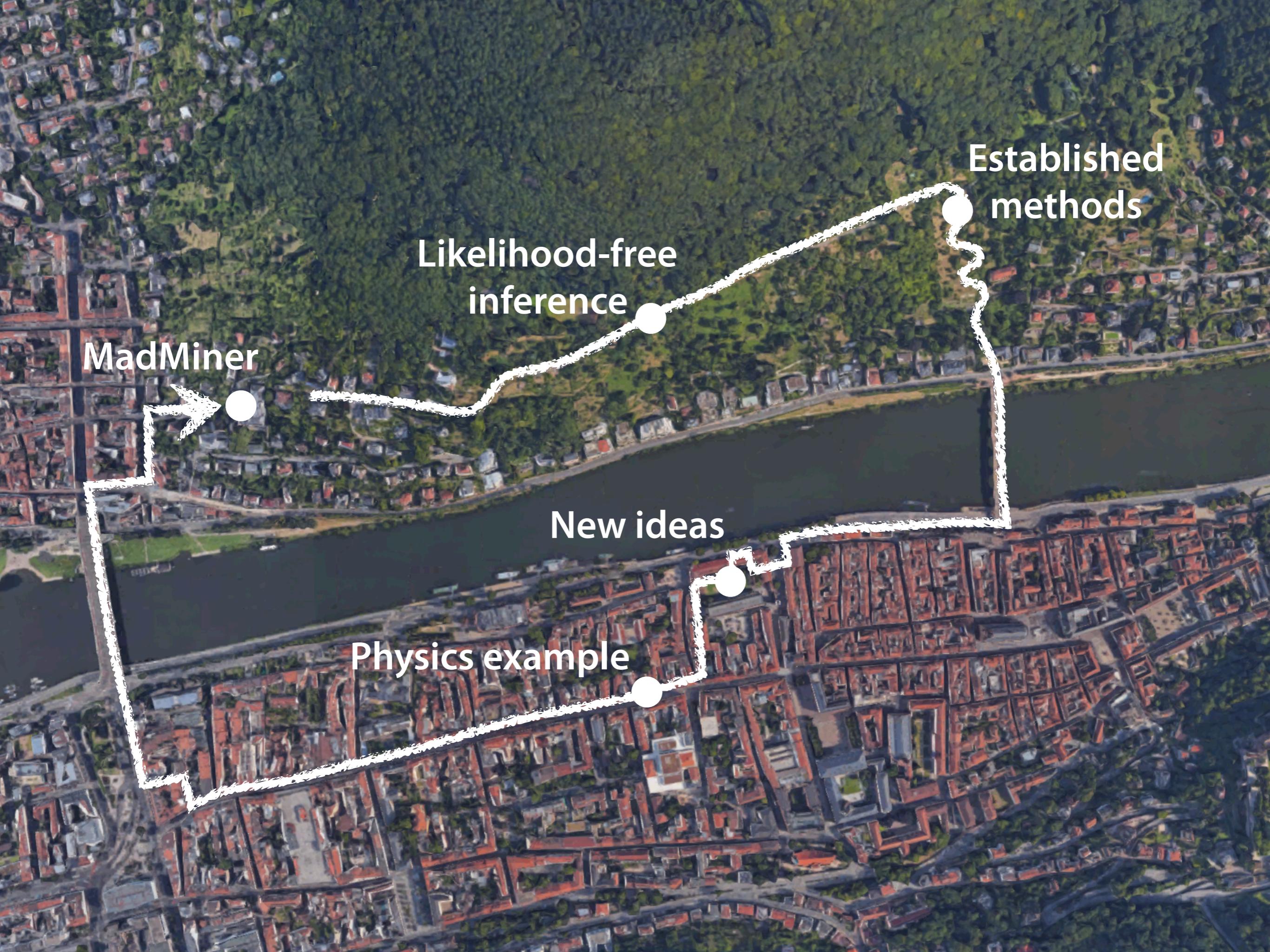


# Learning to constrain new physics

Johann Brehmer

New York University

Heidelberg  
August 21, 2018



MadMiner

Likelihood-free  
inference

Established  
methods

New ideas

Physics example

# Likelihood-free inference

# The Galton board



[Source: galtonboard.com]

# The Galton board



[Source: galtonboard.com]

# The Galton board



FIG. 7.

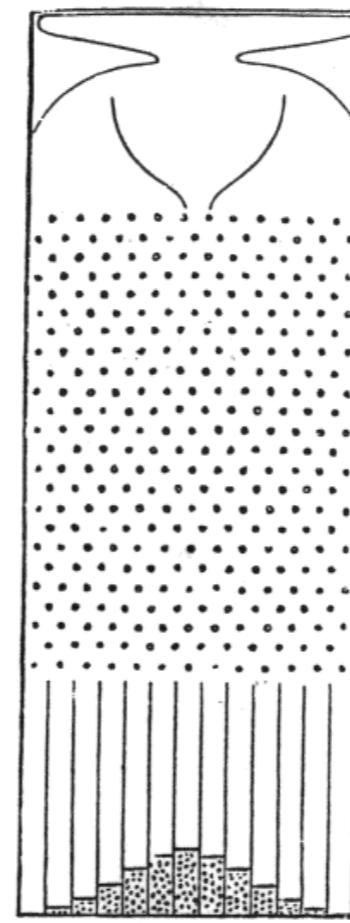


FIG. 8.

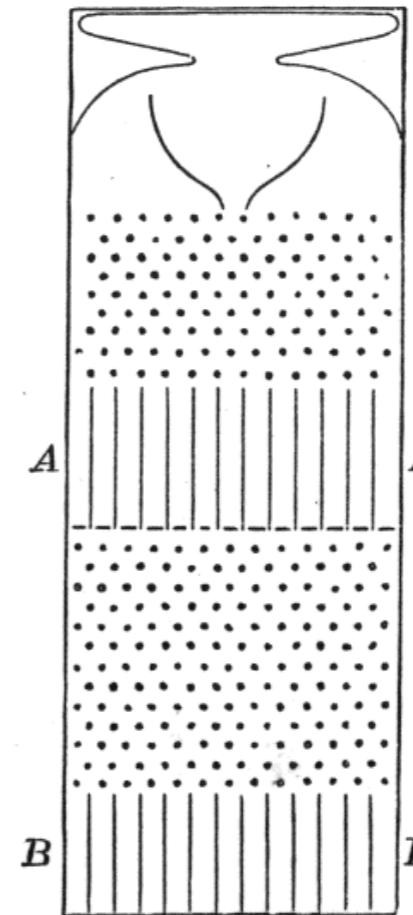
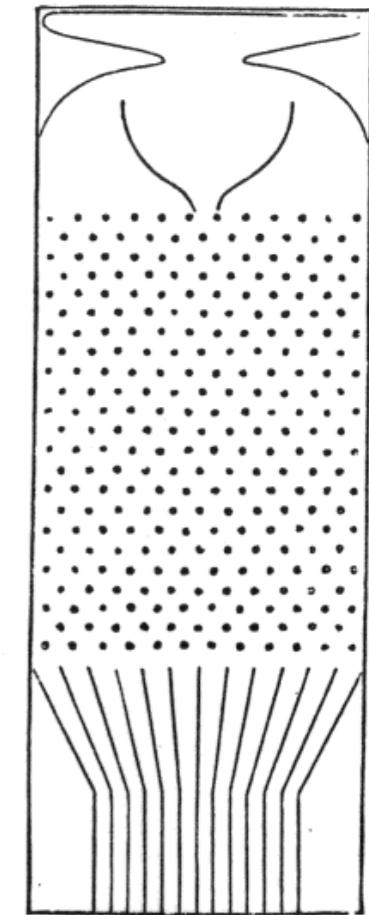
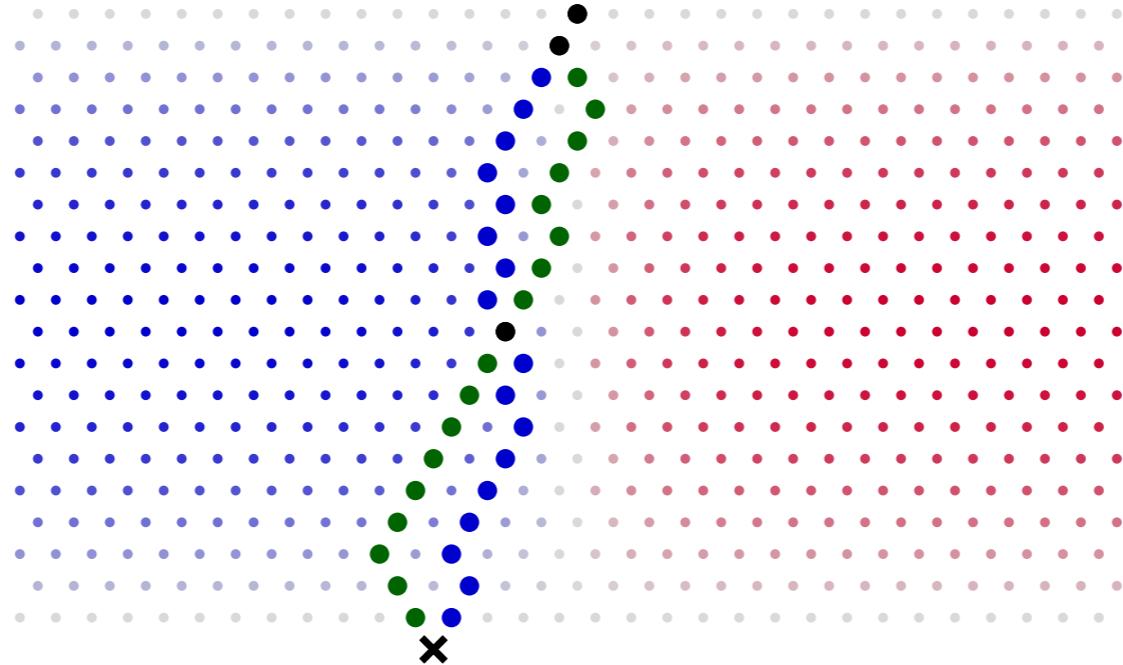


FIG. 9.



[Source: F. Galton 1889]

# Probabilities



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

# The generalized Galton board

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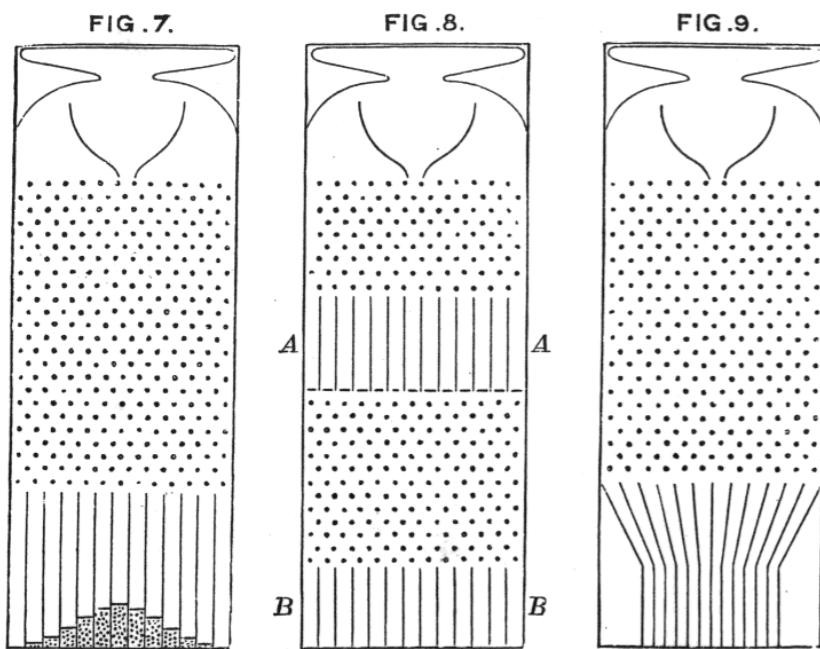
“Easy” problem if we can evaluate likelihood  $p(x_i|\theta)$ . But

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

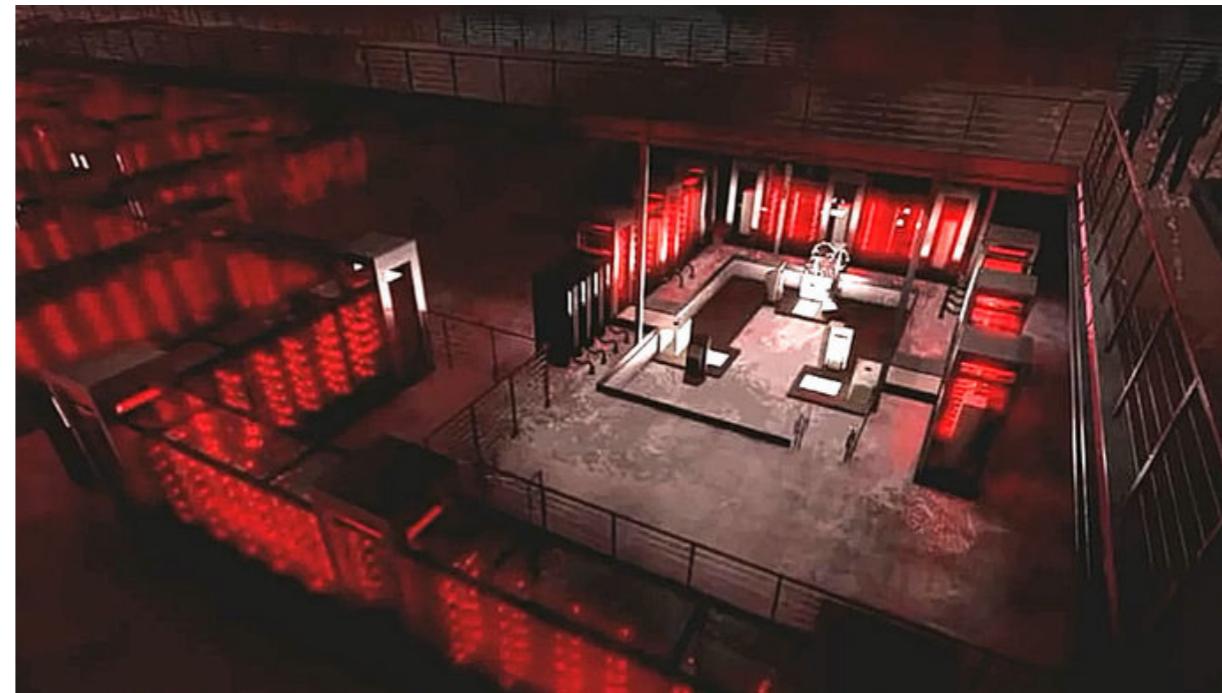
The number of possible **paths**  $z$  can be huge, and it becomes impossible to calculate the integral

⇒ Likelihood not tractable, only implicitly defined through “simulator”

# Galton board: metaphor for simulator-based science



[Source: F. Galton 1889]



[Source: HBO 2018]

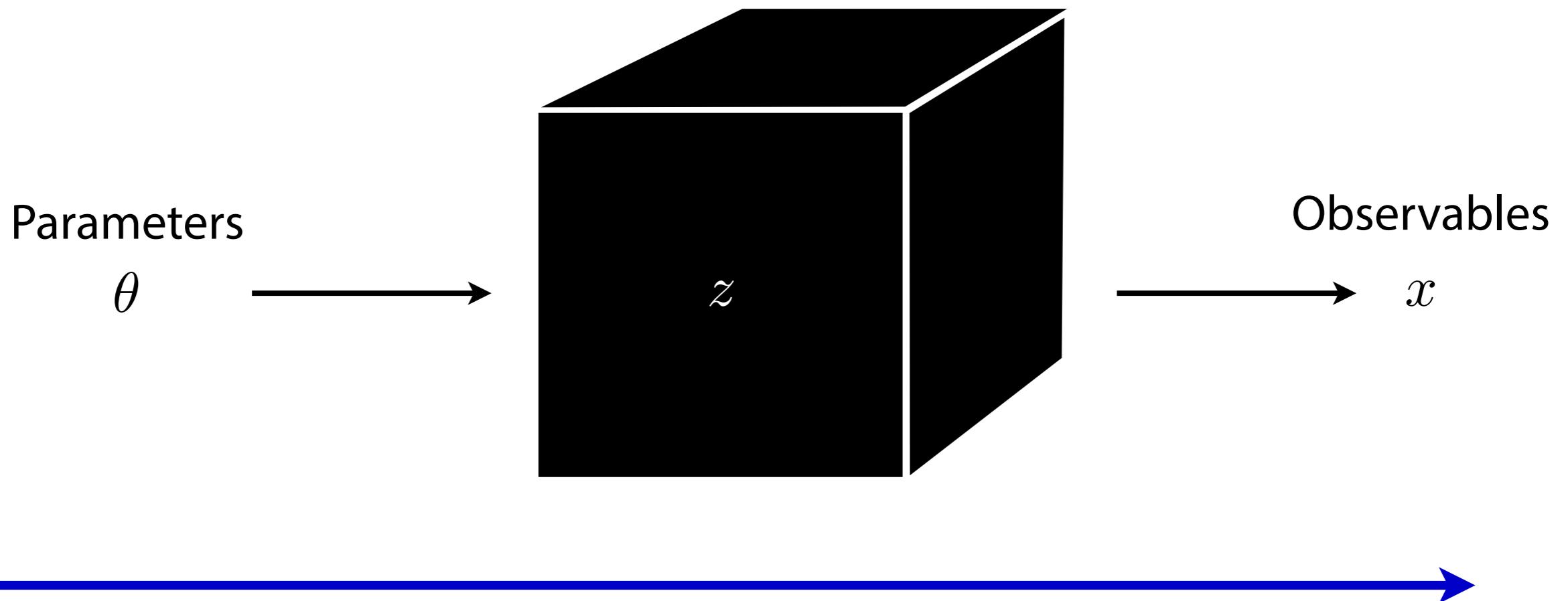
Galton board device → Computer simulation

Parameters  $\theta$  → Parameters of interest  $\theta$

Bins  $x$  → Observables  $x$

Path  $z$  → Latent variables  $z$   
(stochastic execution trace through simulator)

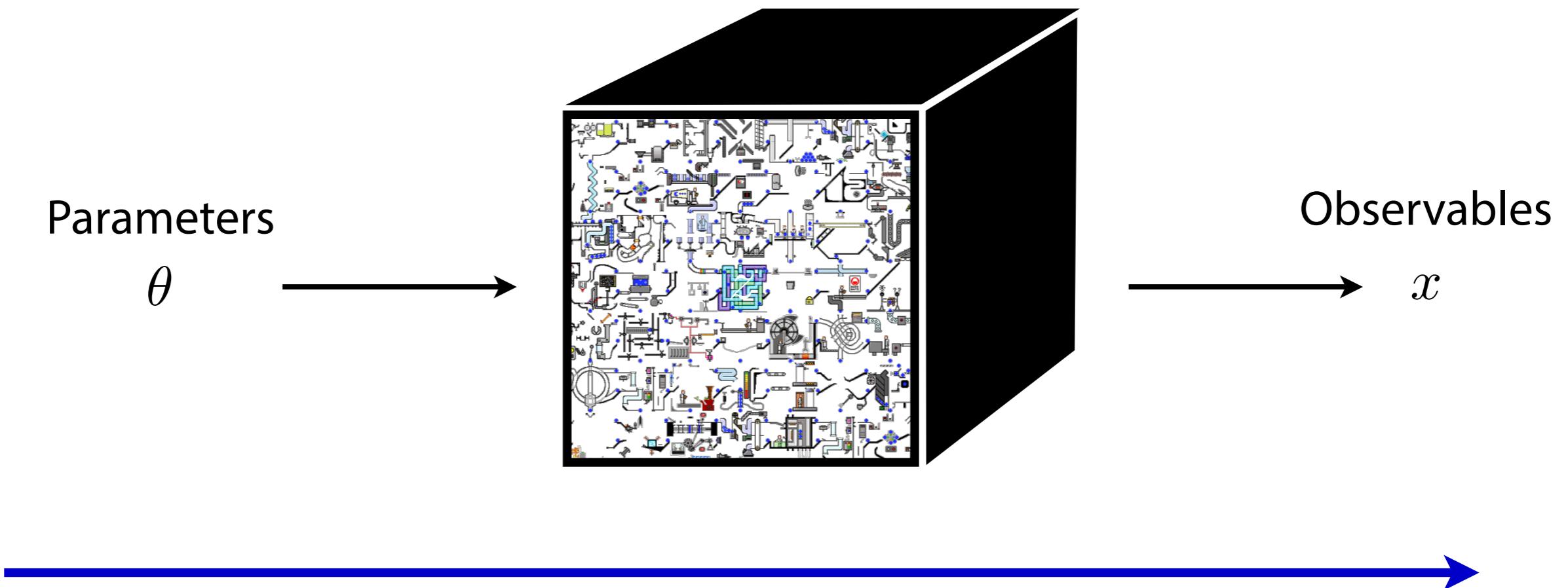
# Likelihood-free inference



Prediction (simulation):

- Well-understood mechanistic model
- Simulator can generate samples

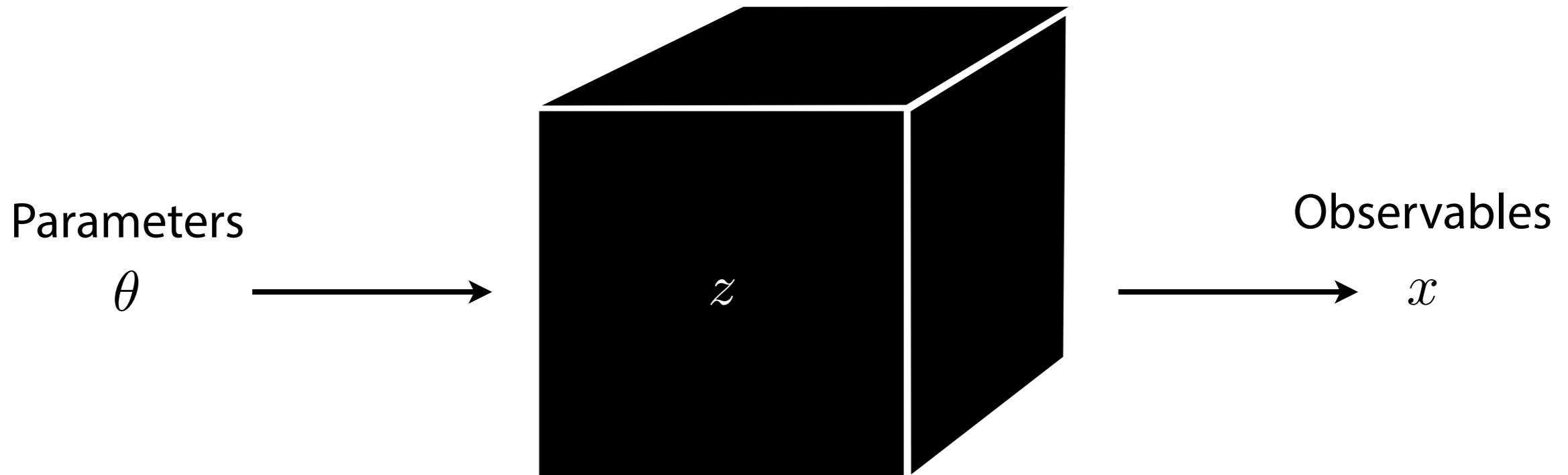
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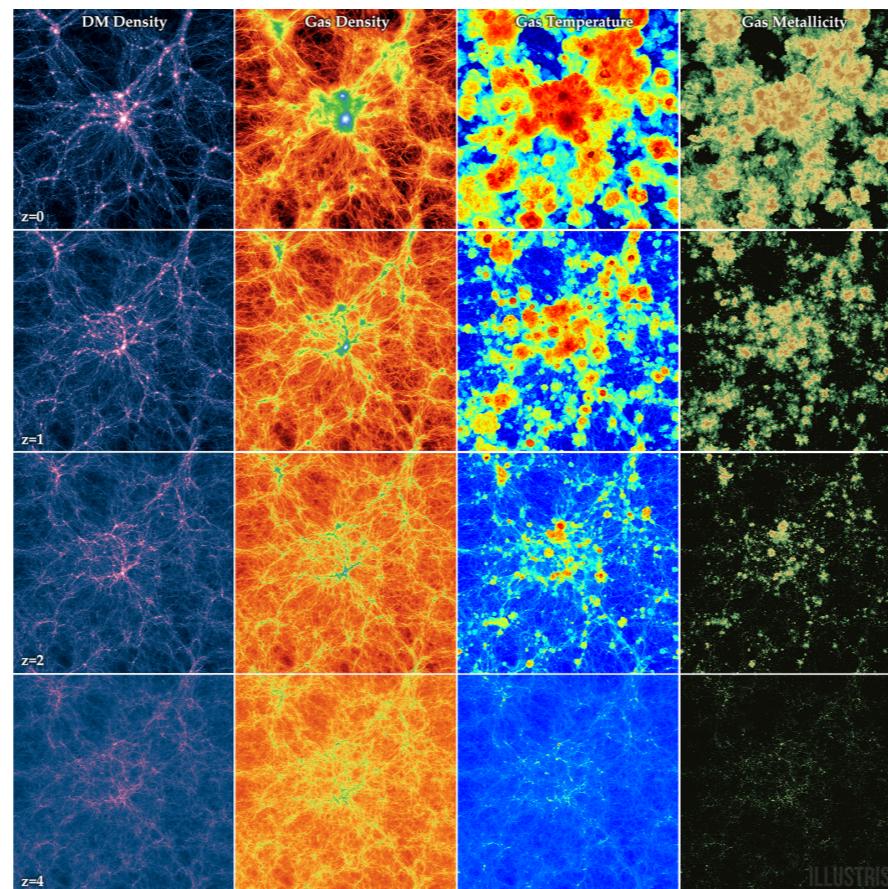
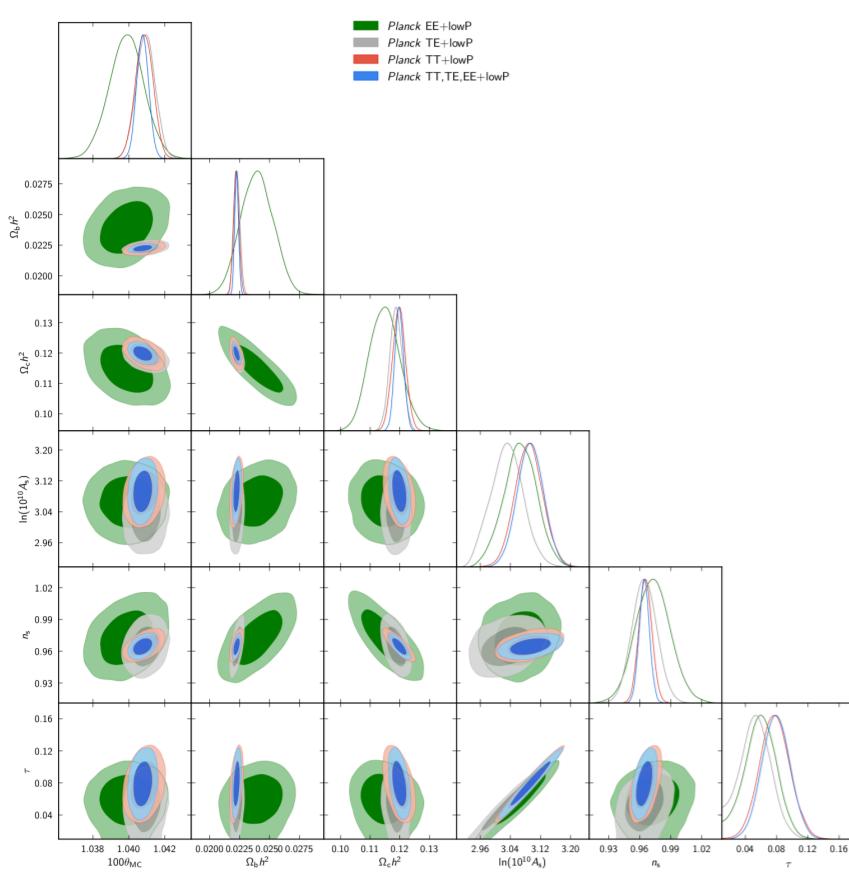
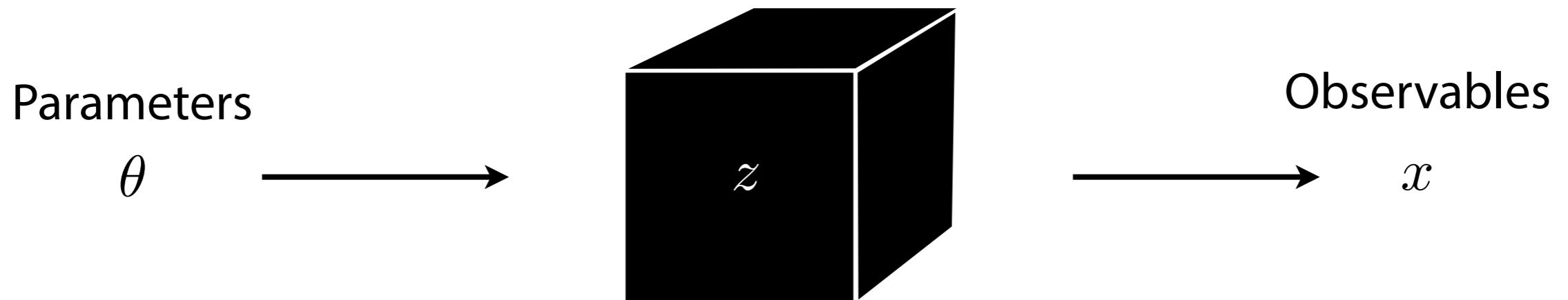
Prediction (simulation):

