Bringing together simulations, physics insight, and machine learning to constrain new physics

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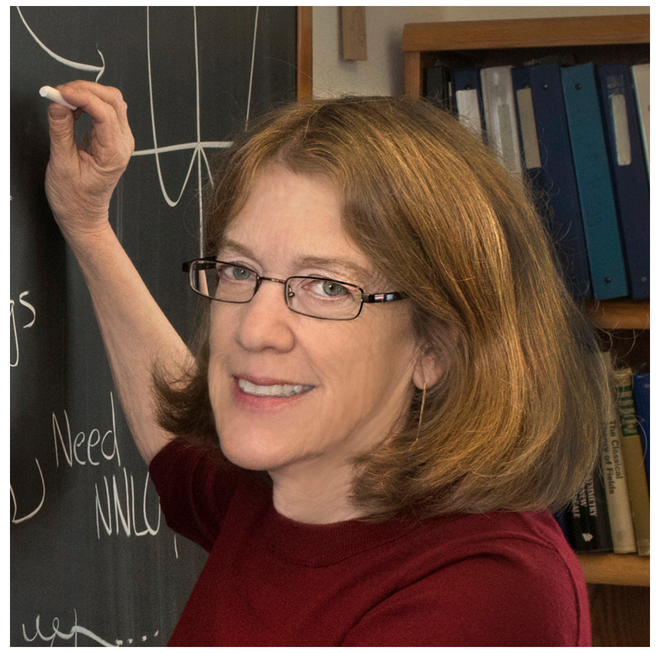
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The SCAILFIN Project
scailfin.github.io

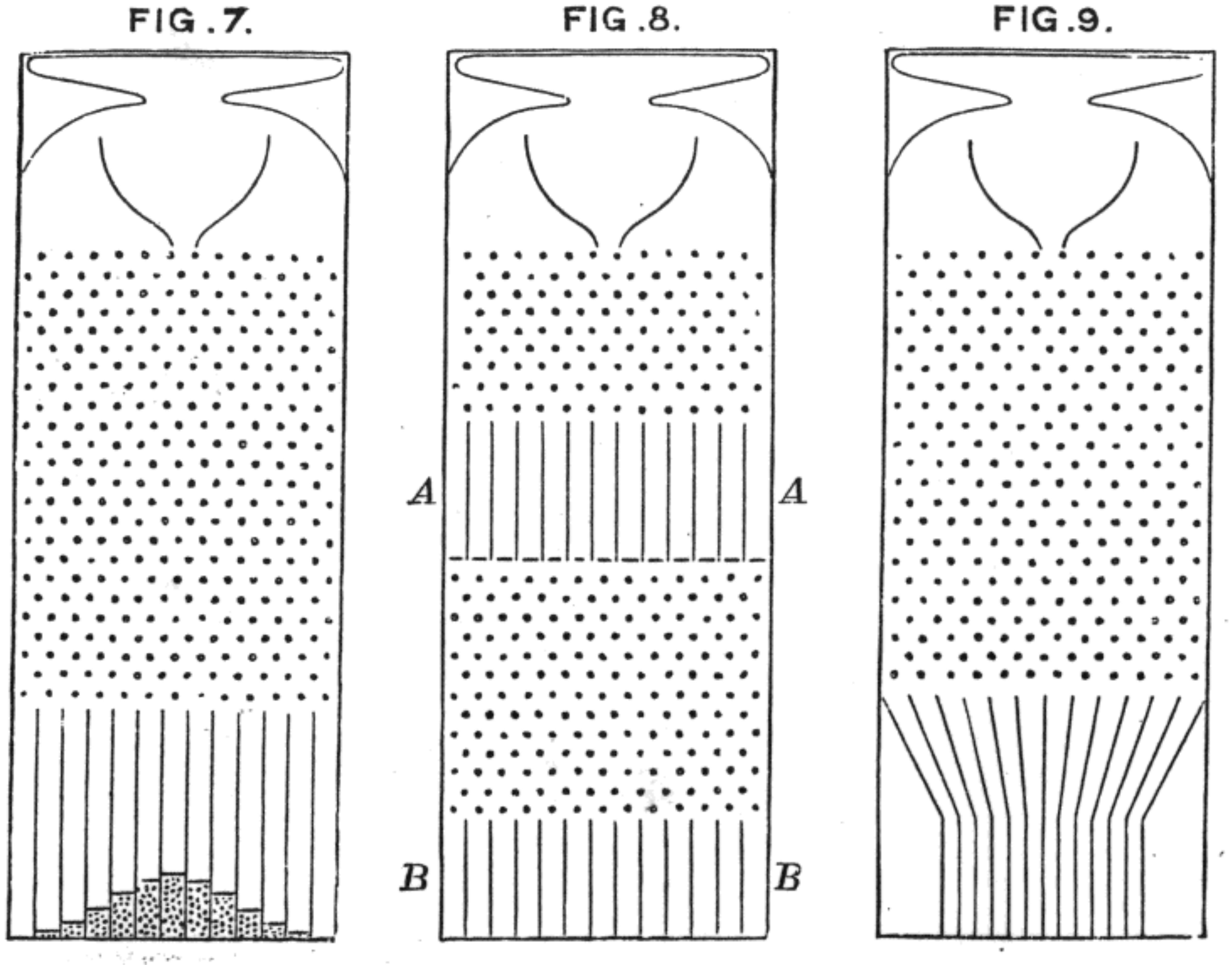

5. Particle physics example
4. Learning optimal summary statistics
3. “Mining gold”: a new approach
2. Existing solutions
1. The problem of
likelihood-free inference

The problem of
“likelihood-free” inference

The Galton board

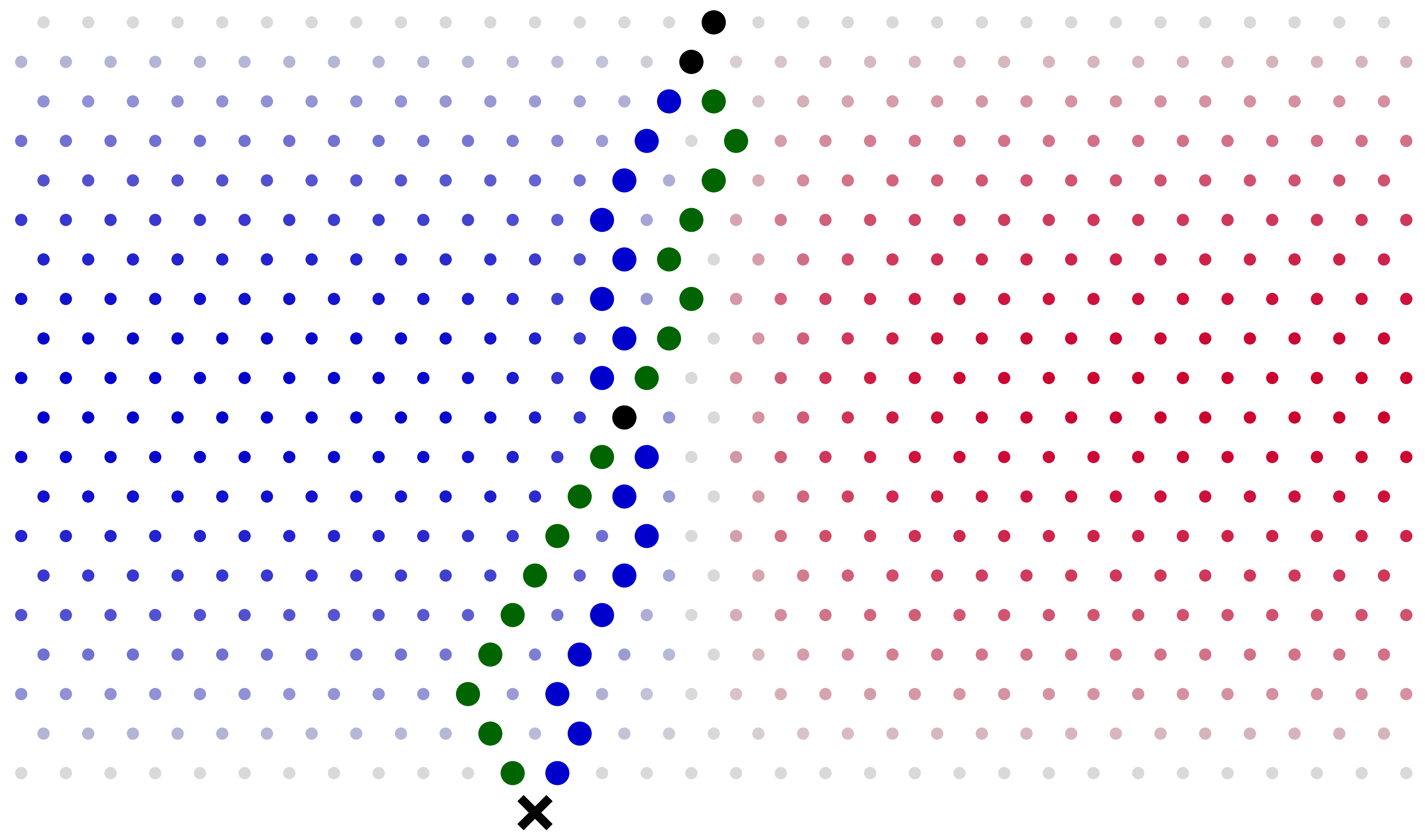
[galtonboard.com]

The Galton board



[F. Galton 1889]

Probabilities from integrating trajectories



Probability of ending in bin x : $p(x) = \int \mathrm{d}z \; p(x, z)$

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 θ ?

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

  Simple: just drop balls!

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 θ ?

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

  Simple: just drop balls!

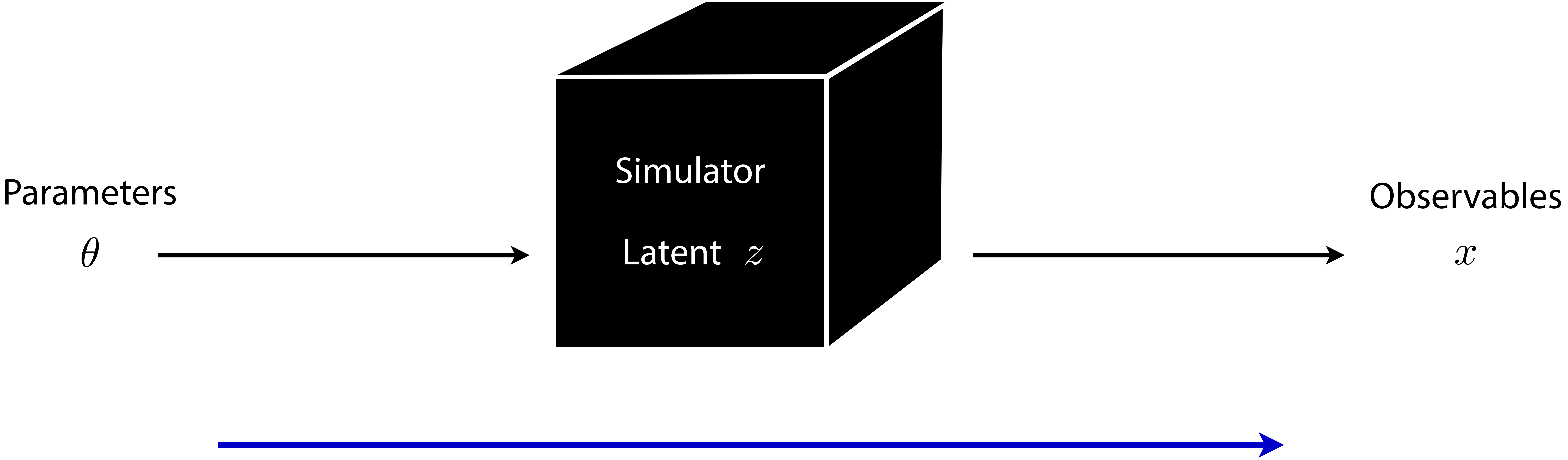
- Inference: given observations $\{x_i\}$, what are the most likely values for θ ?

  Usually we solve this with the likelihood

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

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

“Likelihood-free inference”

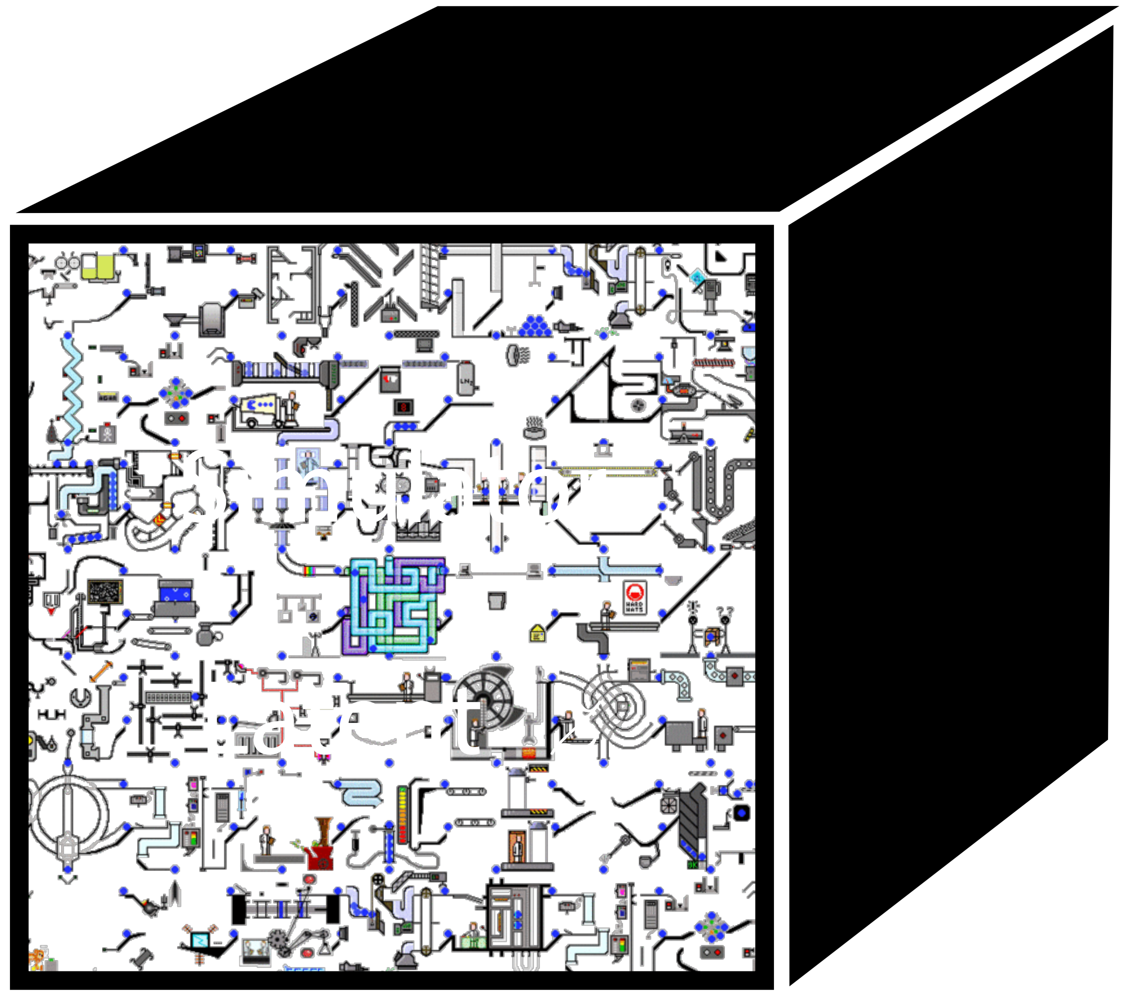


Prediction:

- Well-understood mechanistic model
- Simulator can generate samples

“Likelihood-free inference”

Parameters
θ



Observables
x

Prediction:
- Well-understood mechanistic model
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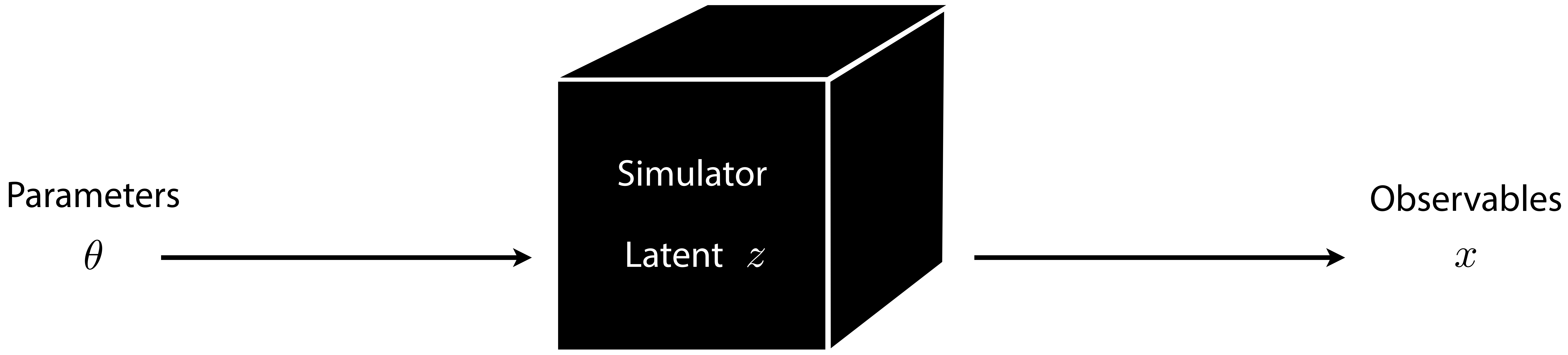
“Likelihood-free inference”



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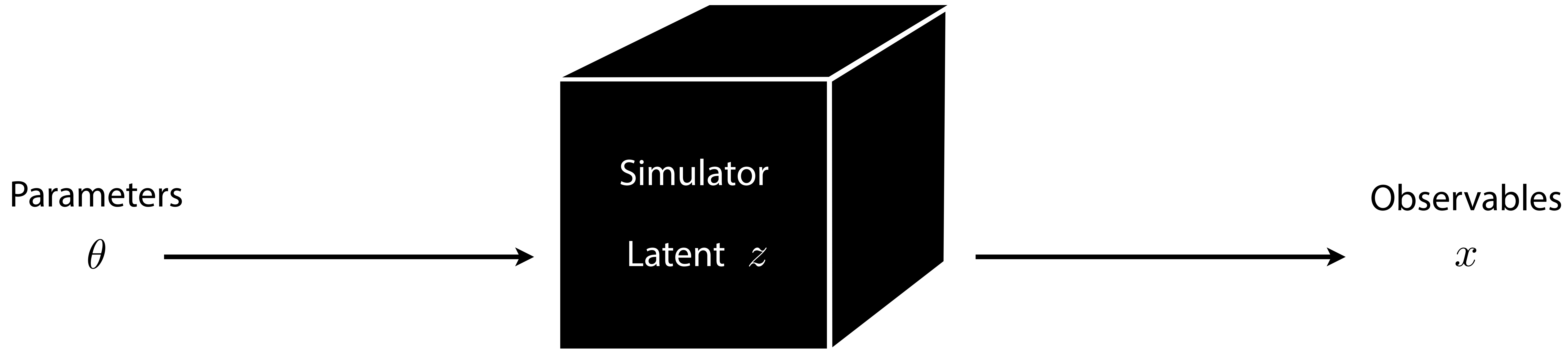


