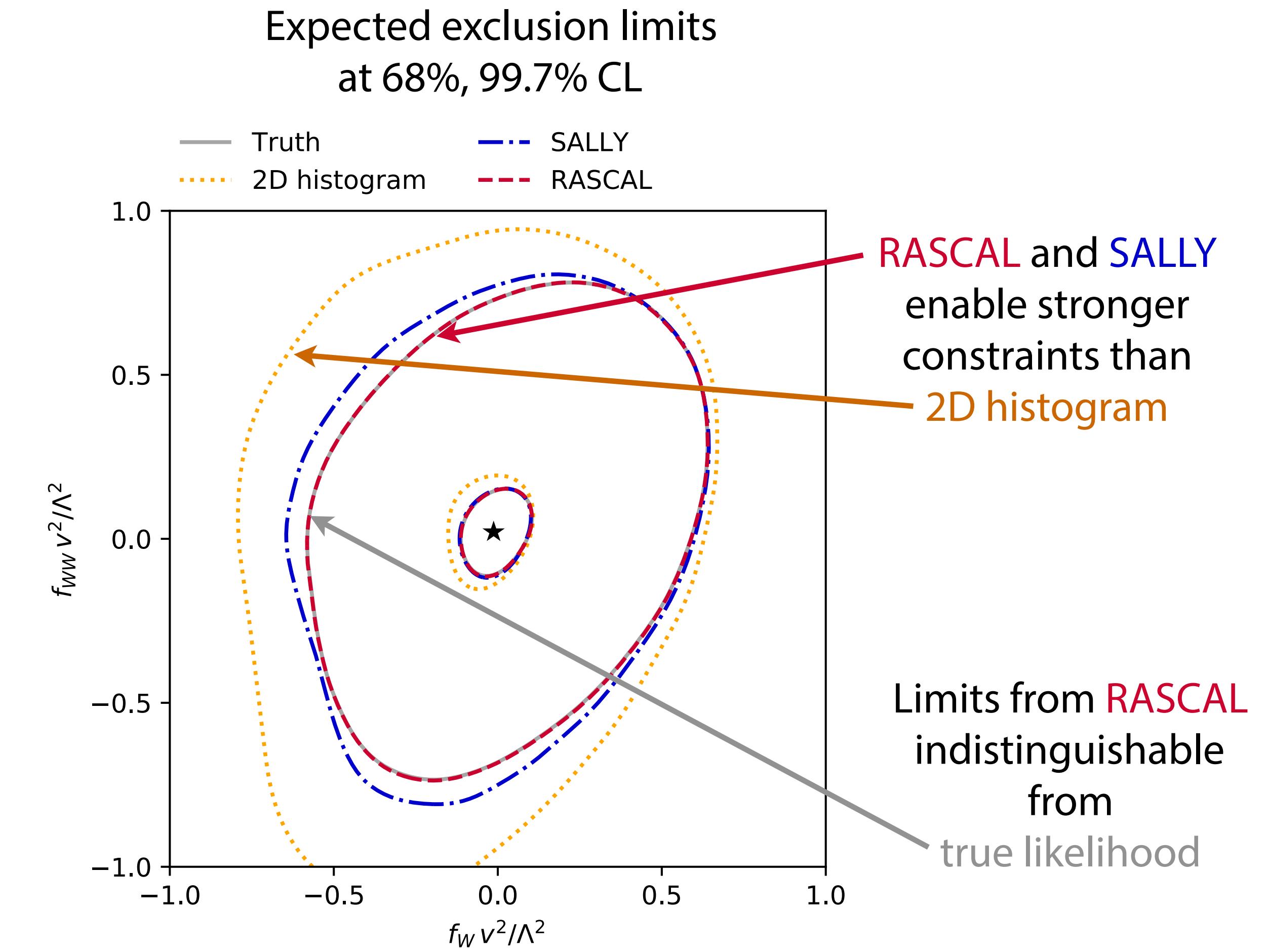
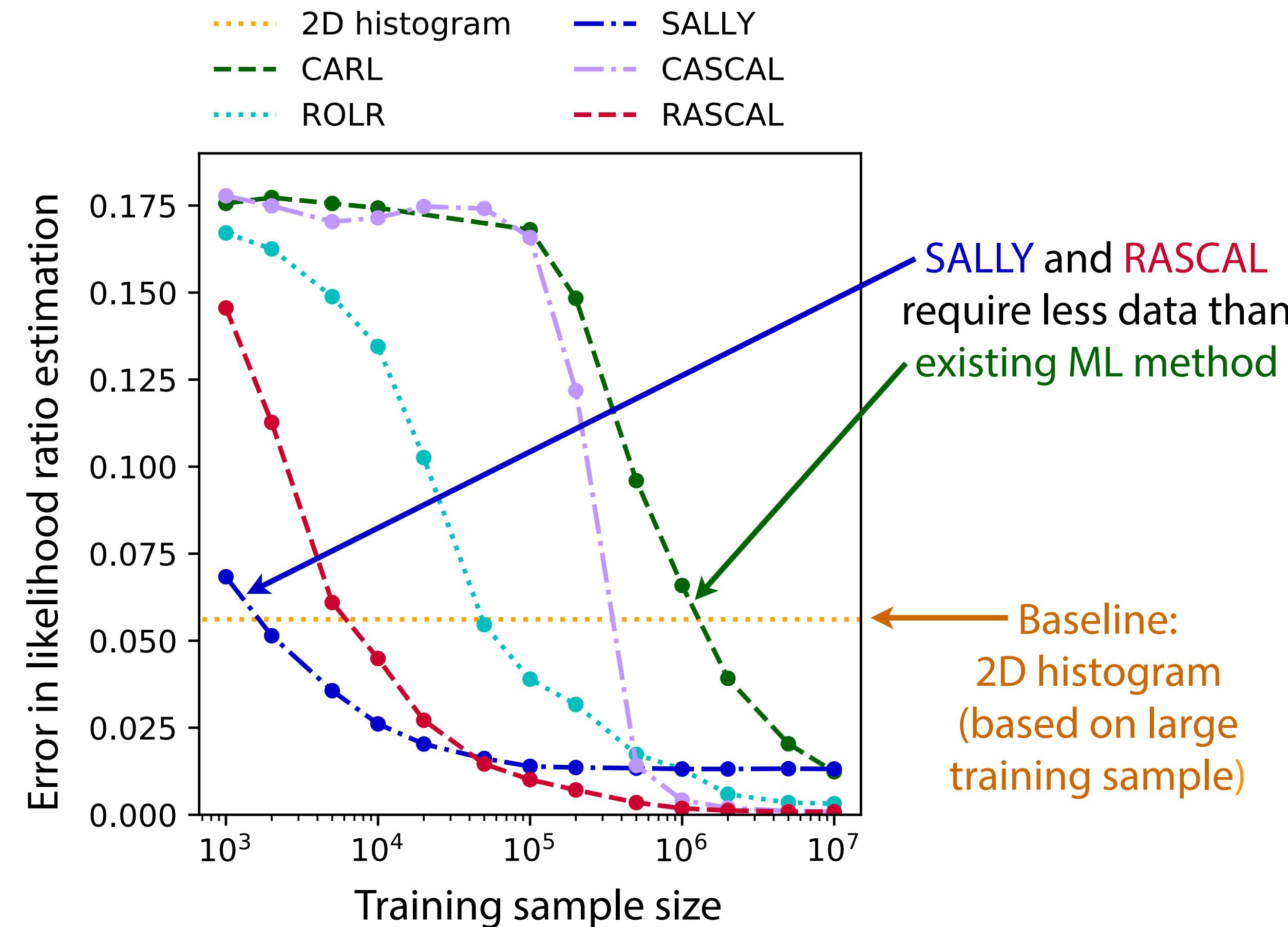
Stronger constraints with less training data



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Stronger constraints with less training data