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Inference:

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

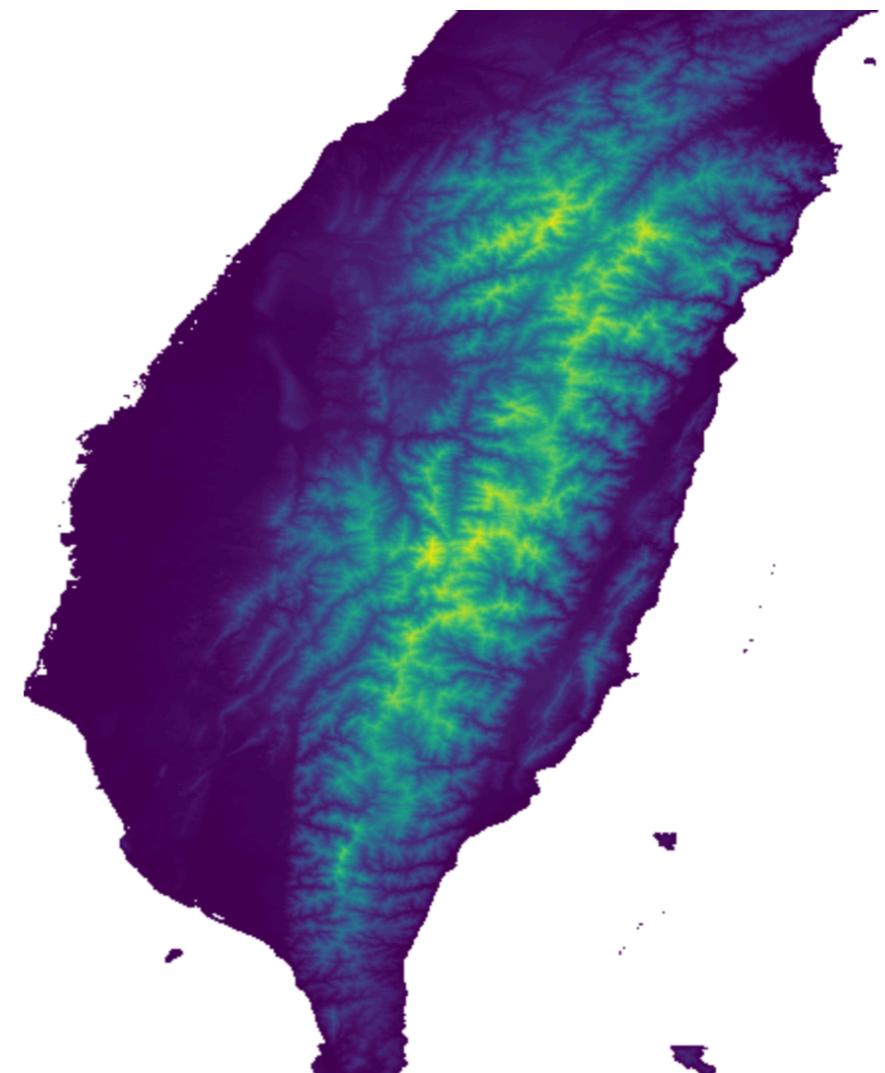
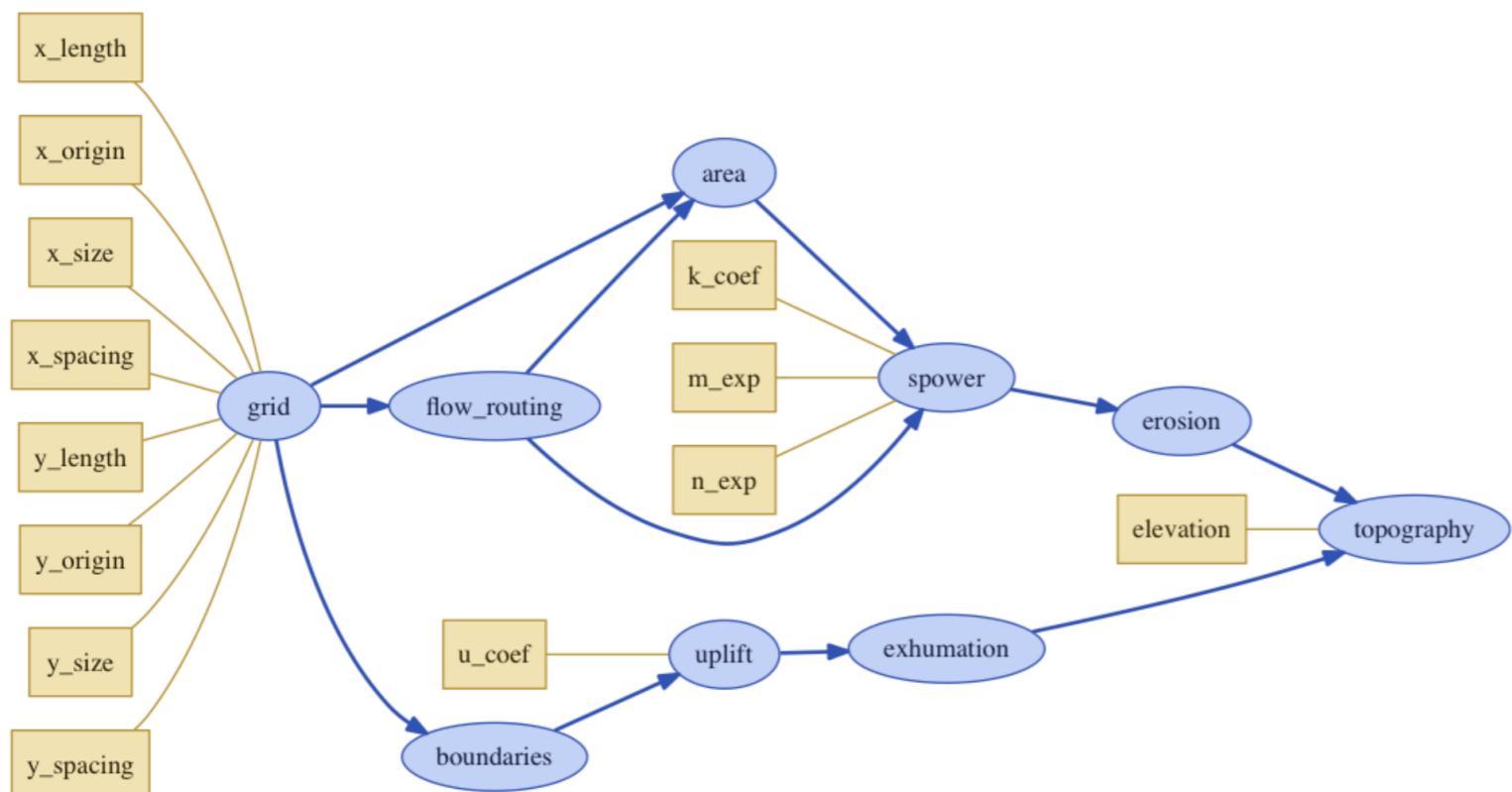
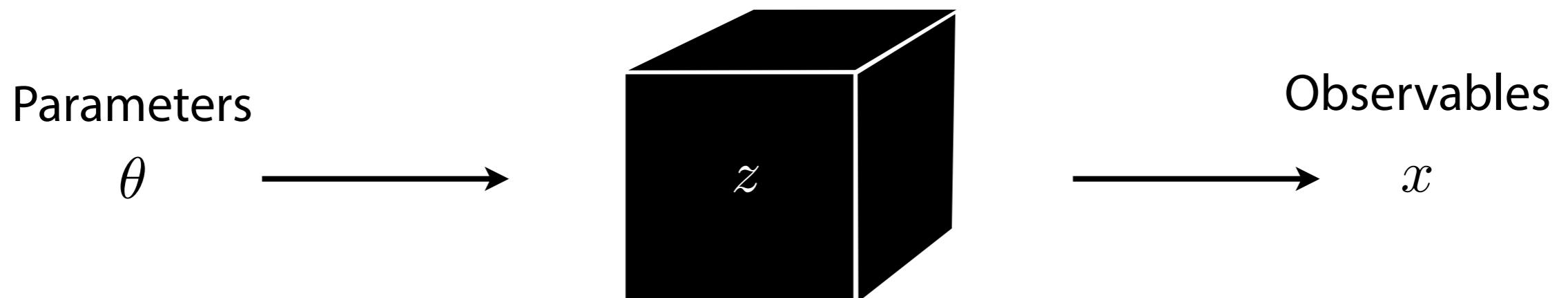
# Cosmological N-body simulations



[Source: Planck 1502.01589]

[Source: Illustris 1405.2921]

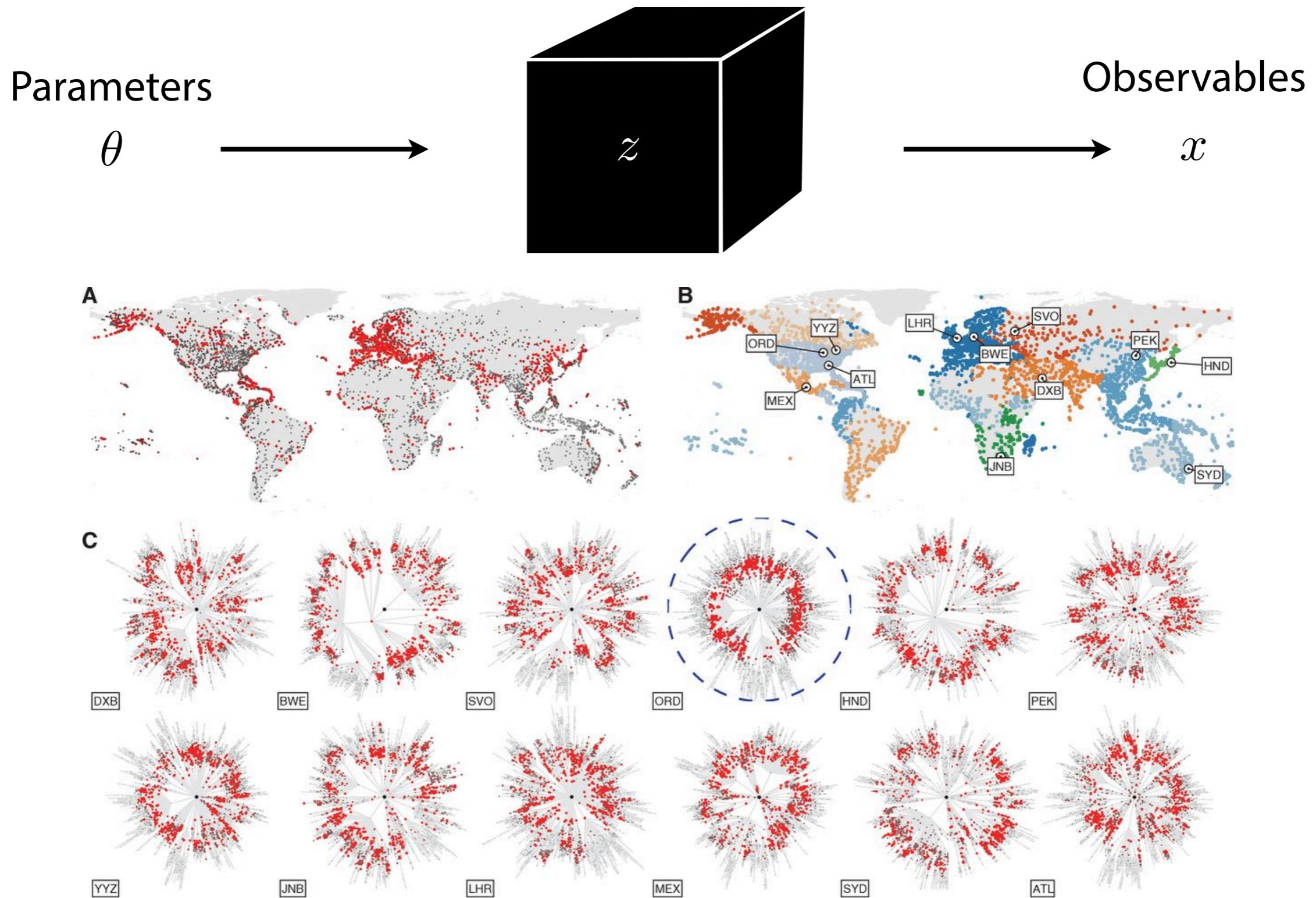
# Computational topography



[Source: Benoit Bovy]

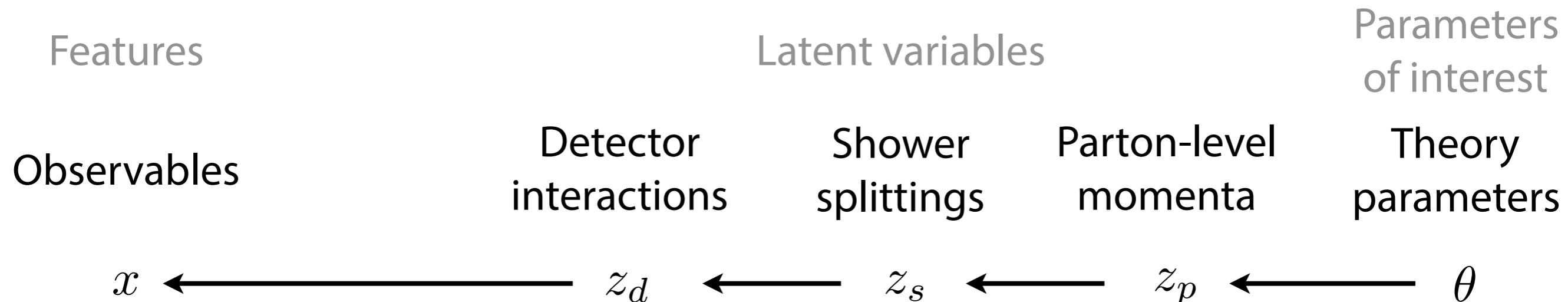
10/40

# Epidemiology

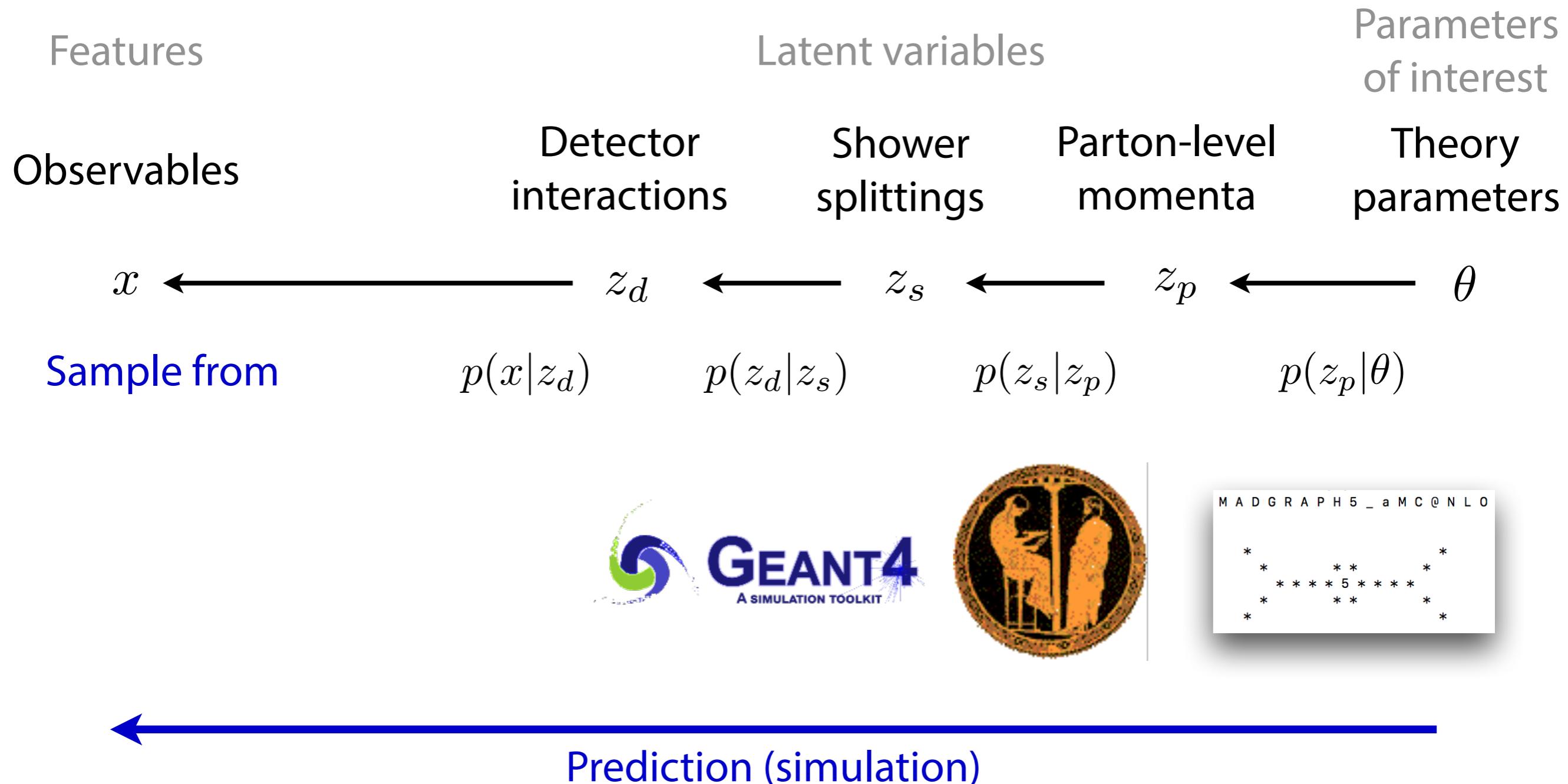


[Source: D. Brockmann, D. Helbing 2013]

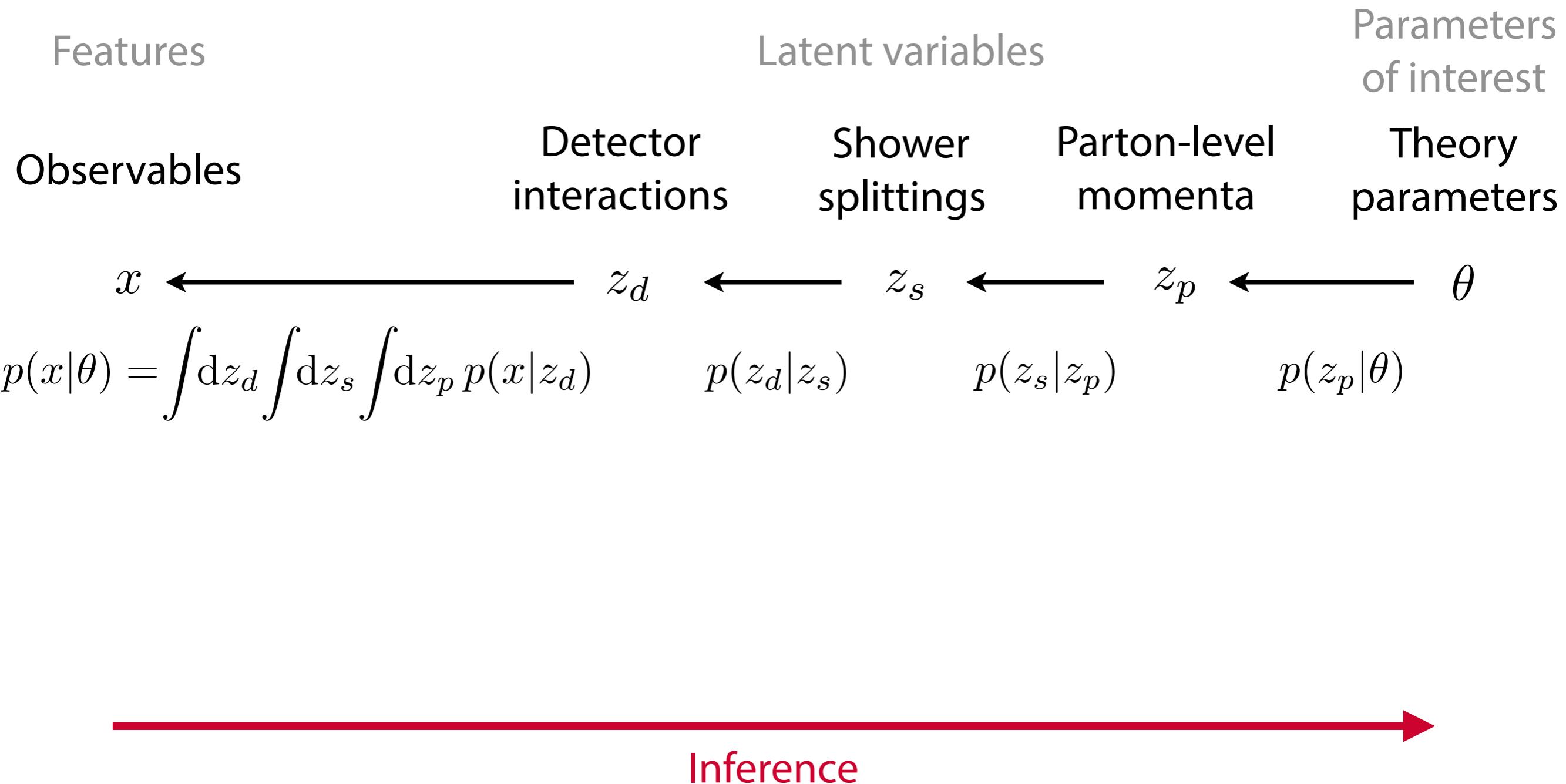
# Particle physics processes: simulation



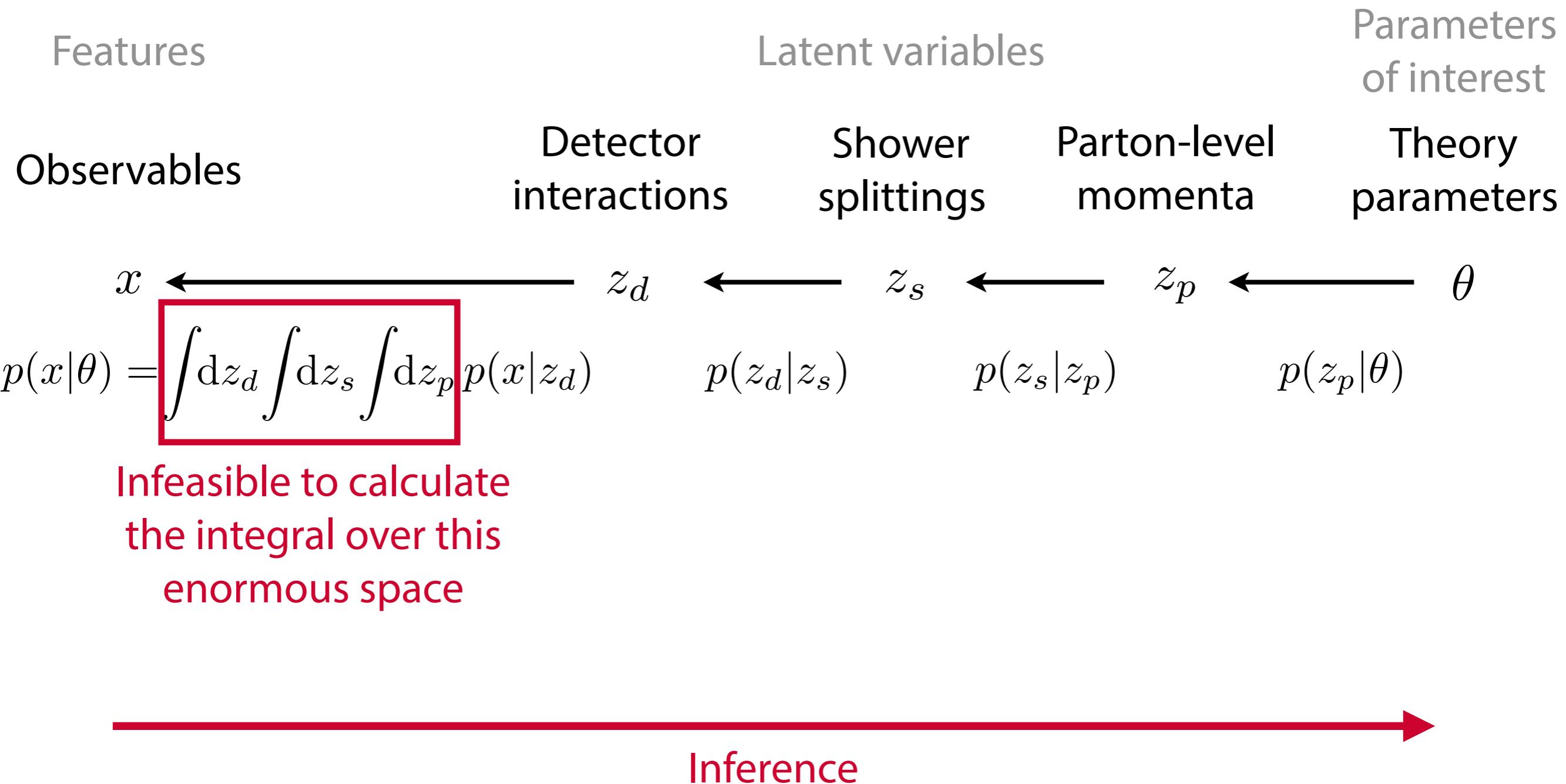
# Particle physics processes: simulation