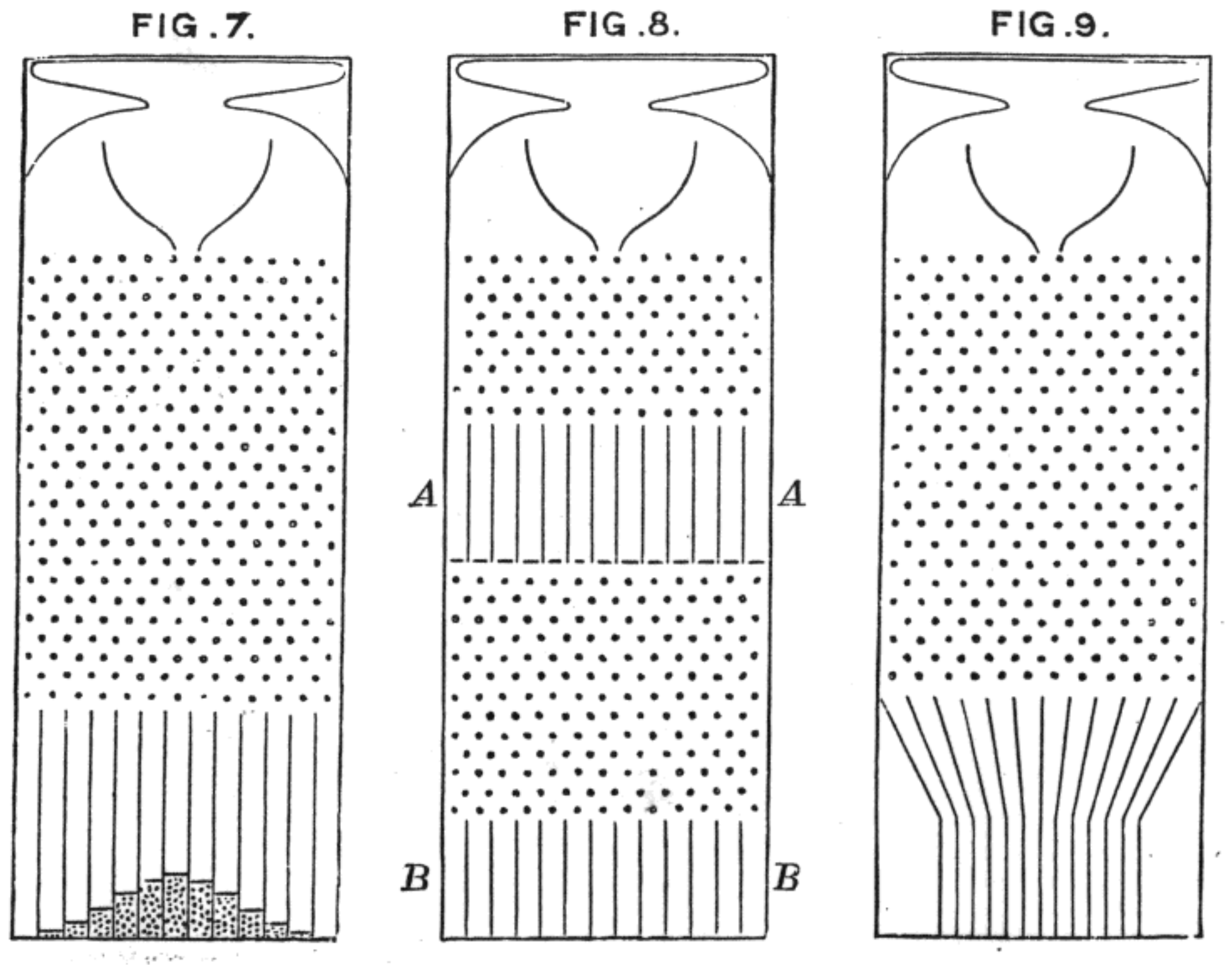
Prediction:

- Well-understood mechanistic model
- Simulator can generate samples

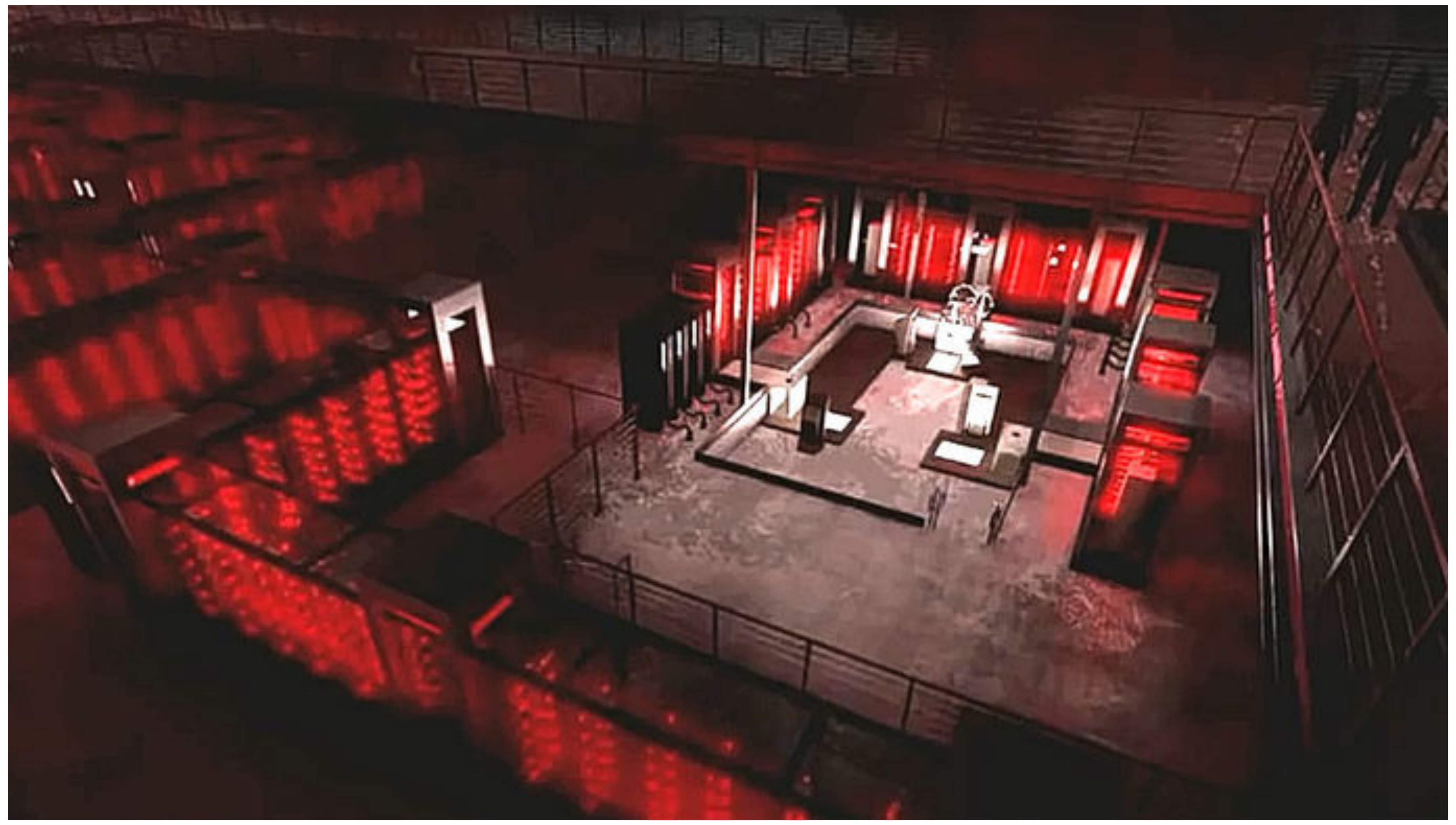
Inference:

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

Galton board: metaphor for simulator-based science



[F. Galton 1889]

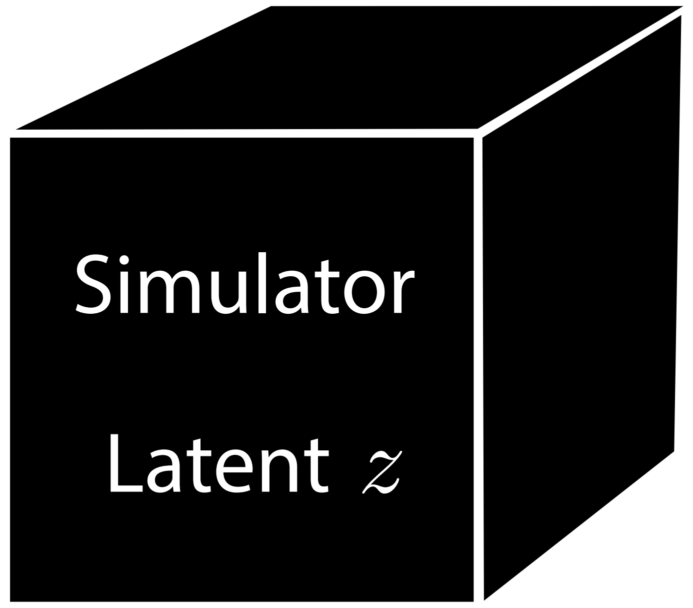


[HBO 2018]

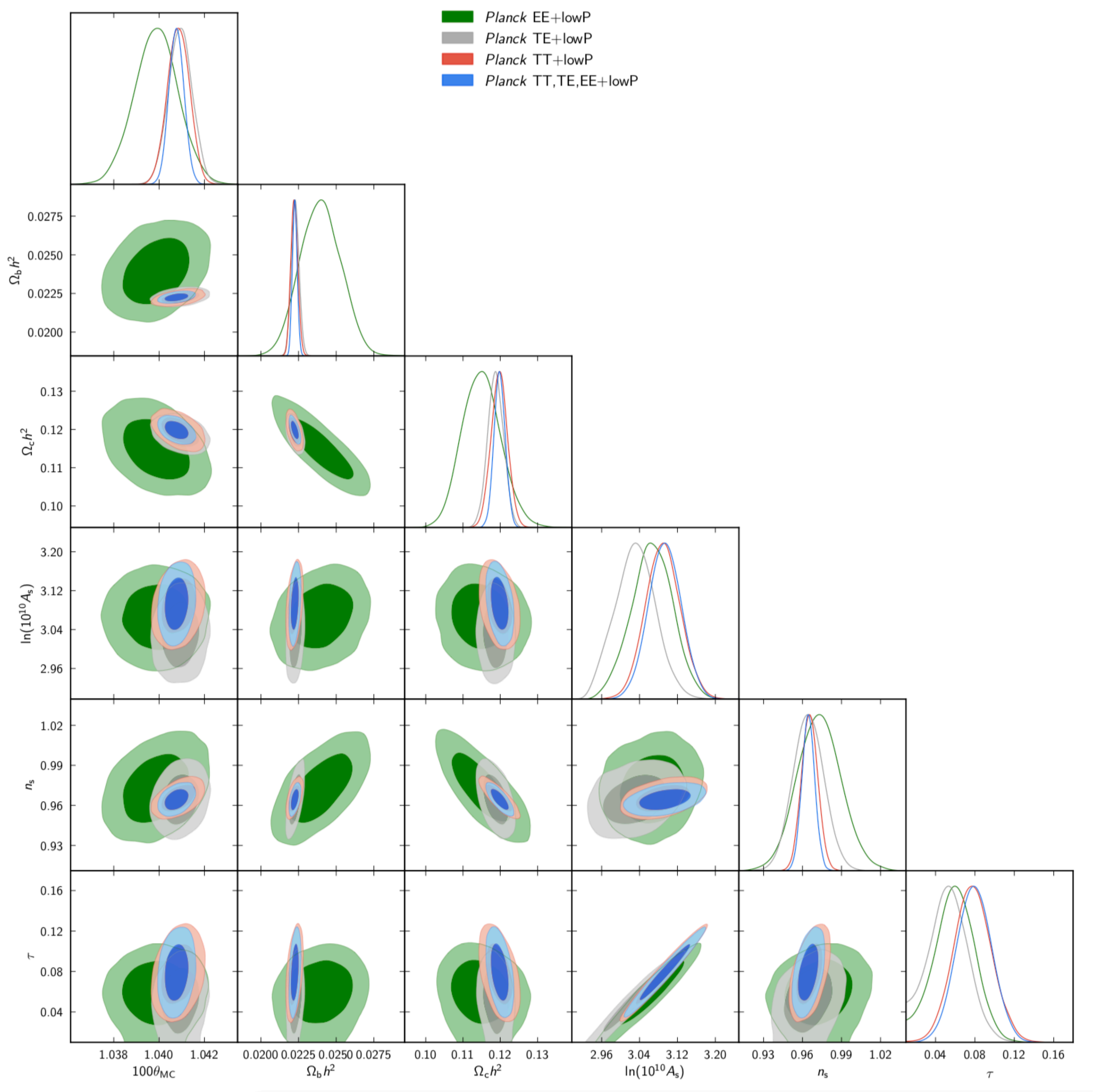
Galton board device	$\longrightarrow$	Computer simulation
Parameters θ	$\longrightarrow$	Model parameters θ
Bins x	$\longrightarrow$	Observables x
Path z	$\longrightarrow$	Latent variables z (stochastic execution trace through simulator)

Cosmological N-body simulations

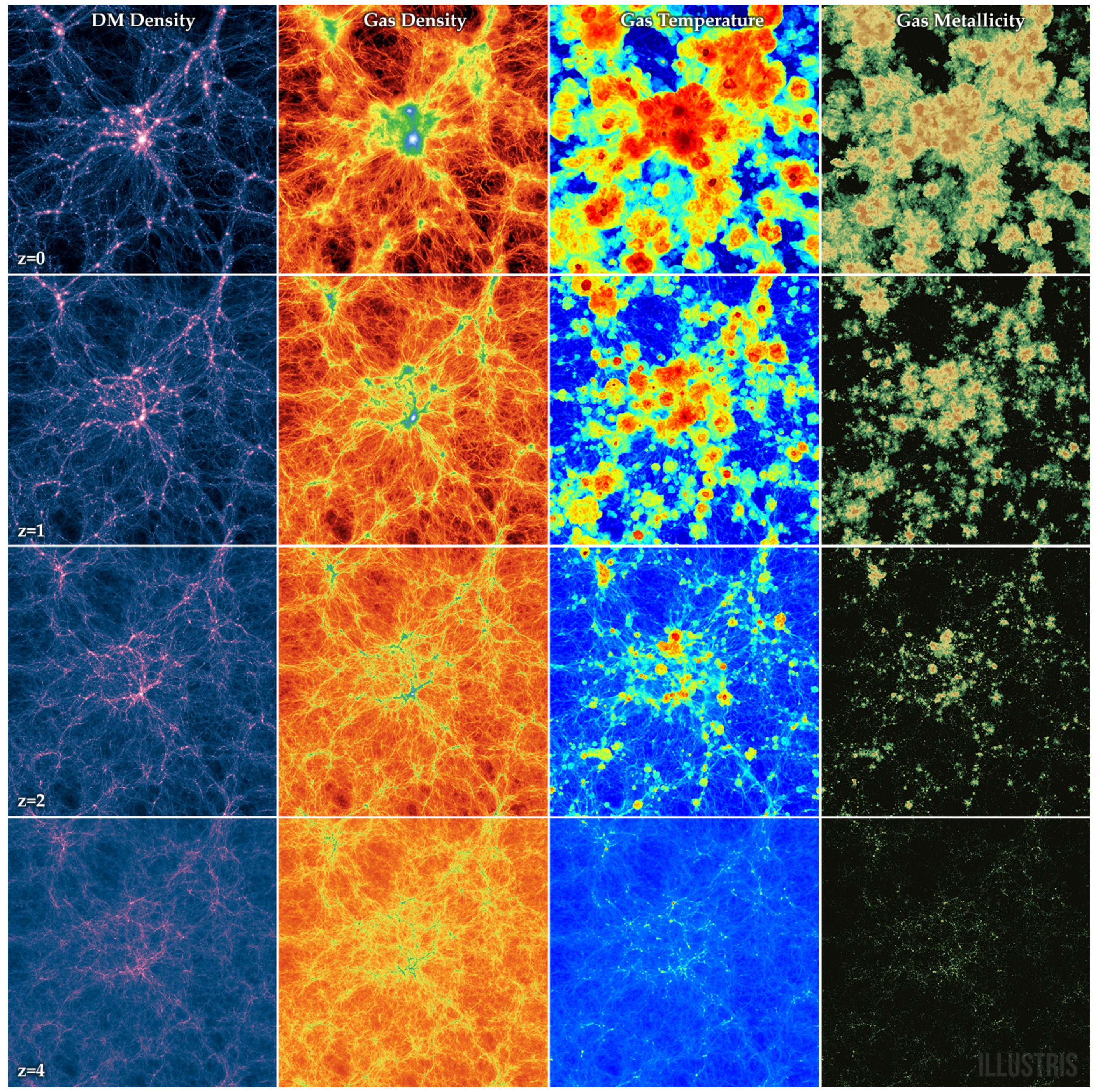
Parameters
θ



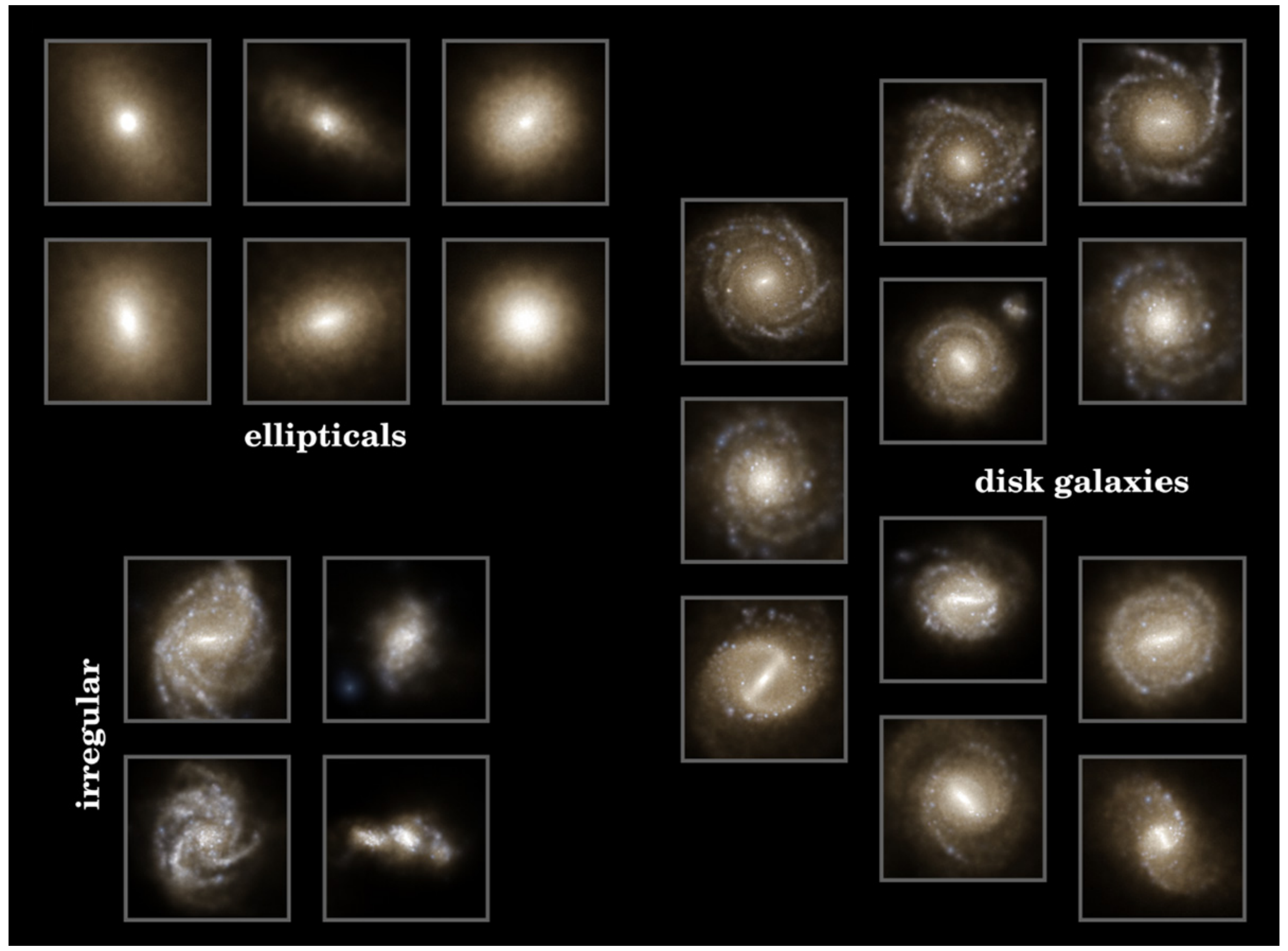
Observables
x



[Planck 1502.01589]