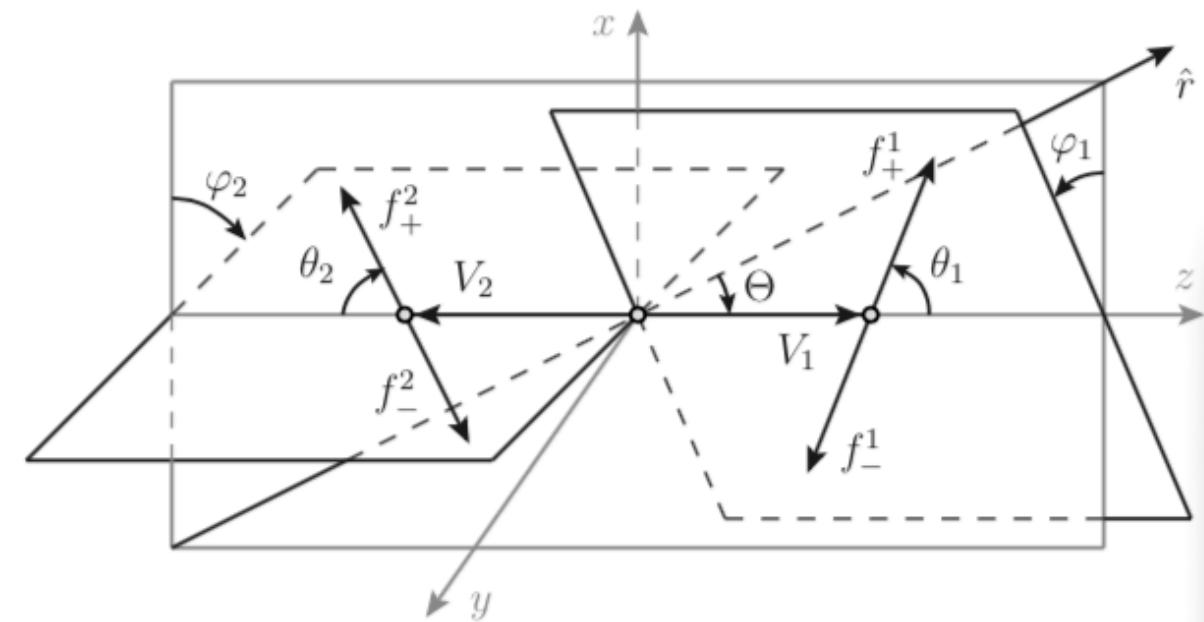


Dibosons

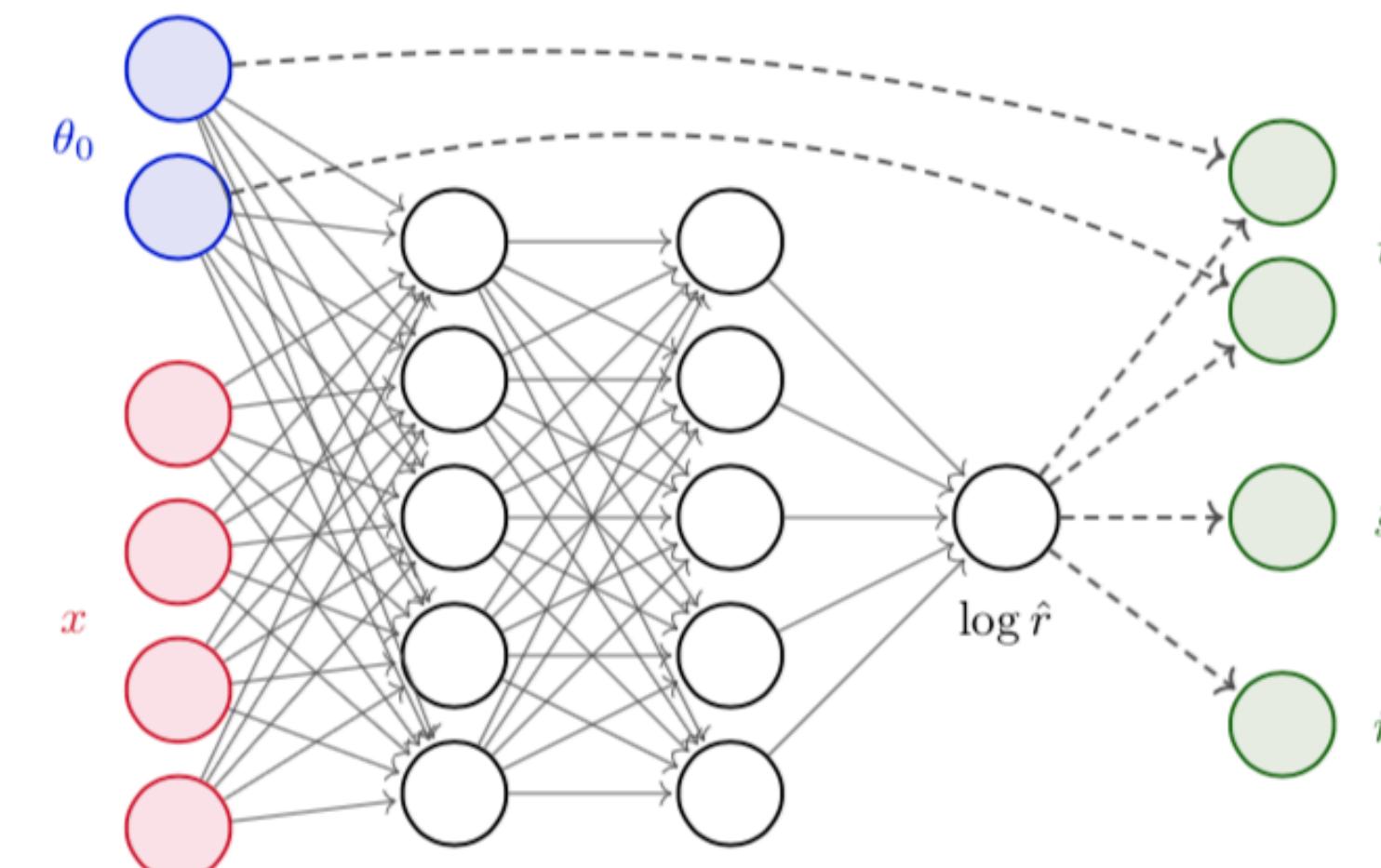
Transverse DiBosons

[Panico, Riva, AW, 2017]

Measuring diboson diff. cross-sections is not enough



Can we get this done by a Machine? (in real world)



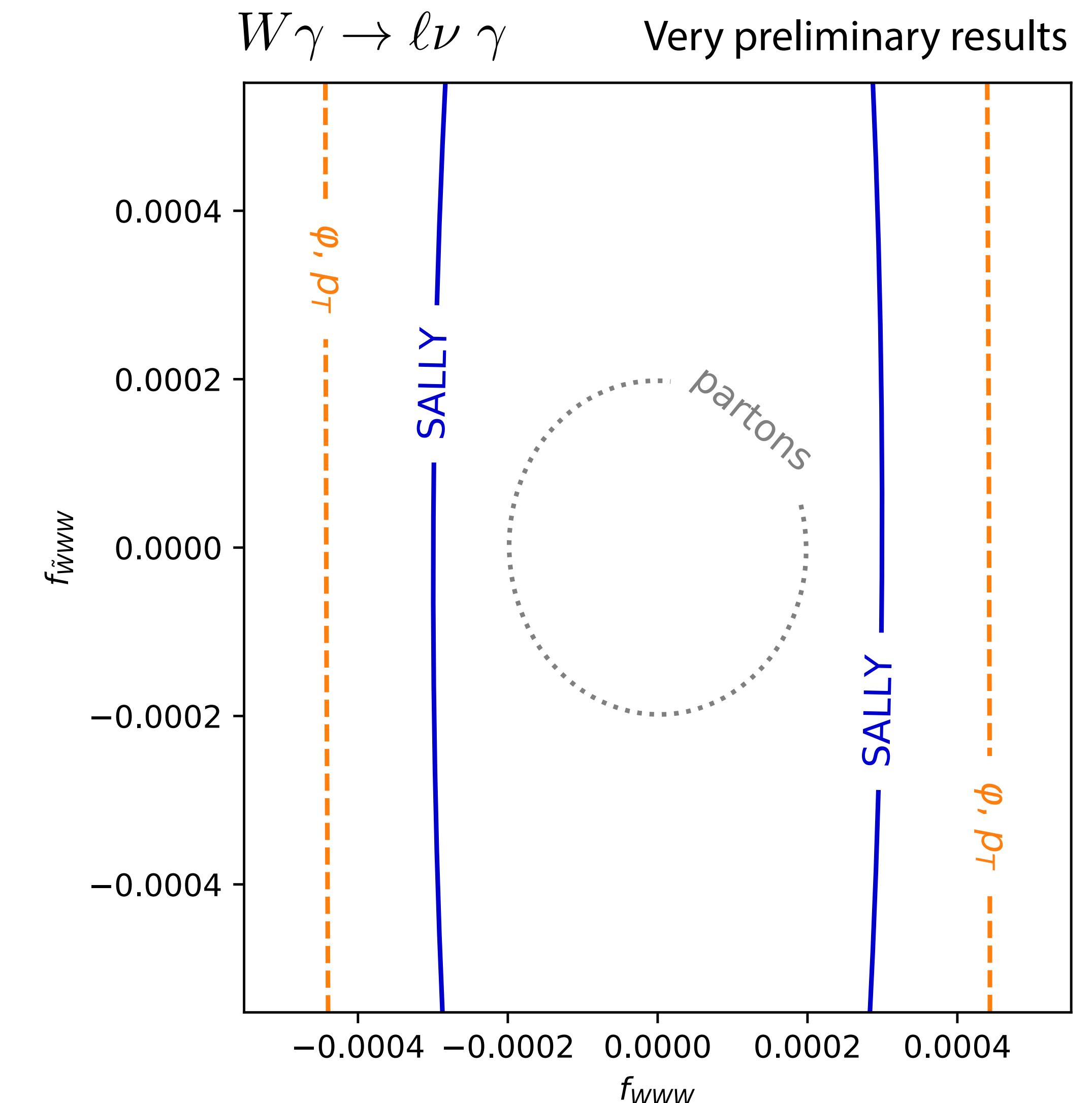
Cranmer et.al., 2018

[from A. Wulzer's talk]

Dibosons

[JB, K. Cranmer, M. Farina, F. Kling, D. Pappadopulo, J. Ruderman in progress]

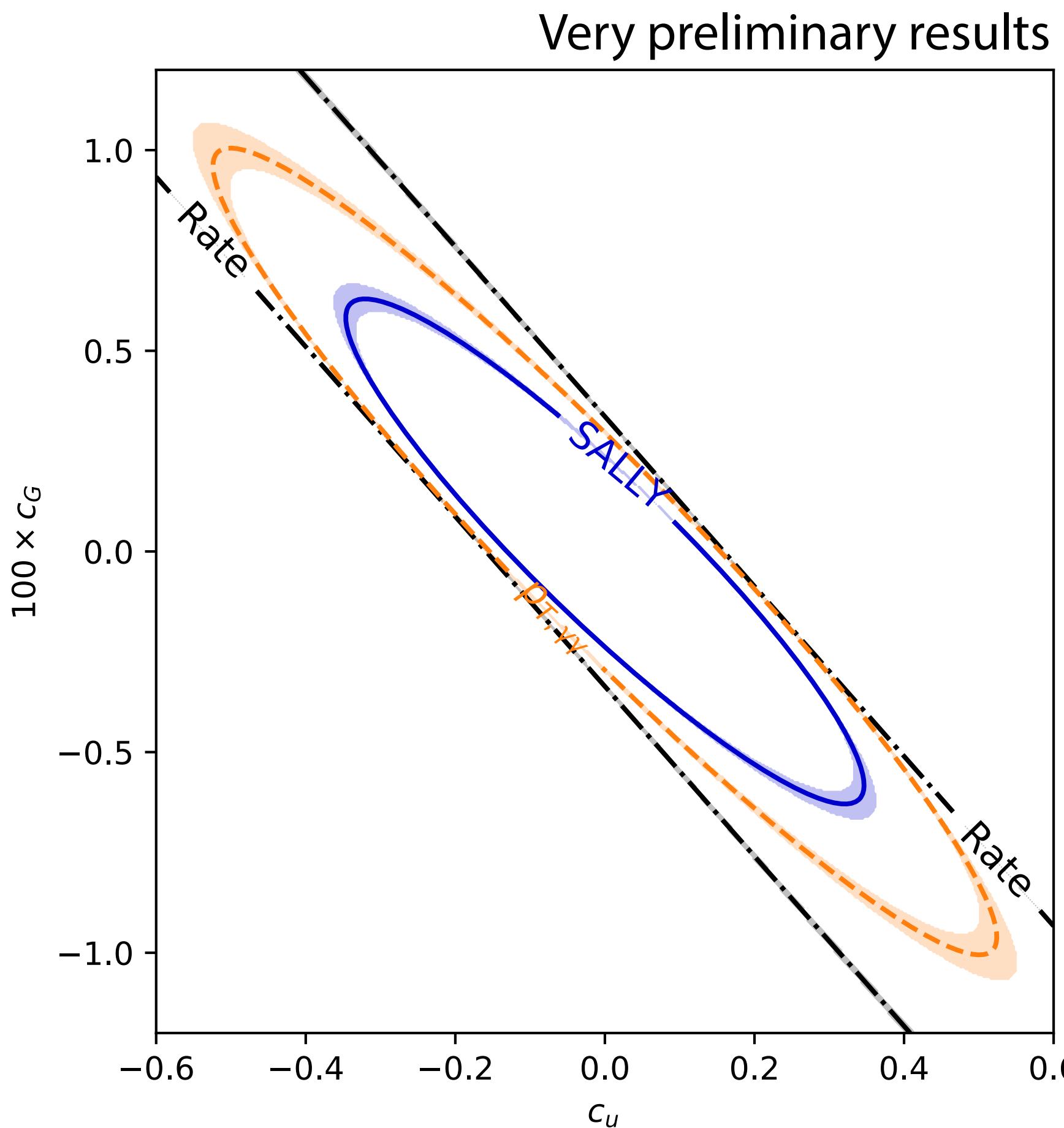
Yes.