# Particle physics processes: inference



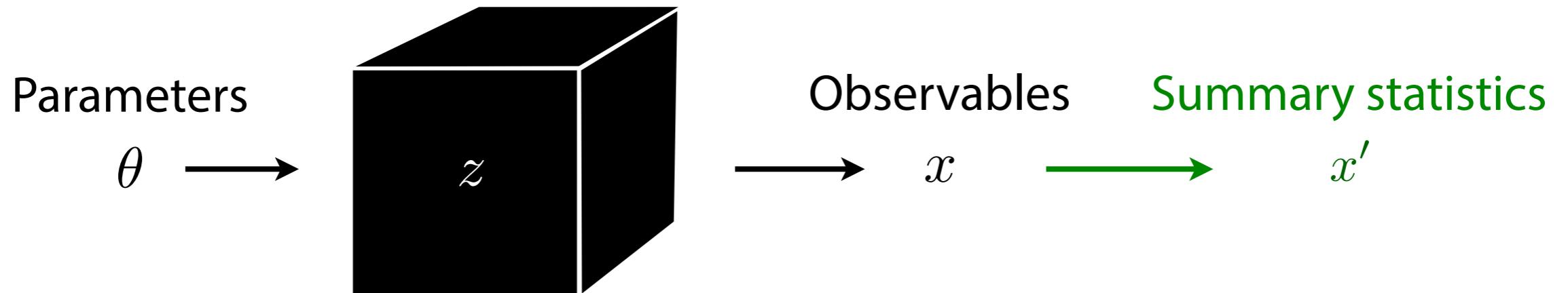
# Particle physics processes: inference



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

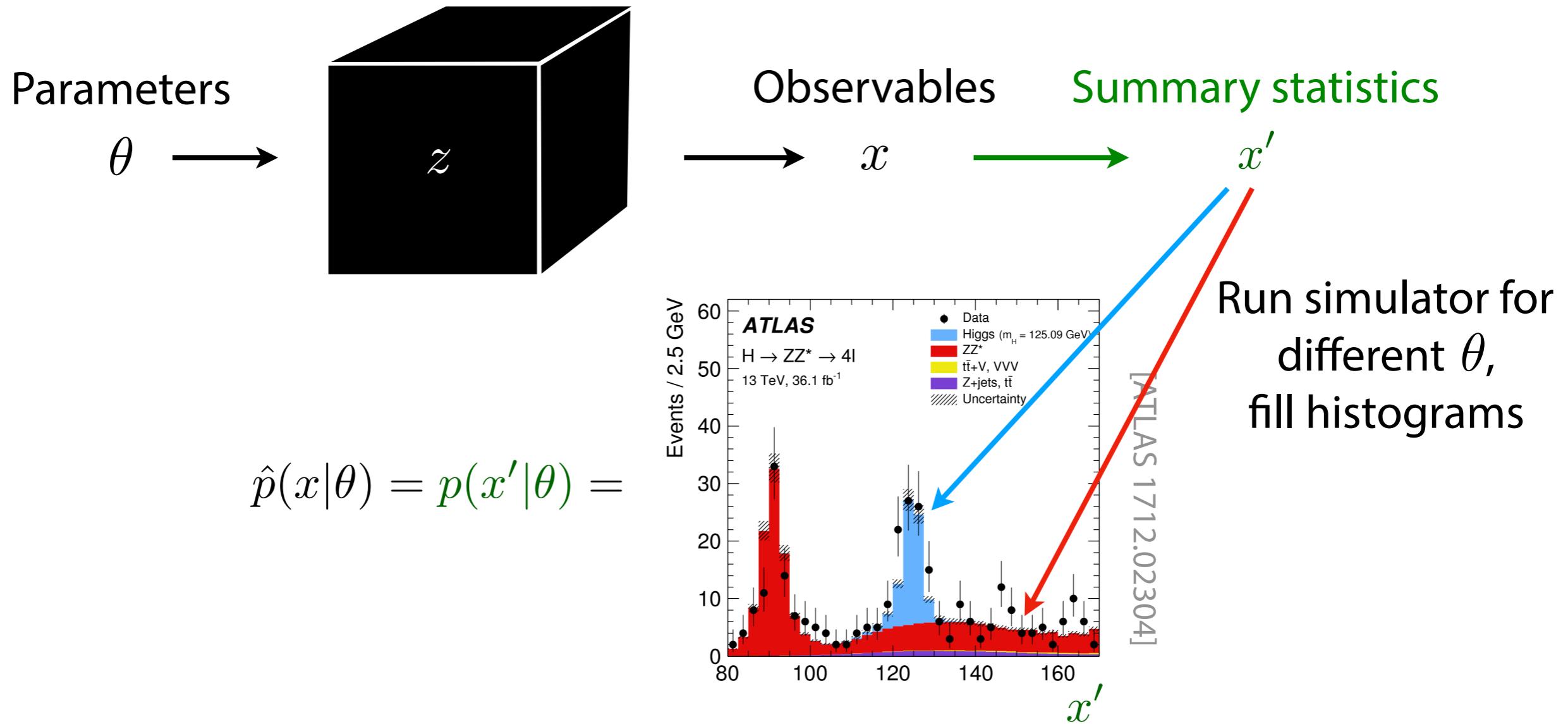
# Why has that not stopped us so far?

- The physicist's way:



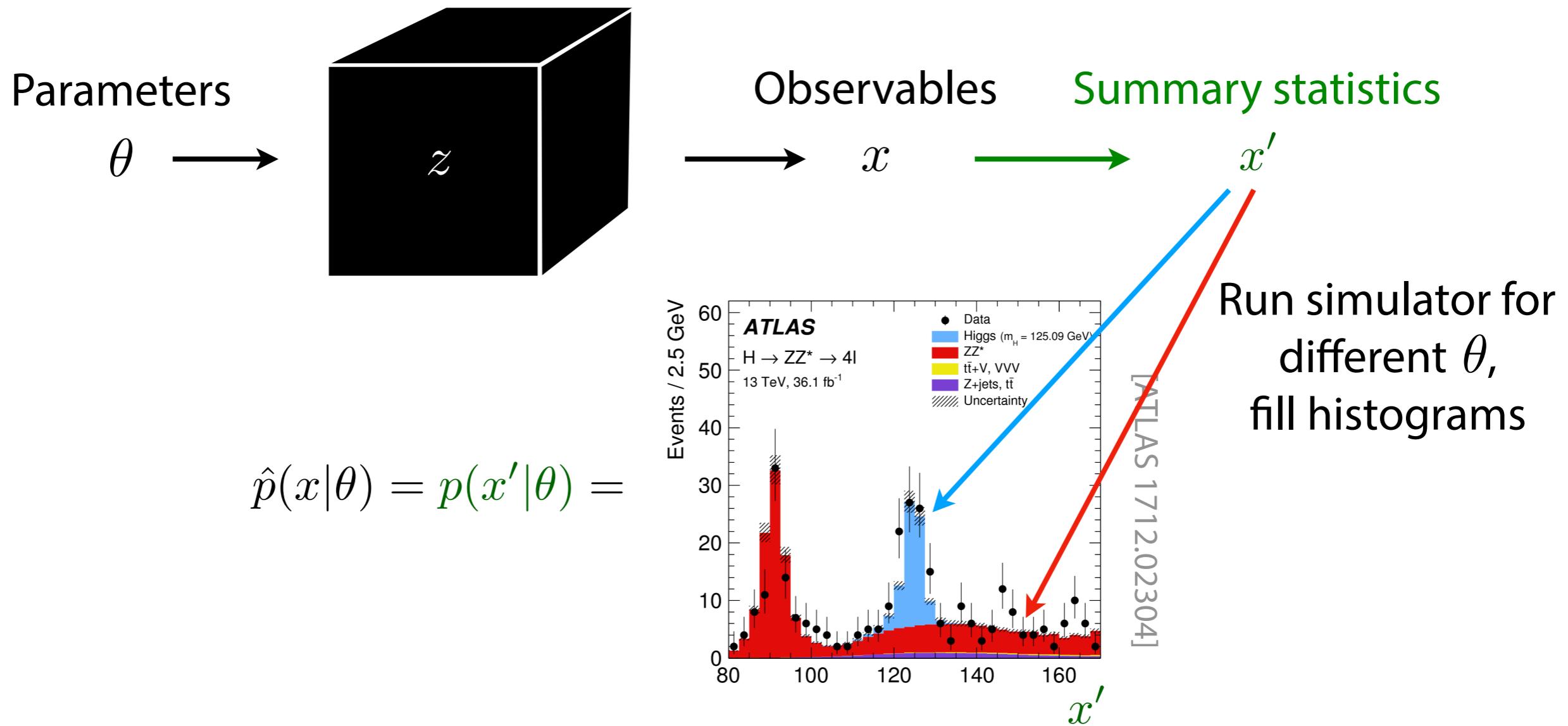
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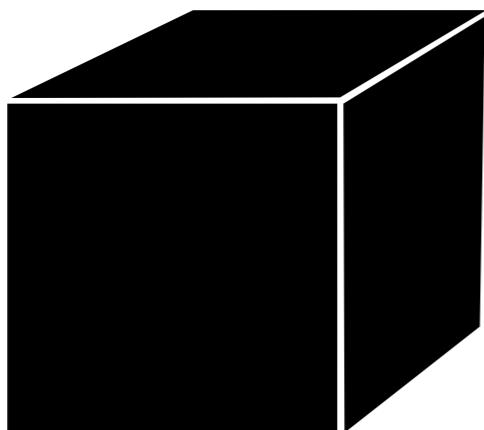


- But how to choose  $x'$ ? Standard variables lose information, analysis of high-dimensional  $x$  (including correlations) often more powerful

# 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, ...



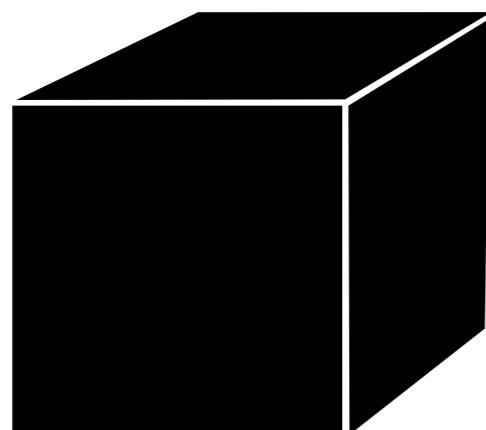
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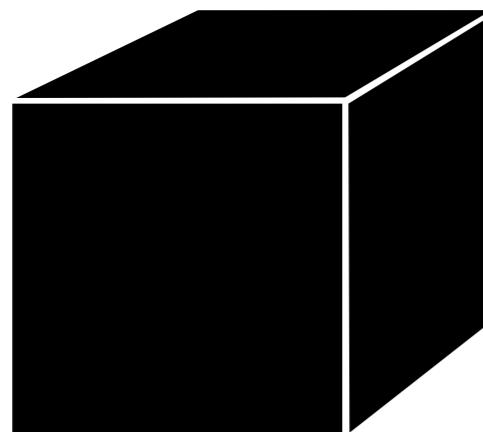
- Matrix Element Method / Optimal  
Observables  
Neglect or approximate shower +  
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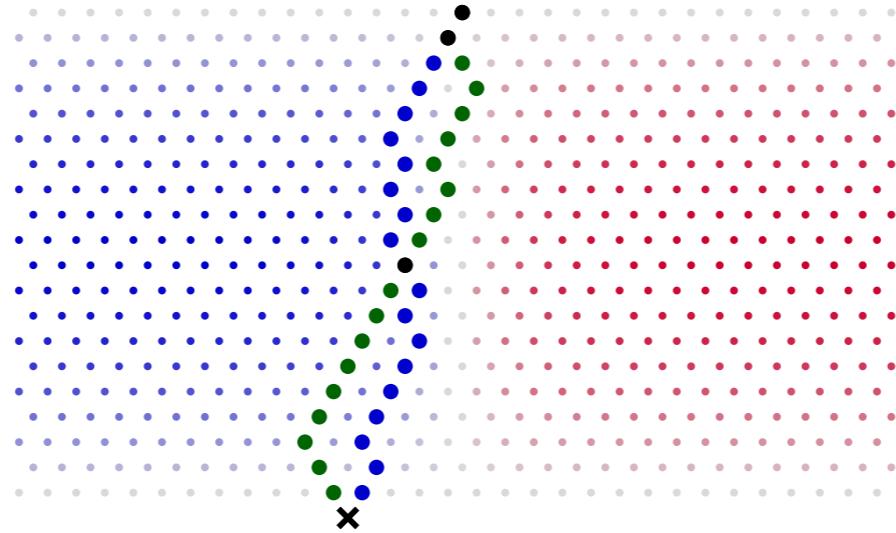
- Matrix Element Method / Optimal  
Observables  
Neglect or approximate shower +  
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- **Mining gold from the simulator**  
Leverage matrix-element information  
+ machine learning
  - ▶ stronger limits
  - ▶ scales to many parameters +  
observables
  - ▶ no approximations on physics  
necessary
  - ▶ evaluation in microseconds

New!

# **Mining gold from the simulator**

# Back to the Galton board



- Likelihood

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

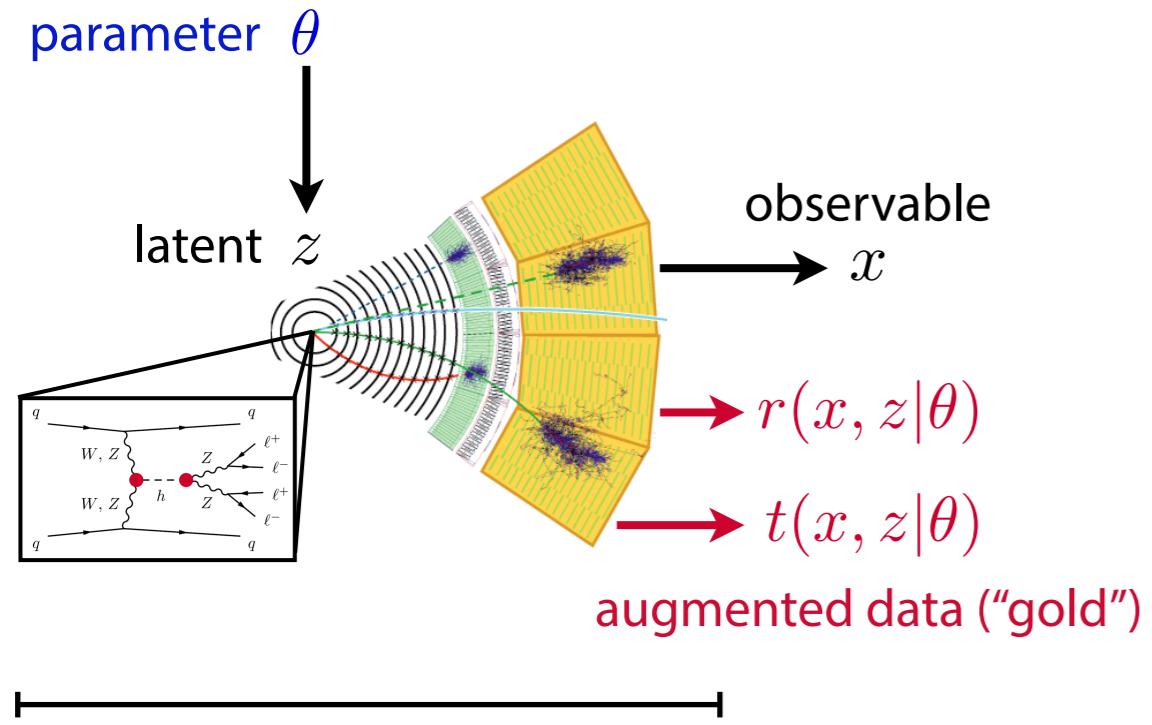
is usually intractable because of the integral over **all possible paths  $z$**

- But: we can calculate the **probability of each individual path**

$$p(x, z|\theta) = \prod_{\text{nails } i} p_i(x, z|\theta)$$

Turns out that that can be useful...

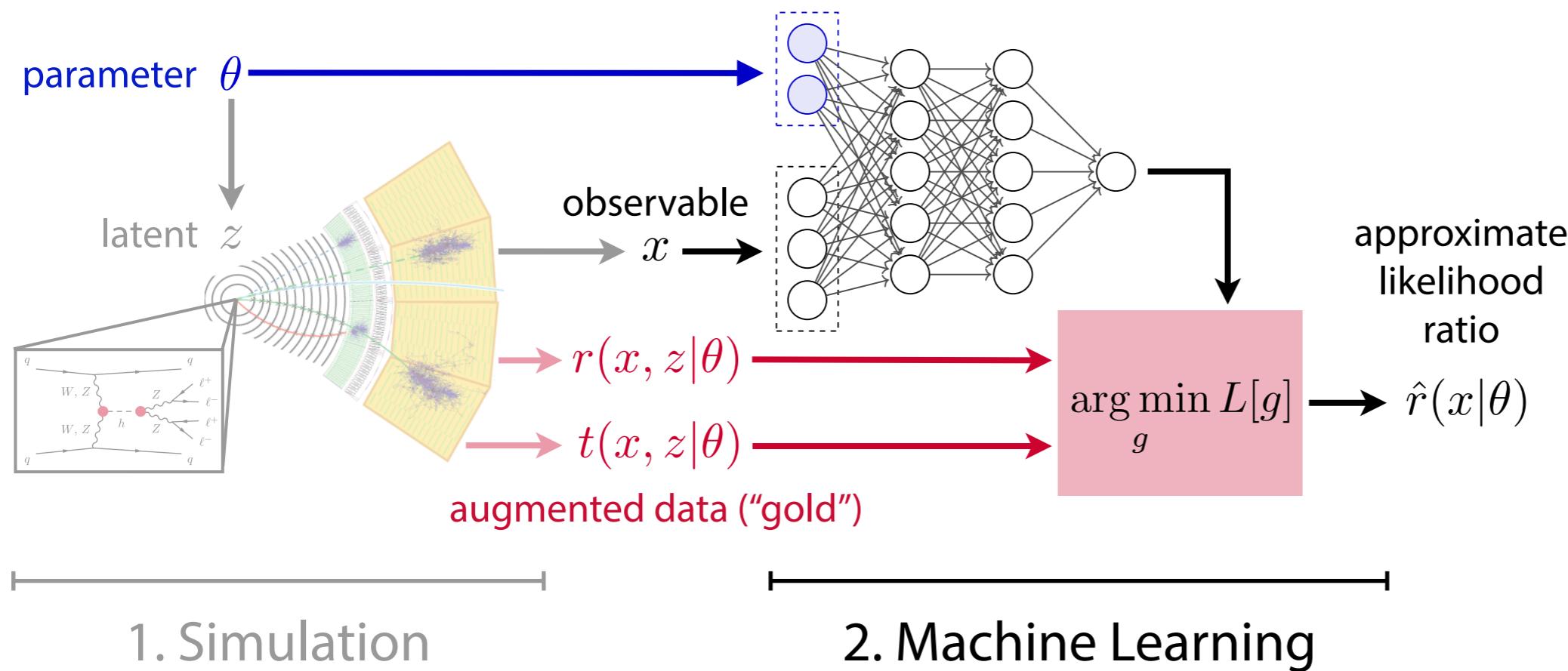
# Bird's-eye view



## 1. Simulation

"Mining gold": Extract additional information from simulator

# Bird's-eye view



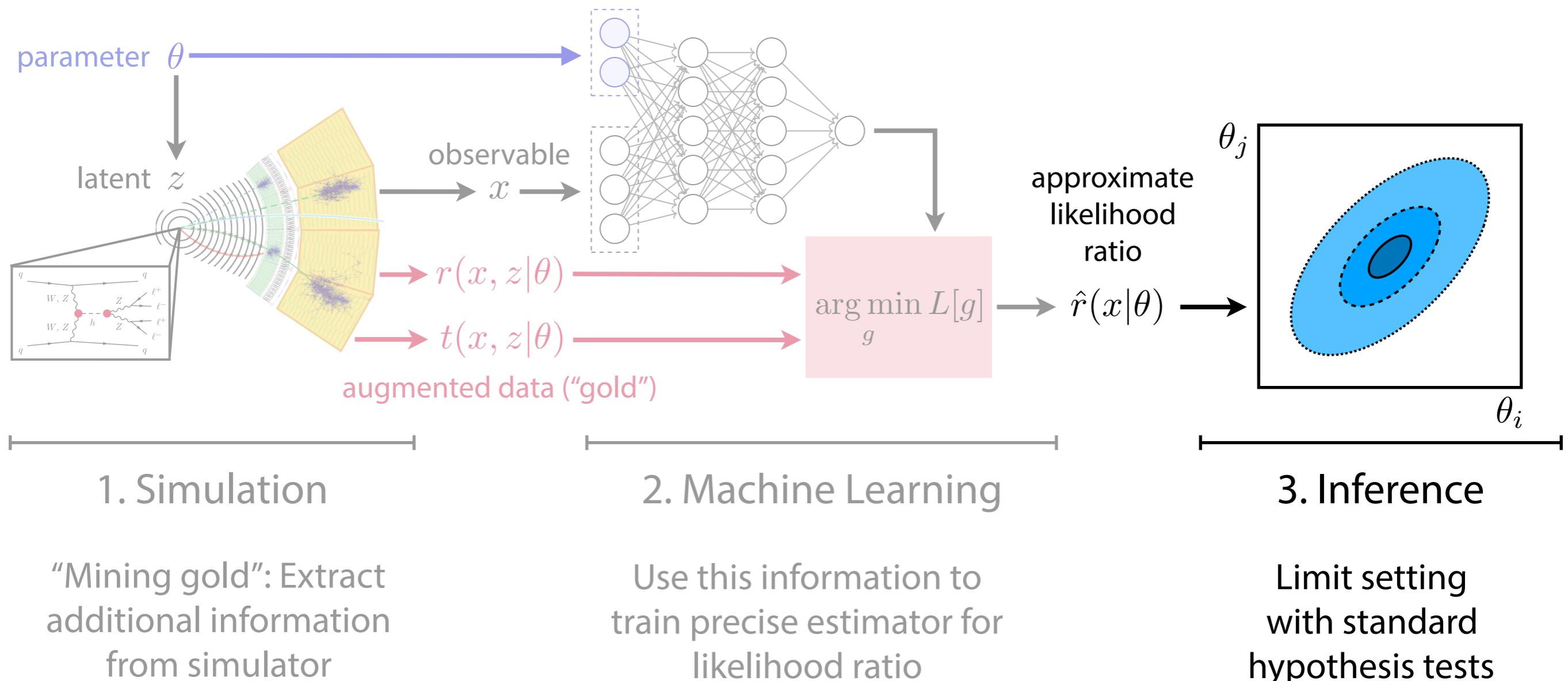
"Mining gold": Extract additional information from simulator