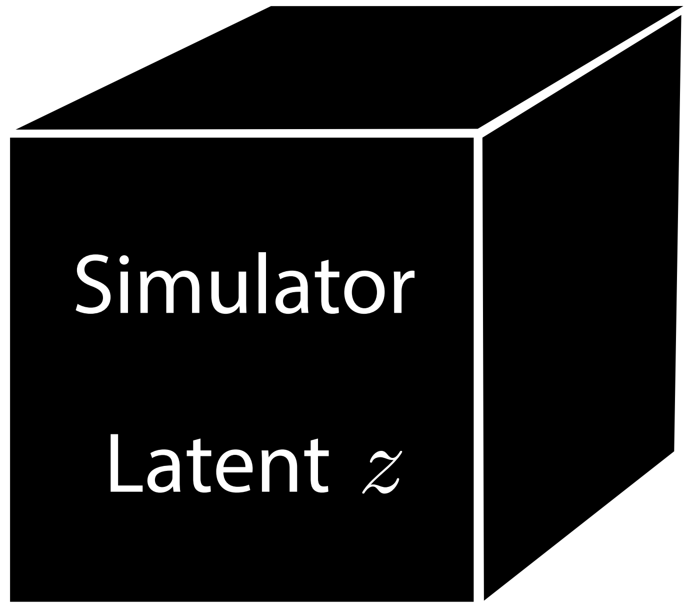
[Illustris 1405.2921]



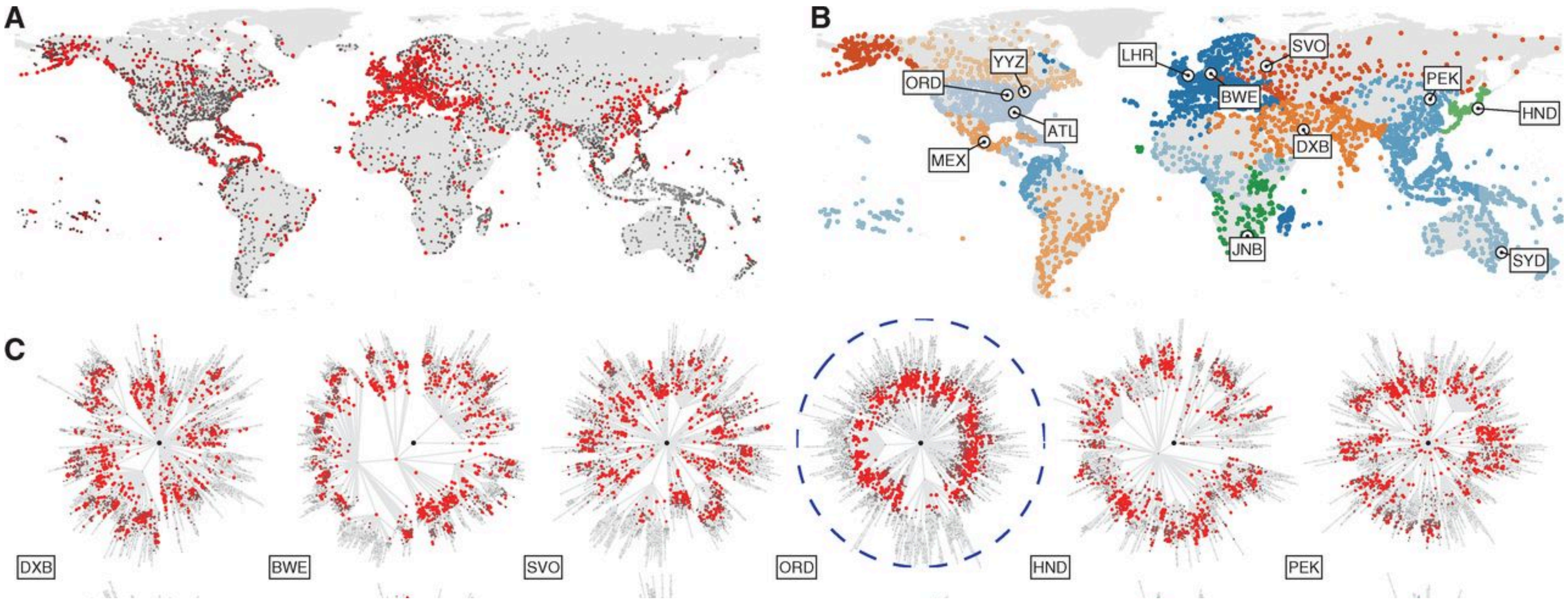
[Illustris 1405.2921]

Epidemiology

Parameters θ $\longrightarrow$

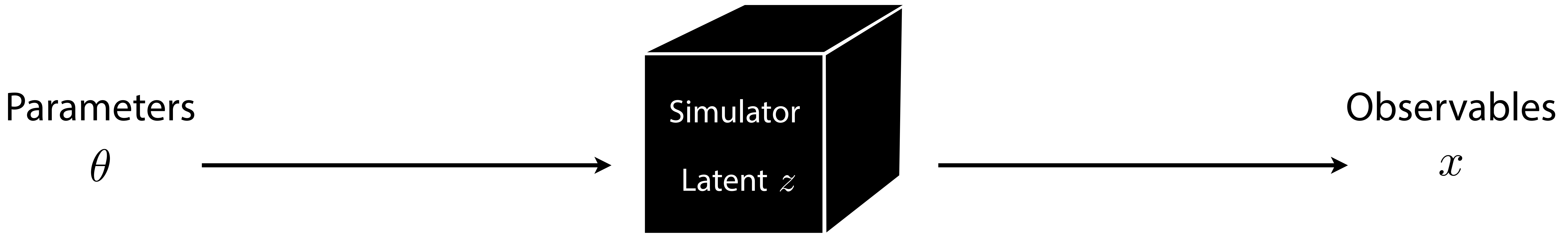


$\longrightarrow$ Observables x

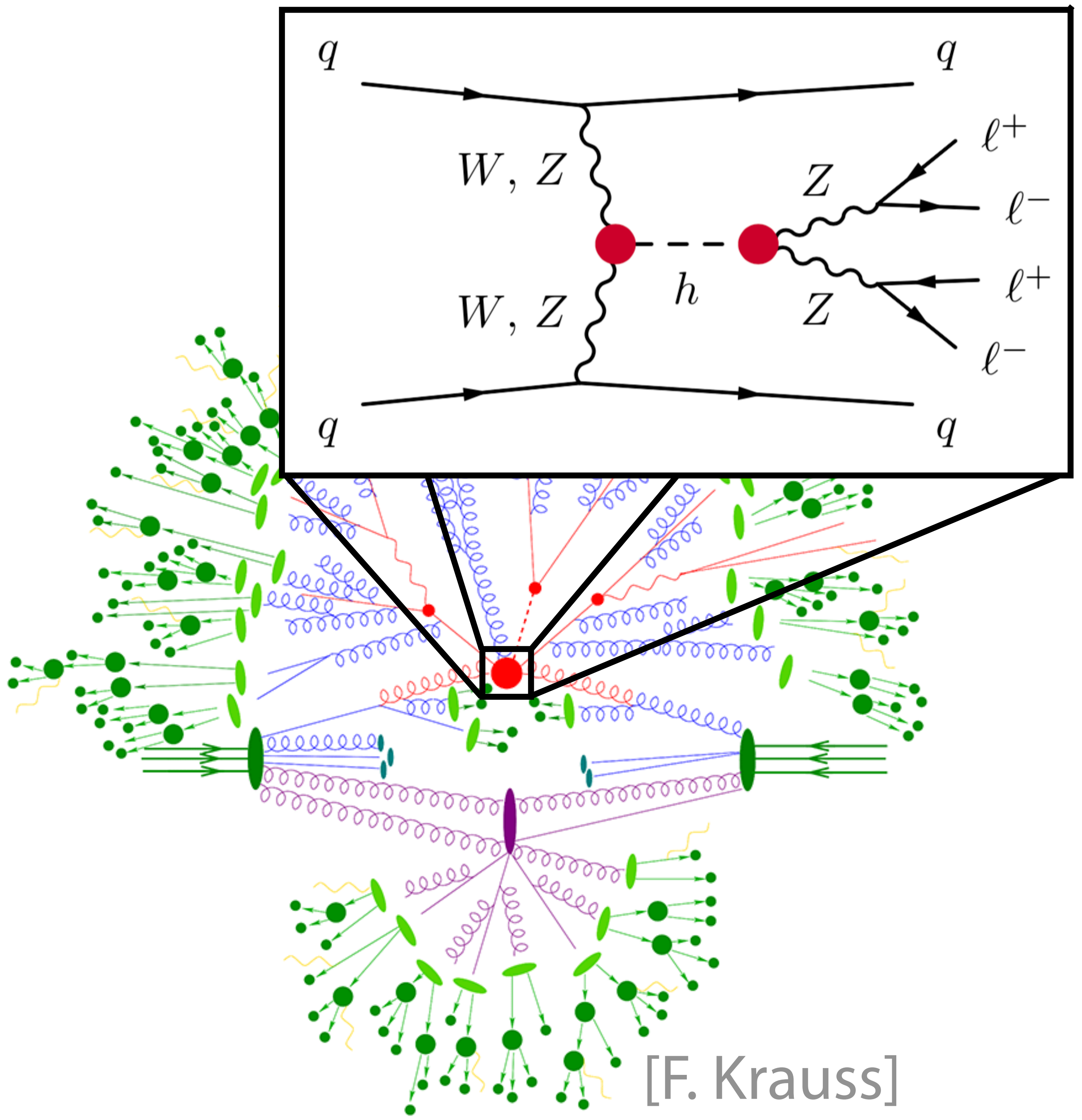


[D. Brockmann, D. Helbing 2013]

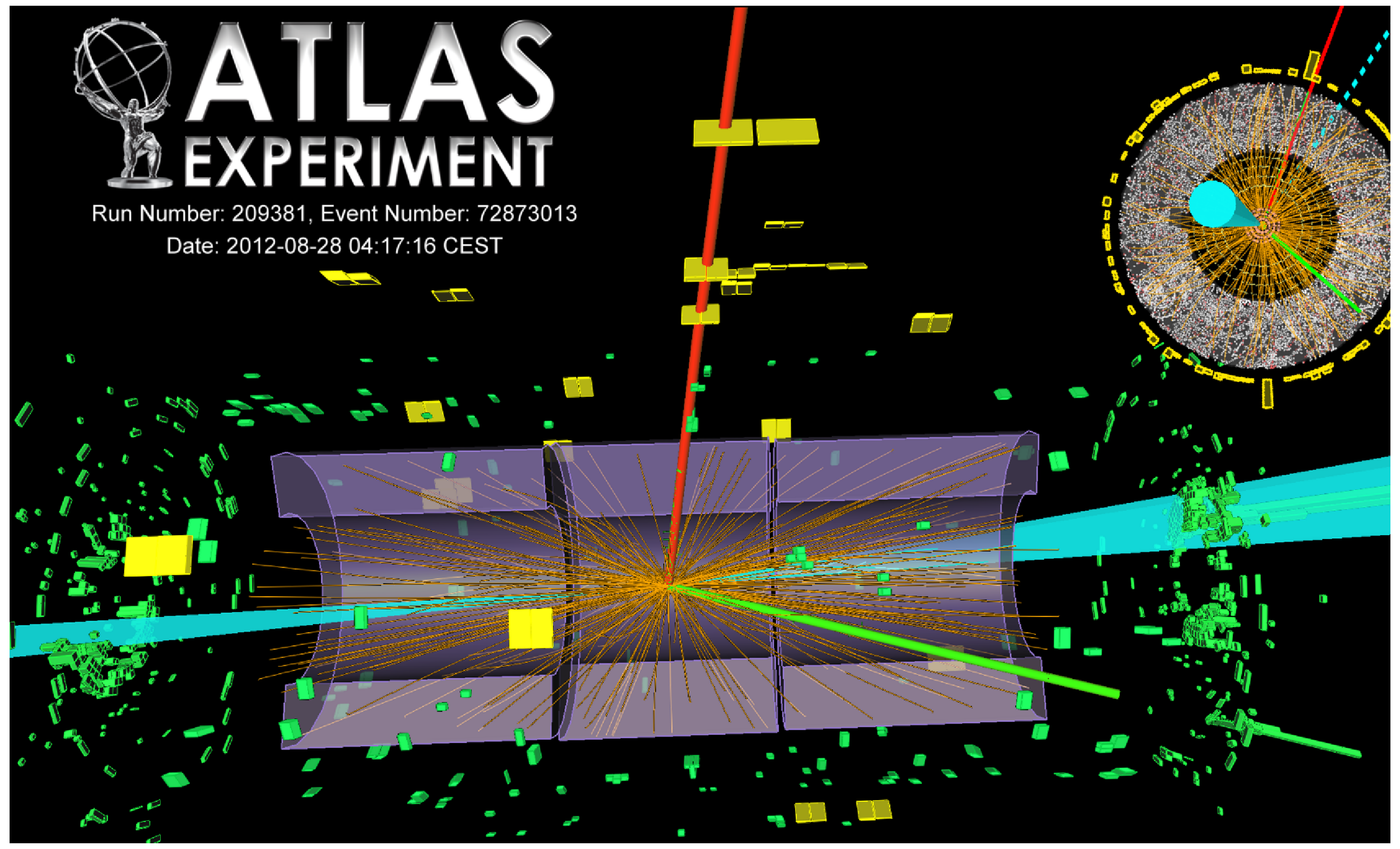
Particle physics



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



[F. Krauss]



[ATLAS 1501.04943]

Why has that not stopped us before?

Solve it by histogramming summary statistics

- Typical particle physicists' solution:

Solve it by histogramming summary statistics

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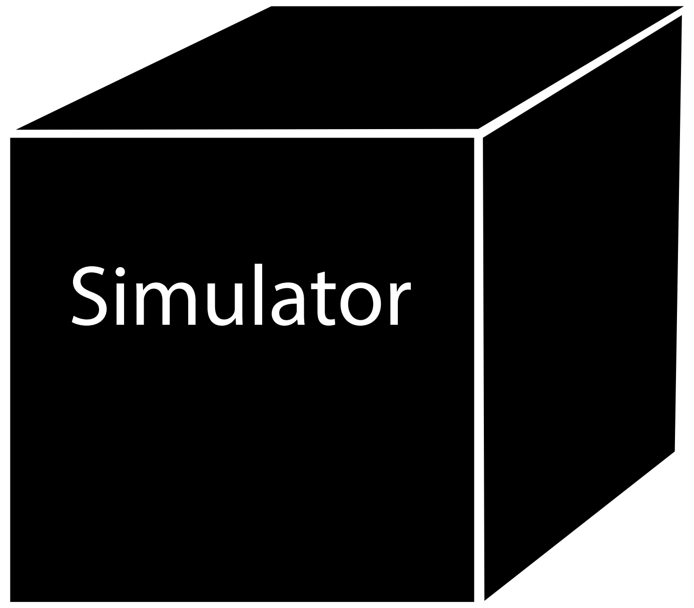
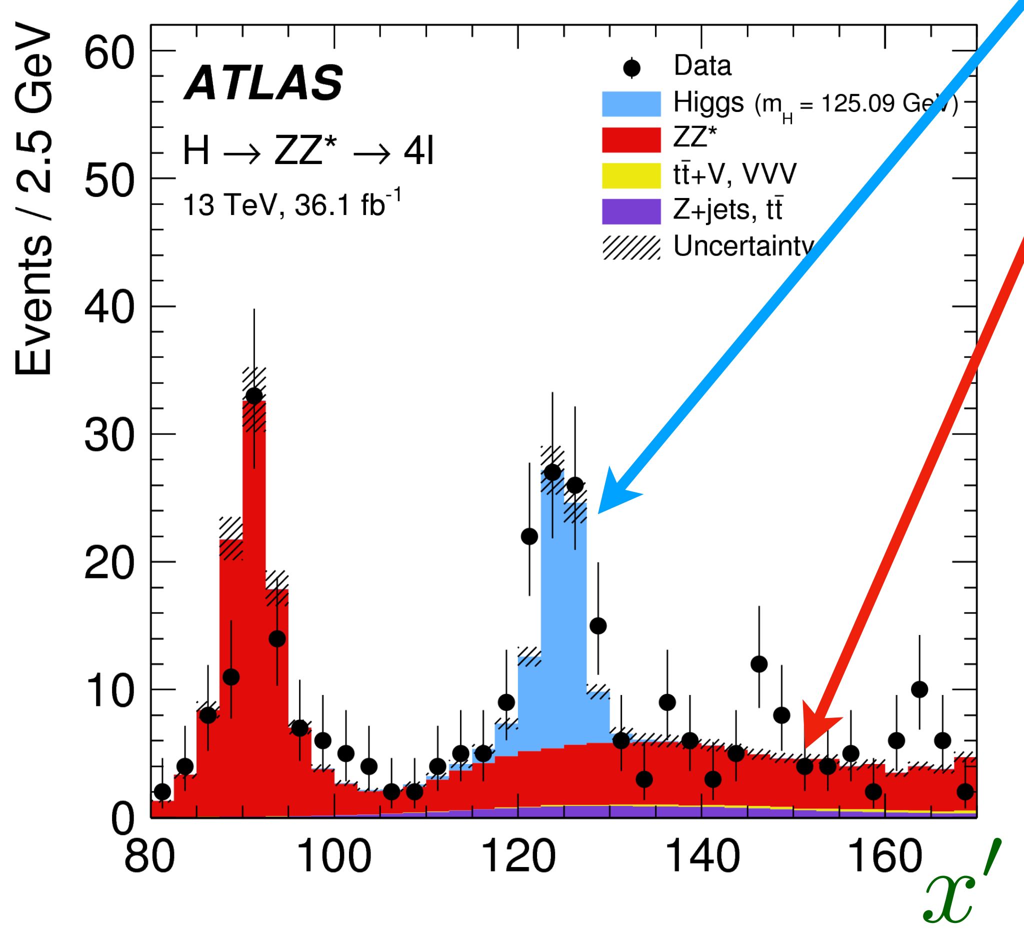
Parameters

θ $\longrightarrow$



$\longrightarrow$ Observables x $\longrightarrow$ Summary statistics x'

$$\hat{p}(x|\theta) = p(x'|\theta) =$$



[ATLAS 1712.02304]