Higgs measurements

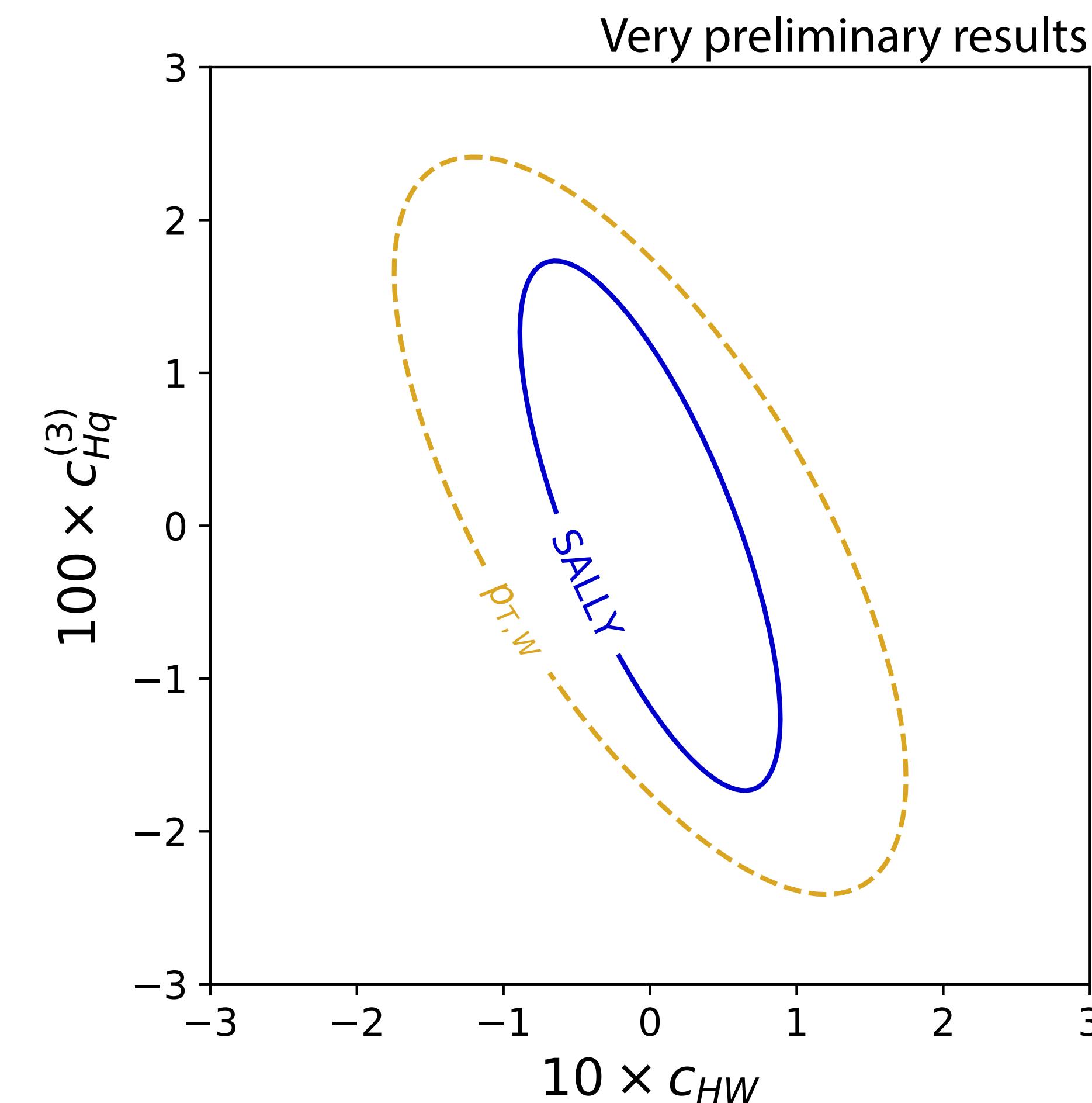
$$t\bar{t}h \rightarrow (b\ell^+\nu)(b\ell^-\bar{\nu})(\gamma\gamma)$$

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

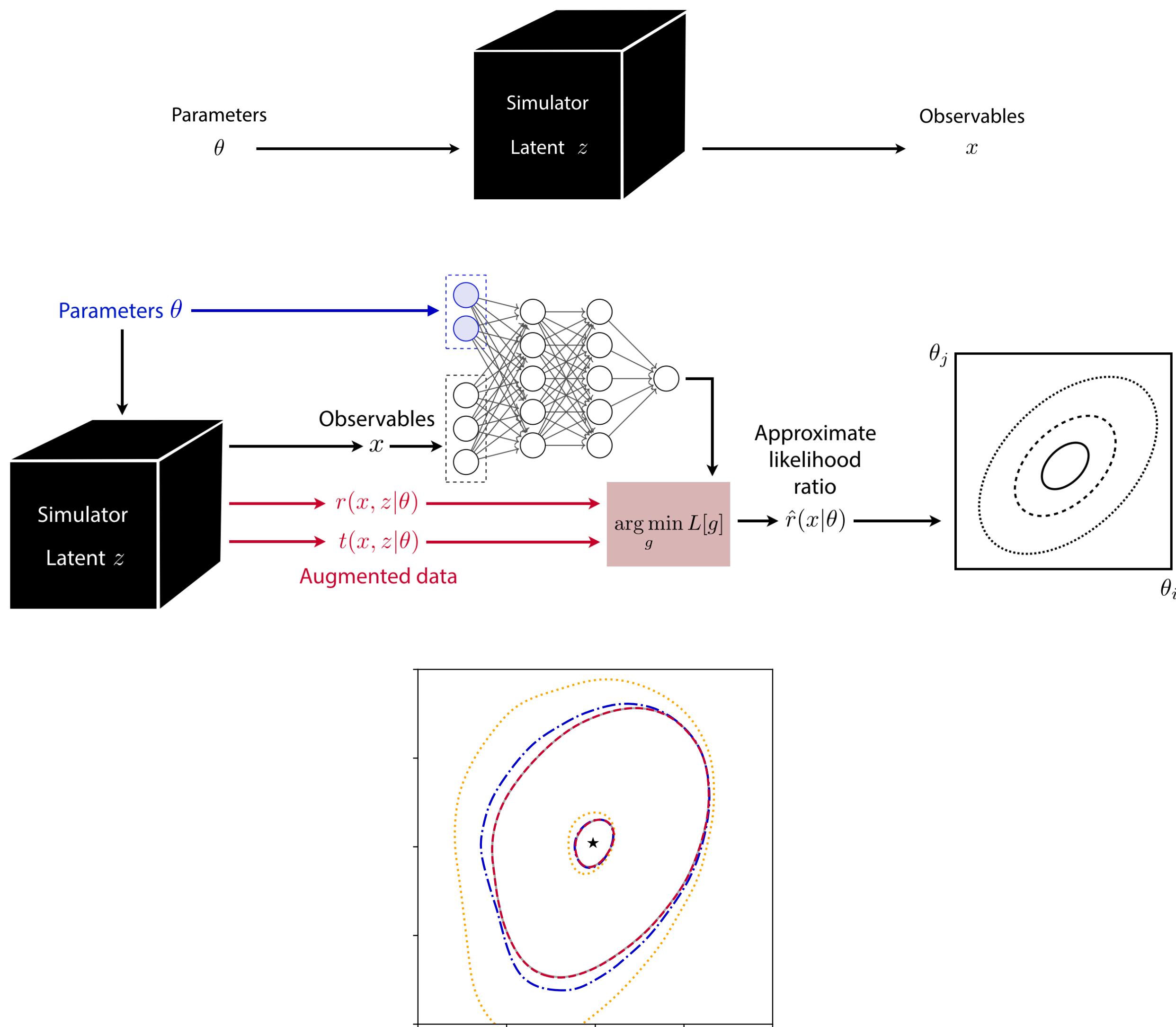


$$Wh \rightarrow (\ell\nu)(b\bar{b})$$

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



A new approach to LHC measurements



- LHC measurements with high-dimensional observations have “likelihood-free” structure
- New multivariate inference techniques:
Leverage information in matrix elements + power of machine learning to...
 - estimate the full likelihood function
 - learn optimal summary statistics
- First tests show potential to substantially increase sensitivity to new physics
 - Ideal for EFT measurements

References



Kyle Cranmer



Gilles Louppe



Juan Pavez



Markus Stoye



Felix Kling



Irina Espejo

- | | | |
|----------------------------|--|-------------------------------|
| JB, KC, GL, JP: | Constraining Effective Field Theories with Machine Learning | [PRL, 1805.00013] |
| JB, KC, GL, JP: | A Guide to Constraining Effective Field Theories with Machine Learning | [PRD, 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, FK, IE, KC: | MadMiner: An inference toolkit for particle physics | [doi: 10.5281/zenodo.1489147] |

Bonus material

Solve it by approximating the integral

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

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

- Matrix Element Method: [K. Kondo 1988]