Use this information to train precise estimator for likelihood ratio

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

observables    model parameters

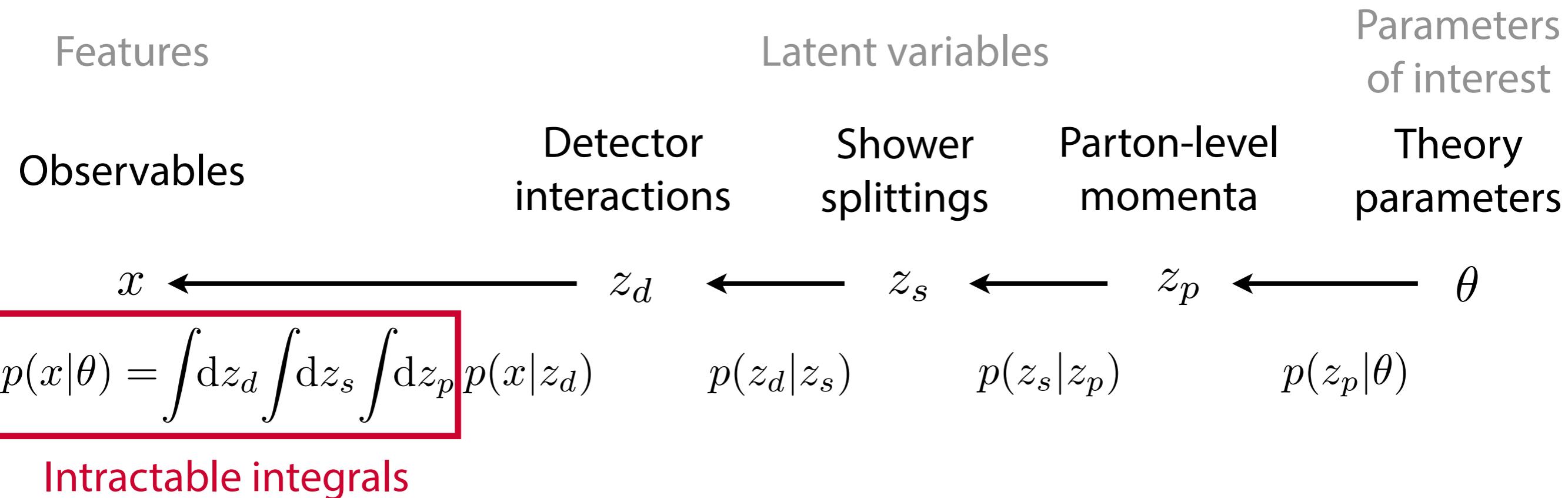
# Bird's-eye view



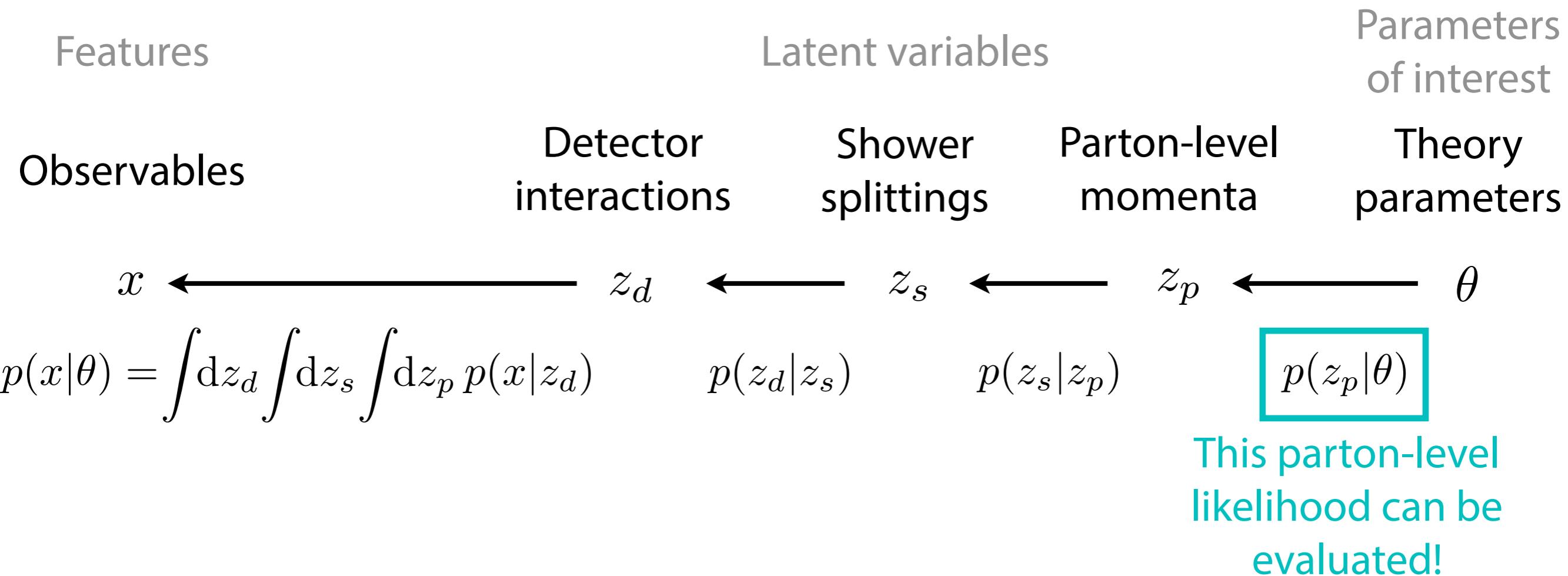




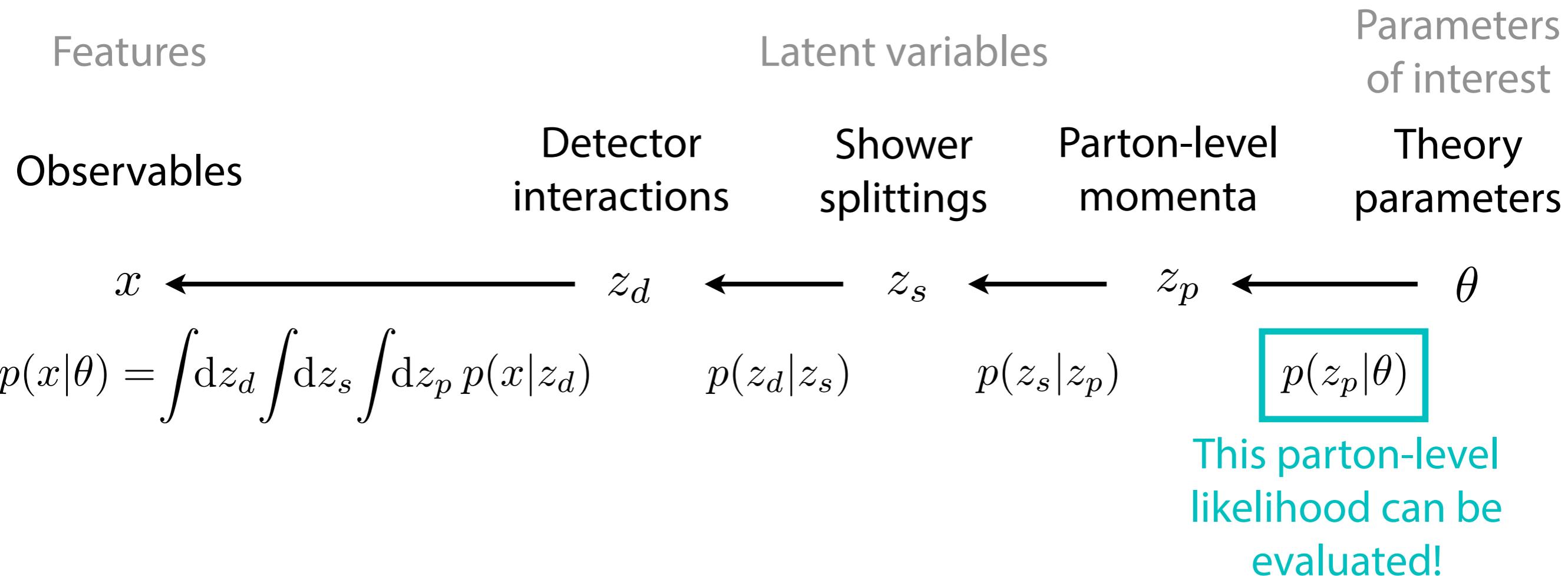
# Mining gold from the simulator



# Mining gold from the simulator



# Mining gold from the simulator



⇒ We can calculate the “joint” likelihood ratio conditional on a 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 have joint likelihood ratio

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



We want likelihood ratio

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

# The value of gold

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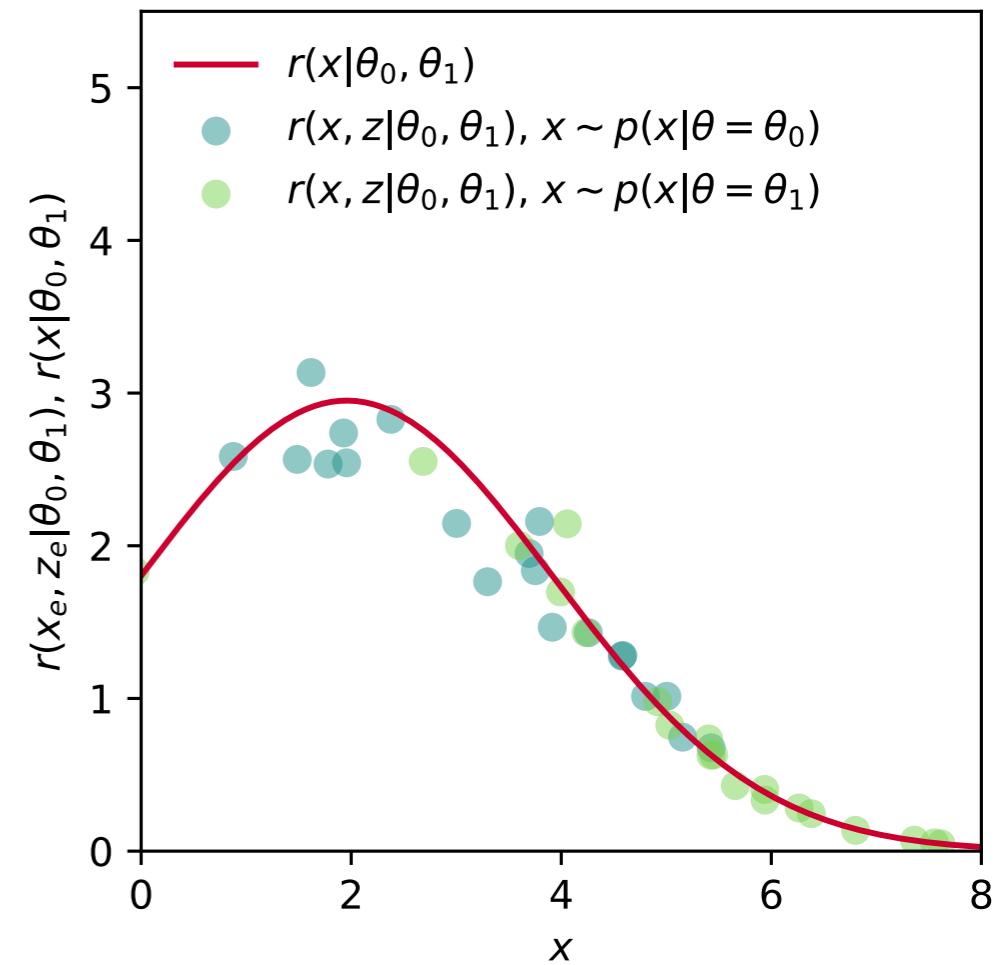
$$r(x, z|\theta_0, \theta_1) \equiv \frac{p(x, z_d, z_s, z_p|\theta_0)}{p(x, z_d, z_s, z_p|\theta_1)}$$



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

We want likelihood ratio

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



# The value of gold

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



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

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

One can show it is minimized by

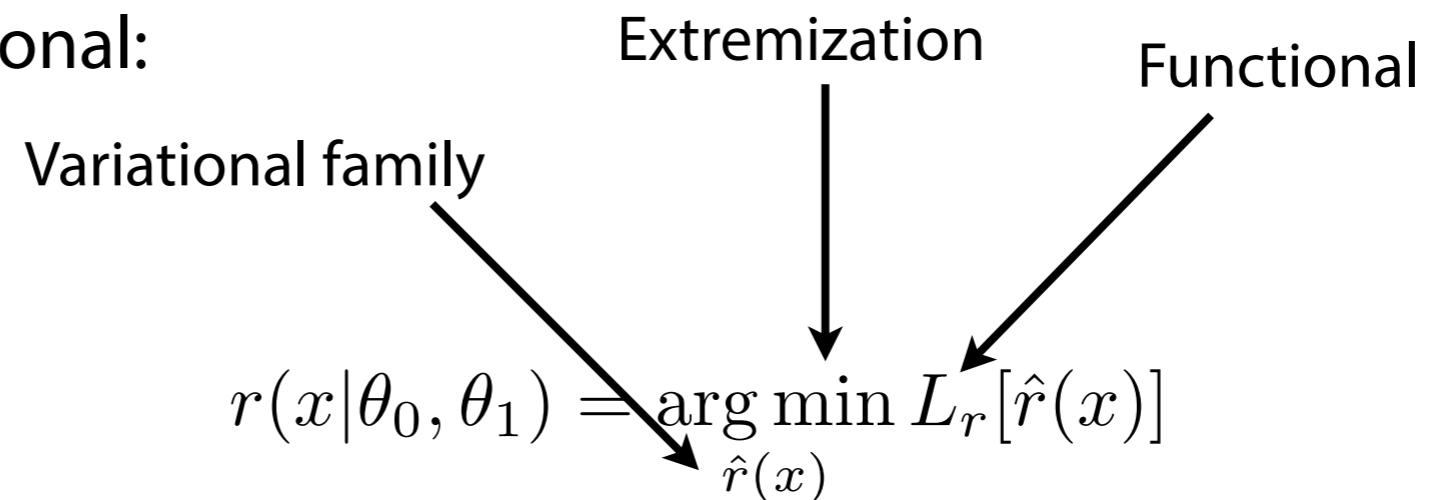
$$\arg \min_{\hat{r}(x)} L_r[\hat{r}(x)] = r(x|\theta_0, \theta_1) !$$

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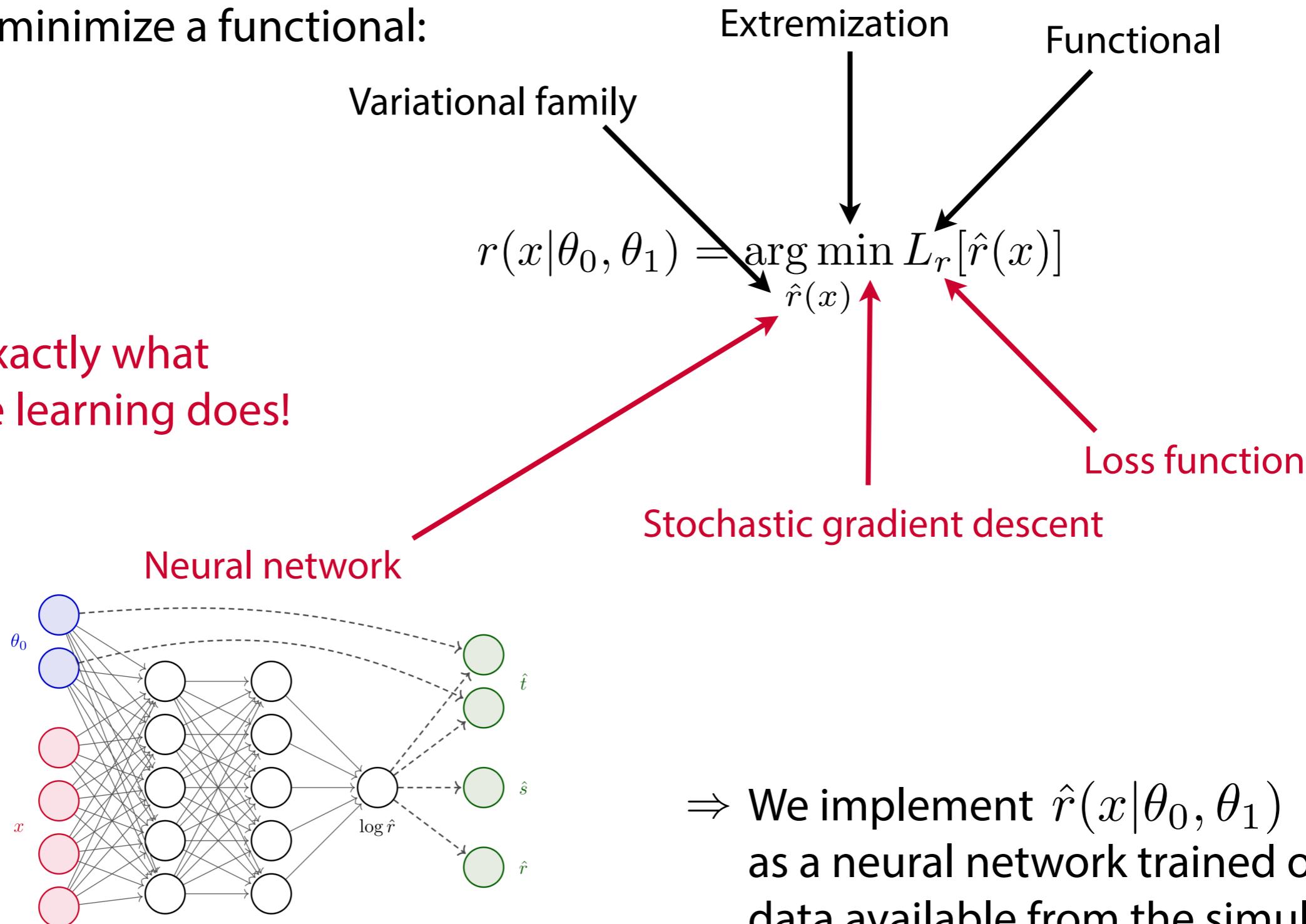
# Machine learning

Need to minimize a functional:



# Machine learning

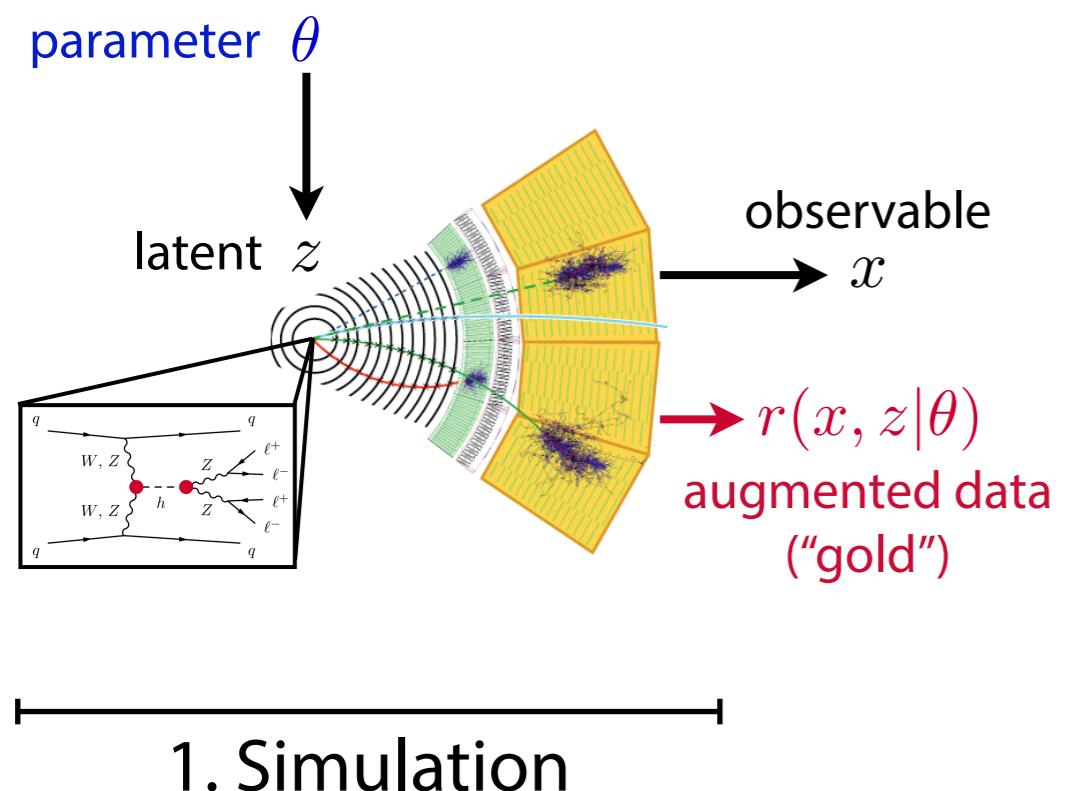
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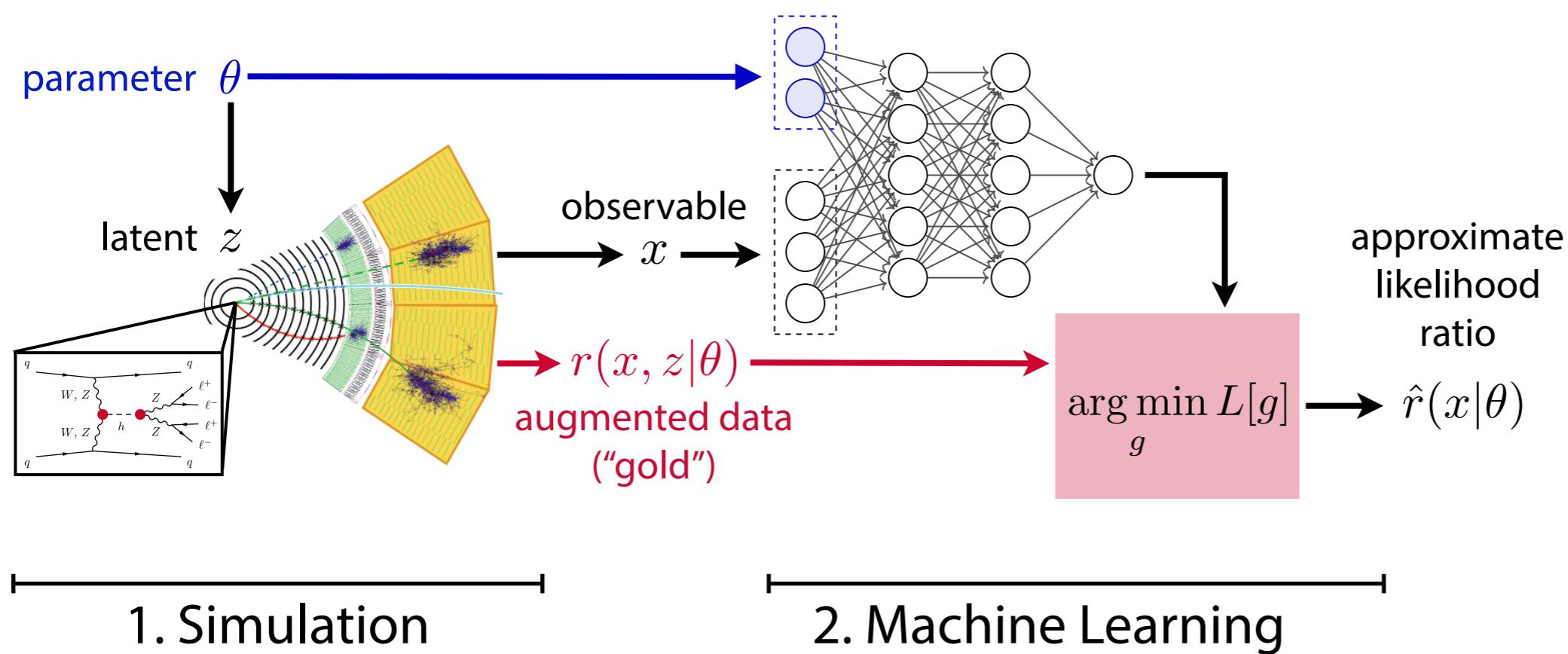
# Parameterized ratio estimators

- Missing: explain parameterized likelihood ratio estimator in detail
- Briefly explain how to get to limits

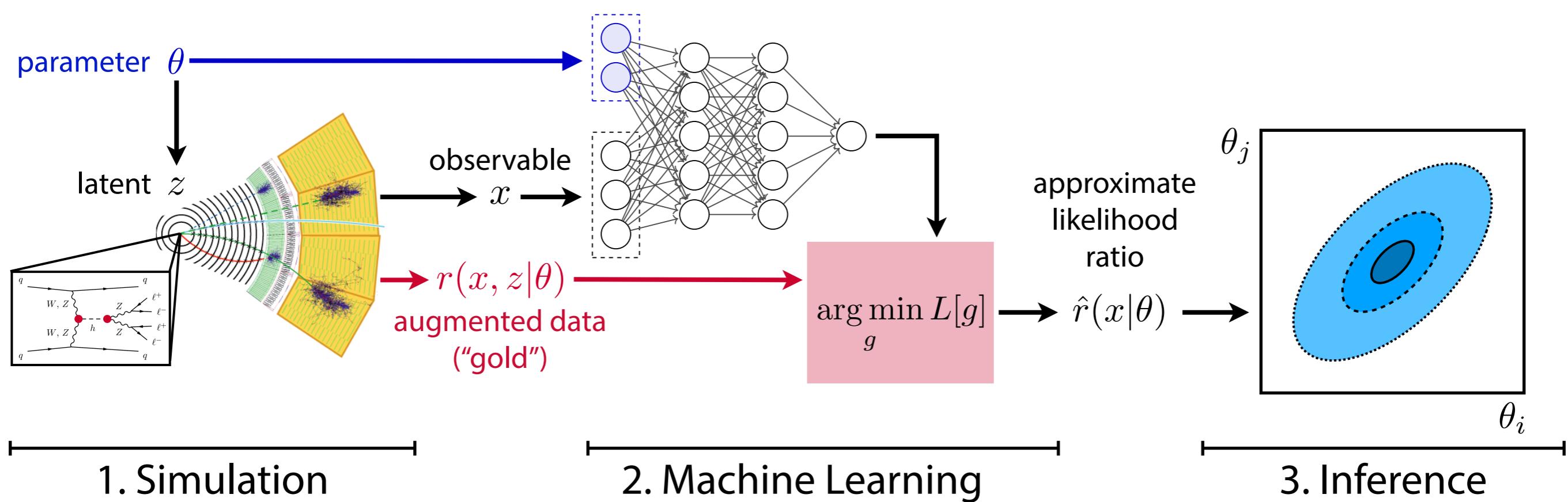
# What we have so far



# What we have so far



# What we have so far



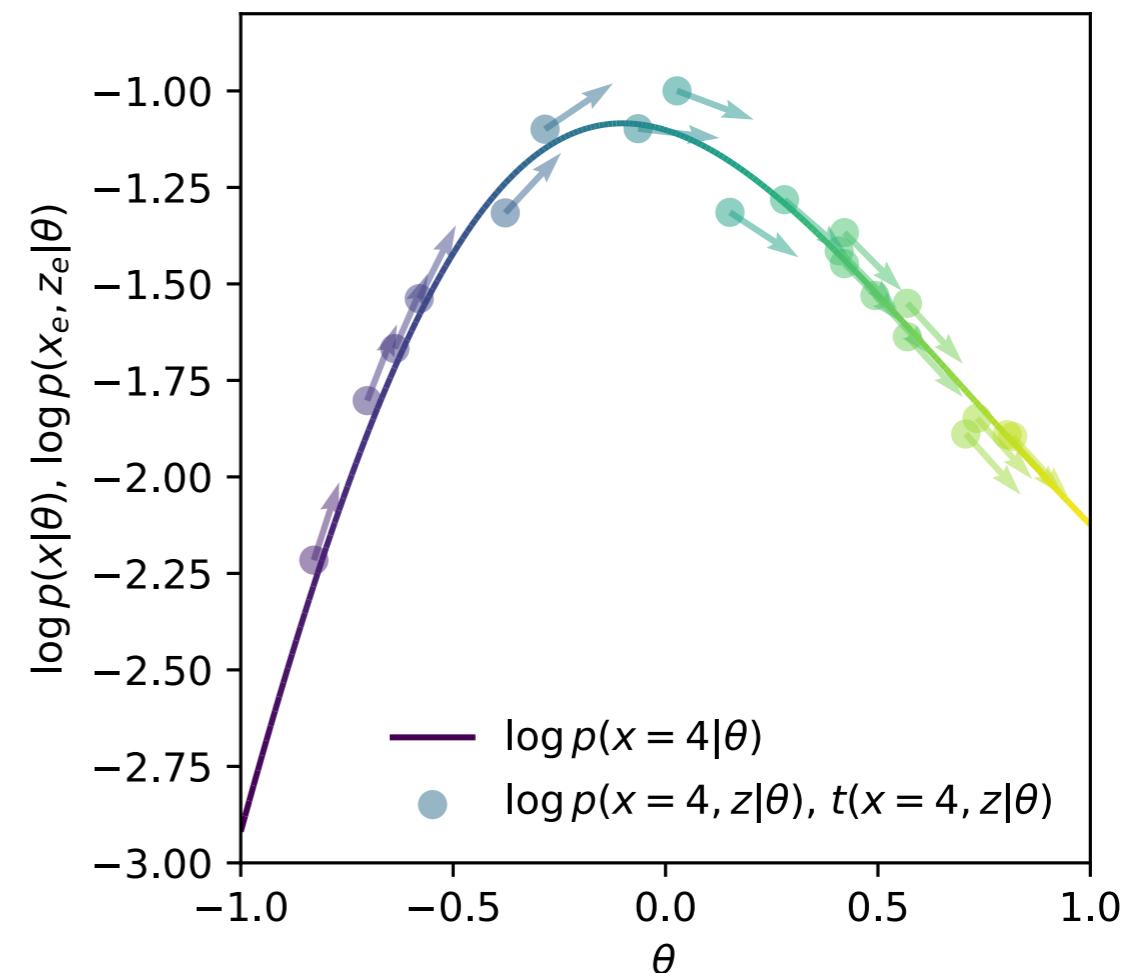
# The score

- Inference just based on the joint likelihood ratio works well, but there is another powerful piece of information
- The **score**

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

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,  
we can calculate the **joint score**

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



We want **score**

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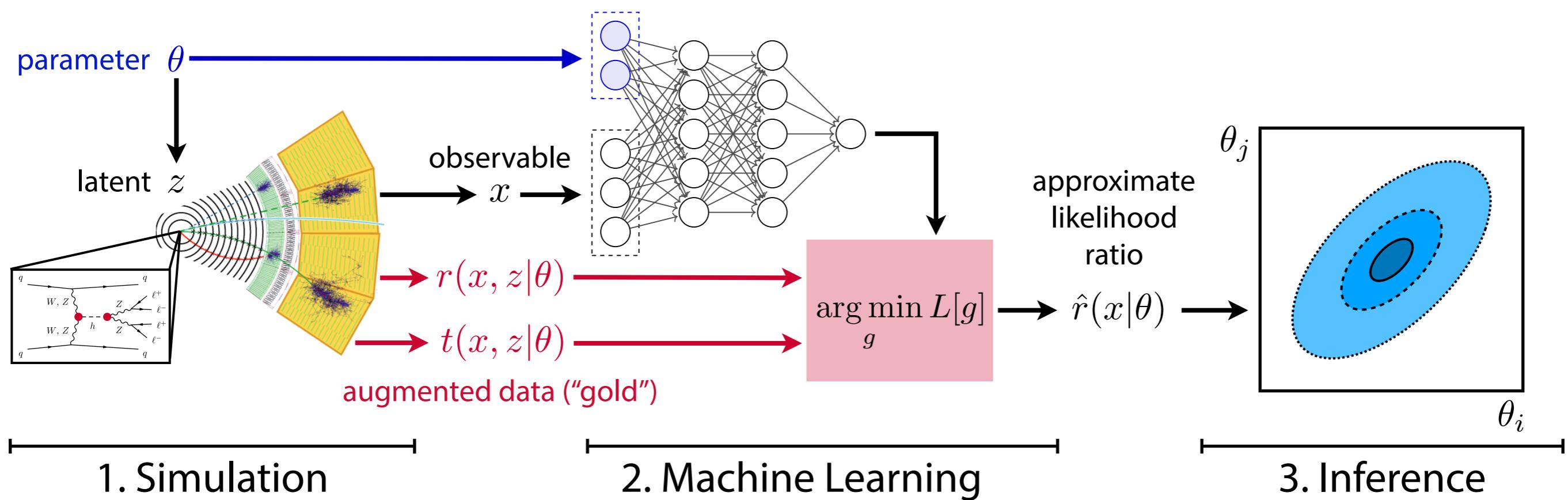
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One can show it is minimized by

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

Again, we implement this  
with machine learning

# Putting the pieces together



# A family of likelihood-free inference strategies

Different strategies to combine the different pieces of information:

Method	$L_{XE}$	$L_{MLE}$	$L_r$	$L_t$	$\theta$ sampling
ABC (Approximate Bayesian Computation)					$\theta \sim \pi(\theta)$
NDE (Neural density estimation)			✓		$\theta \sim \pi(\theta)$
LRT / CARL (Likelihood ratio trick / calibrated approximate ratios of likelihoods)	✓				$\theta \sim \pi(\theta)$
ROLR (Regression on likelihood ratio)				✓	$\theta \sim \pi(\theta)$
SCANDAL (Score augmented neural density approximates likelihood)		✓		✓	$\theta \sim \pi(\theta)$
CASCAL (CARL and score approximate likelihood ratio).	✓			✓	$\theta \sim \pi(\theta)$
RASCAL (Ratio and score approximate likelihood ratio)			✓	✓	$\theta \sim \pi(\theta)$
SALLY (Score approximates likelihood locally)				✓	$\theta = \theta_0$
SALLINO (Score approximates likelihood locally in one dimension)				✓	$\theta = \theta_0$

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RASCAL loss function:

$$L_{\text{RASCAL}}[\hat{r}(x|\theta_0, \theta_1)] = L_r[\hat{r}(x|\theta_0, \theta_1)] + \alpha L_t[\nabla_{\theta_0} \log \hat{r}(x|\theta_0, \theta_1)]$$

# Comparison to established methods

## Likelihood-free inference methods

Treat simulator as black box:

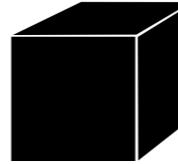
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New!