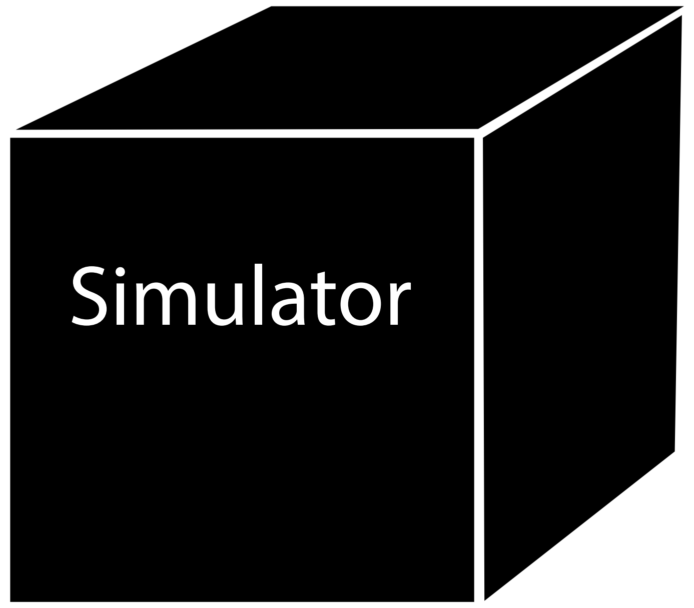
Run simulator for different θ, fill histograms

Solve it by histogramming summary statistics

- Typical particle physicists' solution:

Parameters

θ



Observables

x

Summary statistics

x'

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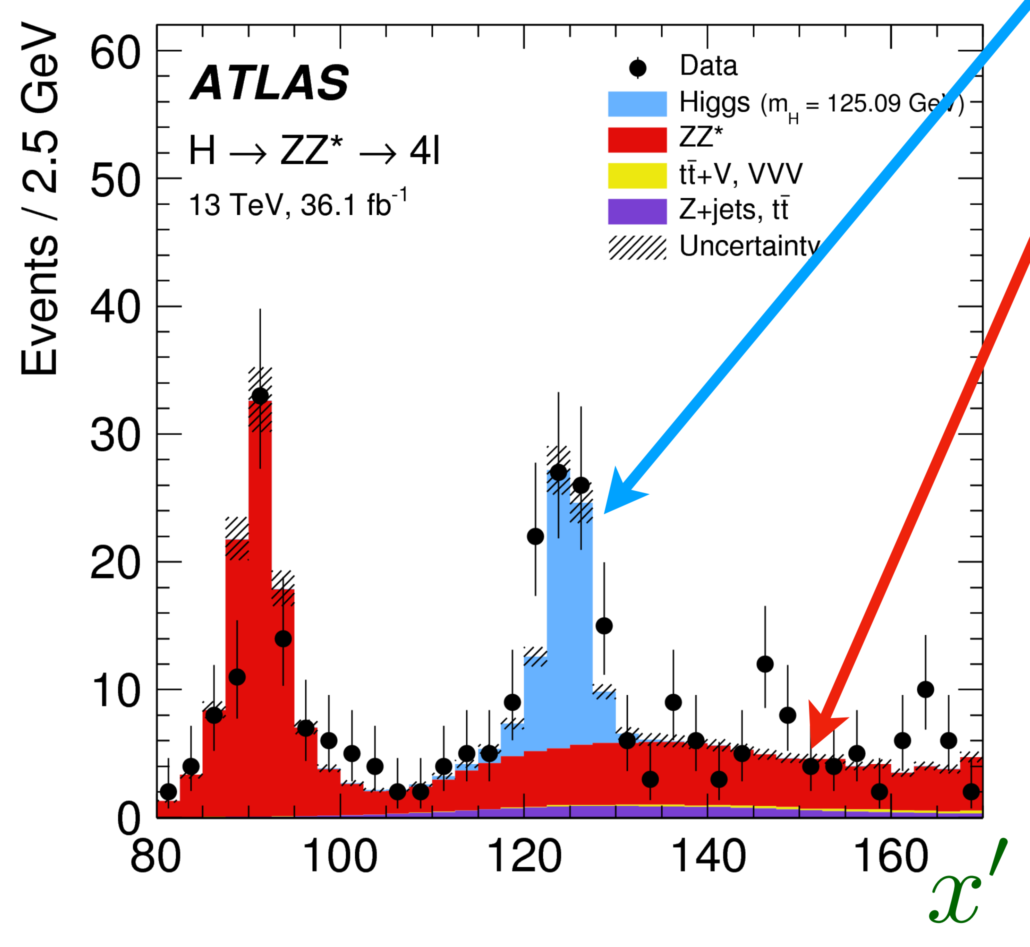
$$\hat{p}(x|\theta) = p(x'|\theta) =$$



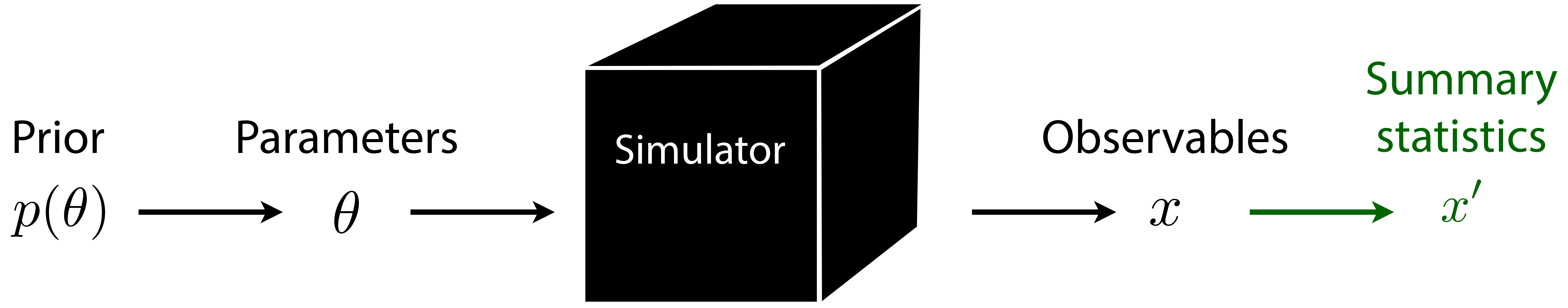
[ATLAS 1712.02304]

- 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 with Approximate Bayesian Computation (ABC)

[D. Rubin 1984]



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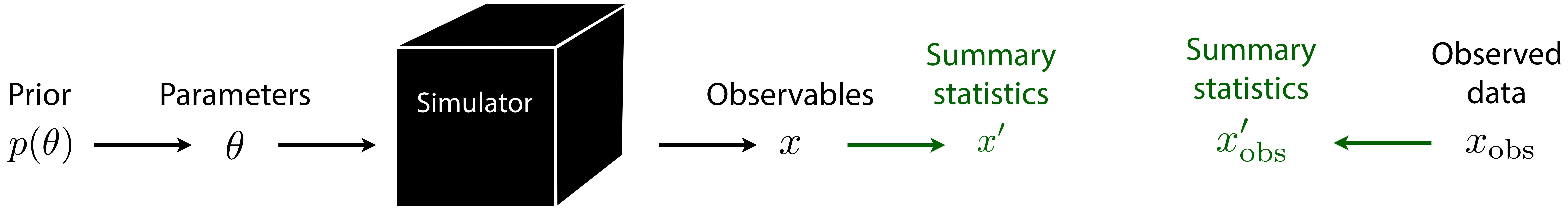

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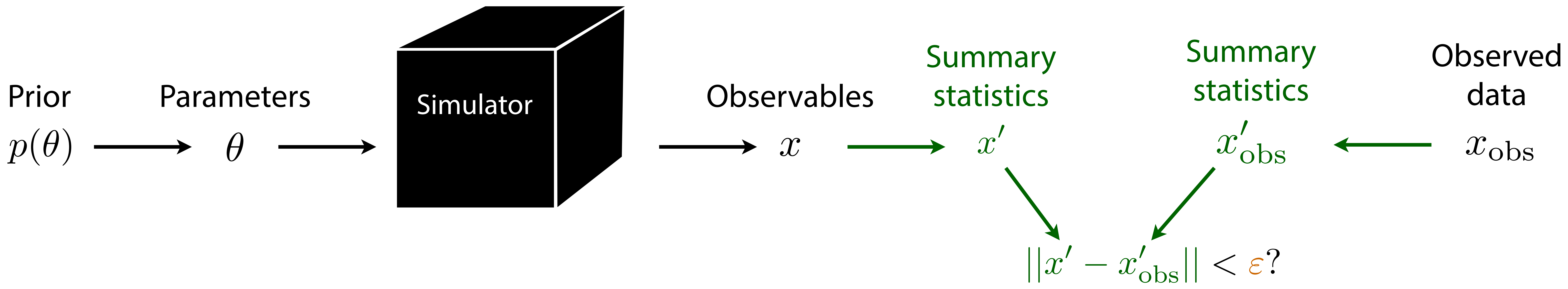

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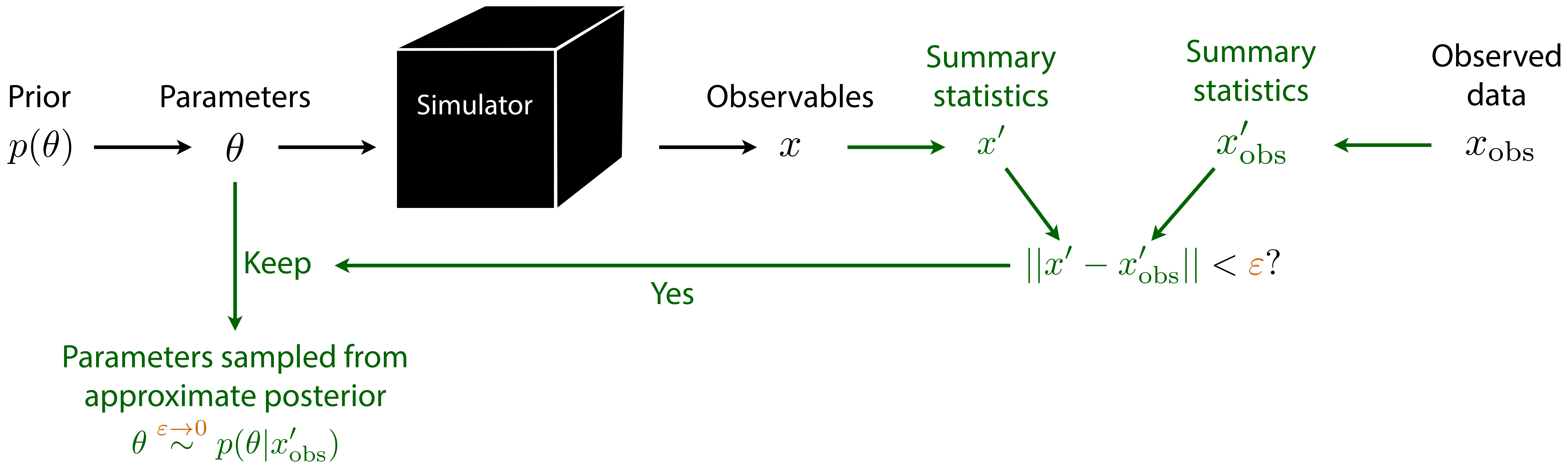

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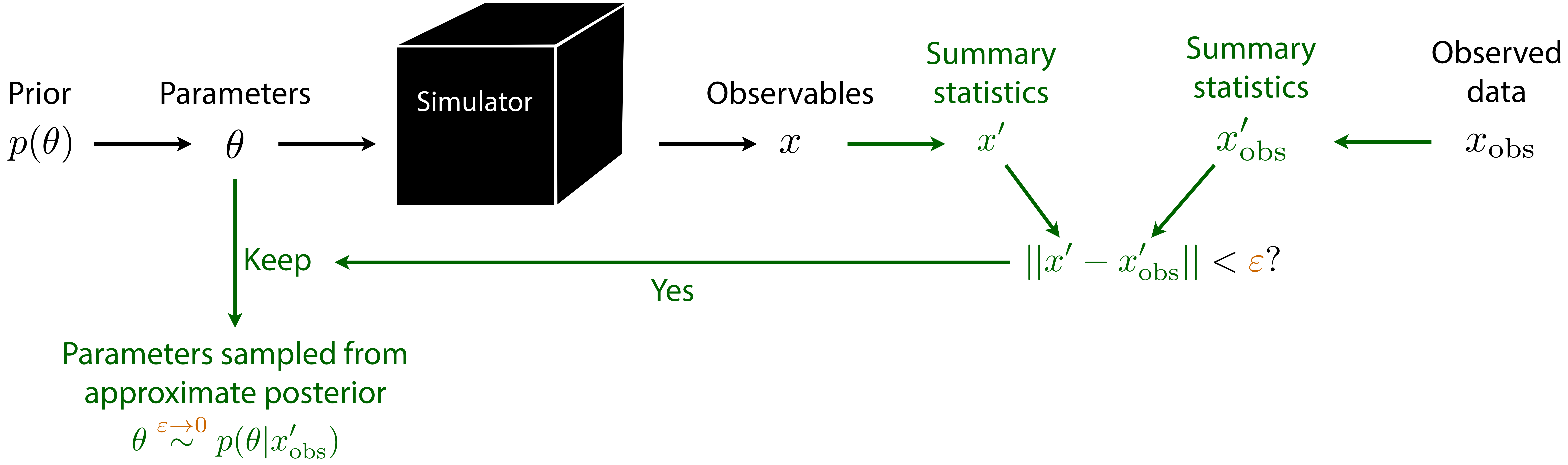


- How to choose x'?
- How to choose ε?
- No tractable posterior
- Need to run new simulations for new data or new prior

"Curse of dimensionality"

Precision vs efficiency tradeoff

Solve it with machine learning classifiers

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

Solve it with machine learning classifiers

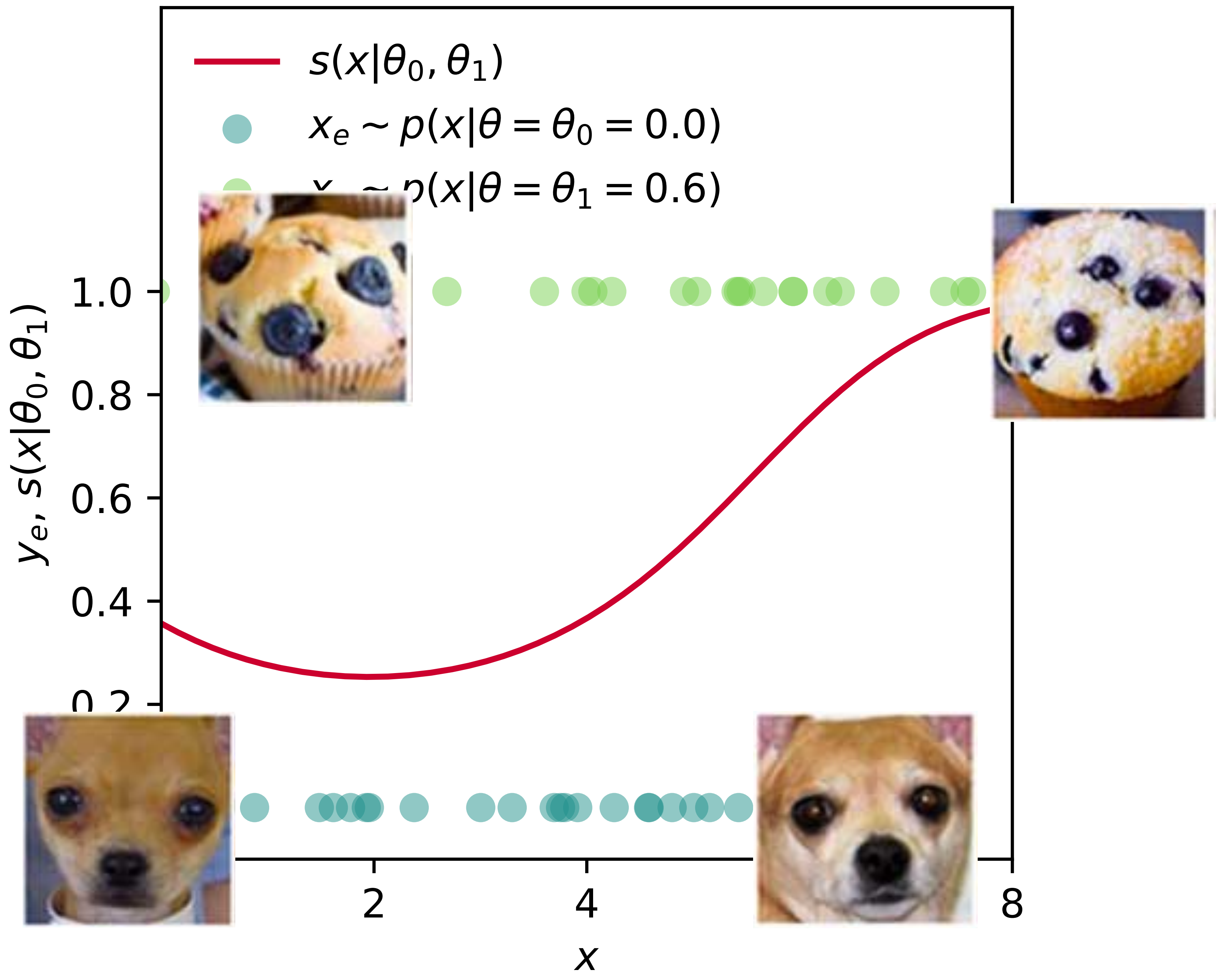
[K. Cranmer, J. Pavez, G. Louppe 1506.02169]

[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)



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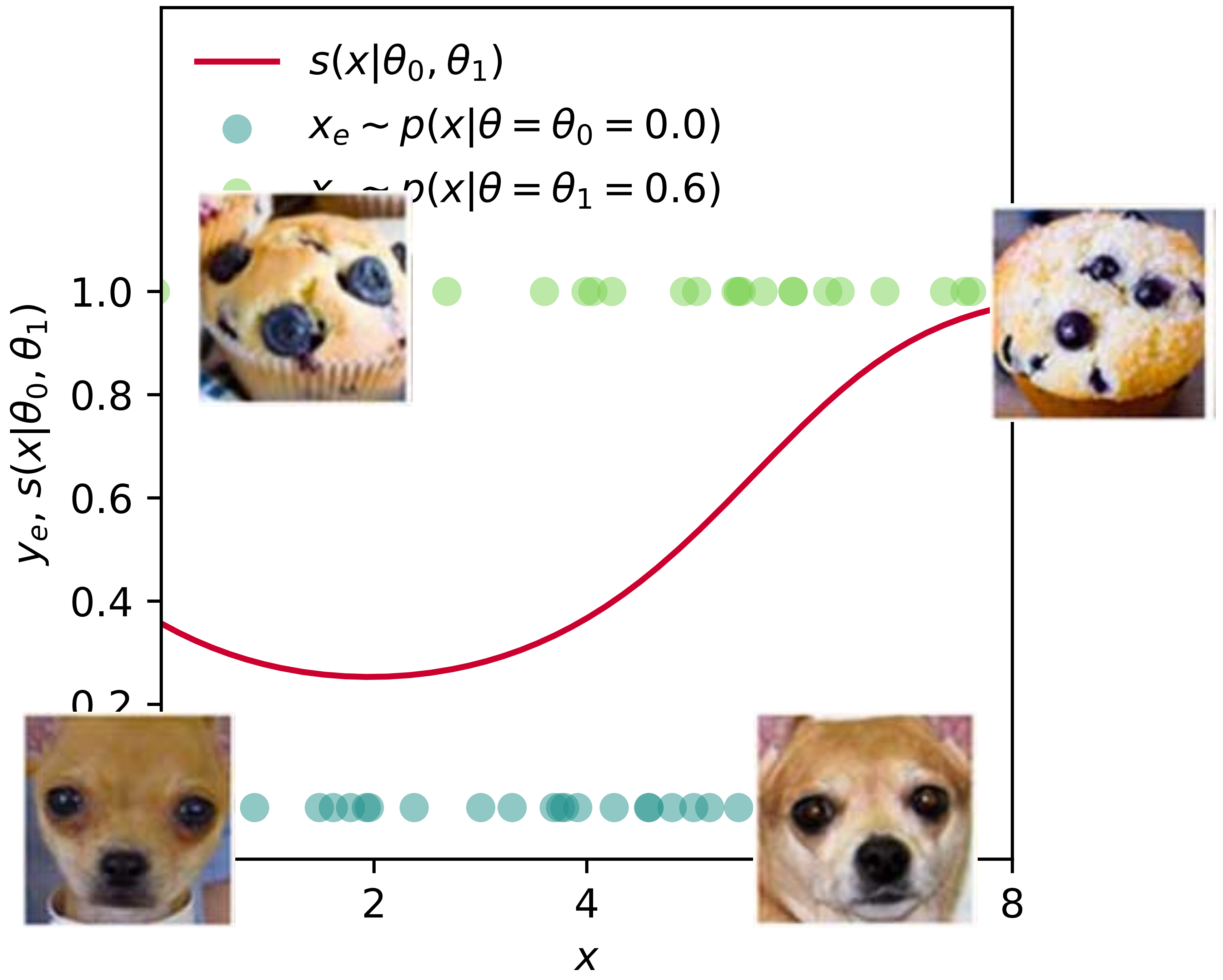