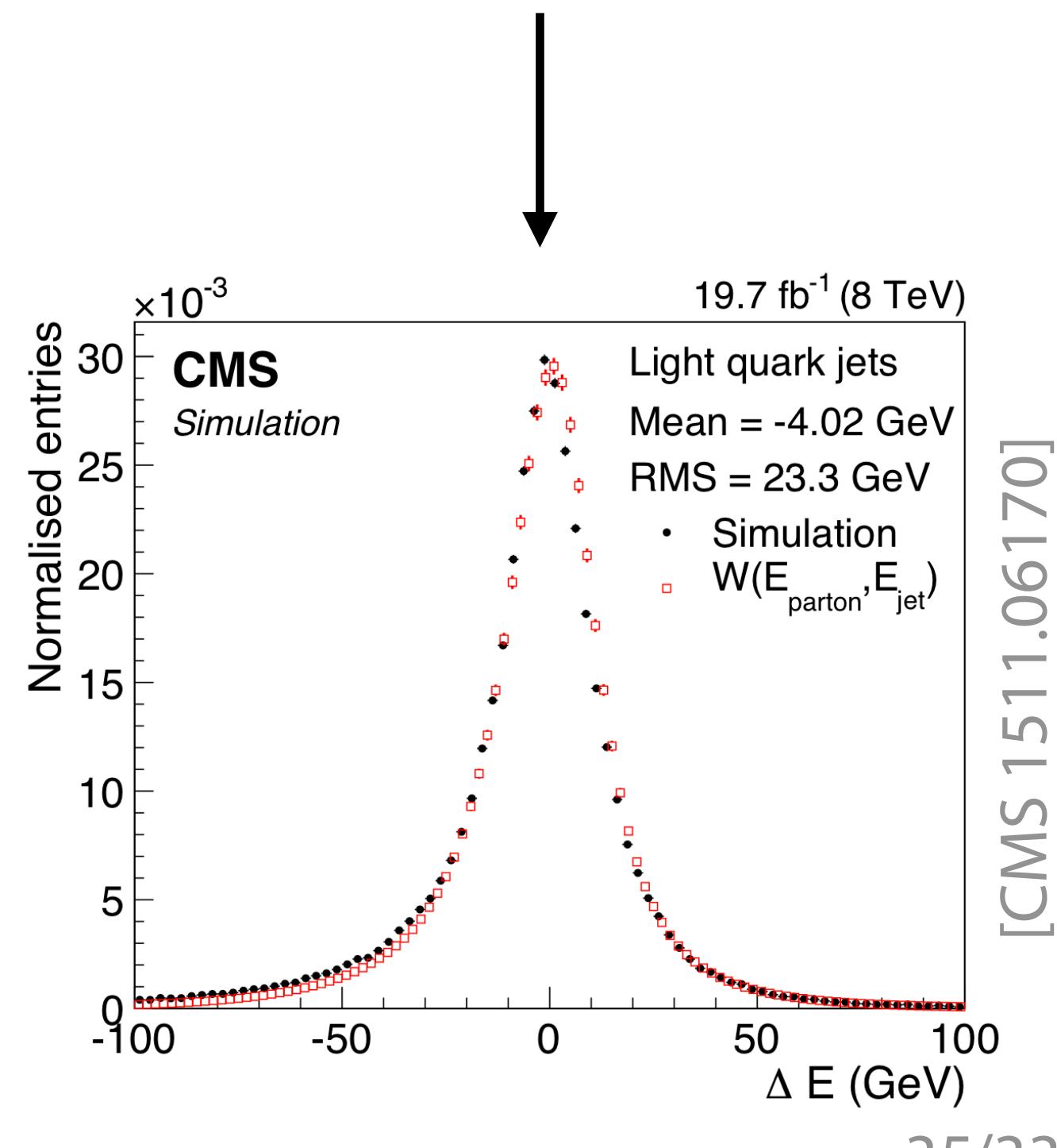
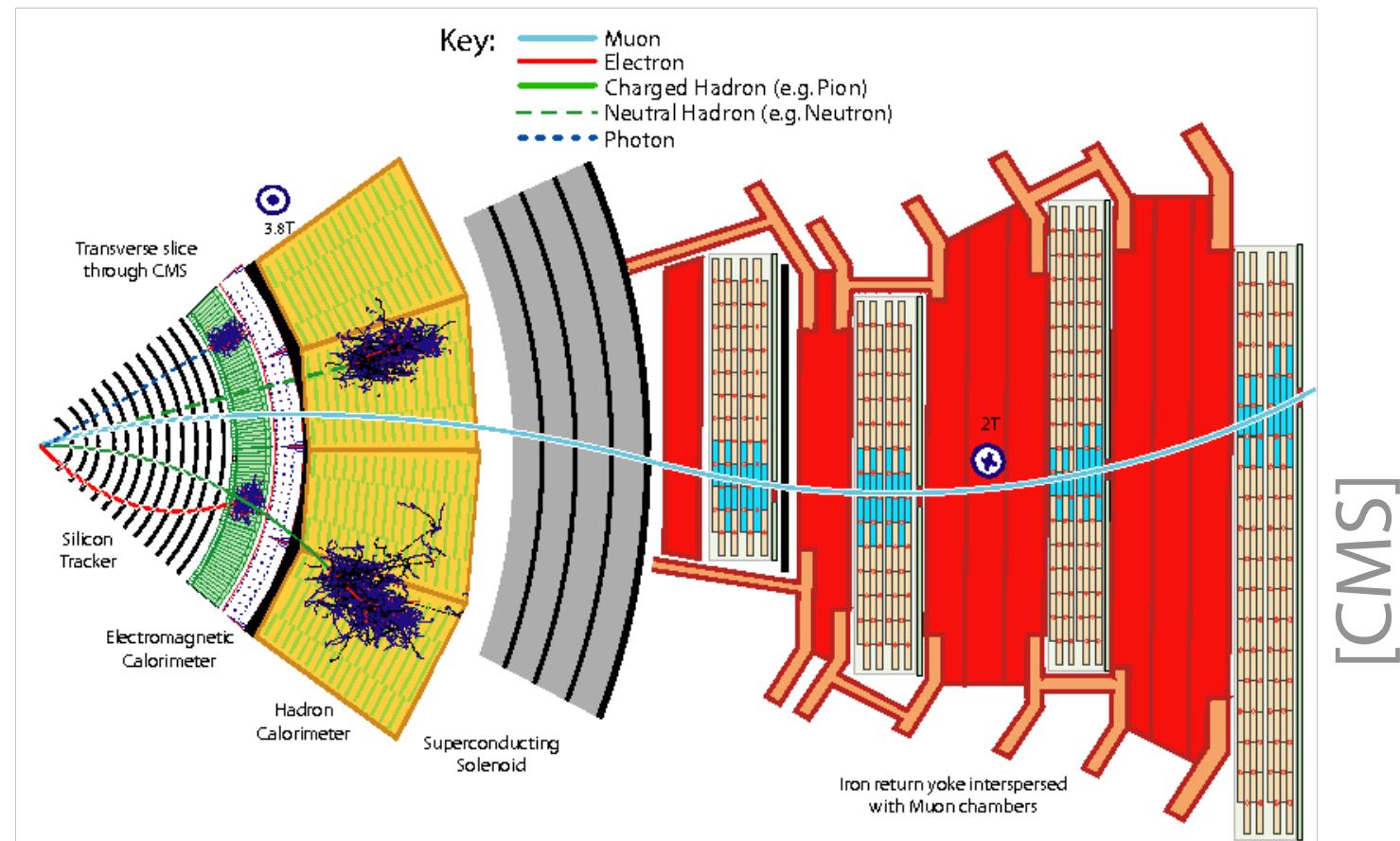
- approximate **shower + detector effects** into **transfer function** $\hat{p}(x|z_p)$
- explicitly calculate remaining integral

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

- Shower / Event Deconstruction [D. E. Soper, M. Spannowsky 1102.3480, 1402.1189]
extend explicit calculation to the shower

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

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



Solve it with machine learning classifiers

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

Solve it with machine learning classifiers

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



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

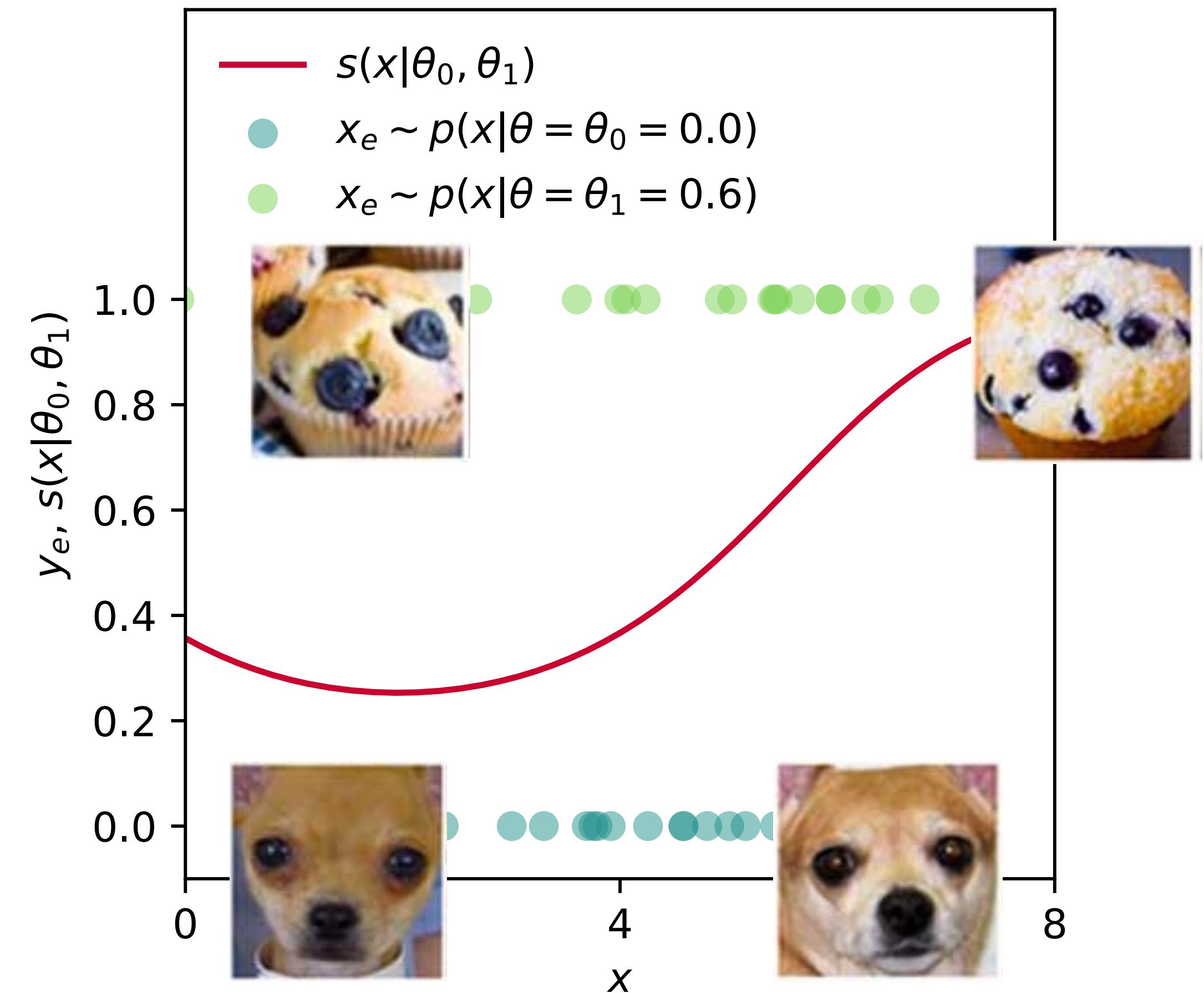
Solve it with machine learning classifiers