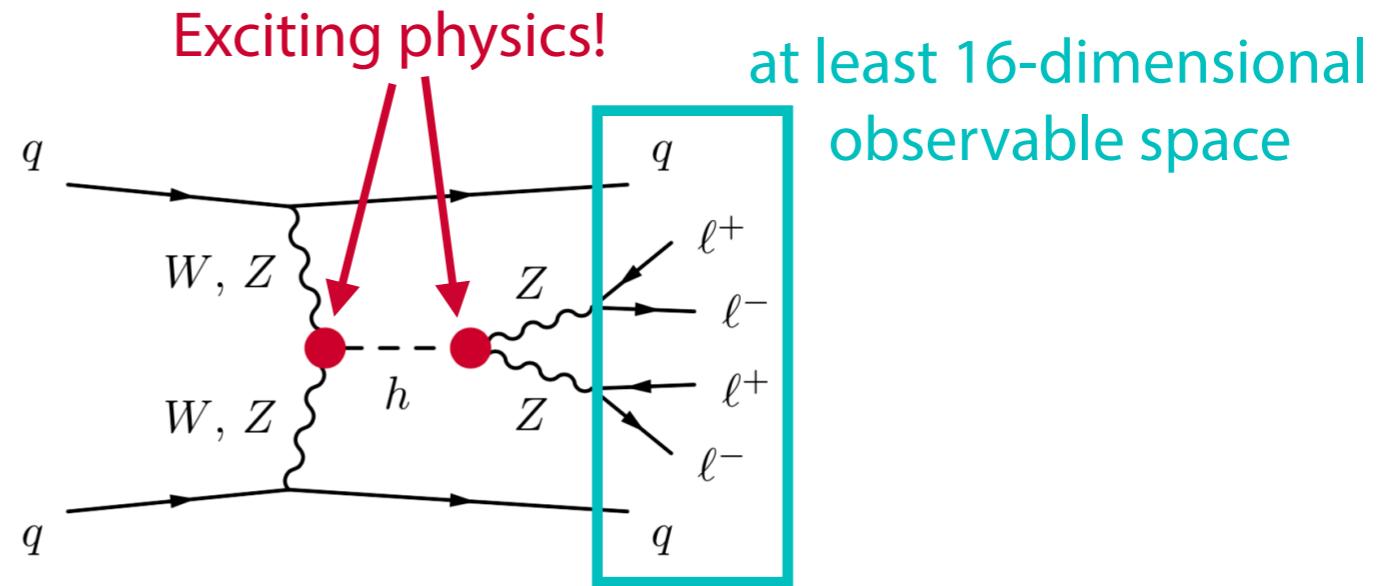
16/40

	Histograms	NDE	MEM / OO	RASCAL etc
High-dimensional observables		✓	✓	✓
Realistic shower, detector sim.	✓	✓		✓
Asymptotically exact		✓		✓
Uses matrix element information			✓	✓
Evaluation	fast	fast	expensive	fast

# Proof of concept

# Proof of concept

- Higgs production in weak boson fusion:

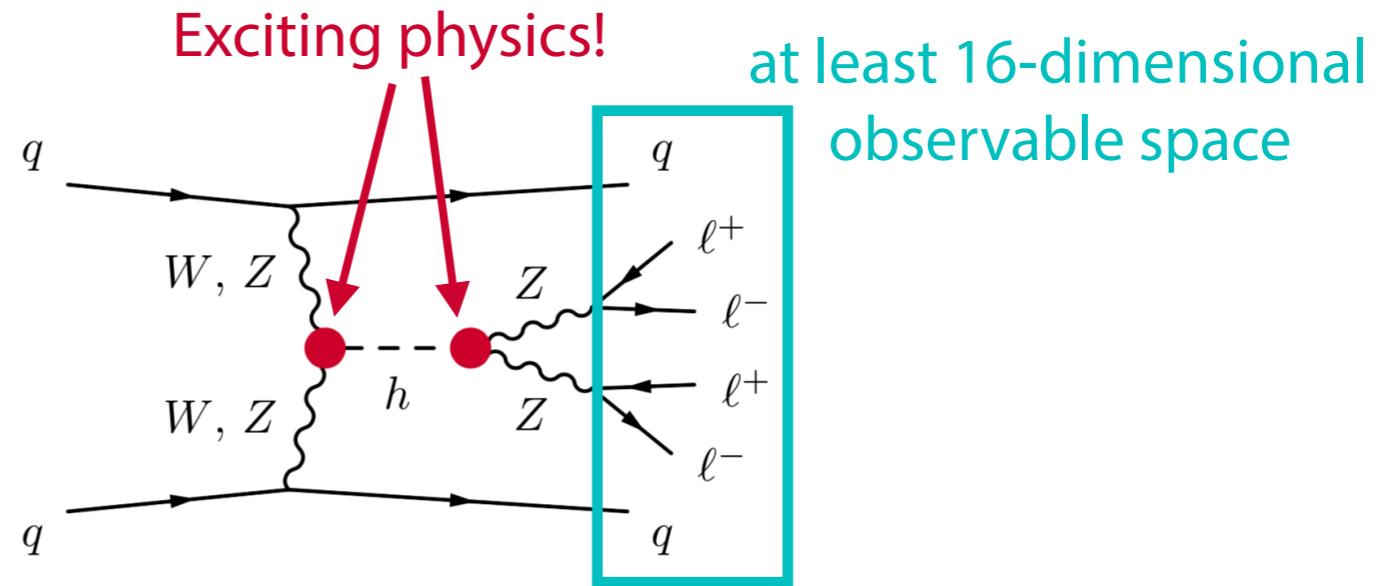


- Goal: constraints on two EFT parameters

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

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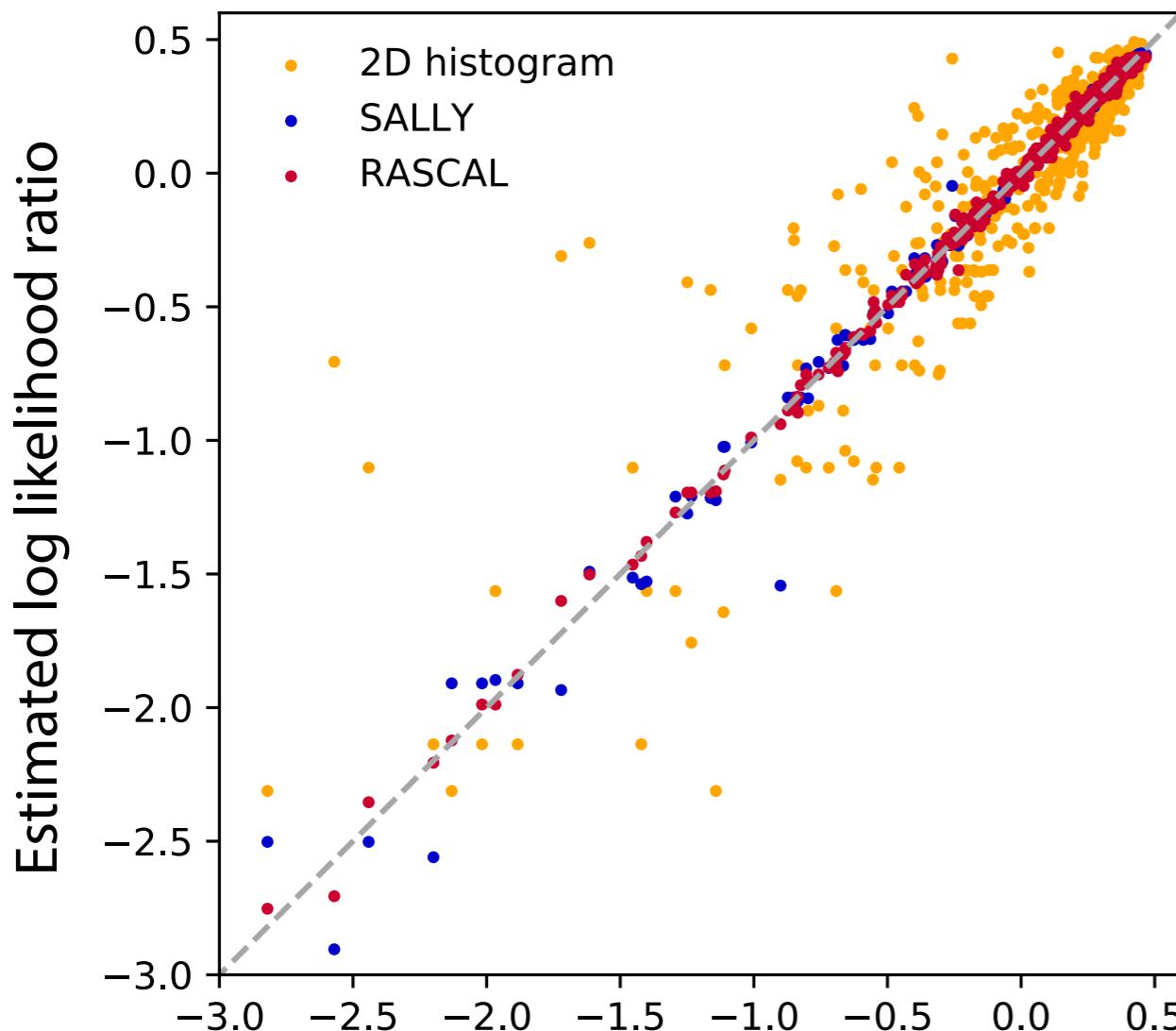
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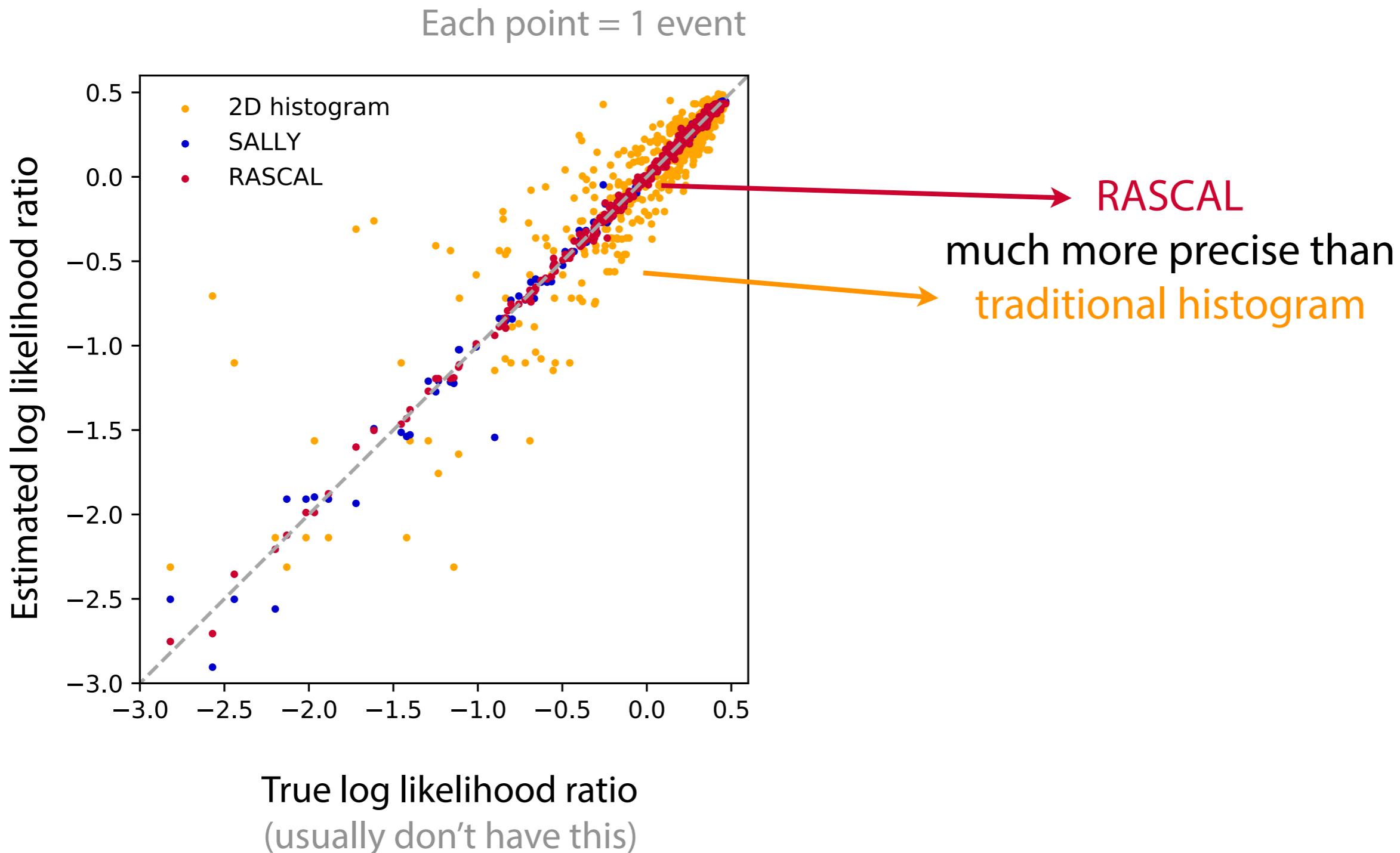
- Two setups:
  - Simplified setup in which we can compare to true likelihood
  - “Realistic” simulation with approximate detector effects
- Simulation: MadGraph [J. Alwall et al. 1405.0301] + MadMax [K. Cranmer, T. Plehn hep-ph/0605268; T. Plehn, P. Schichtel, D. Wiegand 1311.2591]