- Optimal classifier (i.e. minimizing the cross-entropy) converges to

$$s(x) = \frac{p(x|\theta_1)}{p(x|\theta_0) + p(x|\theta_1)} = \frac{1}{1 + \frac{p(x|\theta_0)}{p(x|\theta_1)}} \equiv \frac{1}{1 + r(x|\theta)}$$

- CARL: Turn (calibrated) classifier output $\hat{s}(x)$ into estimator for the likelihood ratio $r(x) \equiv p(x|\theta_0)/p(x|\theta_1)$:

$$\hat{r}(x) = \frac{1 - \hat{s}(x)}{\hat{s}(x)}$$

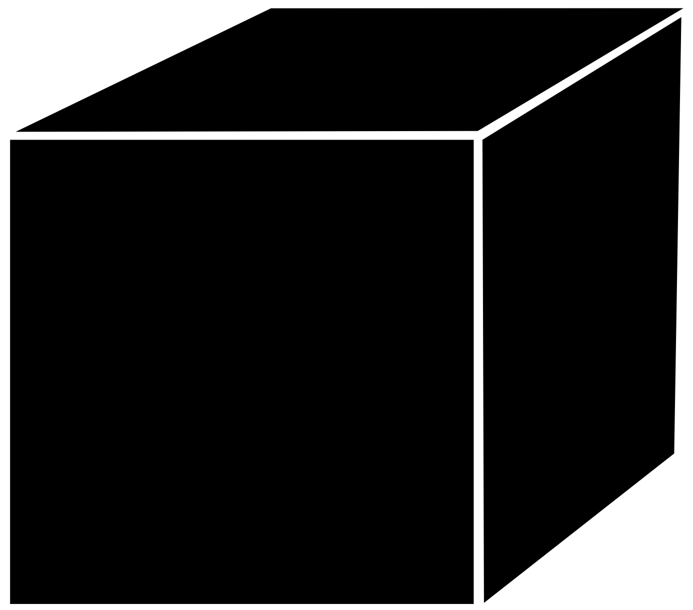
$\Rightarrow$ No summary statistics necessary, very fast evaluation… but may require large training samples

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, …



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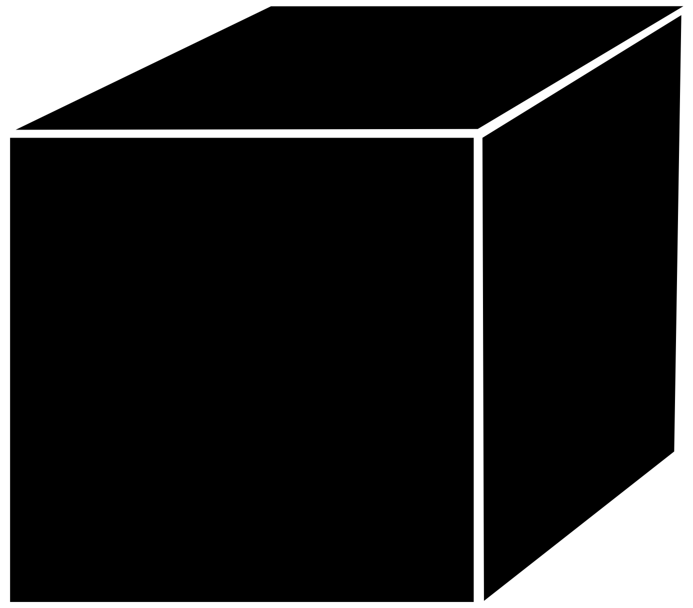
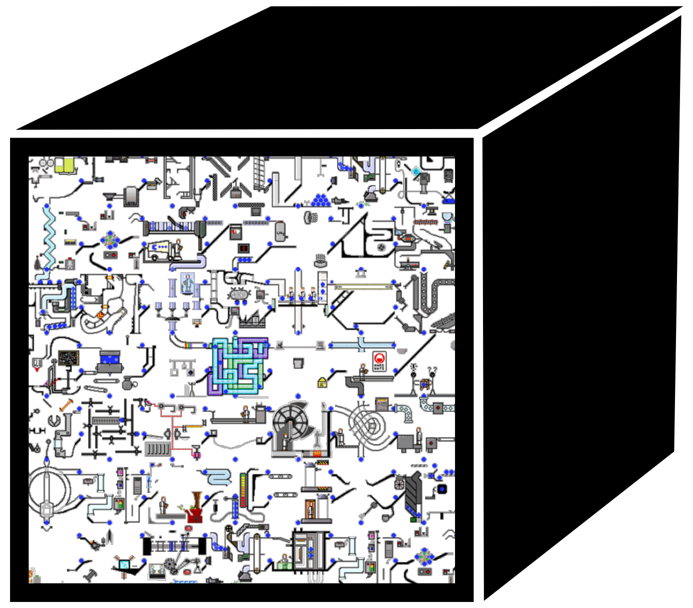


Use latent structure:

- Matrix Element Method, Optimal Observables, Shower Deconstruction, Event Deconstruction
  Specific to particle physics: approximate integrand, explicitly calculate z integral



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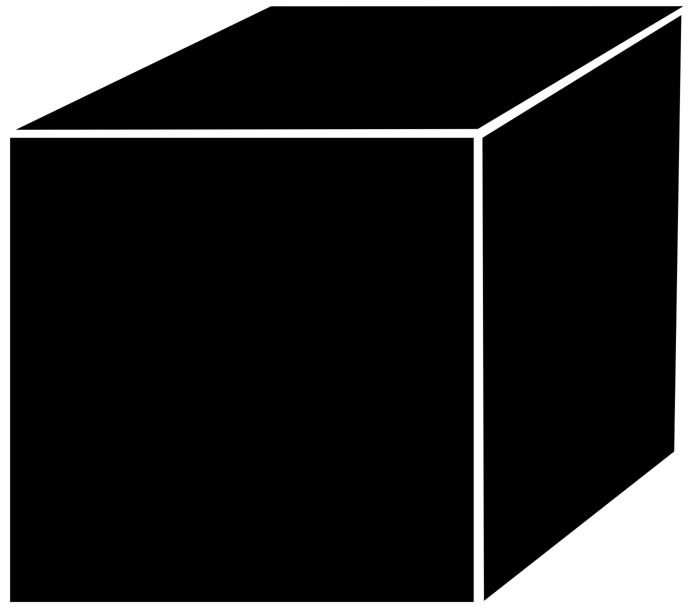

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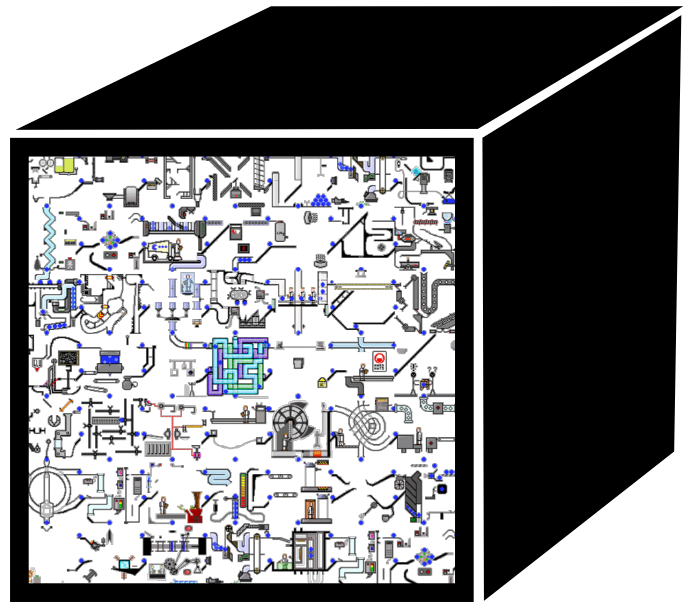
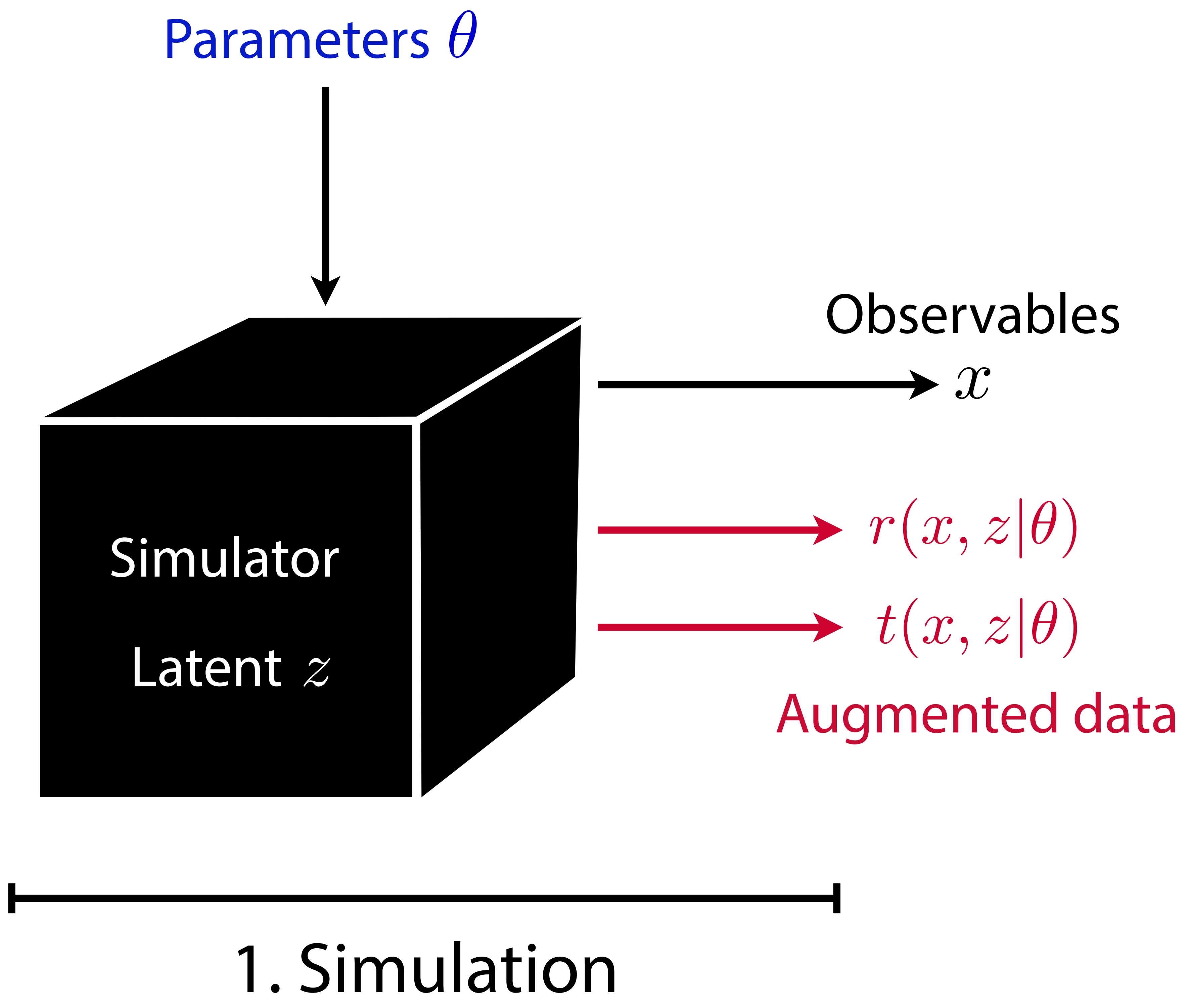
New!

- Mining gold from the simulator
  Leverage physics insight + machine learning



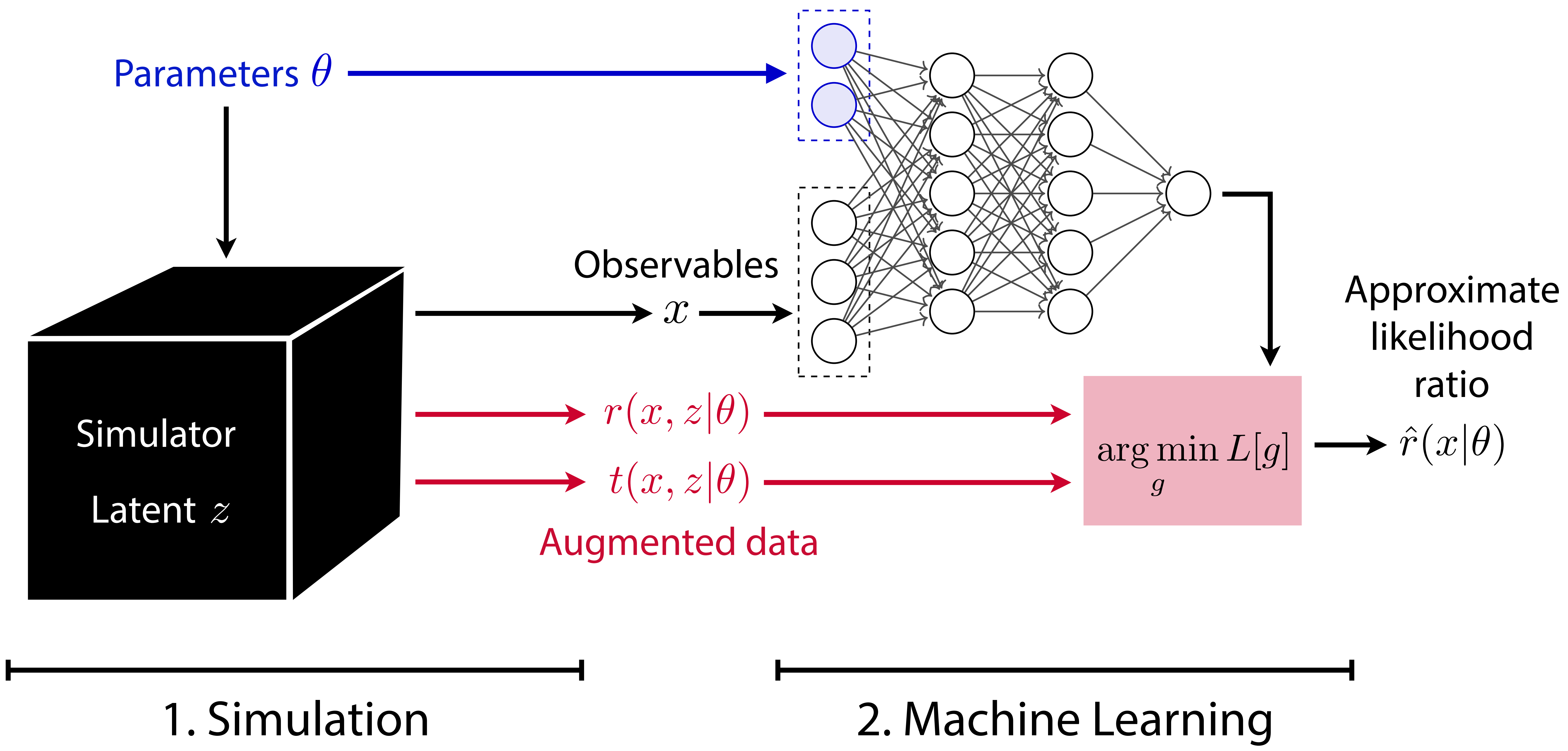
A new approach:
Mining gold from the simulator

Bird's-eye view



"Mining gold": Extract additional information from simulator

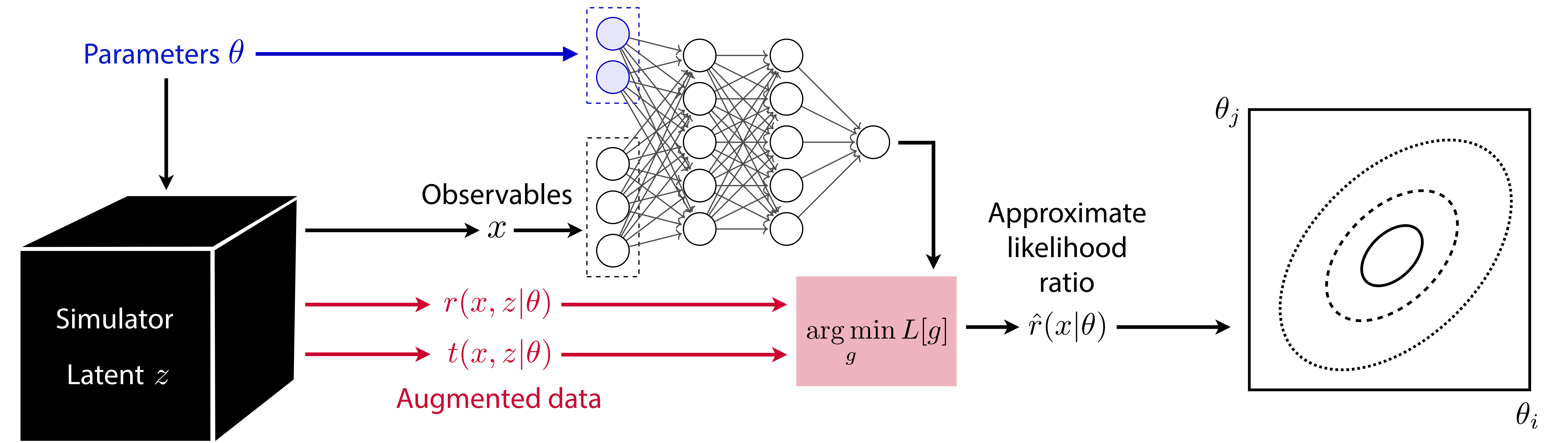
Bird's-eye view



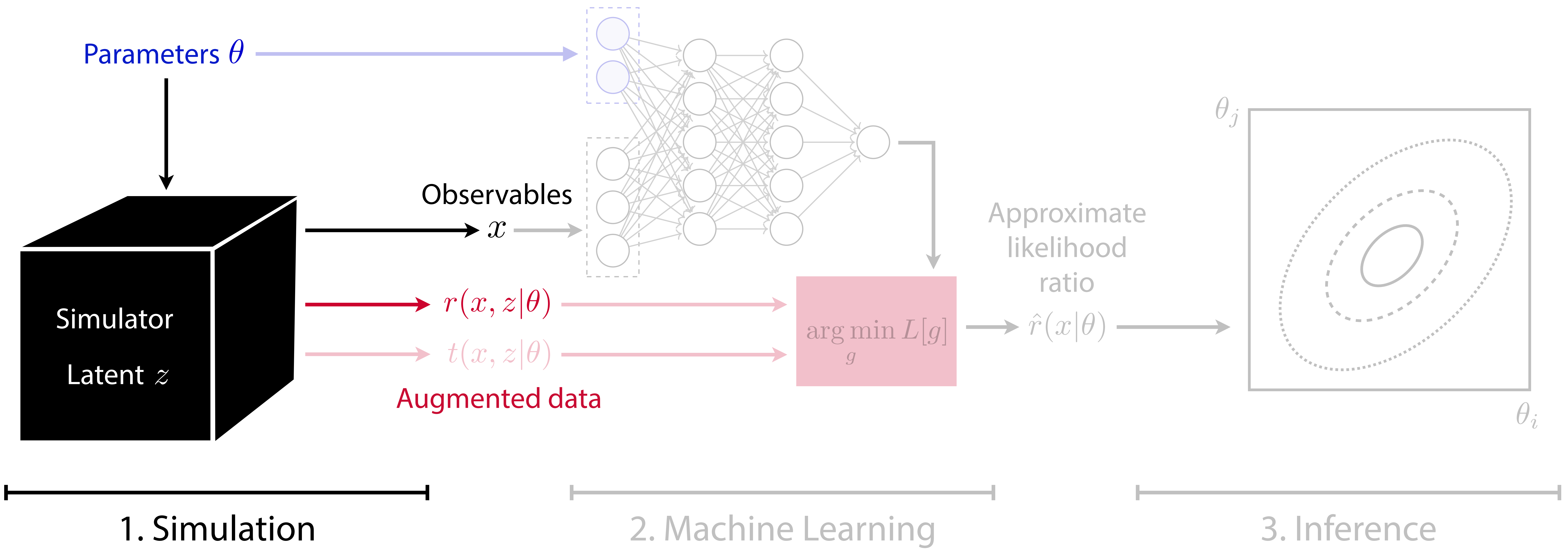
"Mining gold": Extract additional information from simulator