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

- Train neural network (BDT, ...) to tell $x \sim p(x|\theta_0)$ from $x \sim p(x|\theta_1)$
- Classifier output $\hat{s}(x)$ is closer to 0 for θ_0 -like events (closer to 1 for θ_1 -like events)
- CARL: Transform classifier output function $\hat{s}(x)$ into estimator for the likelihood ratio

$$r(x) \equiv p(x|\theta_0)/p(x|\theta_1)$$

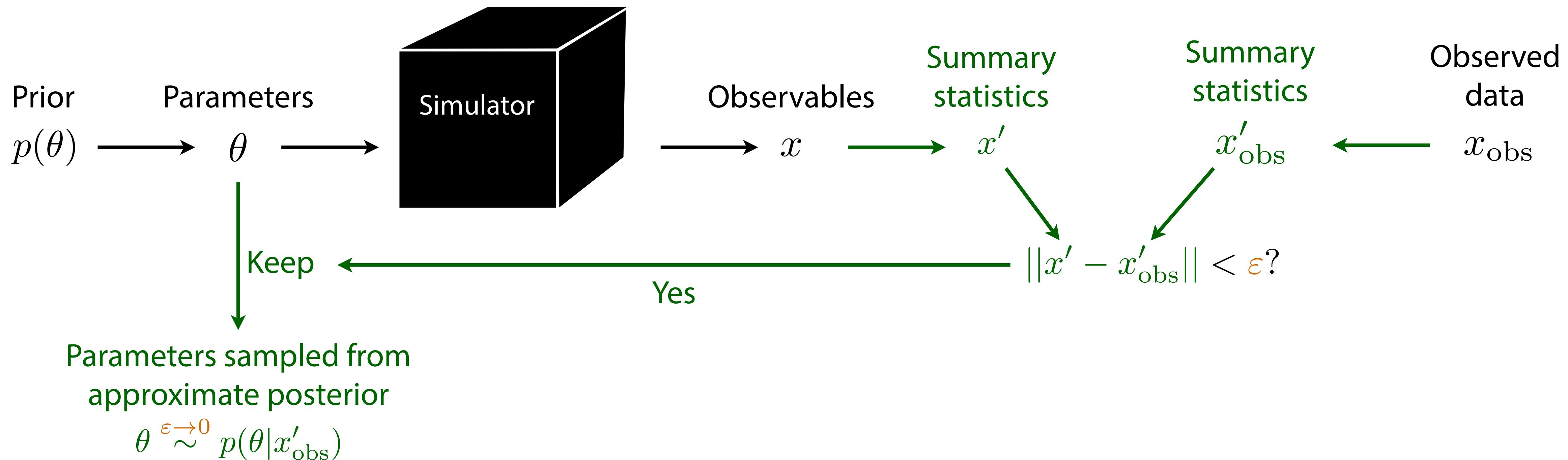
(calibrate estimator with histograms of NN output)



⇒ No summary statistics necessary, very fast evaluation... but may require large training samples

Approximate Bayesian Computation (ABC)

[D. Rubin 1984]



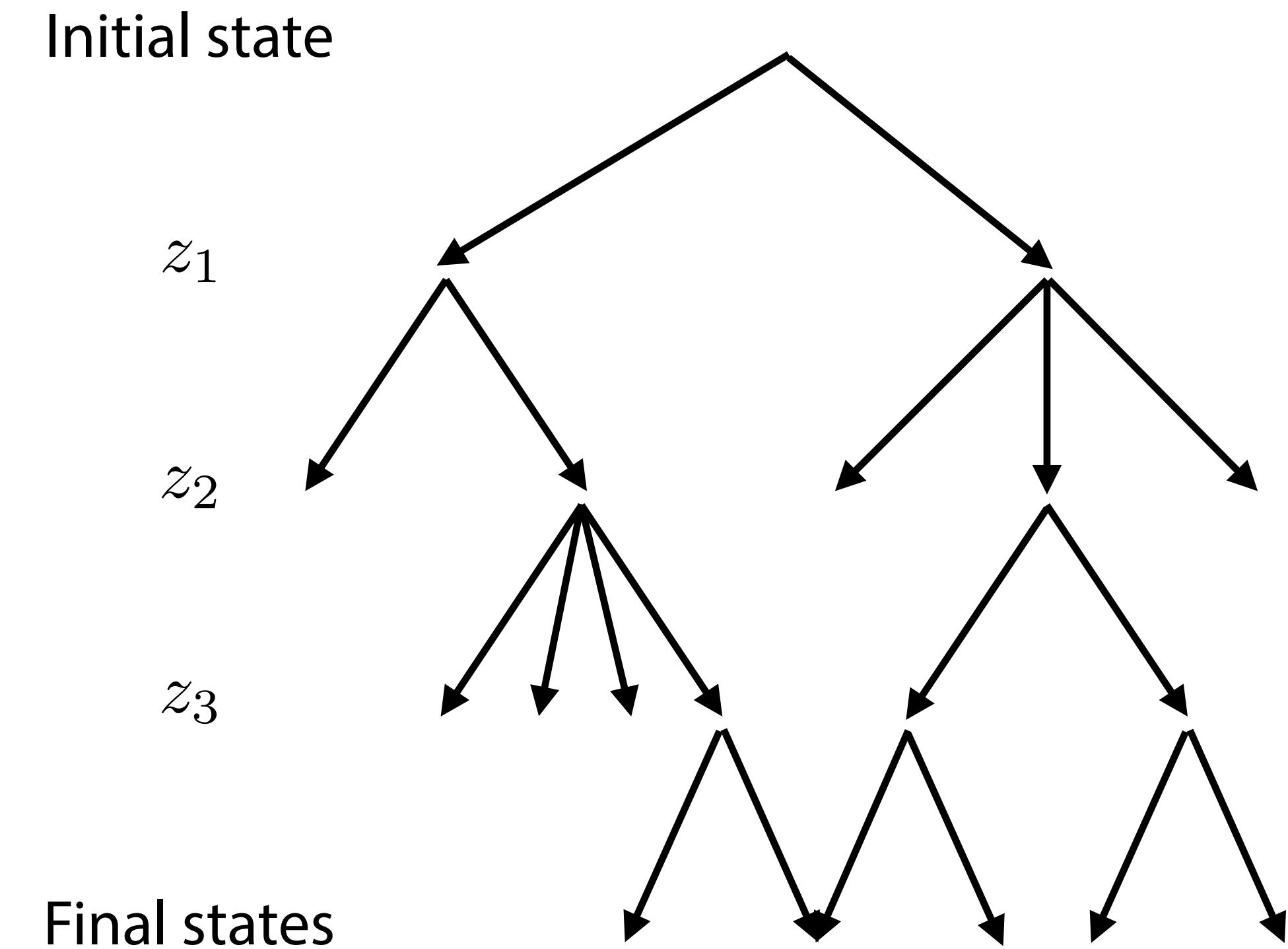
- How to choose x' ?
- How to choose ε ?
- No tractable posterior
- Need to run new simulations for new data or new prior