# Precise likelihood ratio estimates

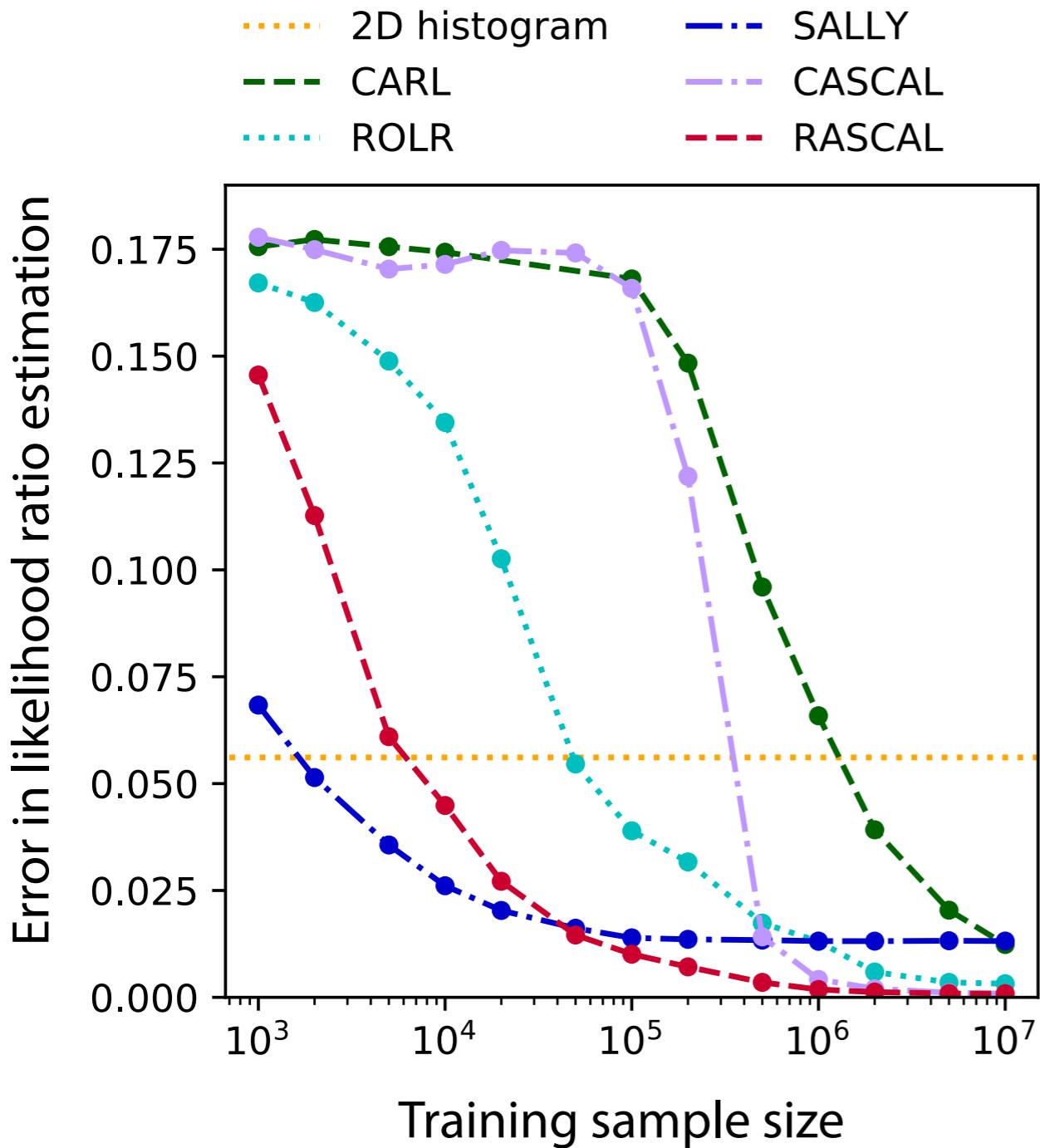
Each point = 1 event



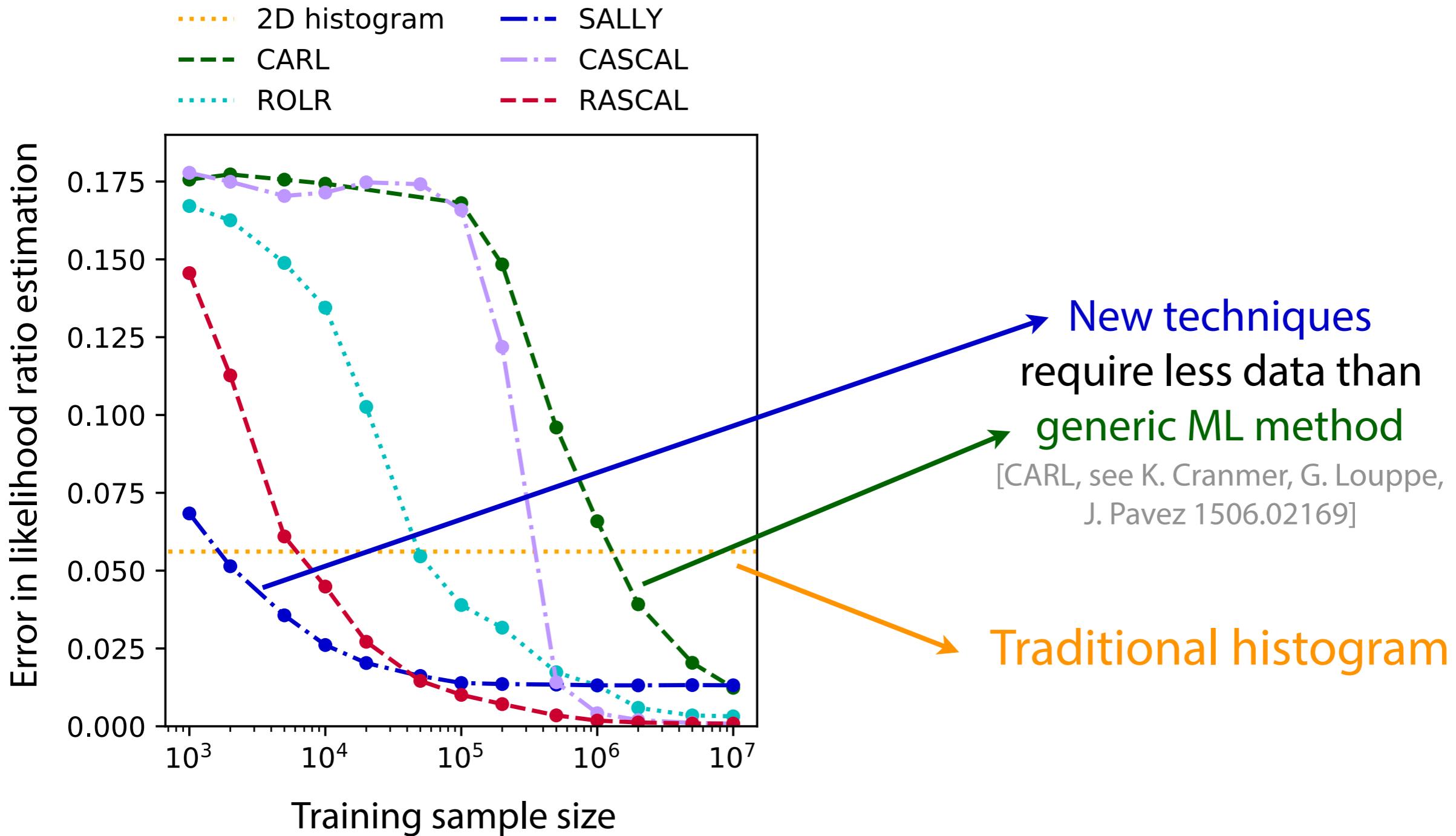
# Precise likelihood ratio estimates



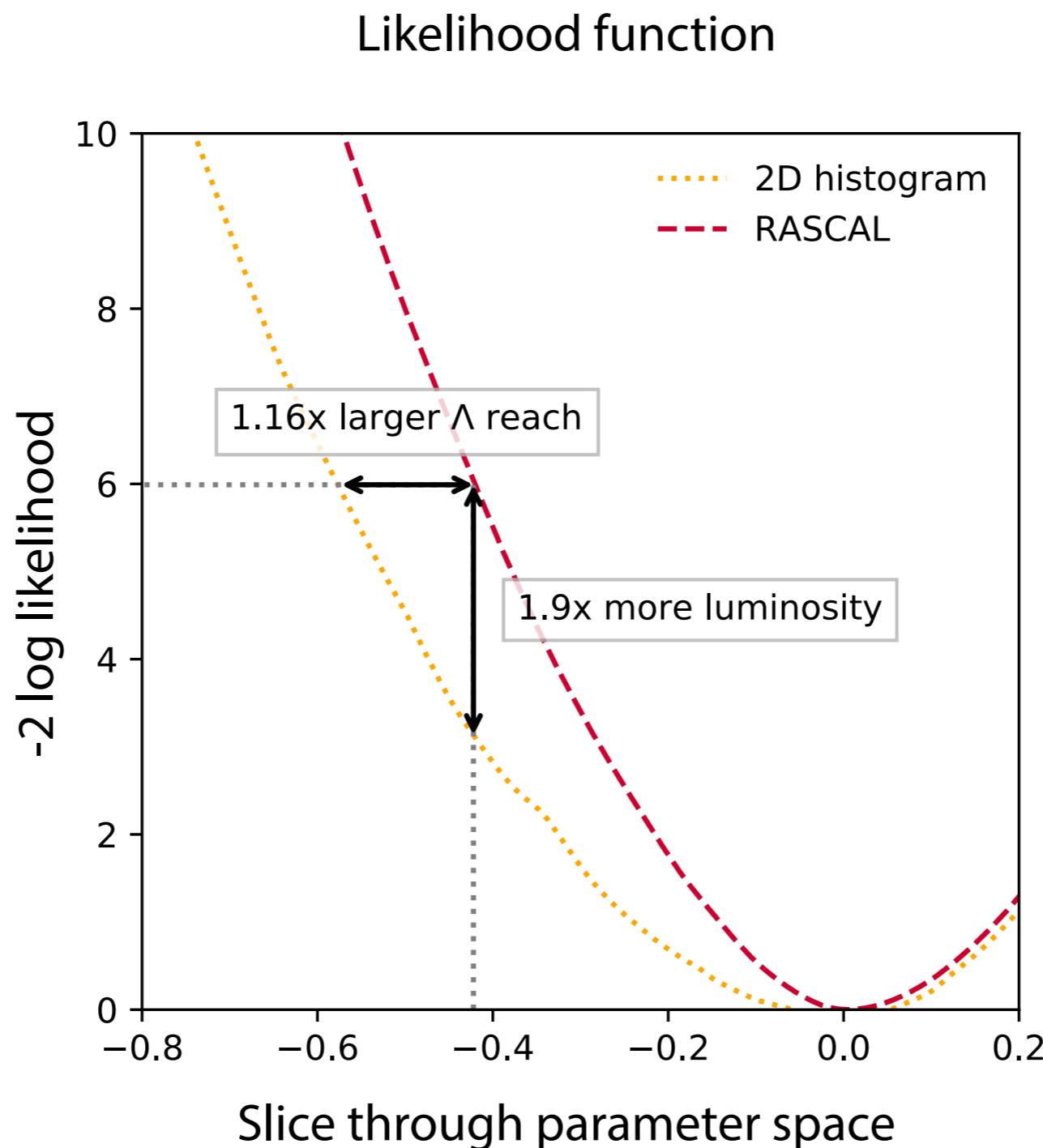
# Less training data needed



# Less training data needed



# Better sensitivity

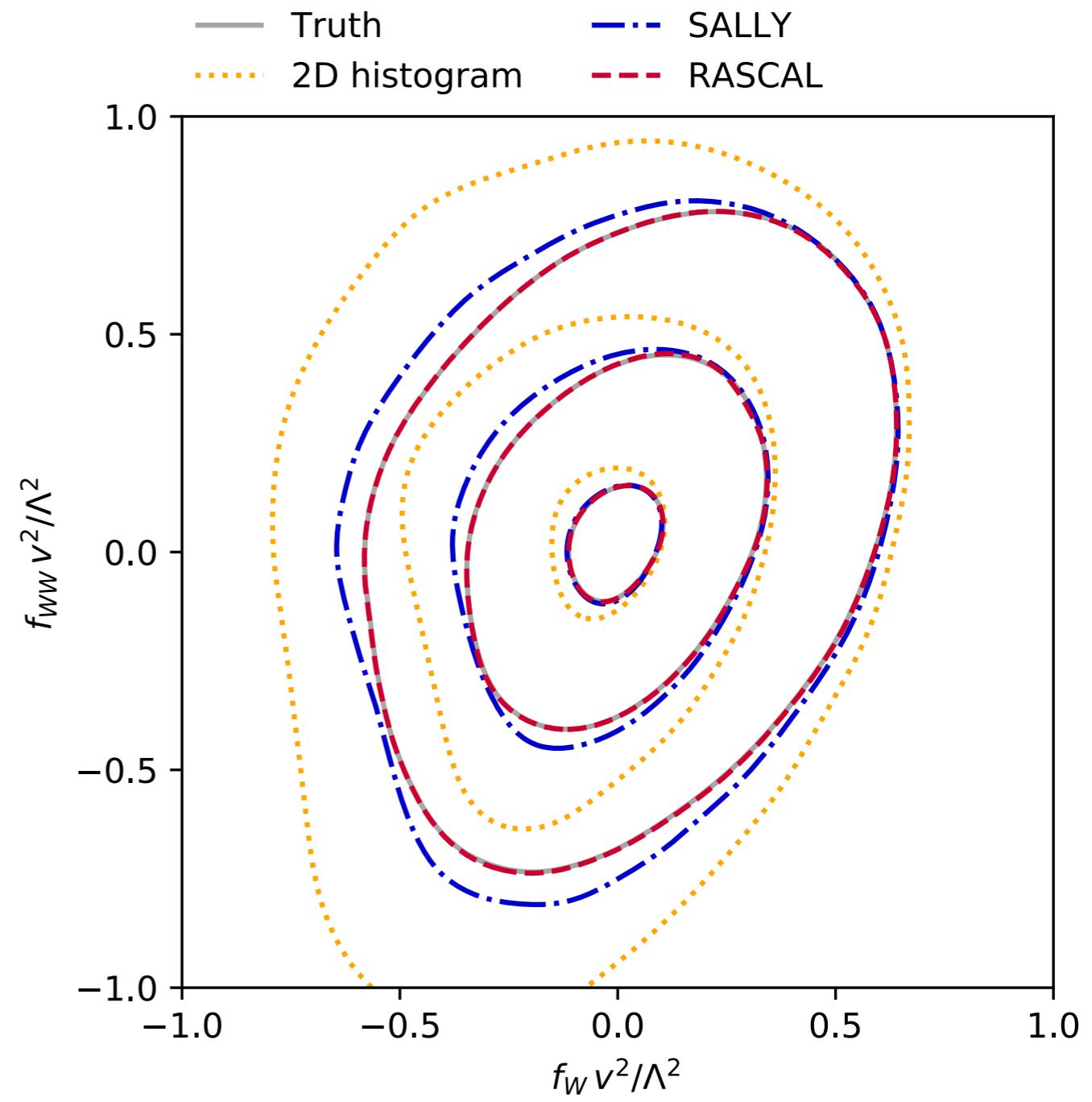


36 events, assuming SM

35/40

# Stronger bounds

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



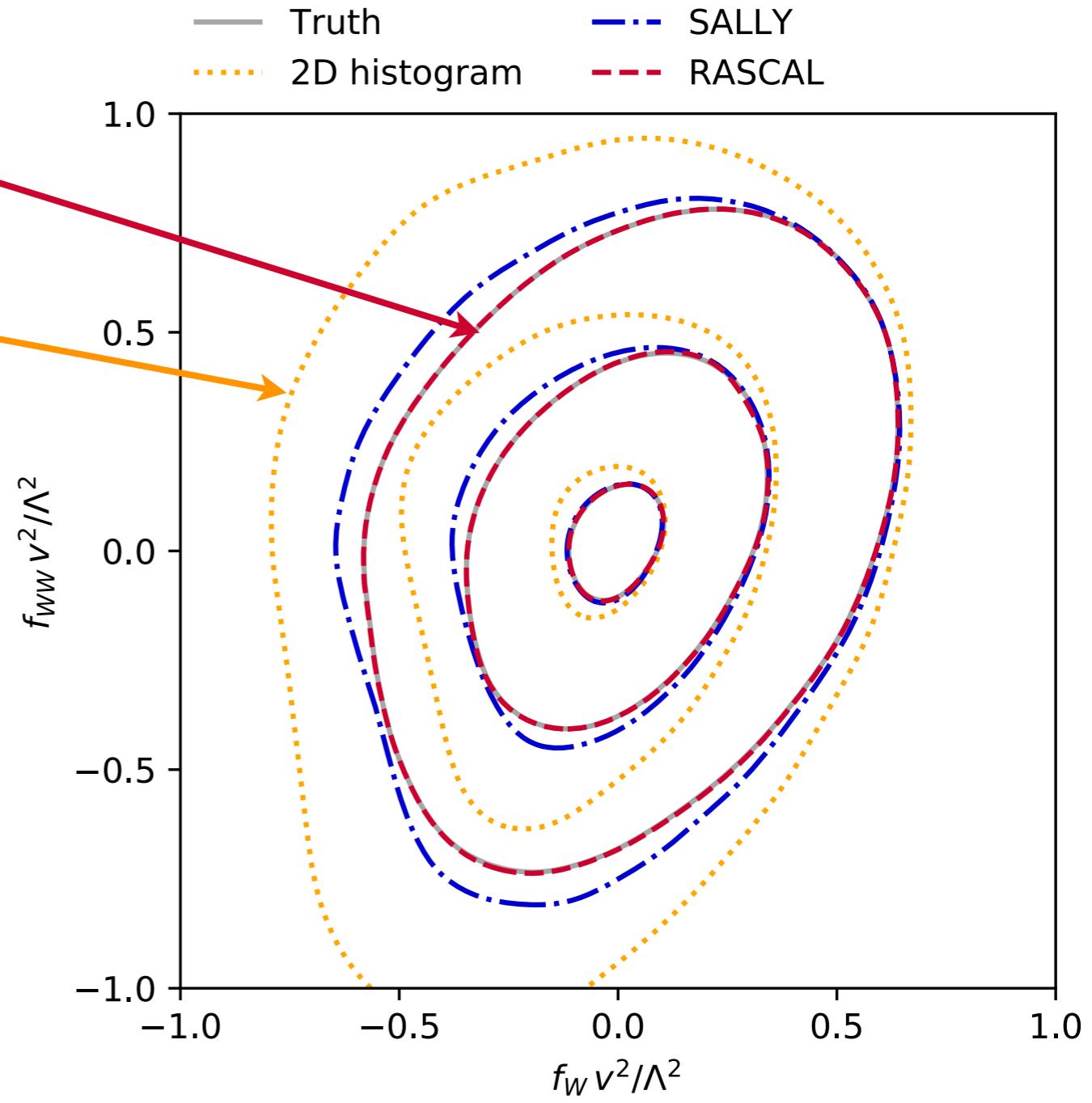
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36/40

# Stronger bounds

RASCAL  
enables stronger  
limits than  
traditional histogram

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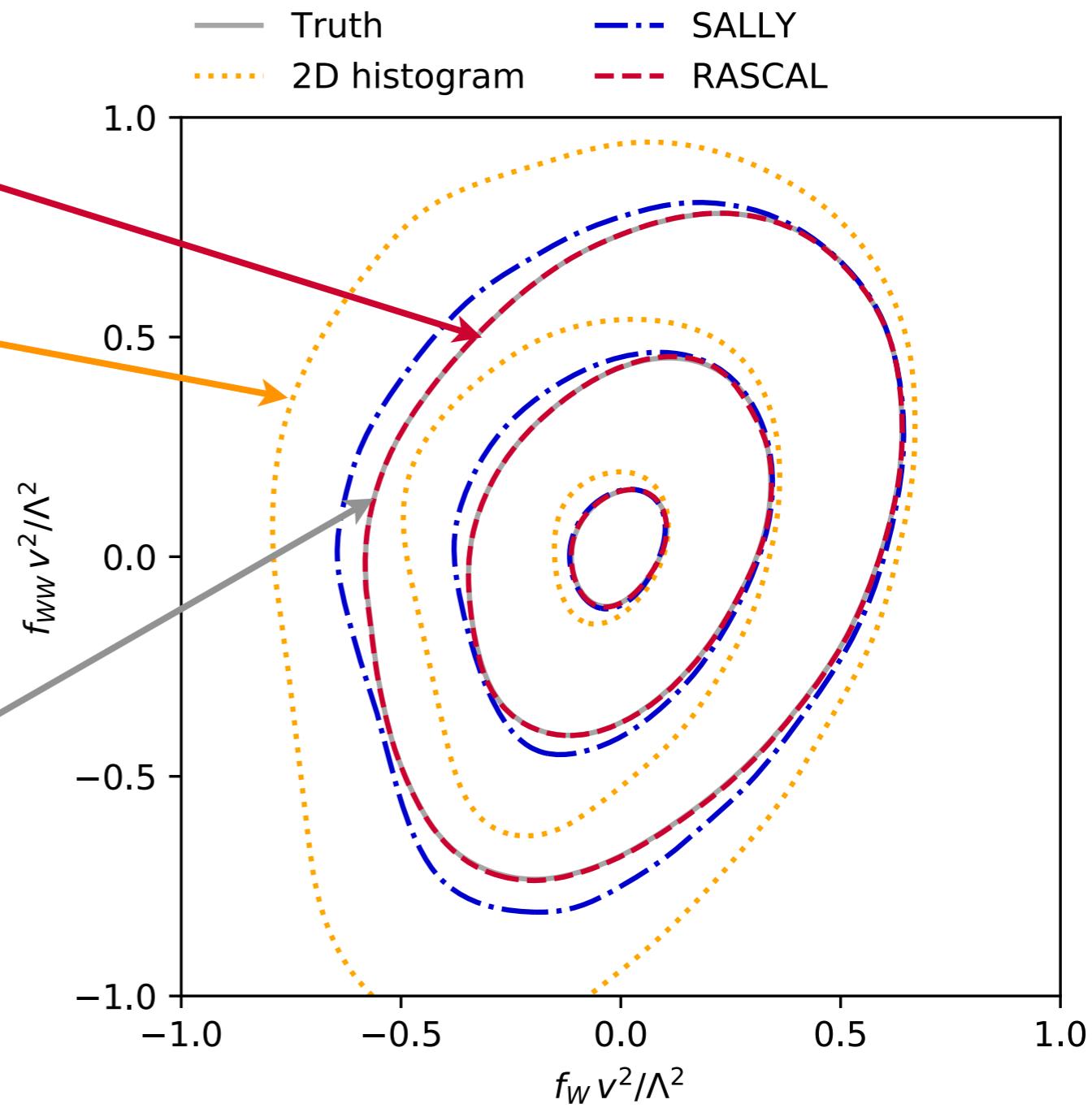
36/40

# Stronger bounds

RASCAL  
enables stronger  
limits than  
traditional histogram

Limits from RASCAL  
virtually indistinguishable  
from true likelihood  
(usually we don't have that)

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



36 events, assuming SM

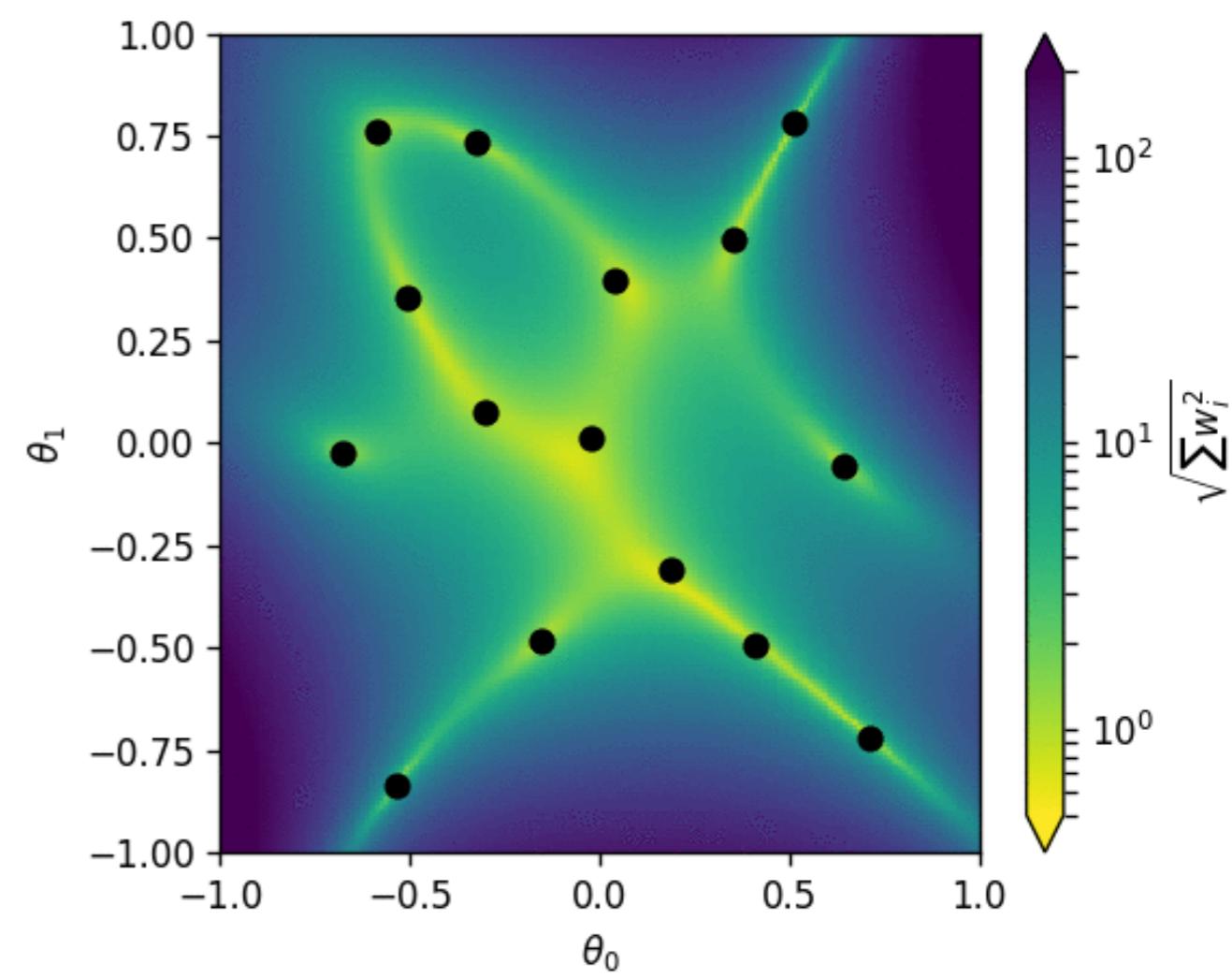
36/40

# MadMiner

# 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)

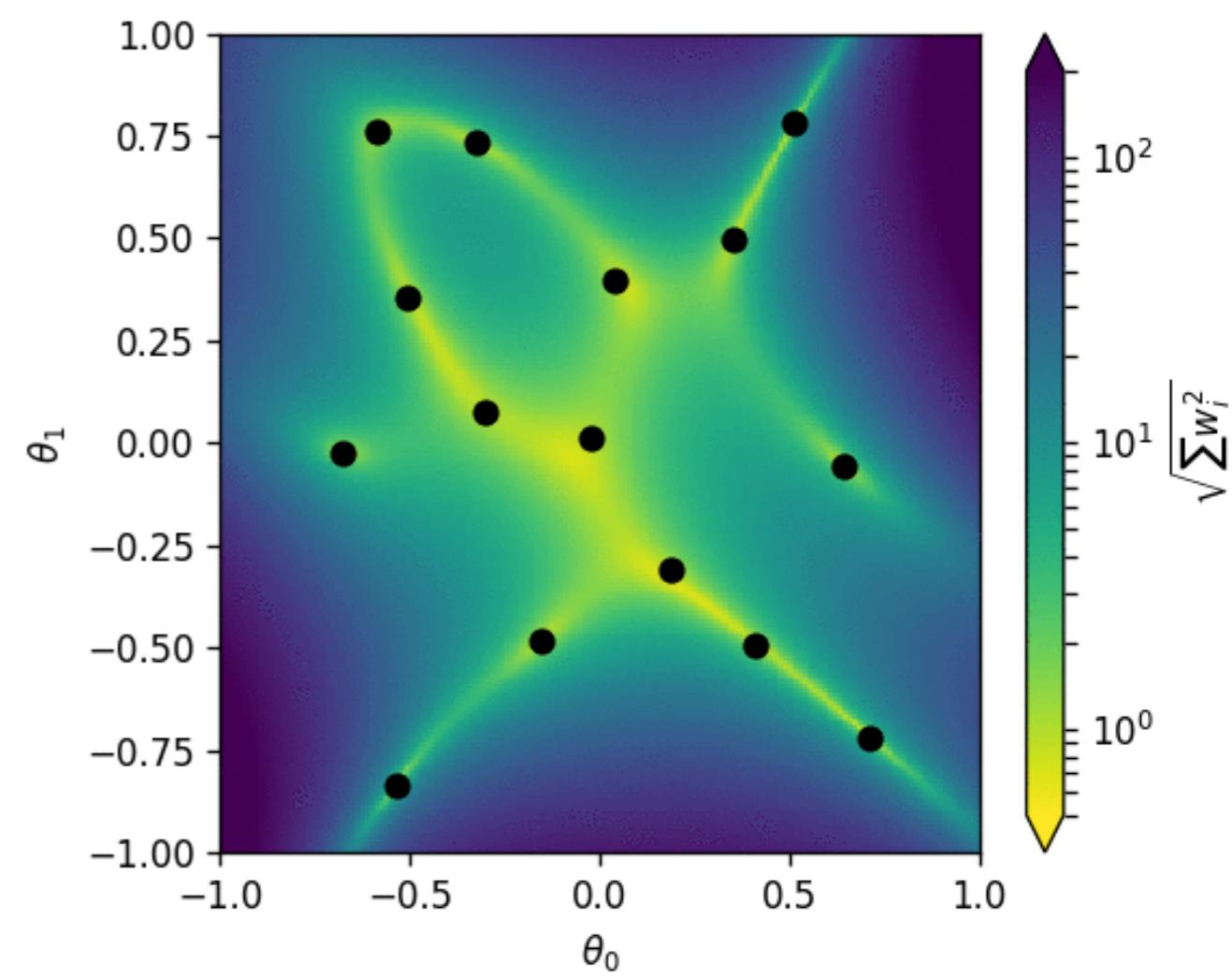


Come visit us at [github.com/johannbrehmer/madminer!](https://github.com/johannbrehmer/madminer)

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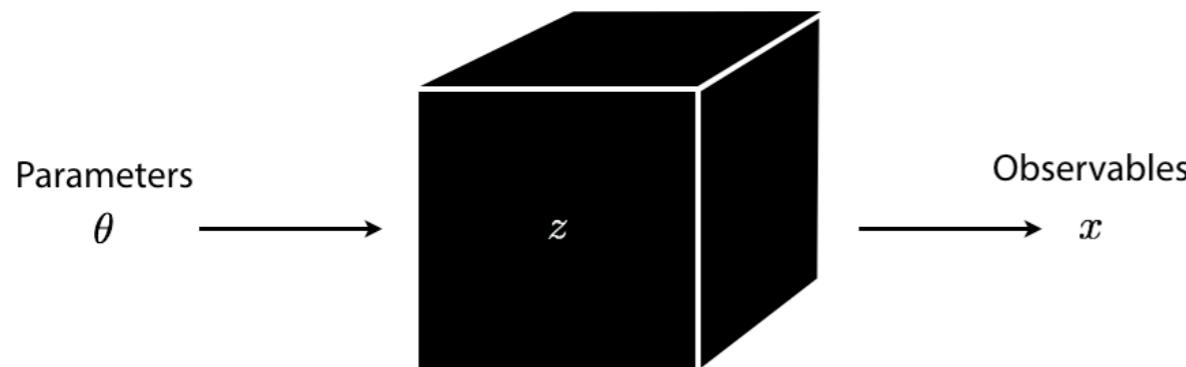
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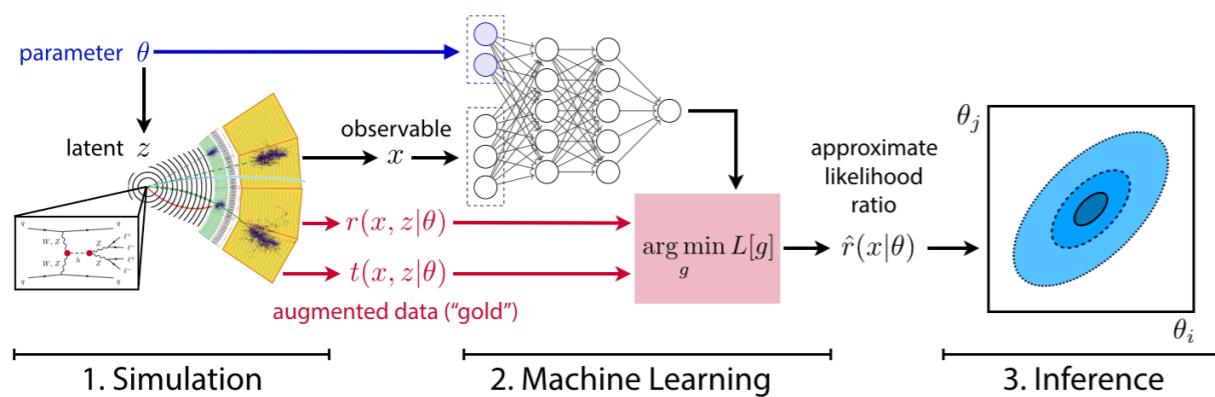
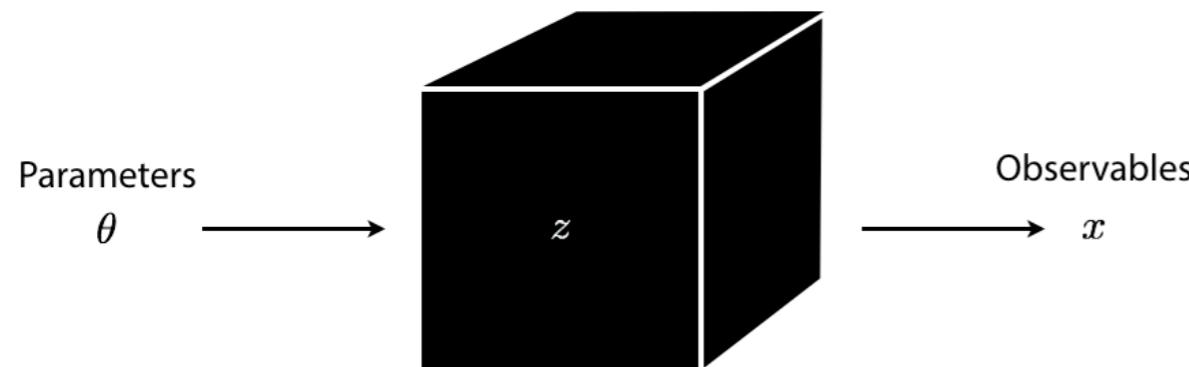
Come visit us at [github.com/johannbrehmer/madminer!](https://github.com/johannbrehmer/madminer)