Use this information to train estimator for likelihood ratio

Bird's-eye view

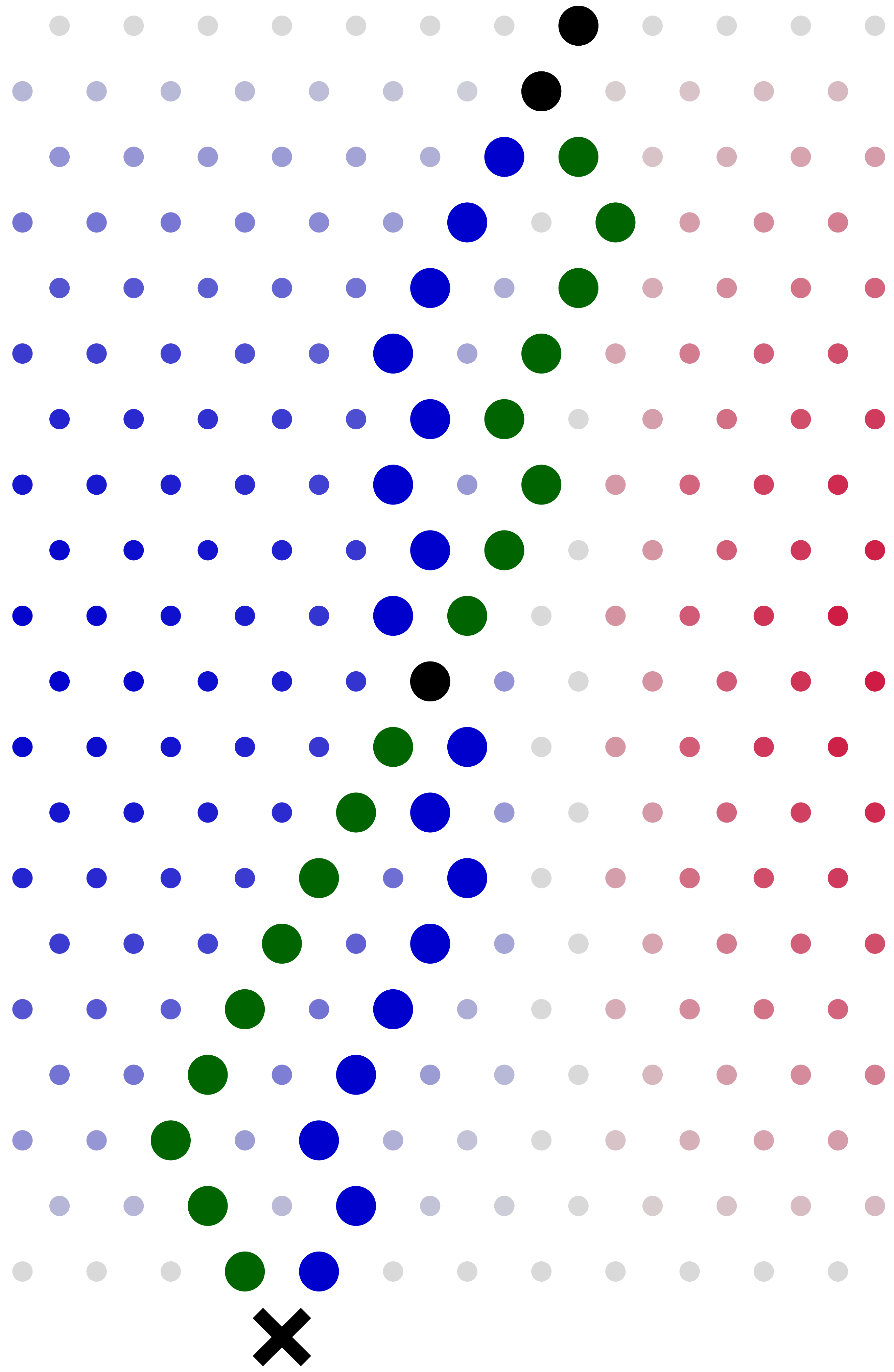


1. Simulation	2. Machine Learning	3. Inference
"Mining gold": Extract additional information from simulator	Use this information to train estimator for likelihood ratio	Limit setting with standard hypothesis tests



Parameters θ
Observables
x
Simulator
Latent z
$r(x, z|\theta)$
$t(x, z|\theta)$
Augmented data
$\arg\min_g L[g]$
Approximate likelihood ratio
$\hat{r}(x|\theta)$
θ_j
θ_i
1. Simulation
2. Machine Learning
3. Inference

Back to the Galton board



- Remember: the likelihood

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

is intractable because of the integral over all possible paths z

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

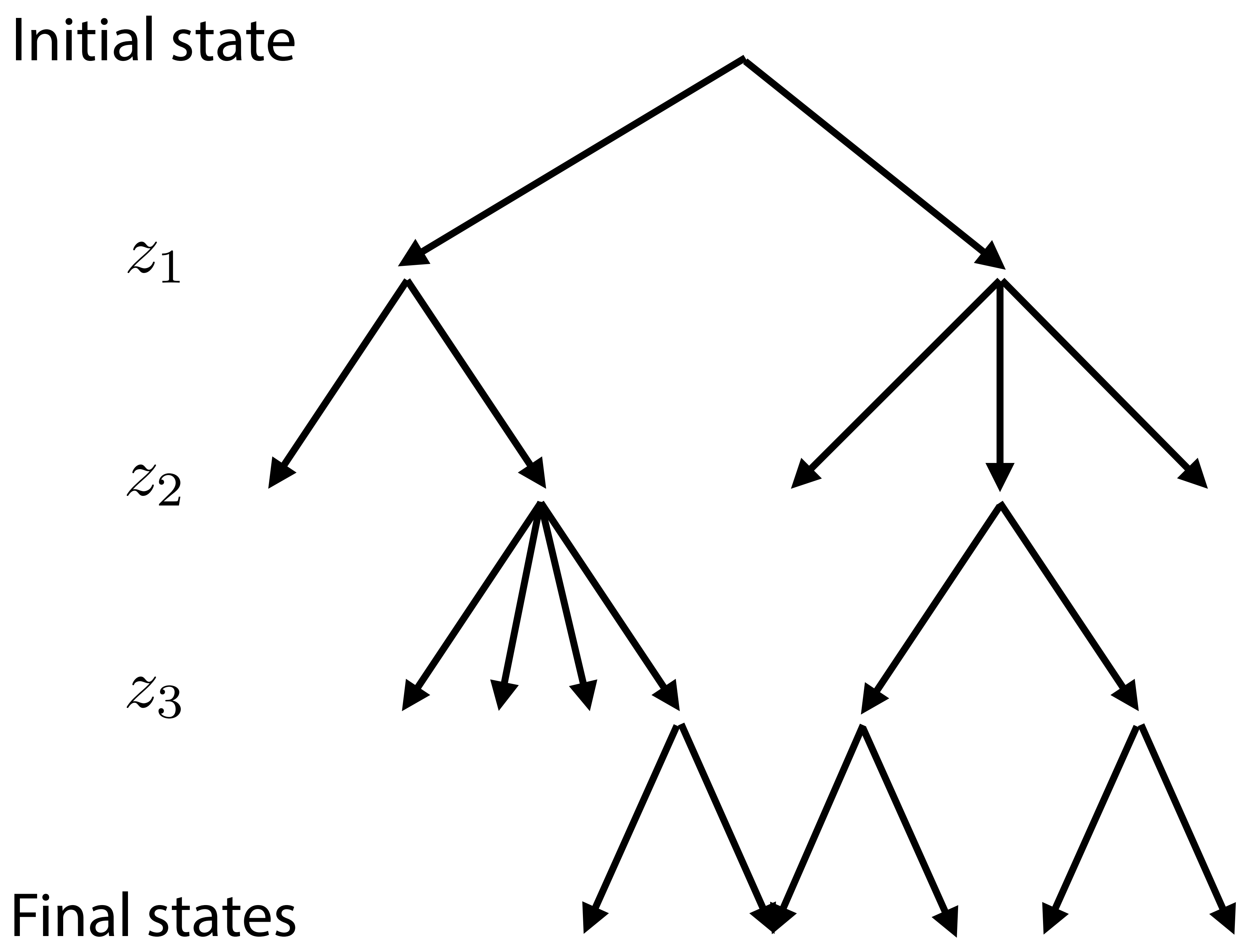
$$p(x, z|\theta) = \prod_{\text{nails } i} p_i(x, z|\theta)$$

and the "joint likelihood ratio" conditional on a particular path

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

Generalizing this idea

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



Generalizing this idea

- 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:
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```

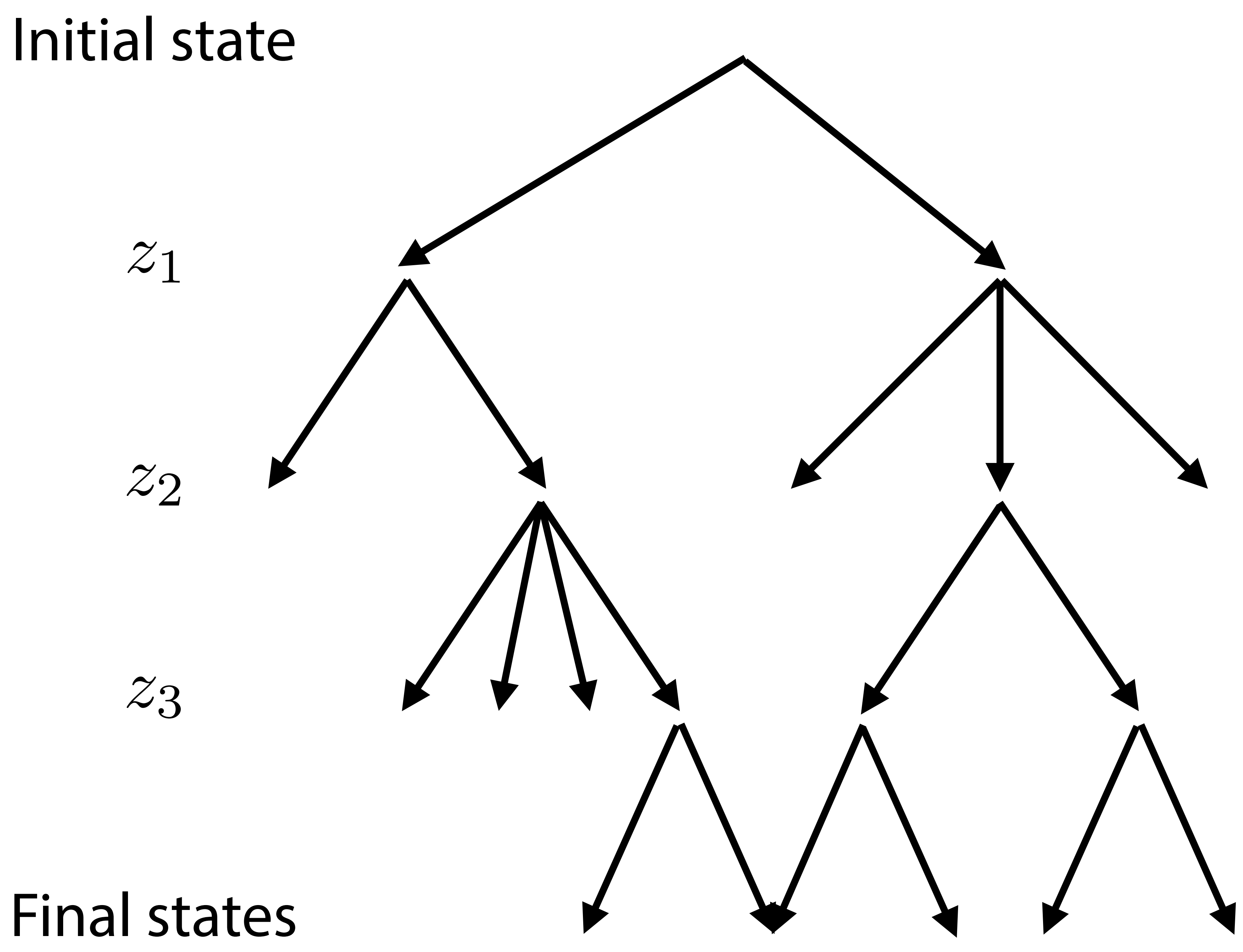

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```
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```
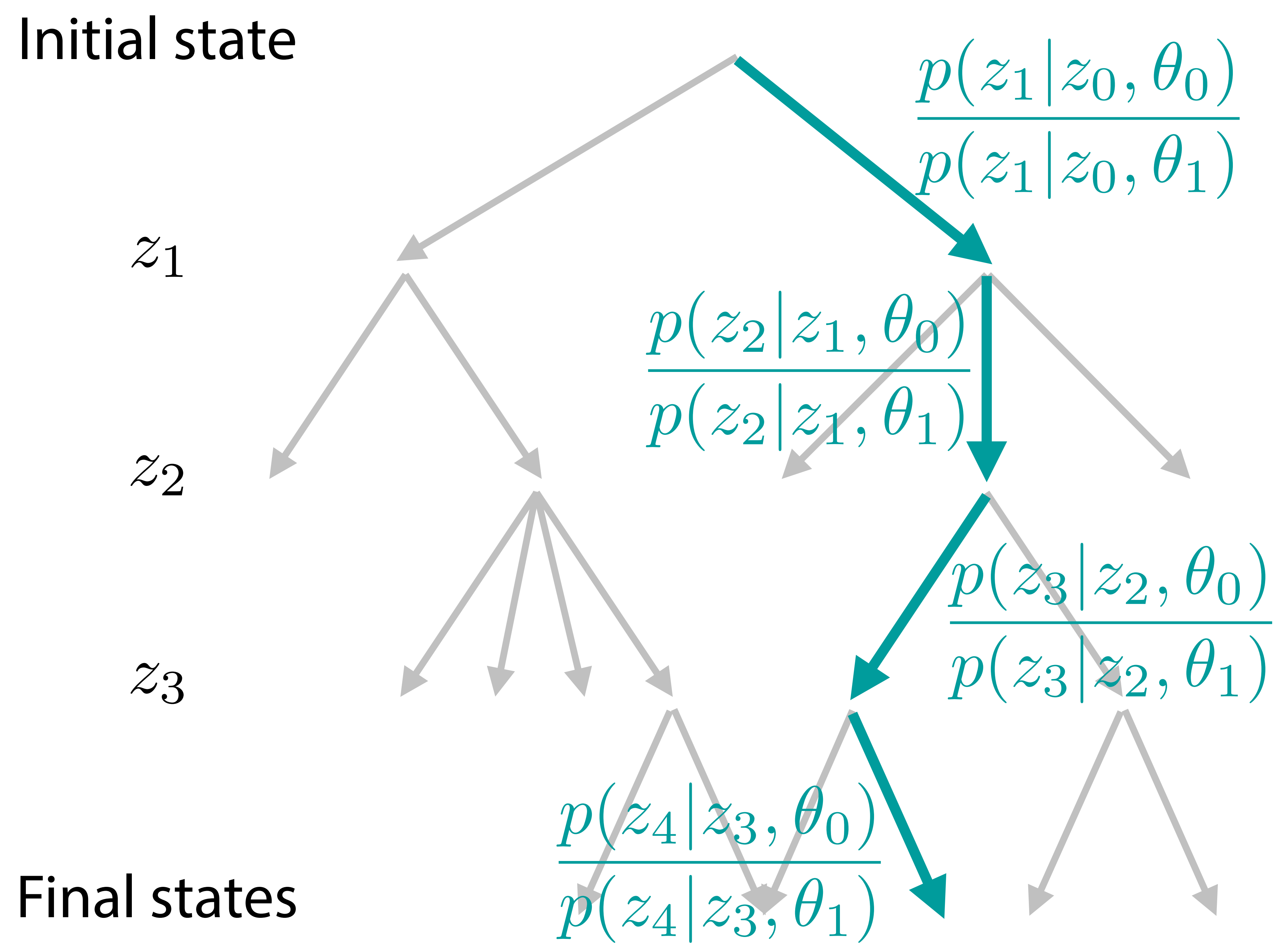
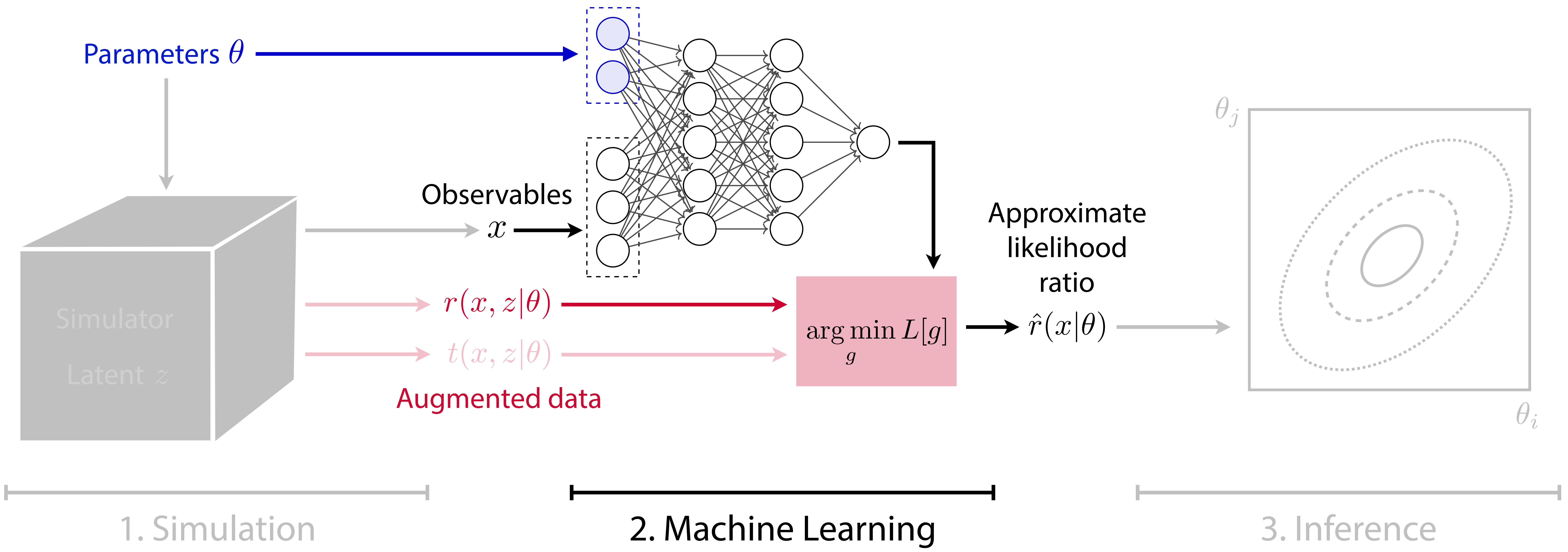