“Curse of dimensionality”
Precision vs efficiency tradeoff

Extracting the joint likelihood ratio from any simulation

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

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



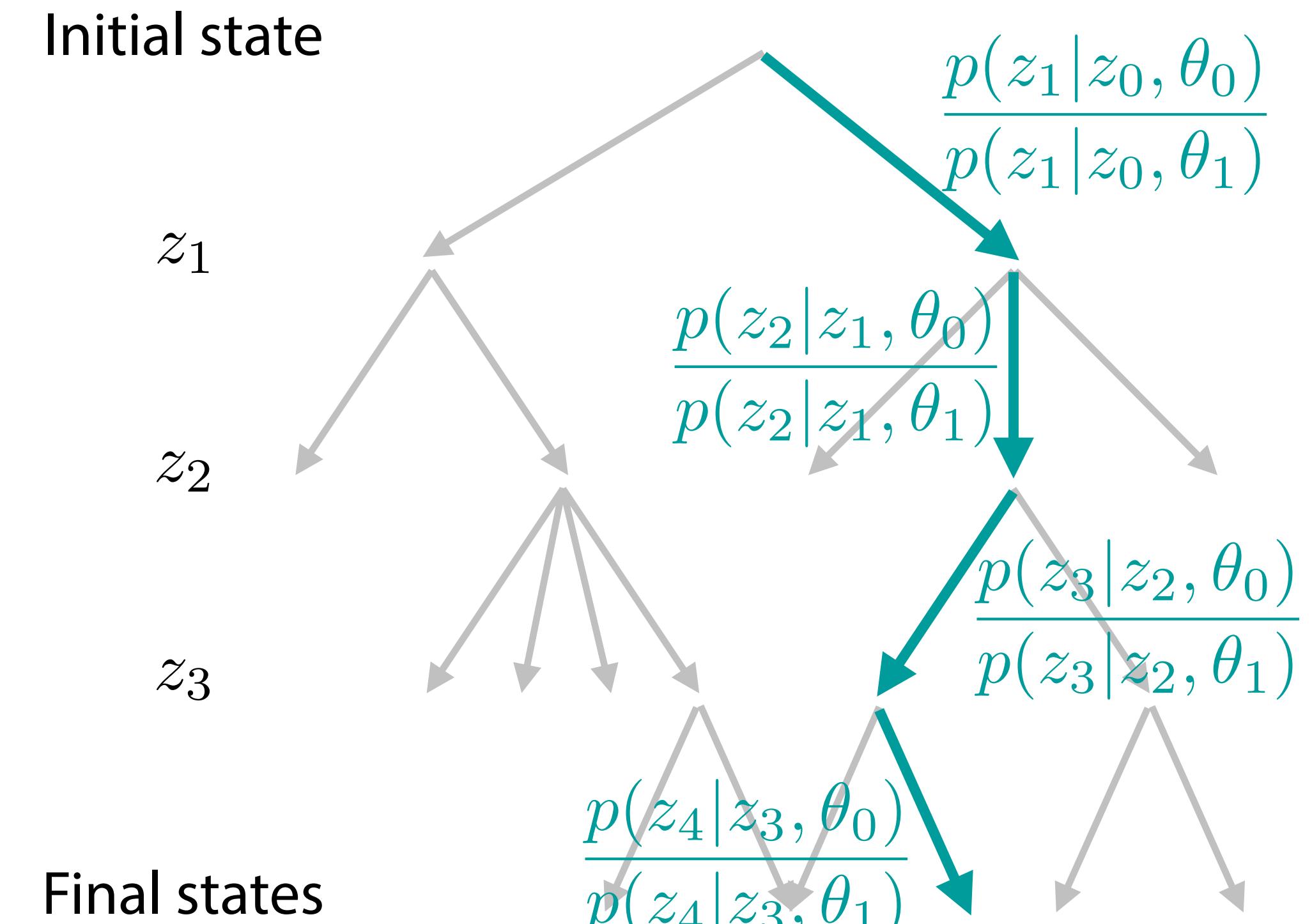
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else:  
    do_another_thing()
```

- 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**”:

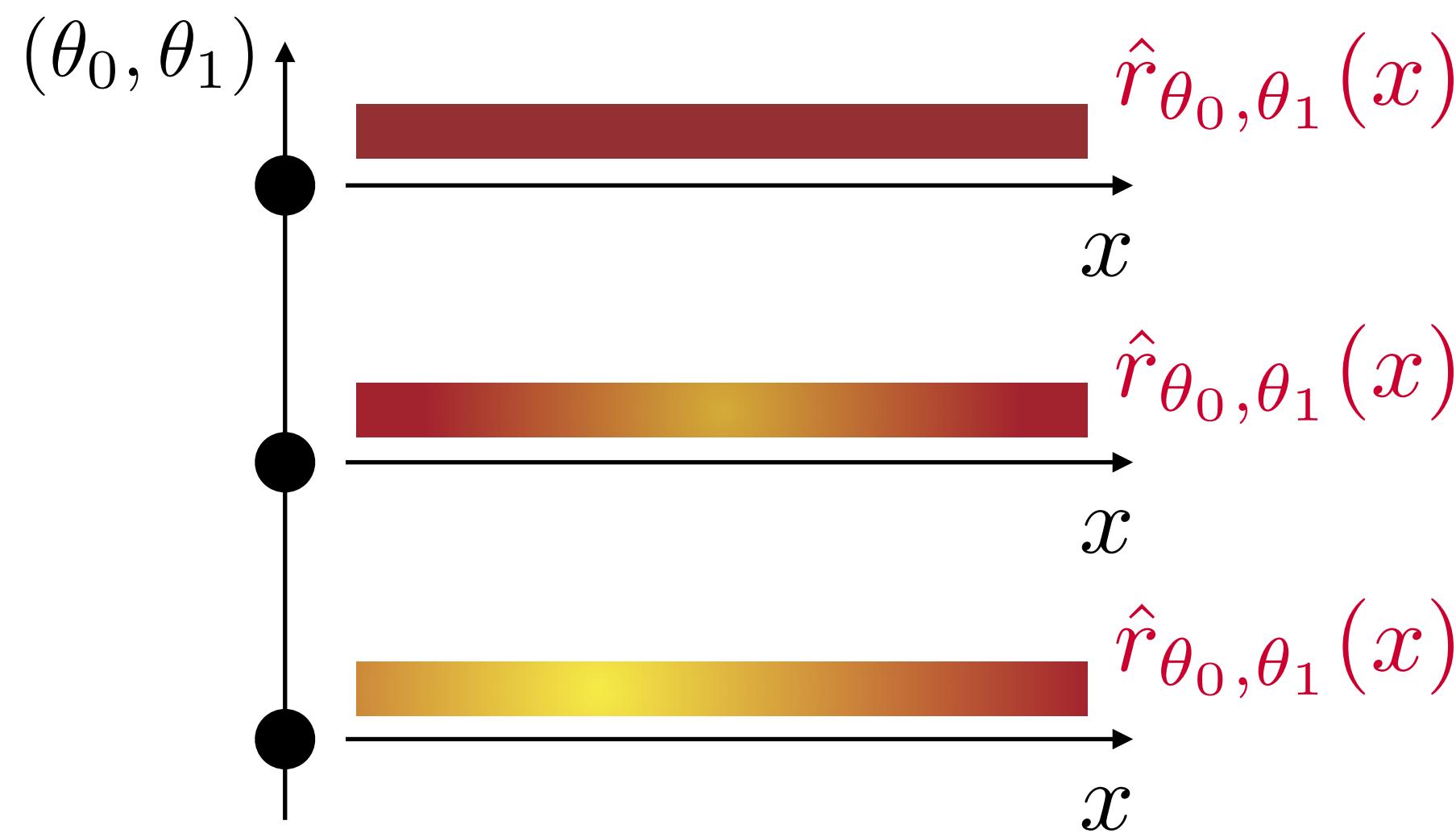
$$r(x, z|\theta_0, \theta_1) = \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)} = \prod_i \frac{p(z_i|z_{i-1}, \theta_0)}{p(z_i|z_{i-1}, \theta_1)}$$



Two types of likelihood ratio estimators

A) Point by point:

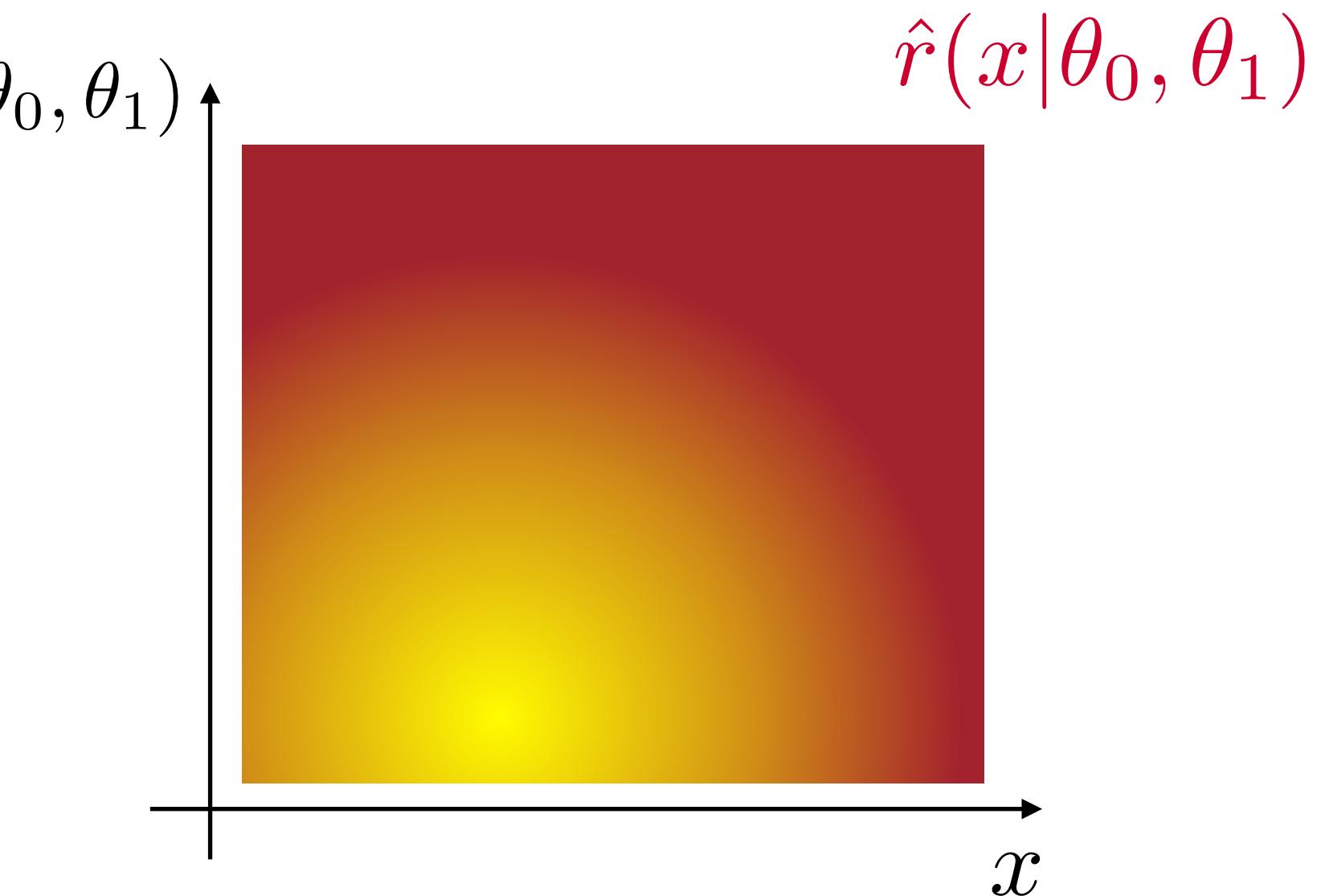
- first, define grid of parameter points $\{(\theta_0, \theta_1)\}$
- for each combination (θ_0, θ_1) ,
create separate estimator $\hat{r}_{\theta_0, \theta_1}(x)$
- final results can be interpolated between grid points

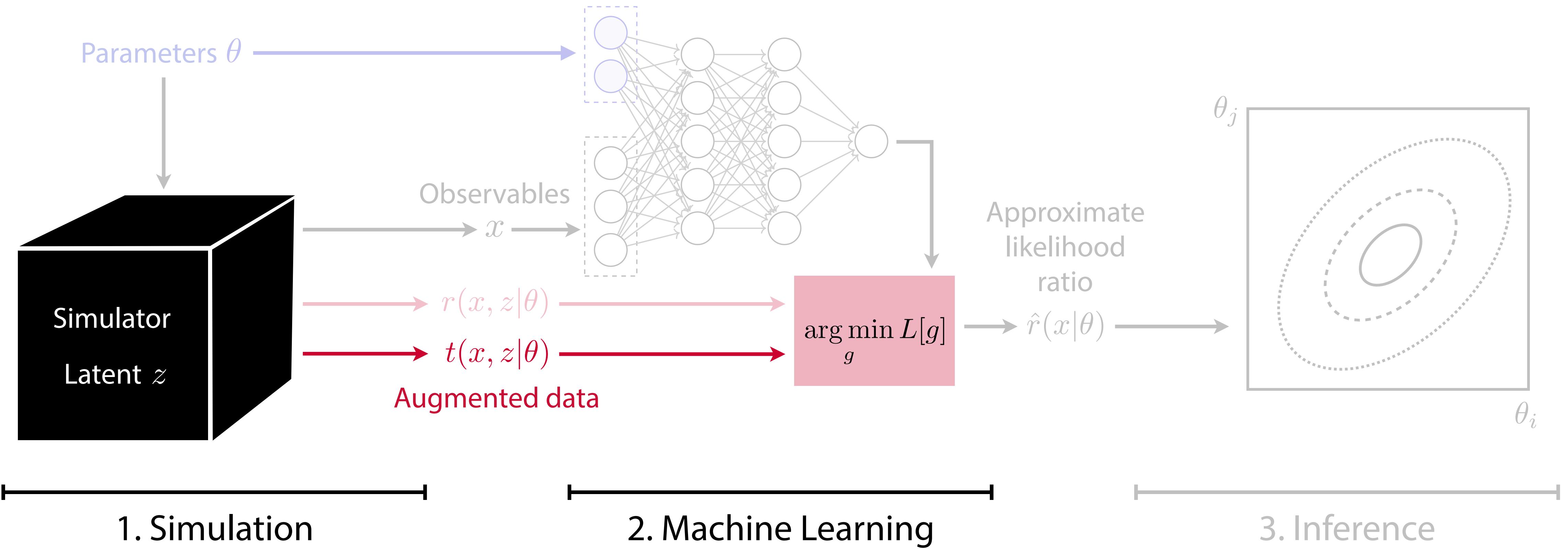


B) Parameterized:

[K. Cranmer, J. Pavez, G. Louppe 1506.02169;
P. Baldi et al. 1601.07913]

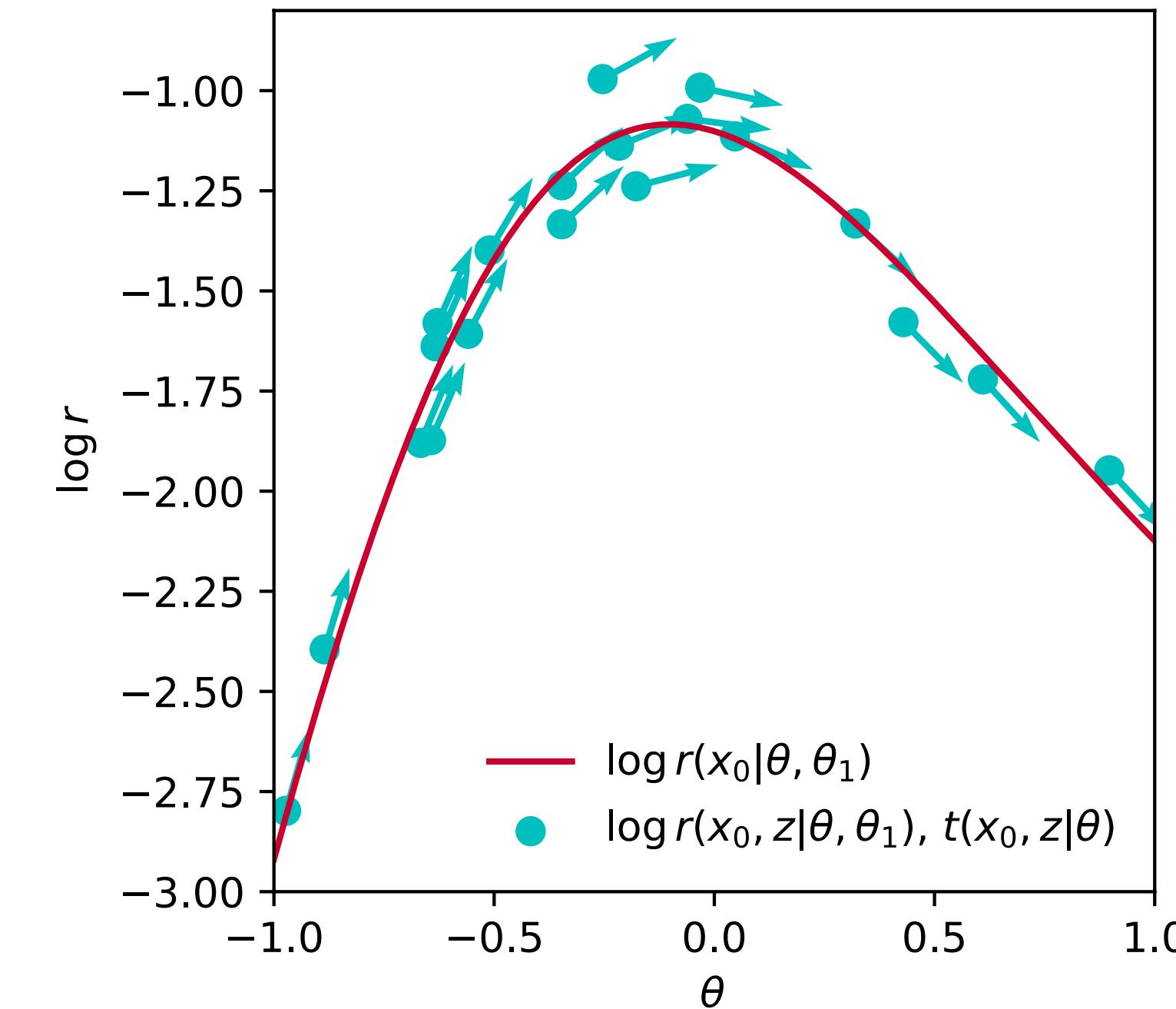
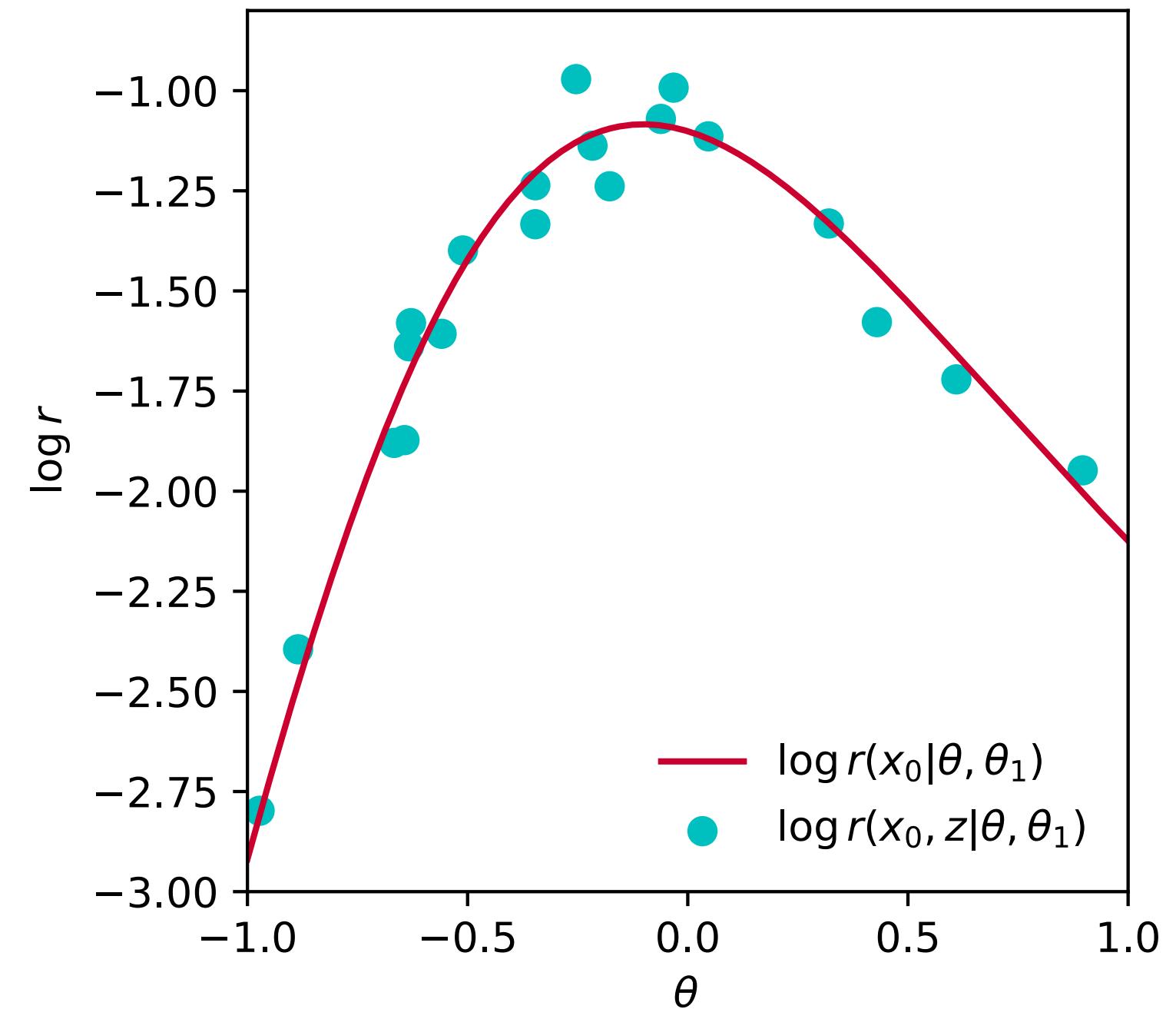
- create one estimator $\hat{r}(x|\theta_0, \theta_1)$ that is a function of θ_0 and θ_1