# A new approach to simulator-based inference



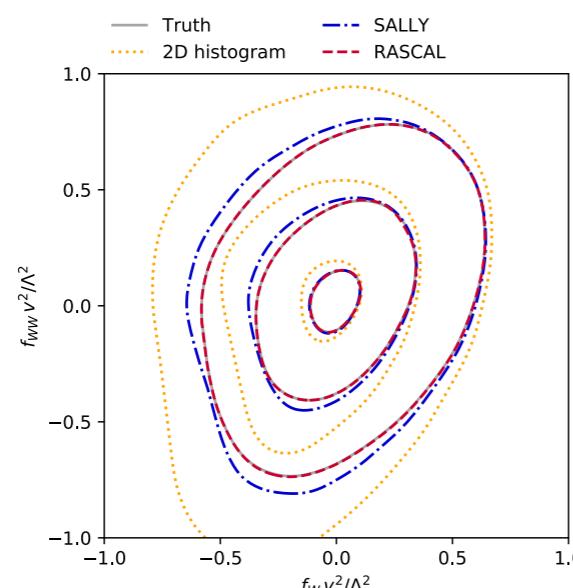
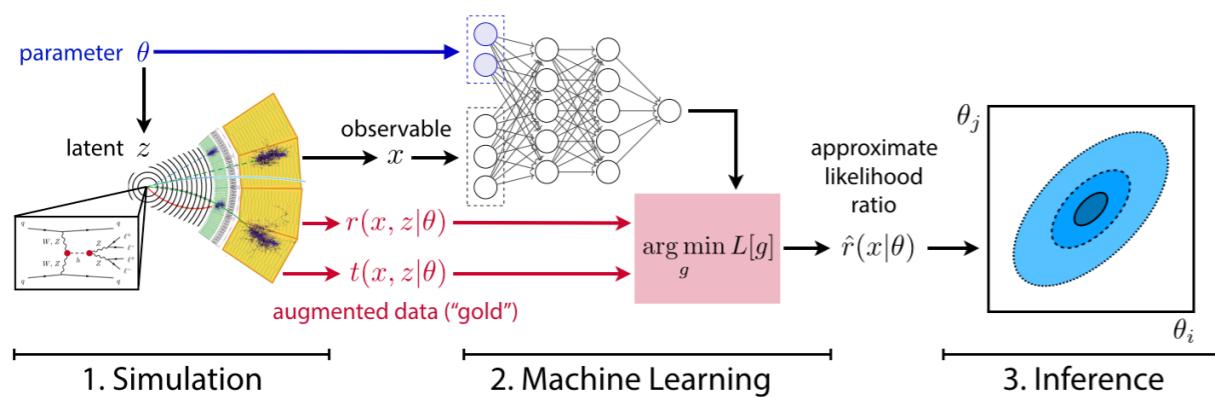
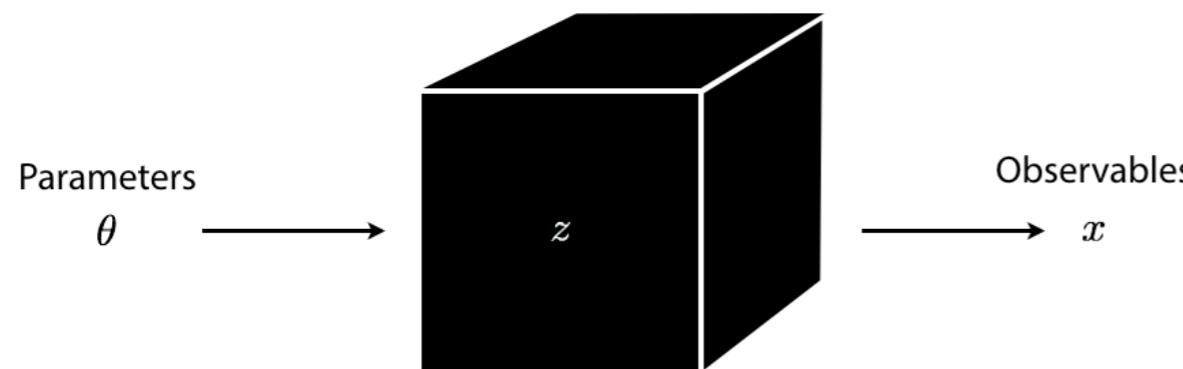
- Many LHC analyses (and much of modern science) are based on simulations, “likelihood-free”
- Established inference methods treat simulator as black box

# A new approach to simulator-based inference



- Many LHC analyses (and much of modern science) are based on simulations, “likelihood-free”
- Established inference methods treat simulator as black box
- New 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”
- Established inference methods treat simulator as black box
- New inference techniques: Leverage more information from simulator + power of machine learning
- First application to Higgs physics: Stronger EFT constraints with less data
- The MadMiner package will make this easy to use for everyone

# References



Kyle Cranmer



Gilles Louppe



Juan Pavez



Felix Kling



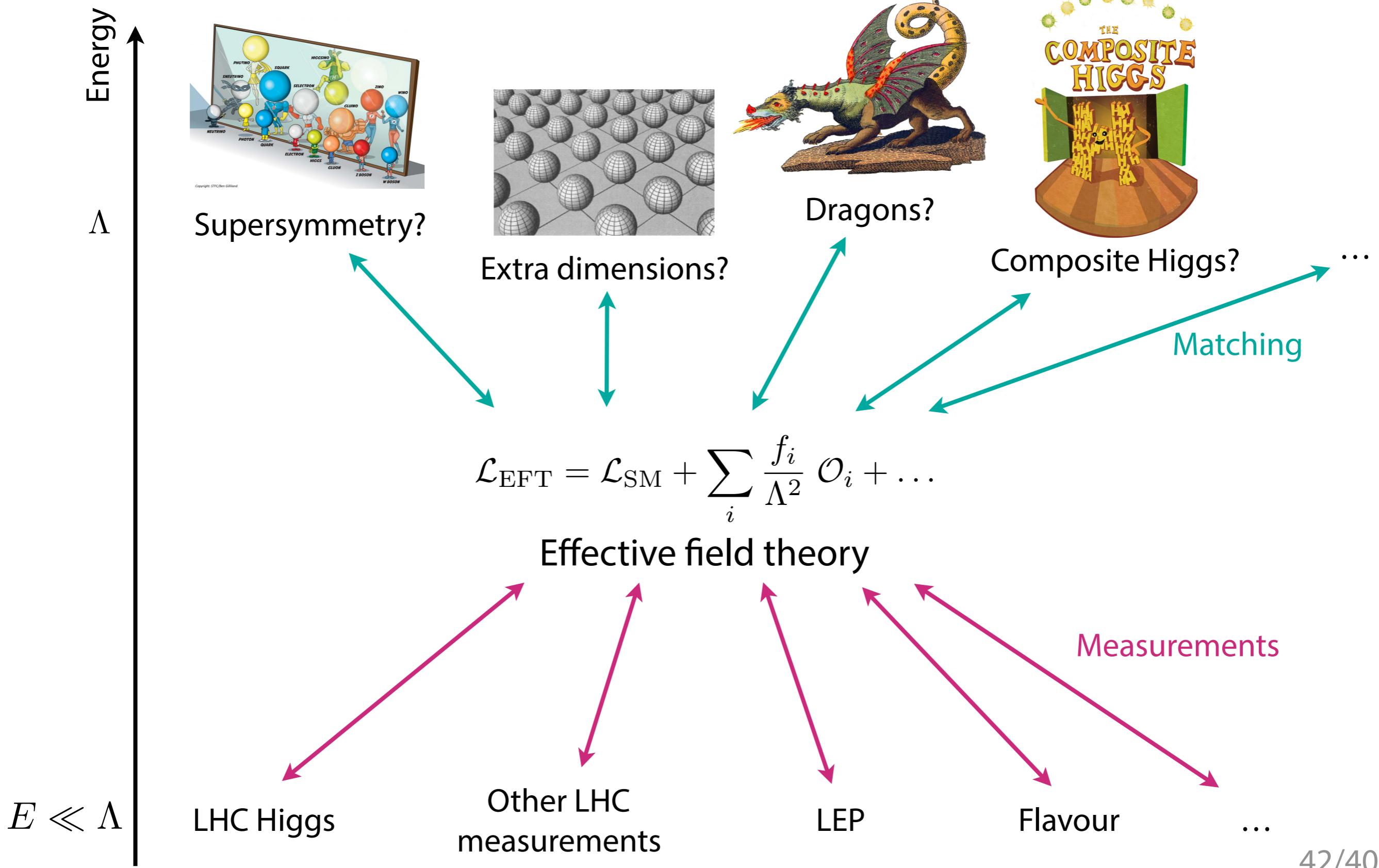
Markus Stoye

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

Thanks to Kyle and Gilles for inspiring many of my slides!

# Bonus material

# Effective field theory



# SMEFT (Standard Model Effective Field Theory)

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

## Operators

- all possible interactions between SM particles mediated by new physics
- fixed by SM particles + SM symmetries + expansion in  $1/\Lambda$ , independent of high-energy physics
- affect rates + kinematics

---

$\mathcal{O}_{\phi,1} = (D_\mu \phi)^\dagger \phi \phi^\dagger D^\mu \phi$	$\mathcal{O}_{GG} = (\phi^\dagger \phi) G_{\mu\nu}^a G^{\mu\nu a}$
$\mathcal{O}_{\phi,2} = \frac{1}{2} \partial_\mu (\phi^\dagger \phi) \partial^\mu (\phi^\dagger \phi)$	$\mathcal{O}_{BB} = -\frac{g'^2}{4} (\phi^\dagger \phi) B_{\mu\nu} B^{\mu\nu}$
$\mathcal{O}_{\phi,3} = \frac{1}{3} (\phi^\dagger \phi)^3$	$\mathcal{O}_{WW} = -\frac{g^2}{4} (\phi^\dagger \phi) W_{\mu\nu}^a W^{\mu\nu a}$
$\mathcal{O}_{\phi,4} = (\phi^\dagger \phi) (D_\mu \phi)^\dagger D^\mu \phi$	$\mathcal{O}_{BW} = -\frac{g g'}{4} (\phi^\dagger \sigma^a \phi) B_{\mu\nu} W^{\mu\nu a}$
	$\mathcal{O}_B = \frac{i g'}{2} (D^\mu \phi)^\dagger D^\nu \phi B_{\mu\nu}$
	$\mathcal{O}_W = \frac{i g}{2} (D^\mu \phi)^\dagger \sigma^a D^\nu \phi W_{\mu\nu}^a$

---

# SMEFT (Standard Model Effective Field Theory)

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

## Operators

- all possible interactions between SM particles mediated by new physics
- fixed by SM particles + SM symmetries + expansion in  $1/\Lambda$ , independent of high-energy physics
- affect rates + kinematics

## Higher-order terms

- suppressed by additional factors of  $E^2 / \Lambda^2$

## Wilson coefficients

- precise measurement of these parameters is one of the most important goals of the LHC
- can be translated to high-energy physics parameters

[W. Buchmuller, D. Wyler 85;  
B. Grzadkowski, M. Iskrzynski, M. Misiak,  
J. Rosiek 1008.4884; ...]

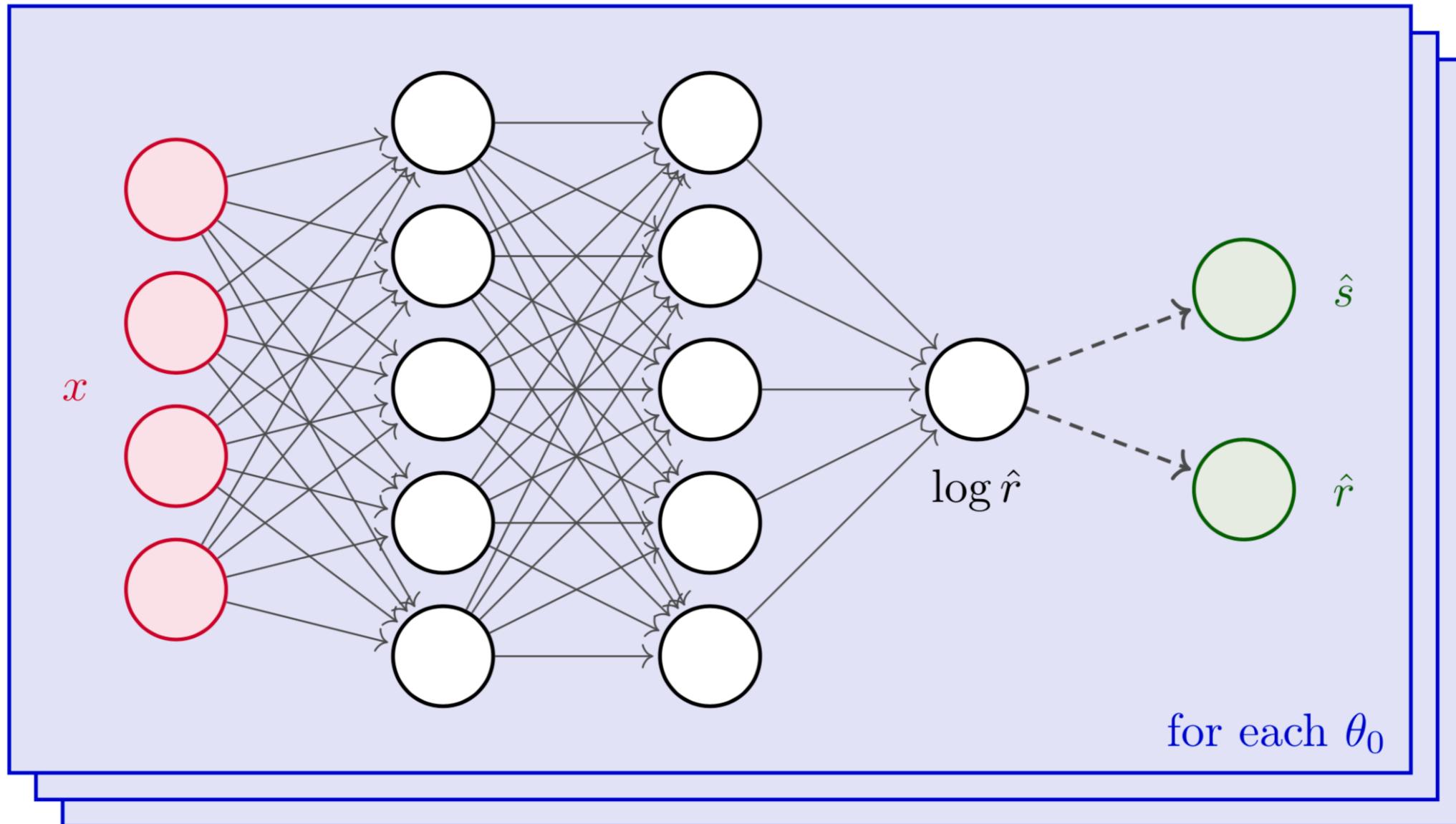
# Variational calculus

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

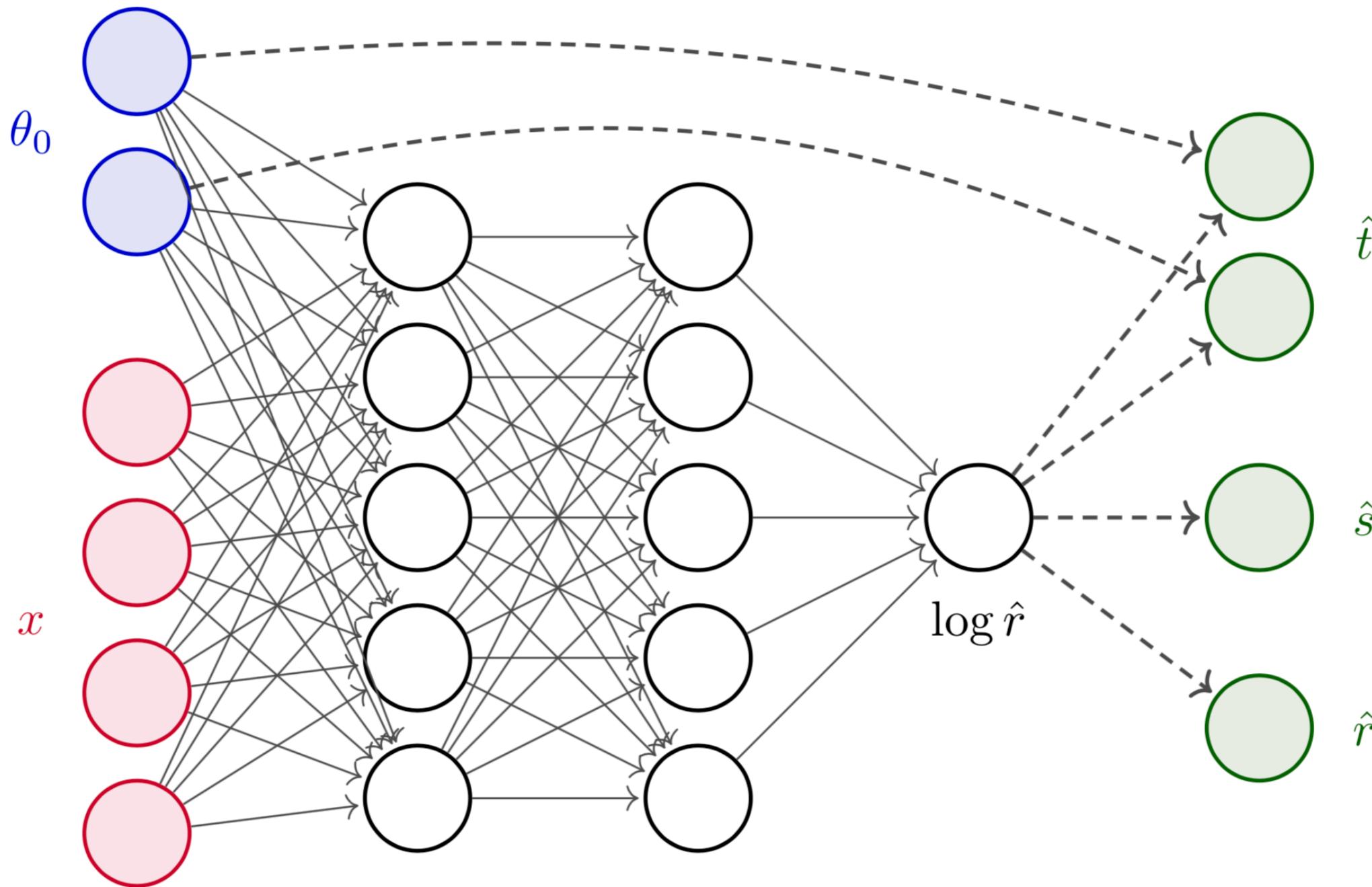
$$0 = \frac{\delta F}{\delta \hat{g}} \Big|_{g^*} = 2\hat{g} \underbrace{\int dz \textcolor{red}{p}(x, z|\theta)}_{=\textcolor{red}{p}(x|\theta)} - 2 \int dz \textcolor{red}{p}(x, z|\theta) g(x, z)$$

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

# Point by point

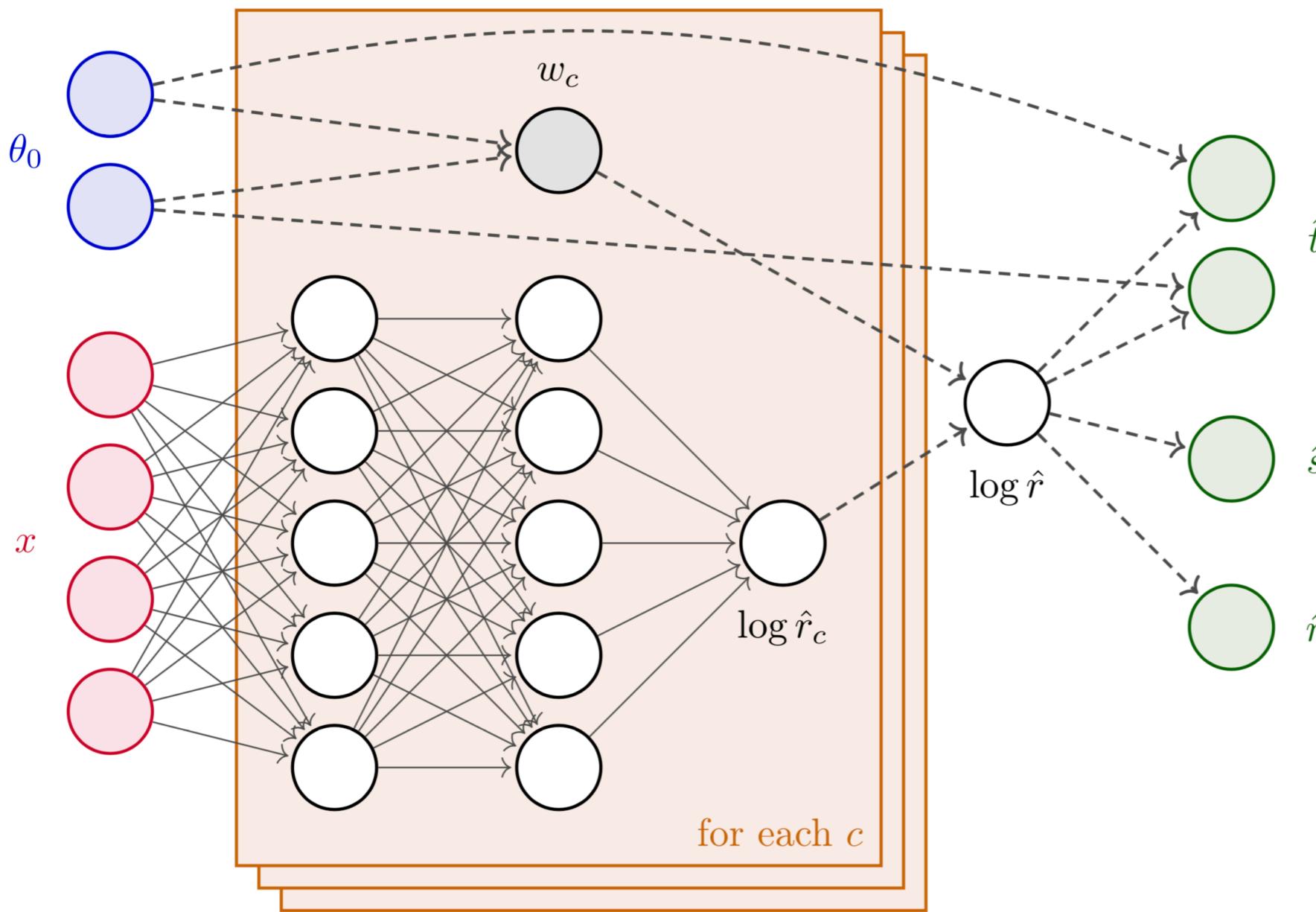


# (Agnostic) parameterized estimators

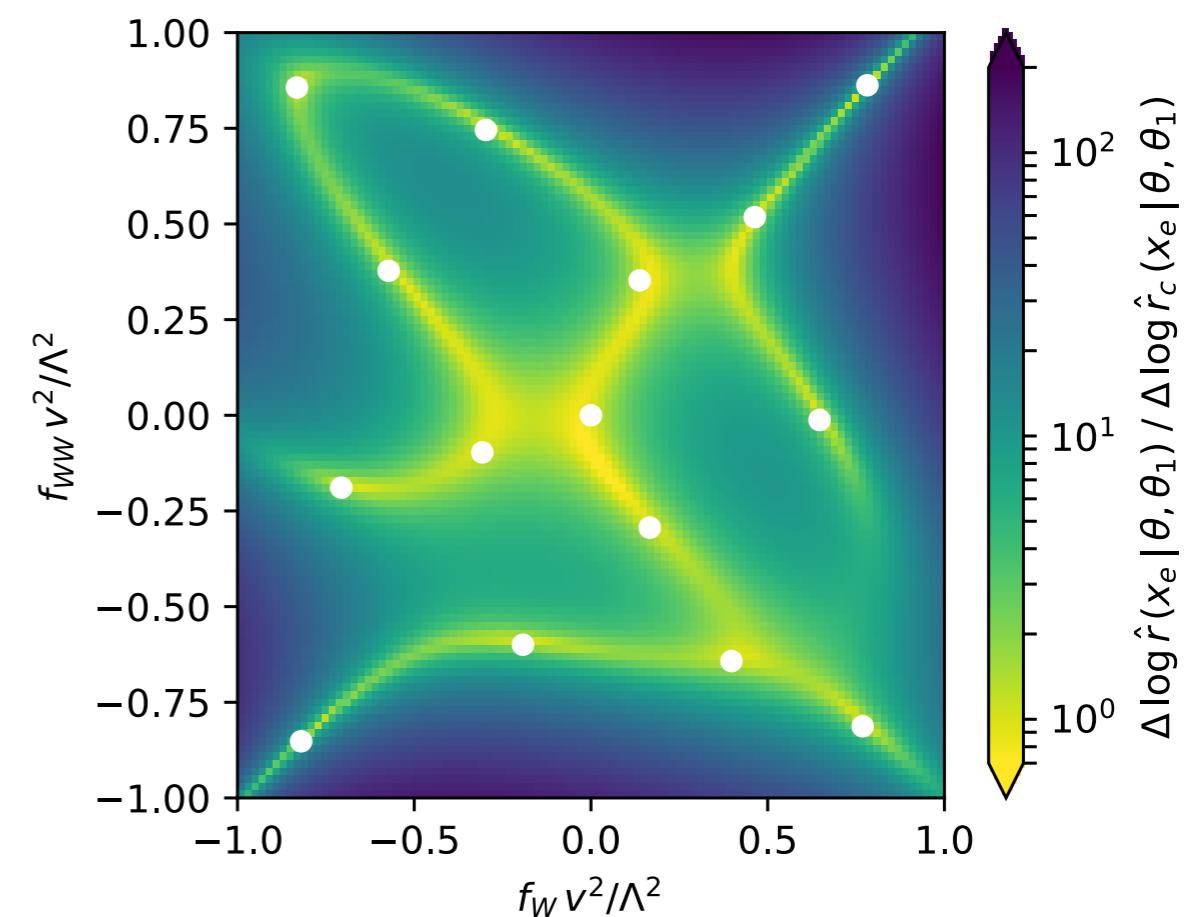
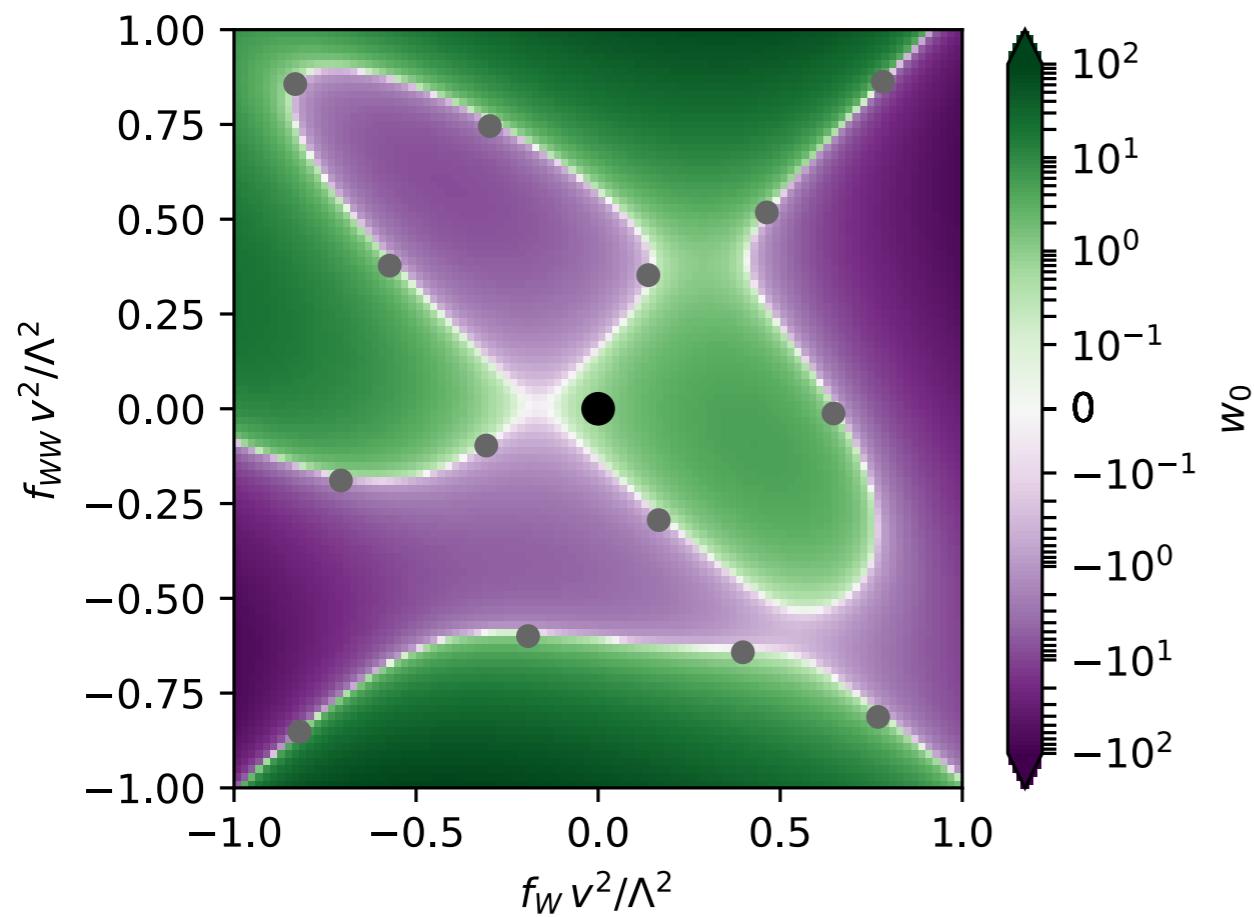