- For each run of the simulator, we can calculate the probability of the chosen path for different values of the parameters, and the "joint likelihood ratio":

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

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Augmented data
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Approximate likelihood ratio
$\hat{r}(x|\theta)$
θ_j
θ_i
1. Simulation
2. Machine Learning
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The value of gold

We can calculate the joint likelihood ratio

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

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

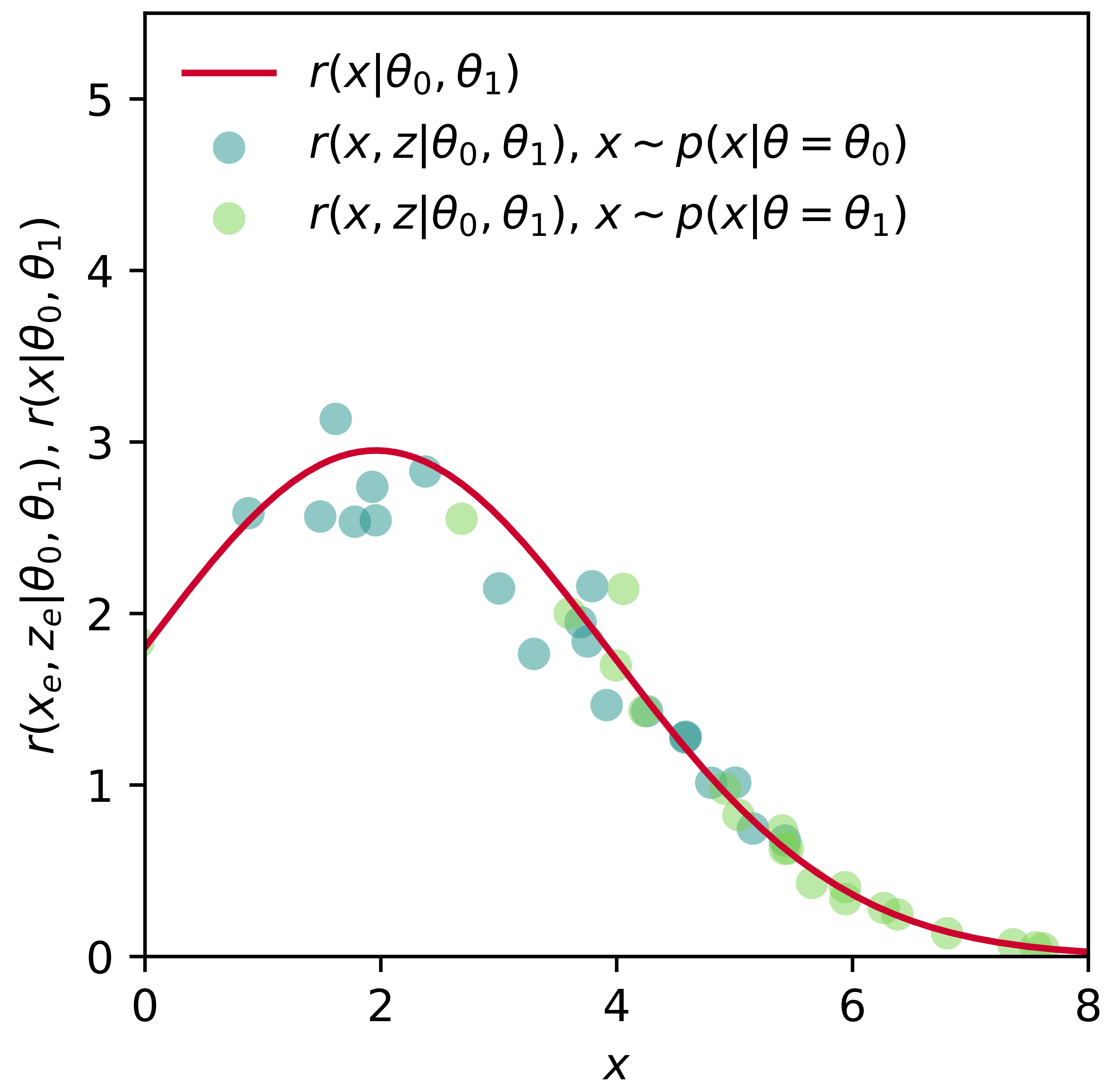
We can calculate the joint likelihood ratio

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

We want the likelihood ratio function

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

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



The value of gold

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

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

$$= \int \mathrm{d}z\; \frac{p(x, z|\theta_1)}{p(x|\theta_1)}\, \frac{p(x, z|\theta_0)}{p(x, z|\theta_1)}$$

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

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

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

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

It is minimized by

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

(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 variatios

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

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

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We do this through machine learning:

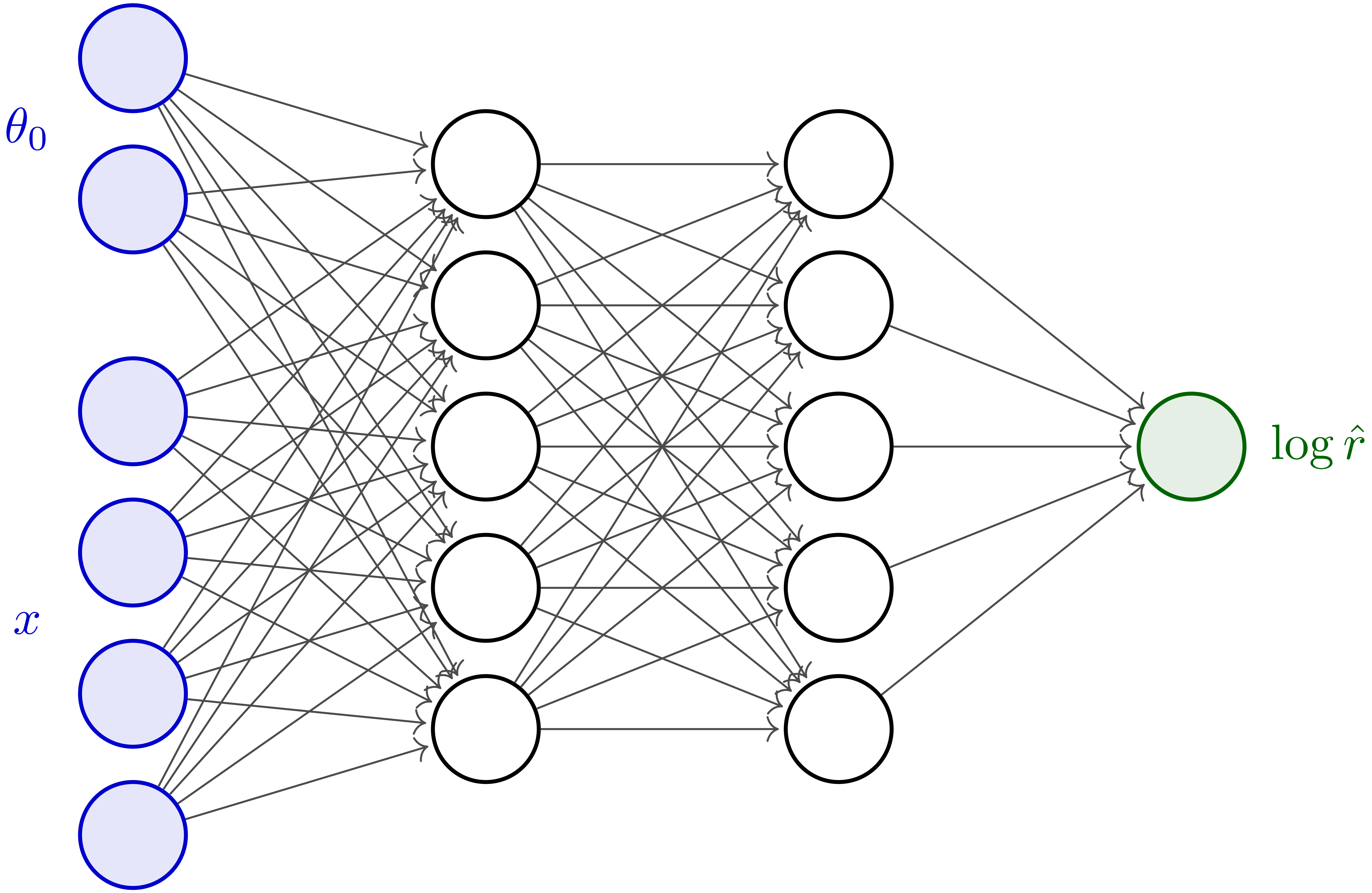
- Functional L_r $\longrightarrow$ Loss function

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

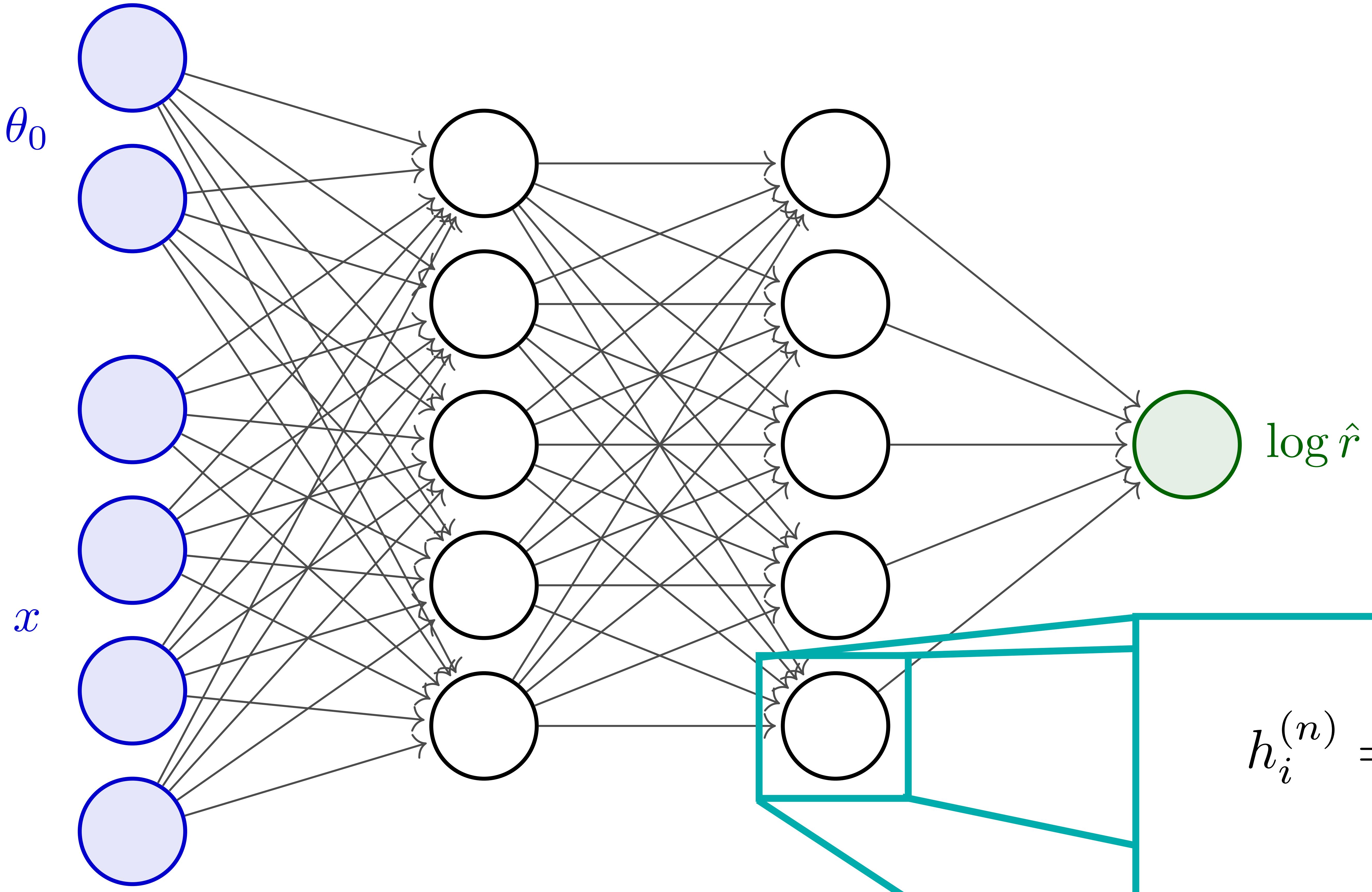
- Variational family $\hat{r}(x|\theta_0,\theta_1)$ $\longrightarrow$ Flexible parametric function (e.g. neural network)
- Exact minimization $\longrightarrow$ Numerical optimization algorithm (e.g. stochastic gradient descent)

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

Neural networks = universal function approximators

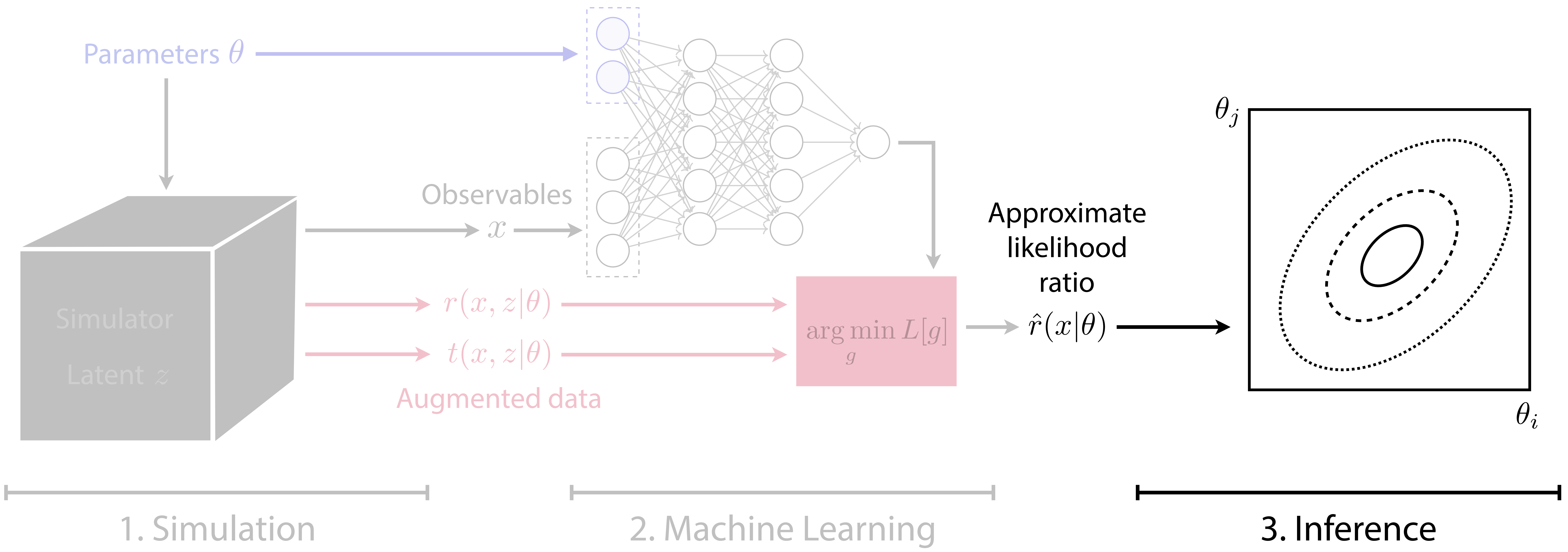


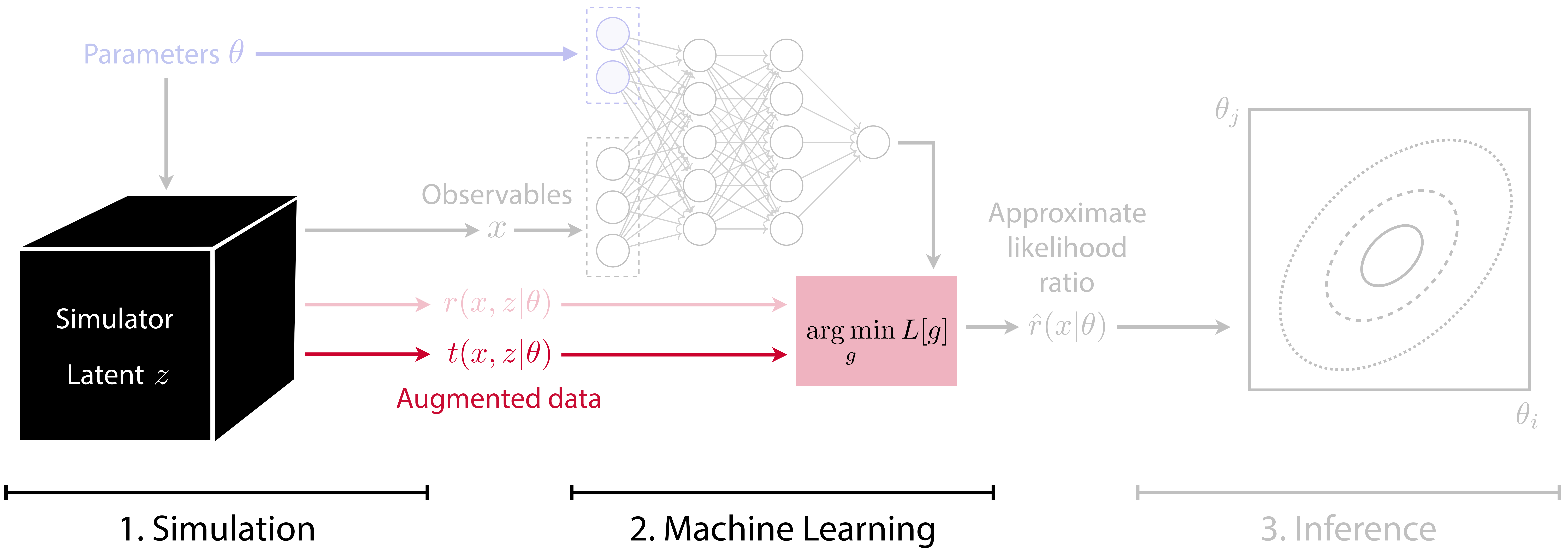
Neural networks = universal function approximators



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

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


Parameters θ
Observables
x
Simulator
Latent z
$r(x, z|\theta)$
$t(x, z|\theta)$
Augmented data
$\arg\min_g L[g]$
Approximate likelihood ratio
$\hat{r}(x|\theta)$
θ_j
θ_i
1. Simulation
2. Machine Learning
3. Inference