- no further interpolation necessary
- “borrows information” from close points





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 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**

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

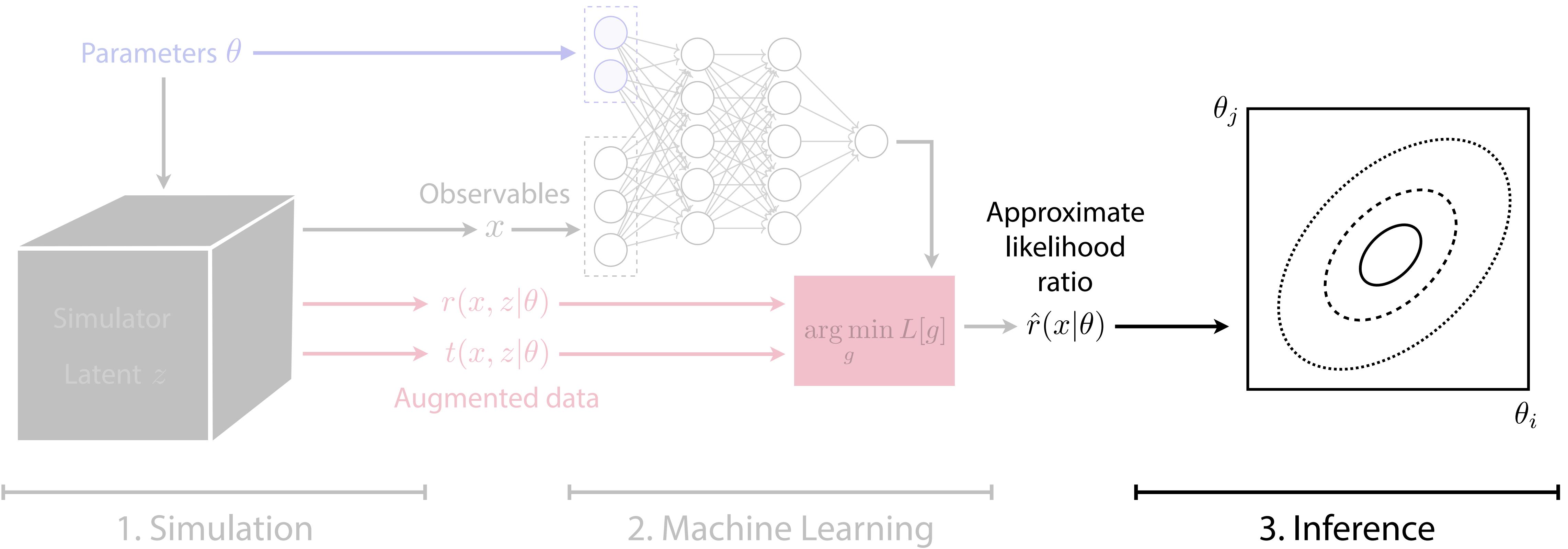
Given $t(x, z|\theta_0)$,
we define the functional

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

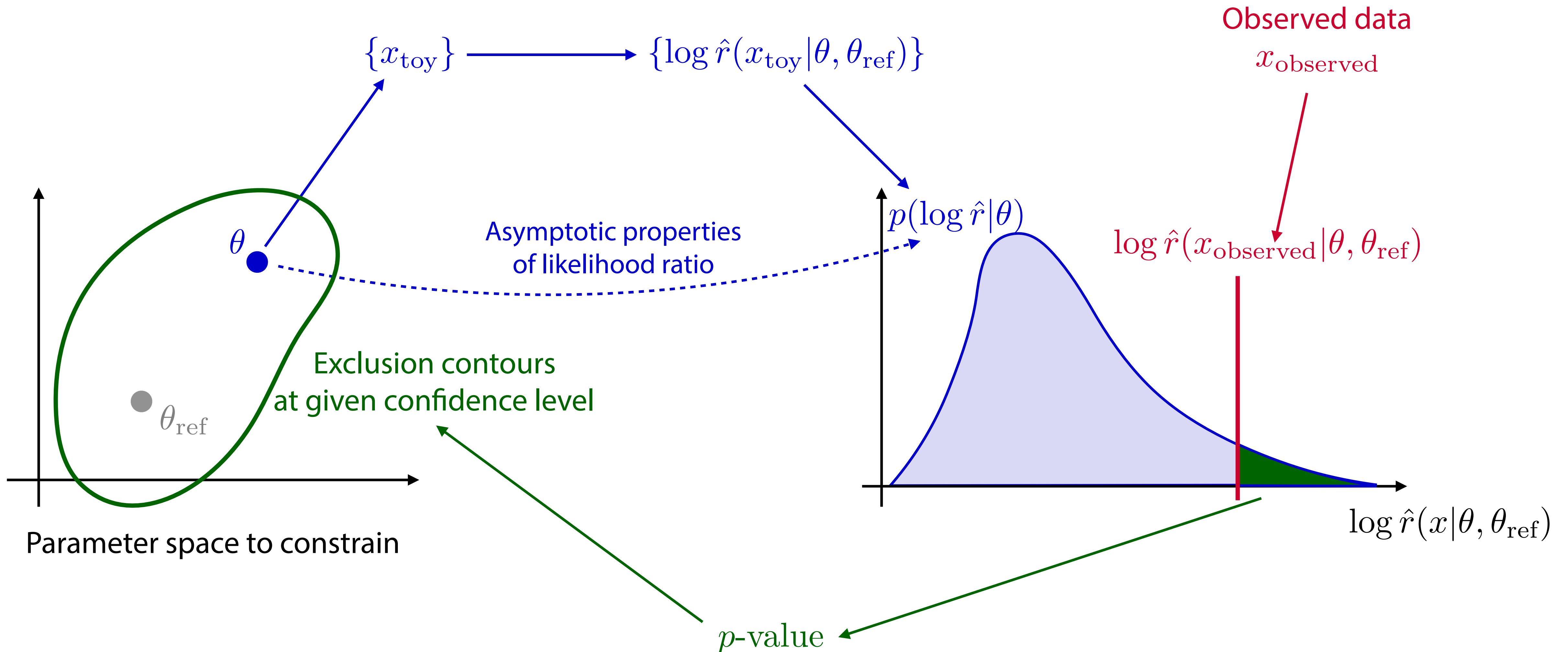
One can show it is minimized by

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

Again, we implement this minimization through machine learning.



Limit setting (frequentist)



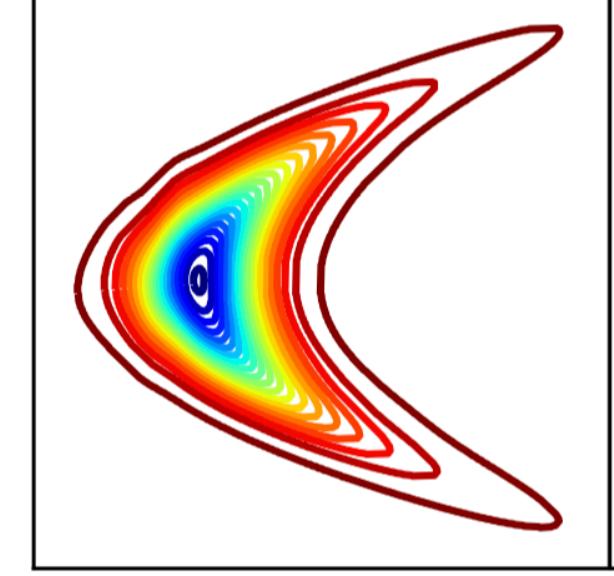
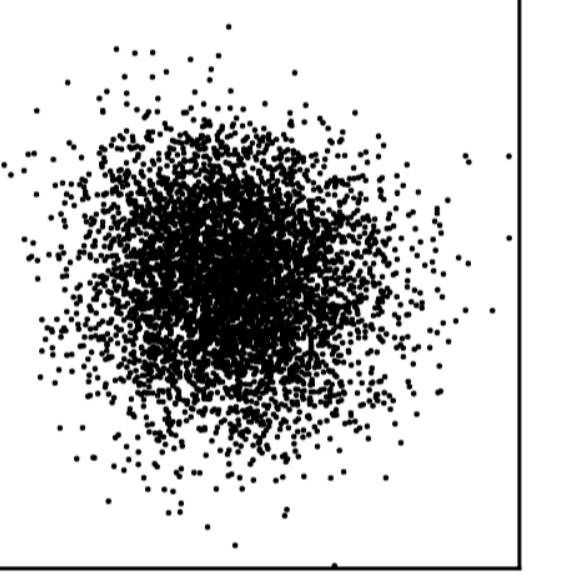
A family of new inference techniques

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

Performance gains with cross-entropy-based loss
 [M. Stoye, JB, K. Cranmer, G. Louppe, J. Pavez 1808.00973]

A family of new inference techniques

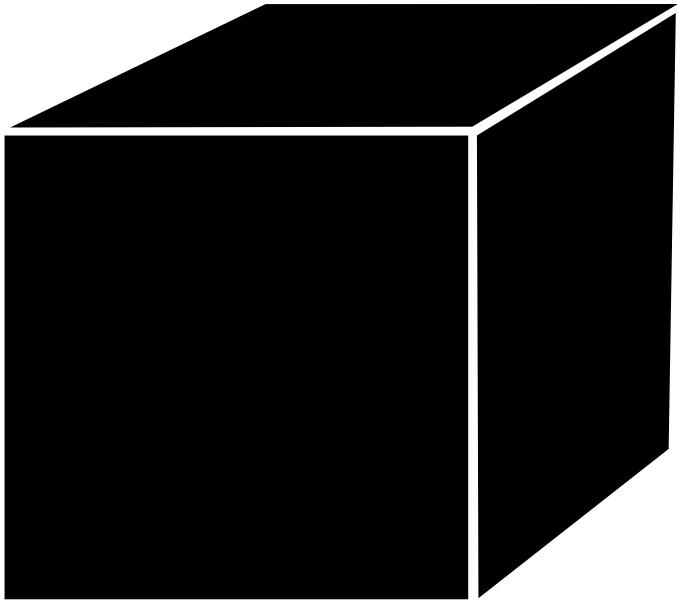
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ROLR	$\theta_0 \sim \pi(\theta), \theta_1$	✓		$\hat{r}(x \theta_0, \theta_1)$	✓	
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RASCAL	$\theta_0 \sim \pi(\theta), \theta_1$	✓	✓	$\hat{r}(x \theta_0, \theta_1)$	✓	