# Morphing-aware parameterized estimators

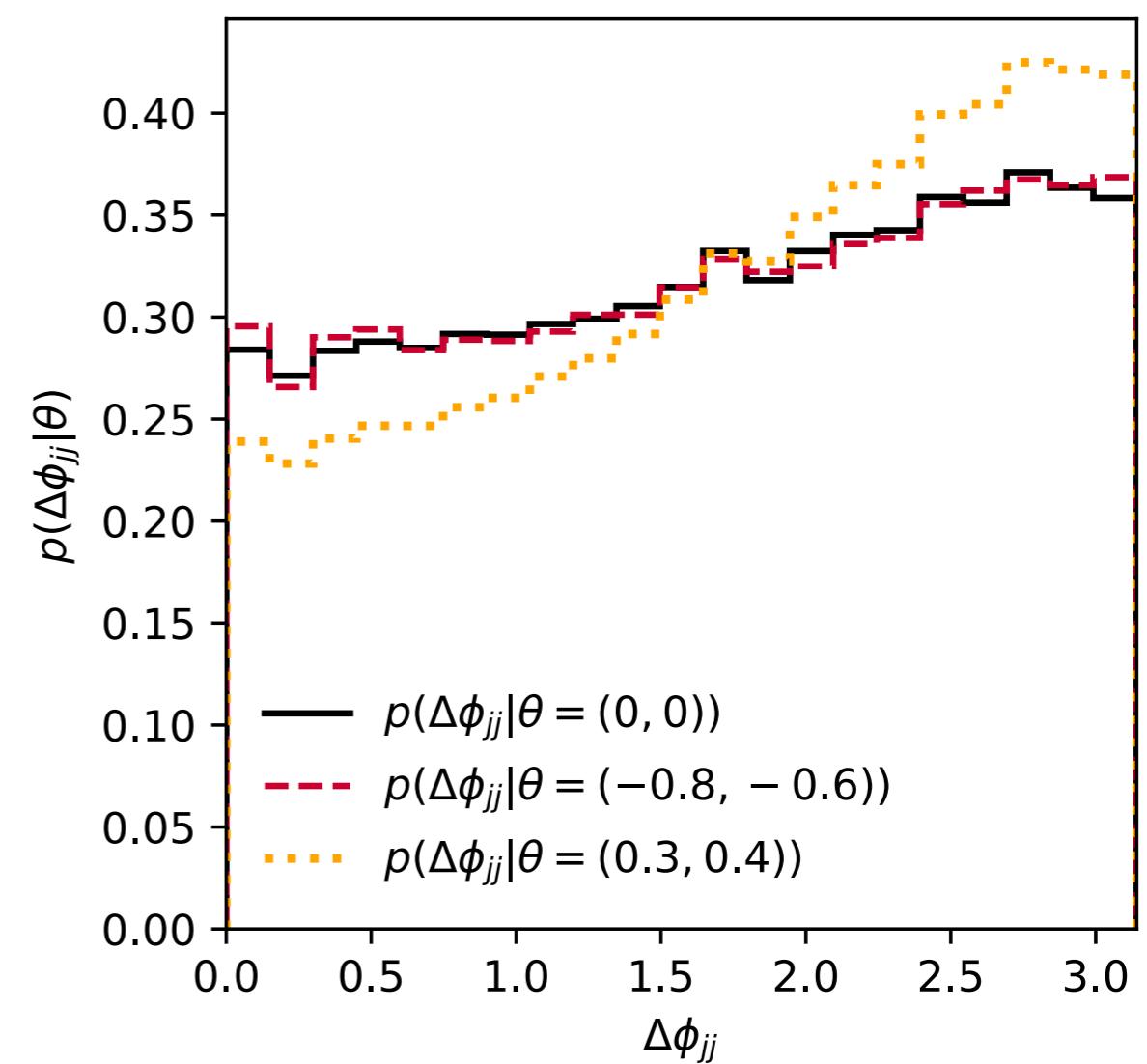
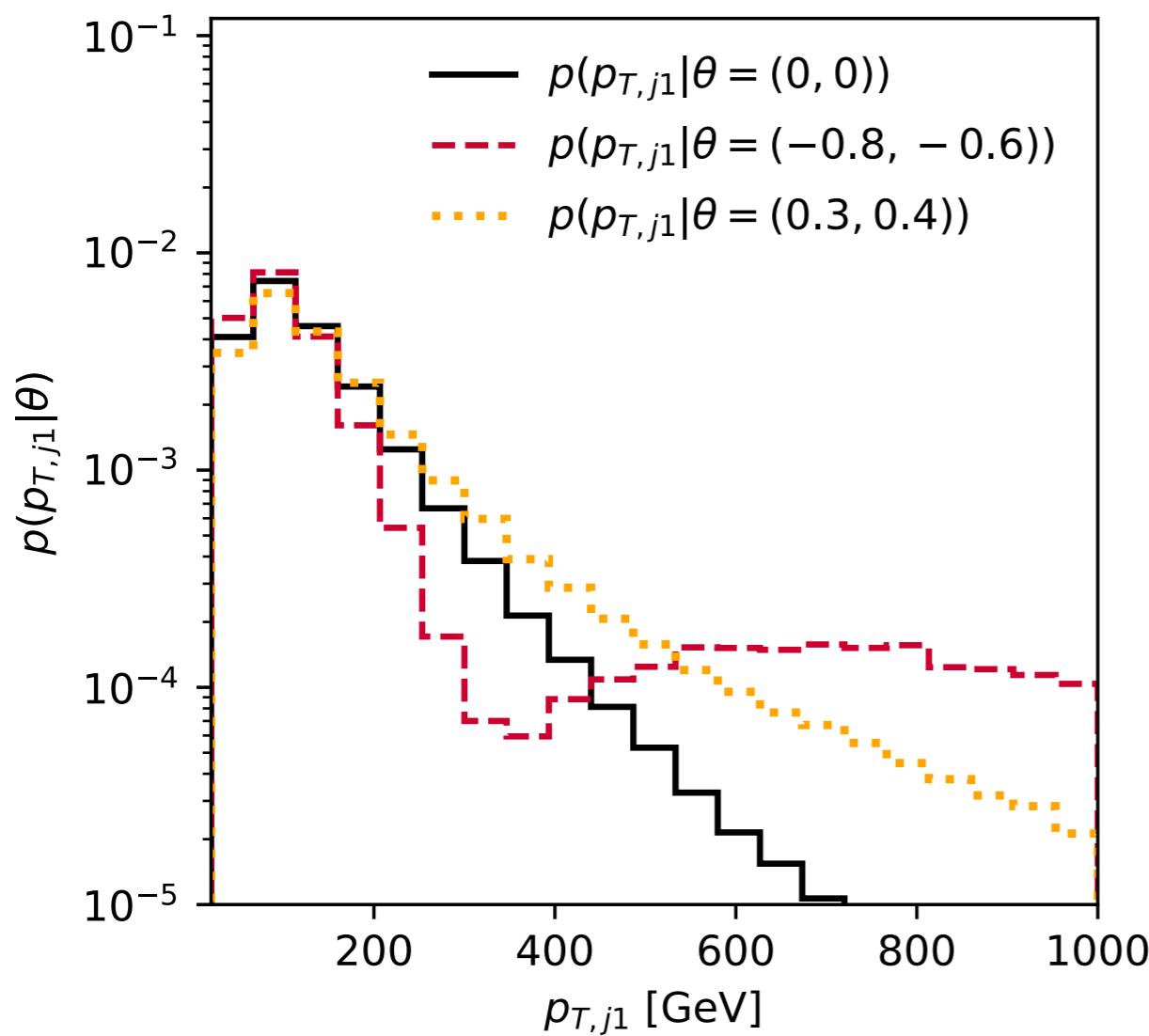
$$\hat{r}(x|\theta_0, \theta_1) = \sum_c w_c(\theta_0) \hat{r}_c(x)$$



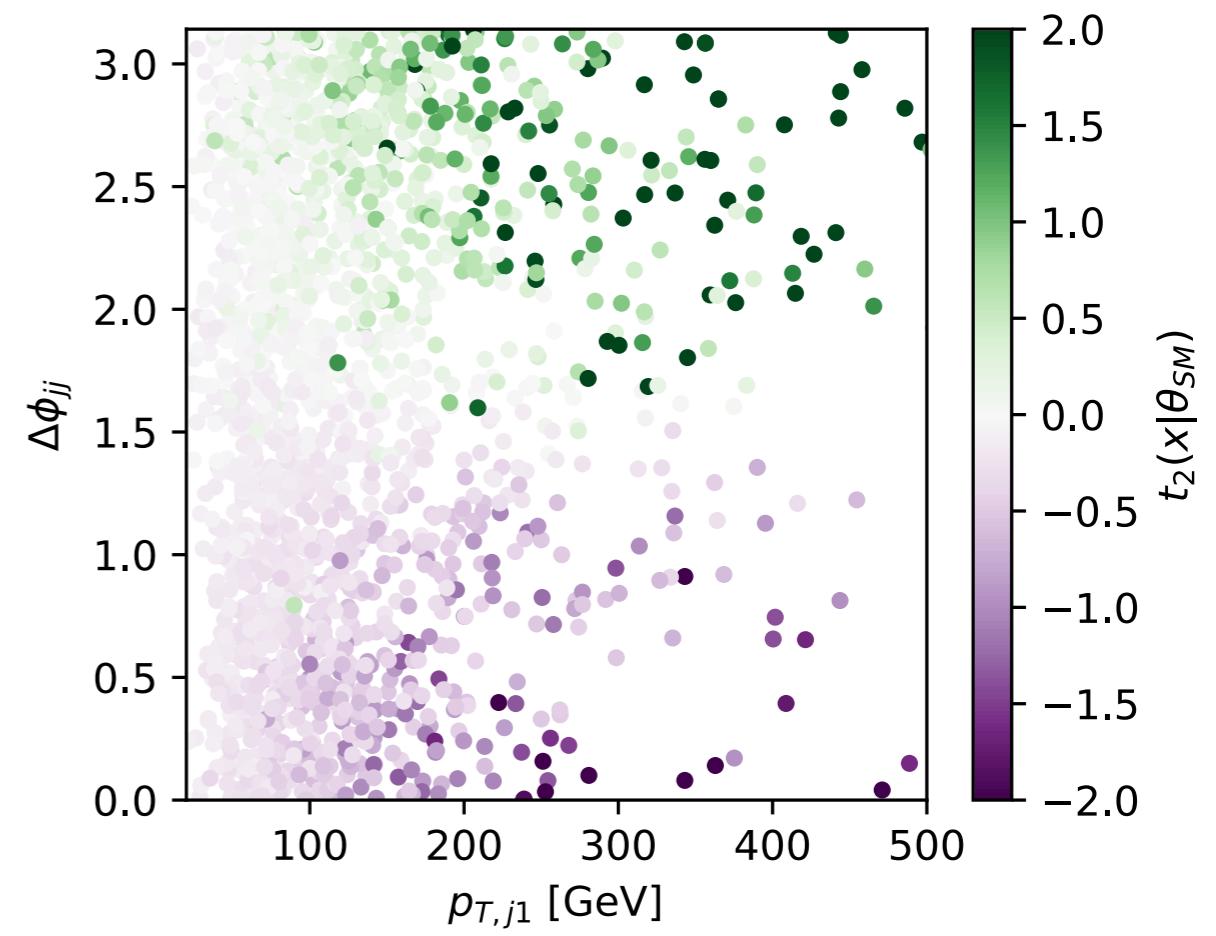
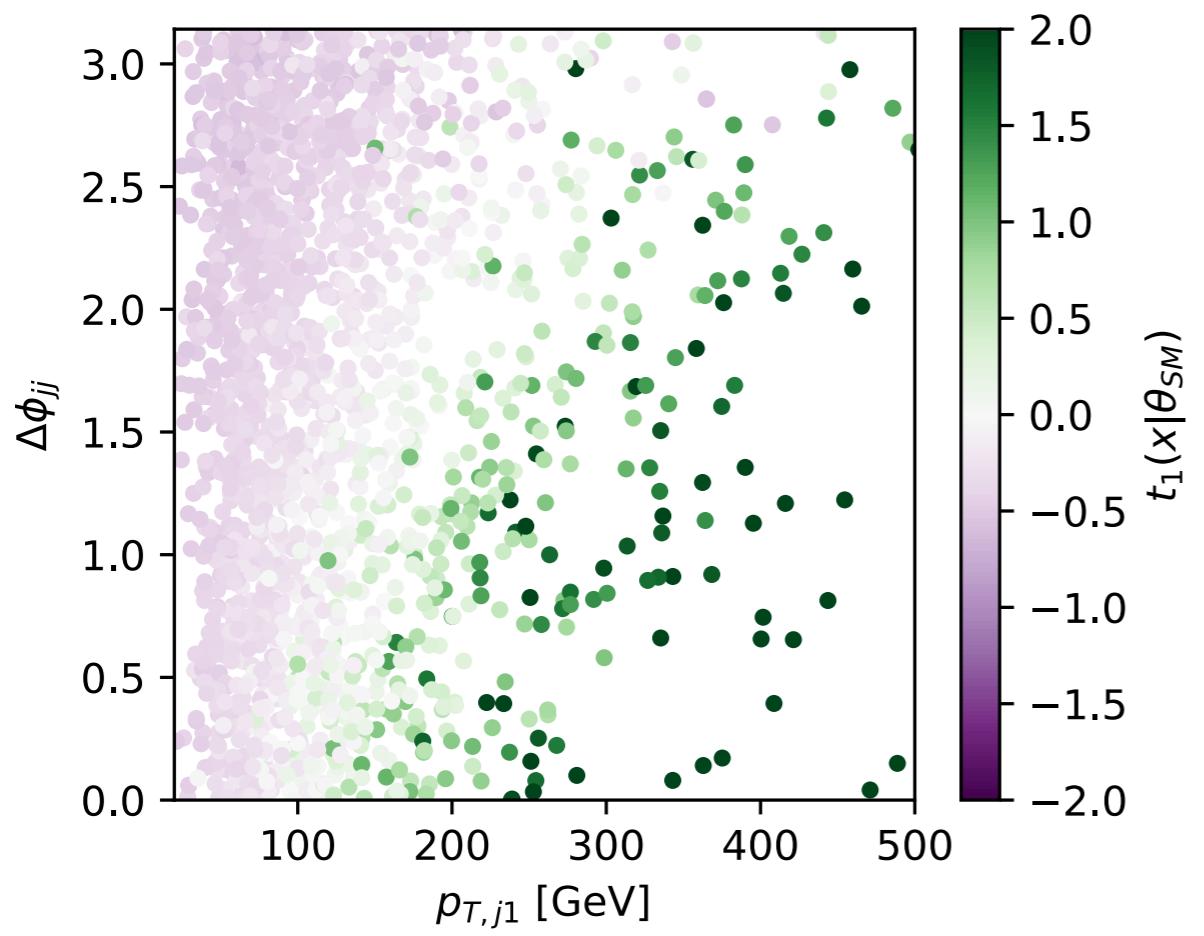
# Morphing coefficients



# Distributions



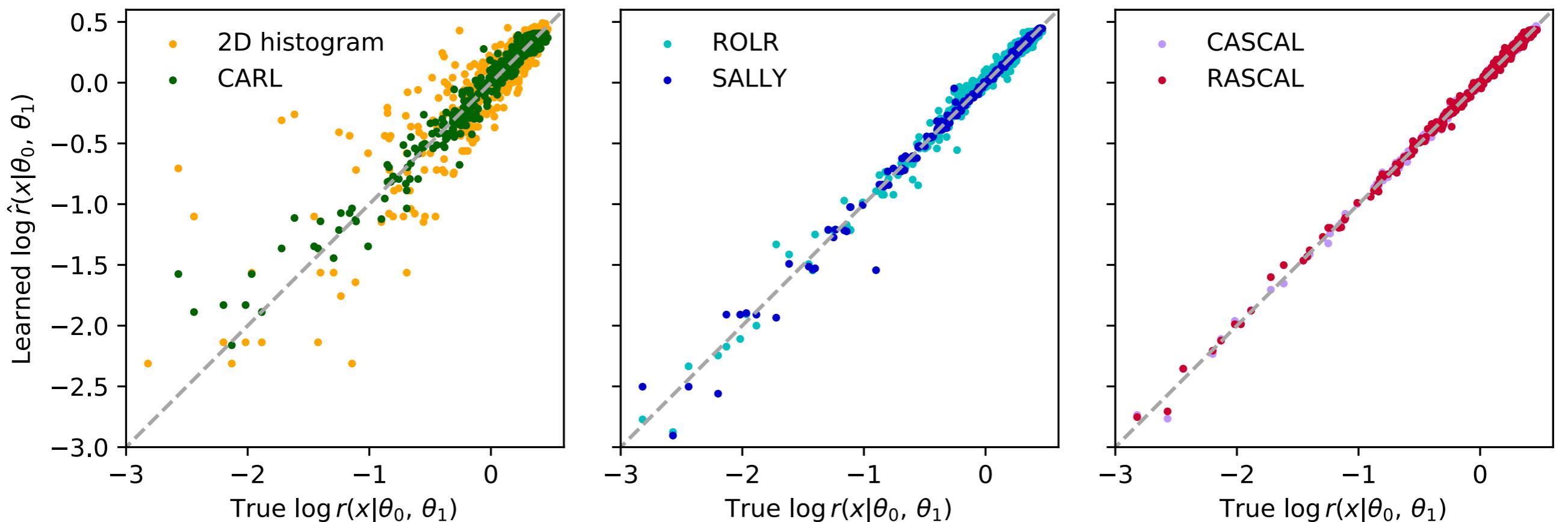
# Score vs observables



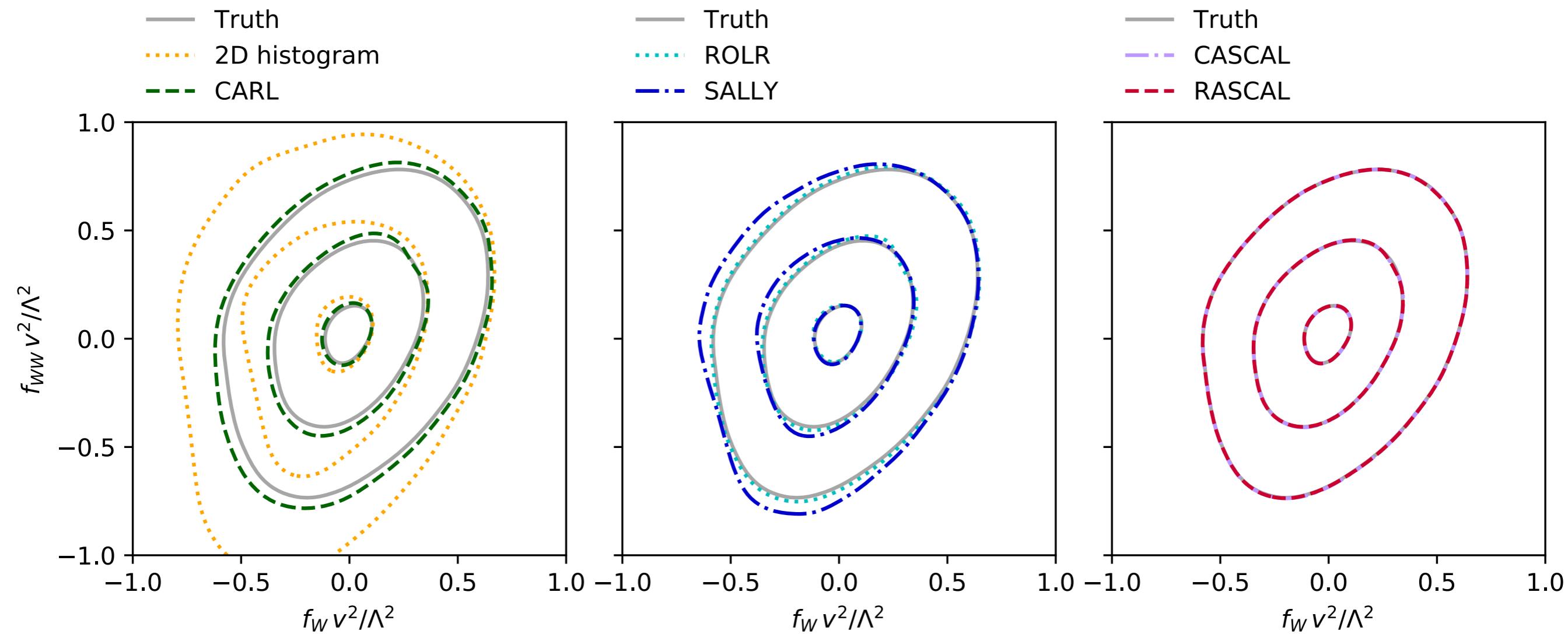
# Results

Strategy	Setup	Expected MSE		Figures
		All	Trimmed	
Histogram	$p_{T,j1}, \Delta\phi_{jj}$	<b>0.056</b>	0.0106	✓
	$p_{T,j1}$	0.088	0.0230	
	$\Delta\phi_{jj}$	0.160	0.0433	
	$p_{T,j1}, \Delta\phi_{jj}$	0.059	<b>0.0091</b>	
AFC	$p_{T,j1}, m_{Z2}, m_{jj}, \Delta\eta_{jj}, \Delta\phi_{jj}$	0.078	0.0101	
CARL (PbP)	PbP	0.030	0.0111	Fig. 12
CARL (parameterized)	Baseline	0.012	<b>0.0026</b>	✓
	Random $\theta$	<b>0.012</b>	0.0028	
	Baseline	0.076	0.0200	Fig. 12
CARL (morphing-aware)	Random $\theta$	0.086	0.0226	
	Morphing basis	0.156	0.0618	
ROLR (PbP)	PbP	0.005	0.0022	
ROLR (parameterized)	Baseline	0.003	0.0017	✓
	Random $\theta$	<b>0.003</b>	<b>0.0014</b>	
	Baseline	0.024	0.0063	
ROLR (morphing-aware)	Random $\theta$	0.022	0.0052	
	Morphing basis	0.130	0.0485	
SALLY		<b>0.013</b>	<b>0.0002</b>	✓
SALLINO		0.021	0.0006	
CASCAL (parameterized)	Baseline	<b>0.001</b>	<b>0.0002</b>	✓
	Random $\theta$	0.001	0.0002	
CASCAL (morphing-aware)	Baseline	0.136	0.0427	
	Random $\theta$	0.092	0.0268	
	Morphing basis	0.040	0.0081	
RASCAL (parameterized)	Baseline	0.001	0.0004	✓
	Random $\theta$	<b>0.001</b>	<b>0.0004</b>	
RASCAL (morphing-aware)	Baseline	0.125	0.0514	
	Random $\theta$	0.132	0.0539	
	Morphing basis	0.031	0.0072	

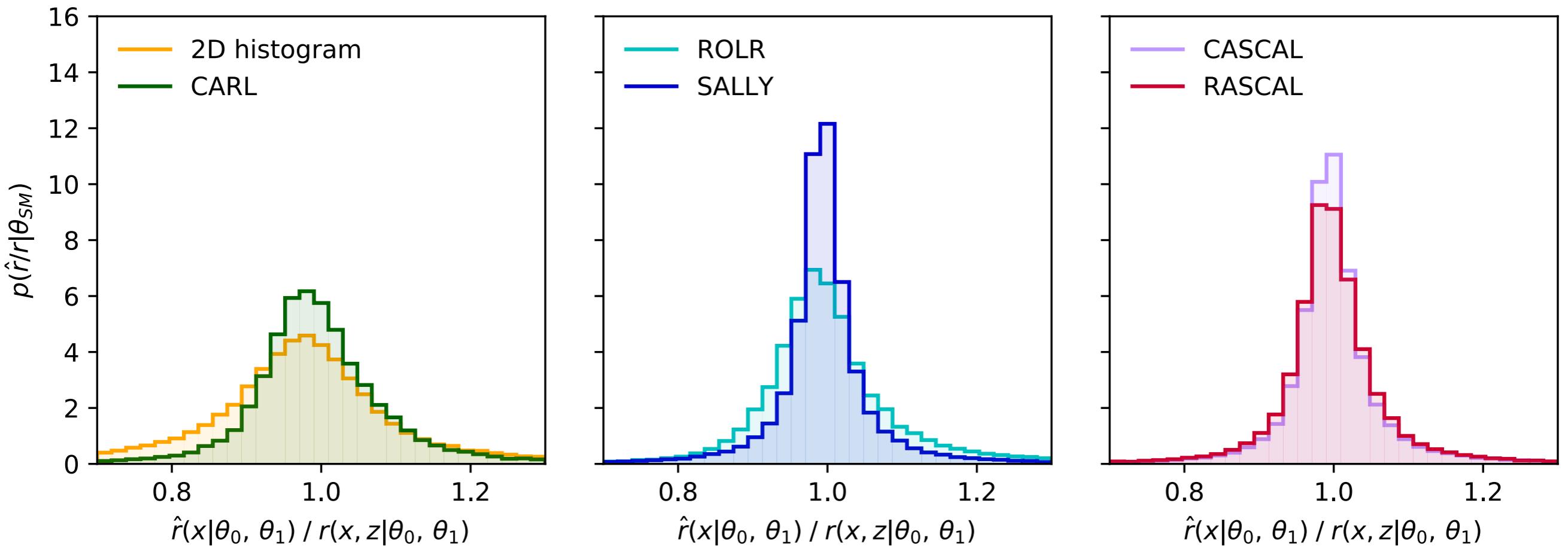
# Precision of estimates



# Expected limits (truth level)



# Detector effects



# Expected limits (with detector effects)