ALICES	$\theta_0 \sim \pi(\theta), \theta_1$	✓	✓	$\hat{r}(x \theta_0, \theta_1)$	✓	
SCANDAL	$\theta \sim \pi(\theta)$		✓	$\hat{p}(x \theta)$	✓	✓
SALLY	θ_{ref}		✓	$\hat{t}(x \theta_{\text{ref}})$	in local approx.	
SALLINO	θ_{ref}		✓	$\hat{t}(x \theta_{\text{ref}})$	in local approx.	

Combination with state-of-the-art conditional neural density estimators, e.g. normalizing flows

[everything by G. Papamakarios:
G. Papamakarios, T. Pavlakou, I. Murray 1705.07057;
G. Papamakarios, D. Sterratt, I. Murray 1805.07226; ...]

Systematics



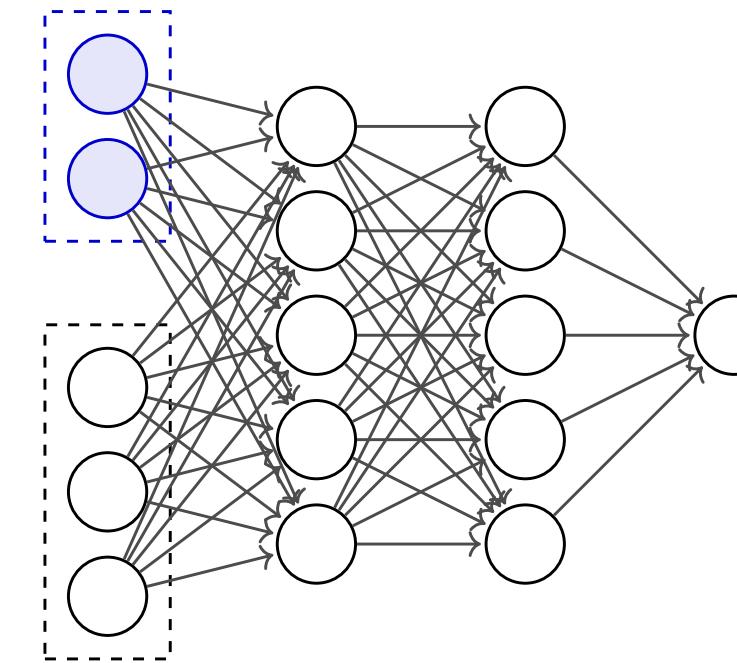
Don't fully trust the simulator?

- Nuisance parameters to model systematic uncertainties
- Methods learn dependence both on parameters of interest and nuisance parameters. Then we can construct profile likelihood and “nuisance-hardened” score

[P. de Castro, T. Dorigo 1806.04743;
J. Alsing, B. Wandelt 1903.01473]

- Alternatively: Robustness to nuisance with adversarial training

[G. Louppe, M. Kagan, K. Cranmer 1611.01046]



Don't blindly trust the neural network?

- Diagnostic cross checks: known expectation values, “critic” tests
- Calibration / Neyman construction with toys: badly trained network can lead to suboptimal limits, but not to wrong limits

WBF Higgs to four leptons with detector effects