Parameters θ
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1. Simulation
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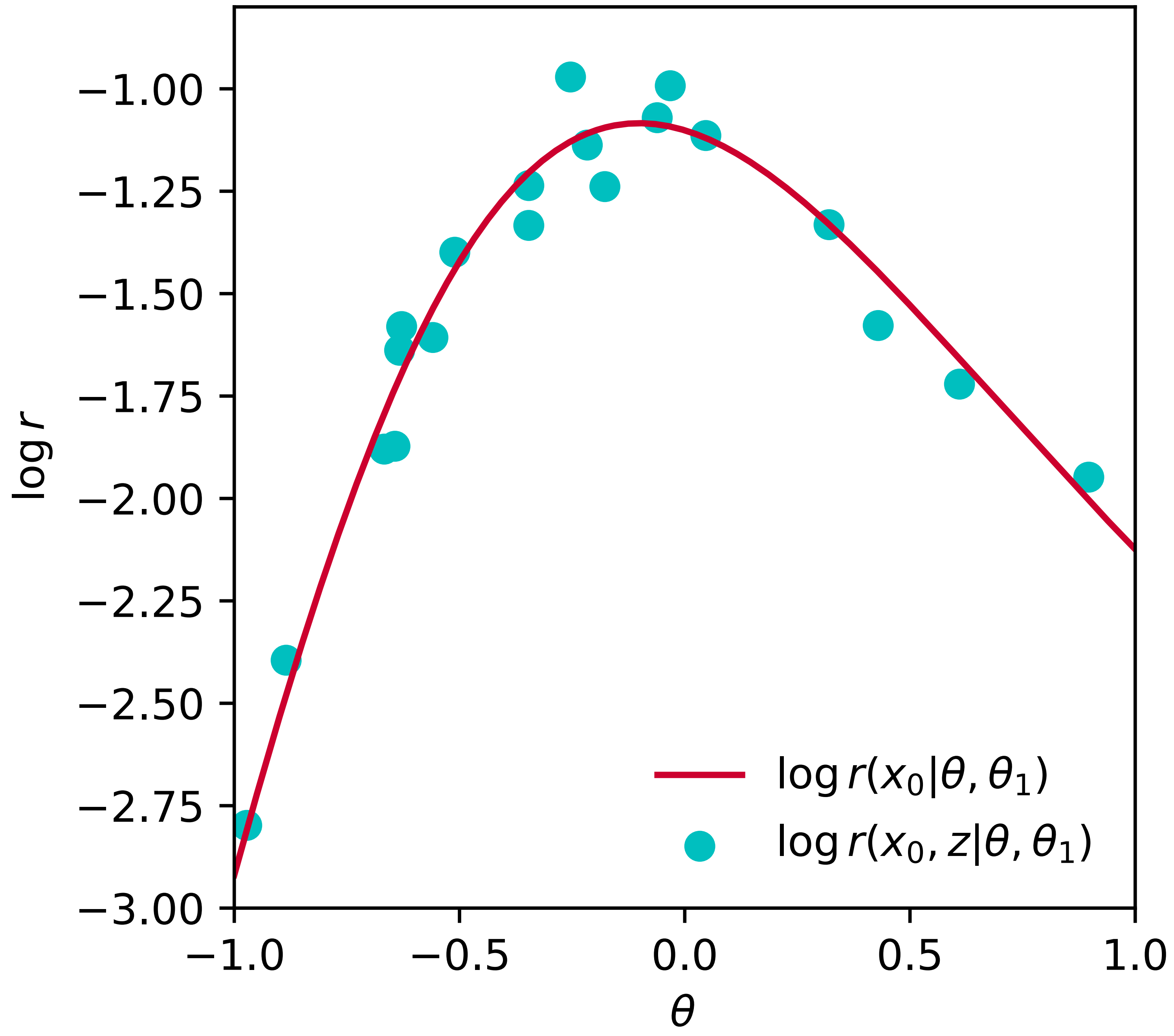
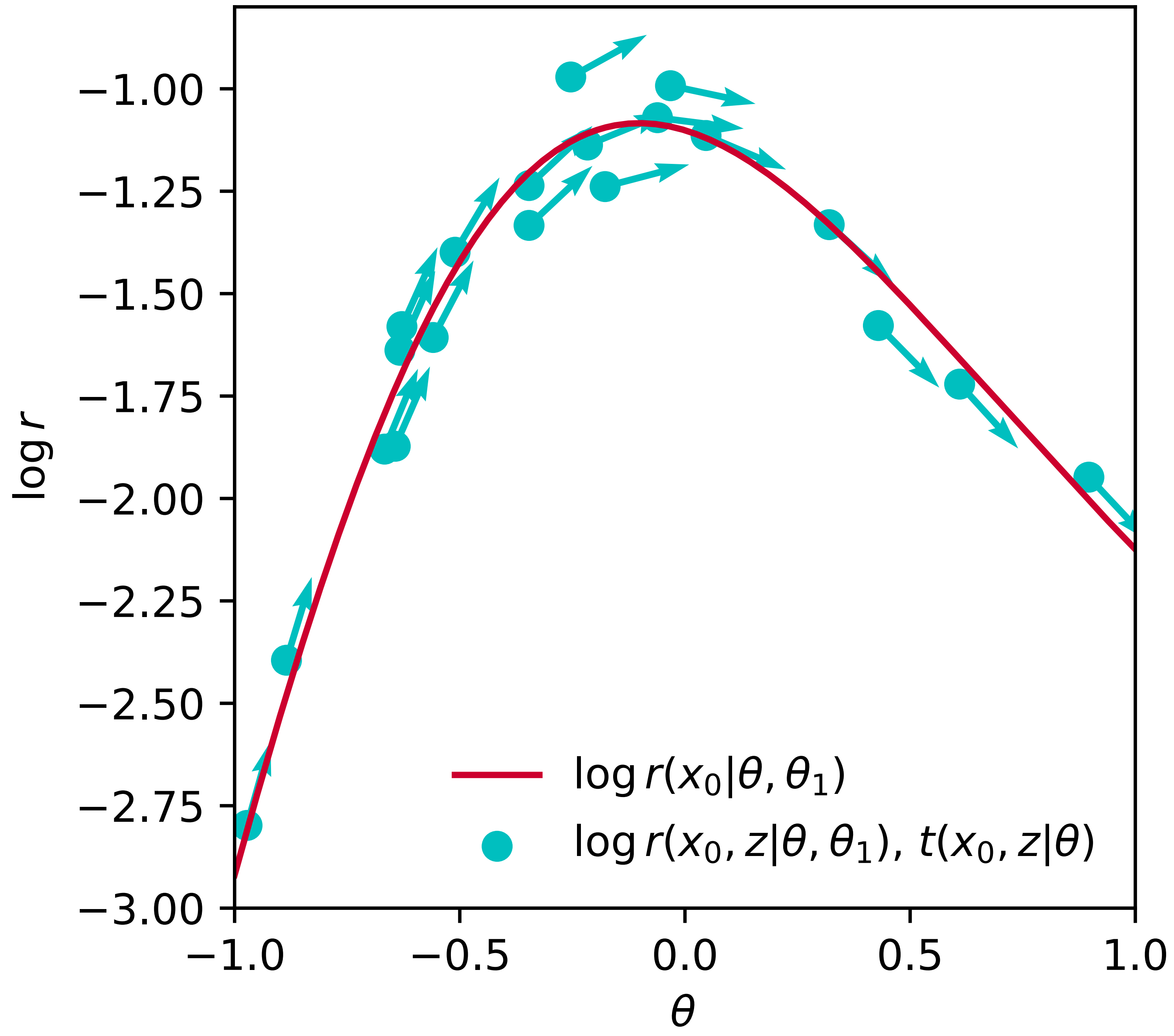
3. Inference

One more piece: the score

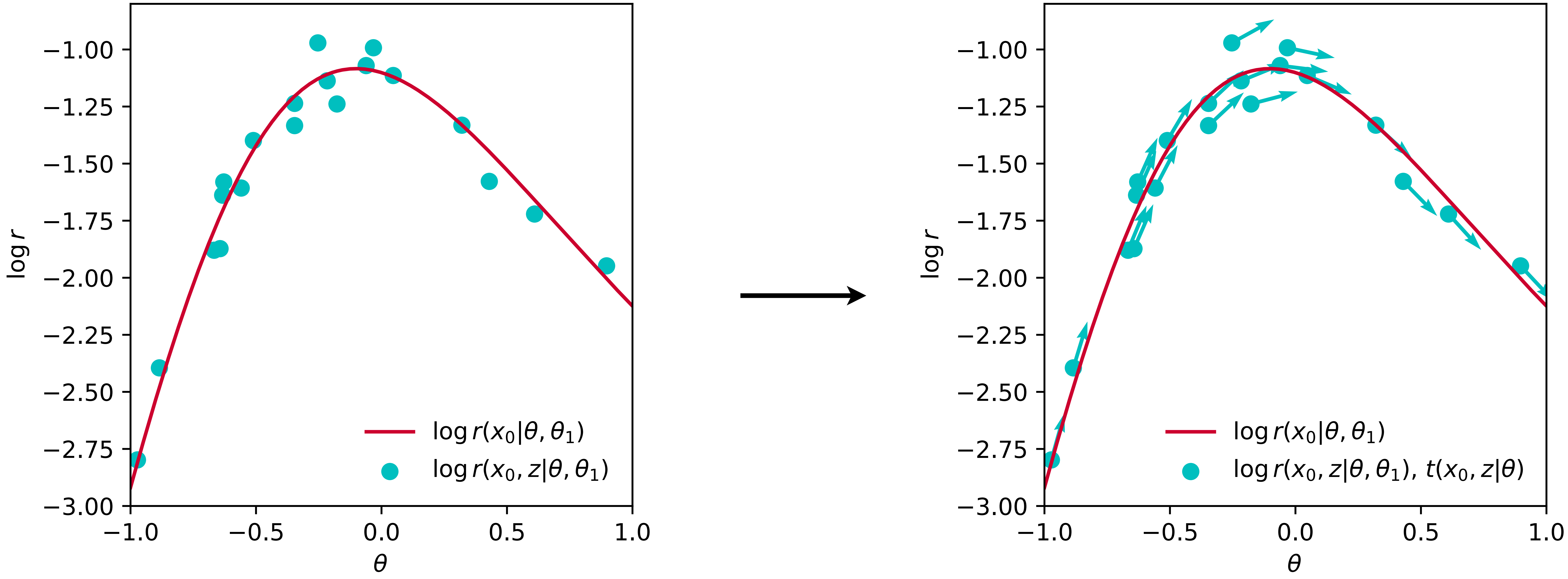
- Knowing derivative often helps fitting:





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 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

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

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

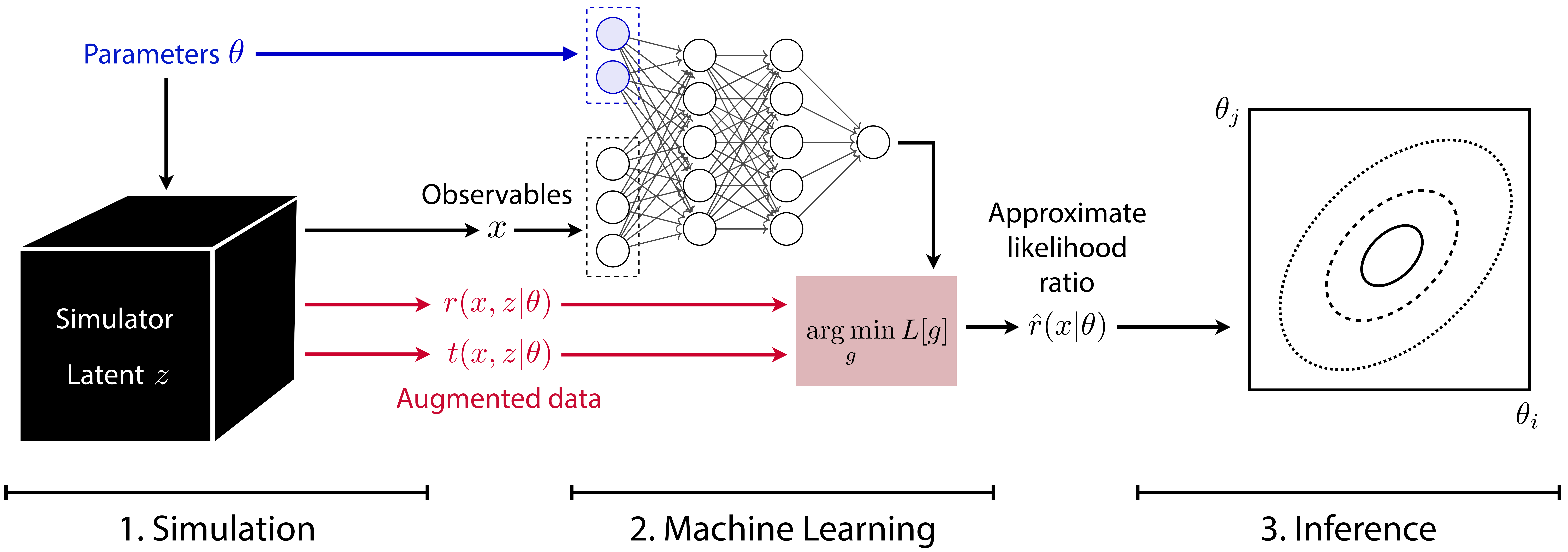
$$L_t[\hat{t}(x|\theta_0)] = \int \mathrm{d}x \int \mathrm{d}z \;\; p(x, z|\theta_0) \, \Big[\Big(\hat{t}(x|\theta_0) - t(x, z|\theta_0)\Big)^2\Big].$$

One can show it is minimized by

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

Again, we implement this minimization through machine learning.

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



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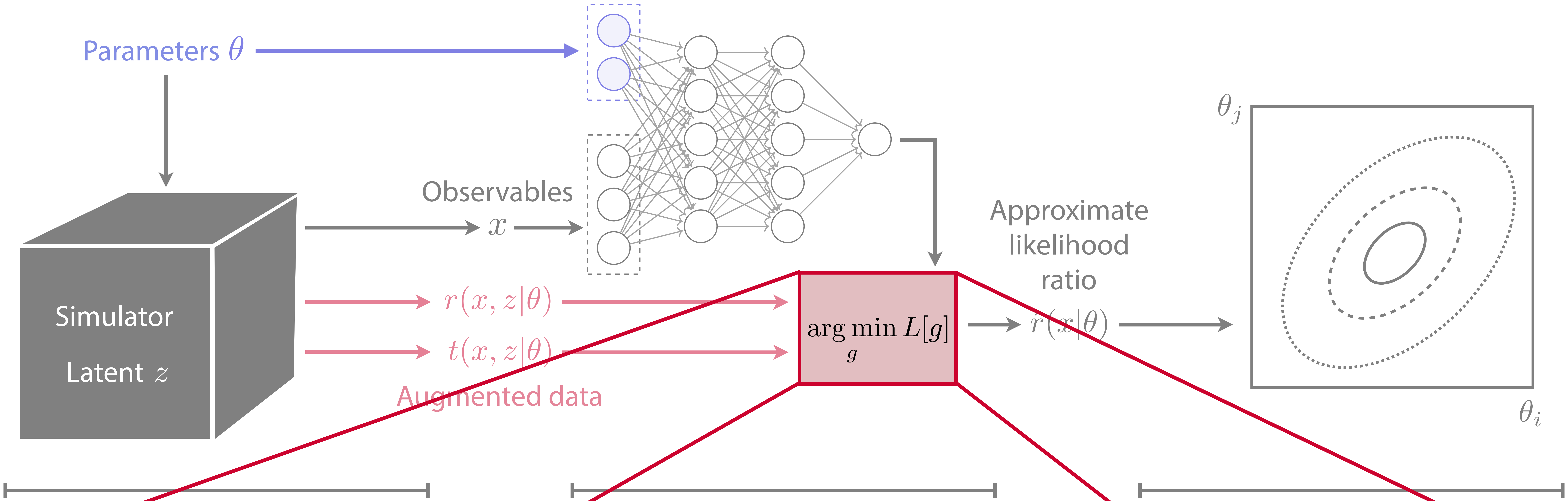
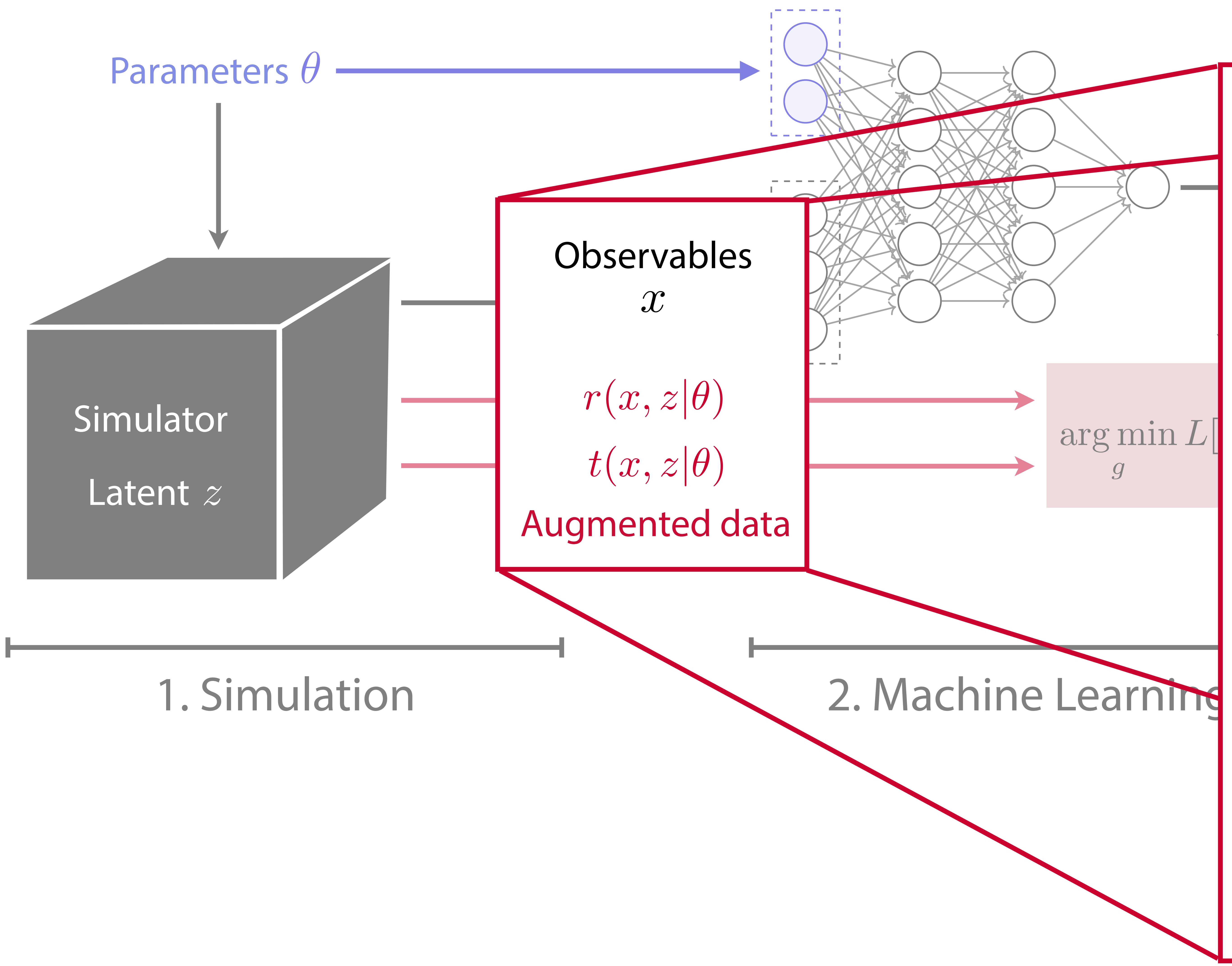


Combining ratio and score information:

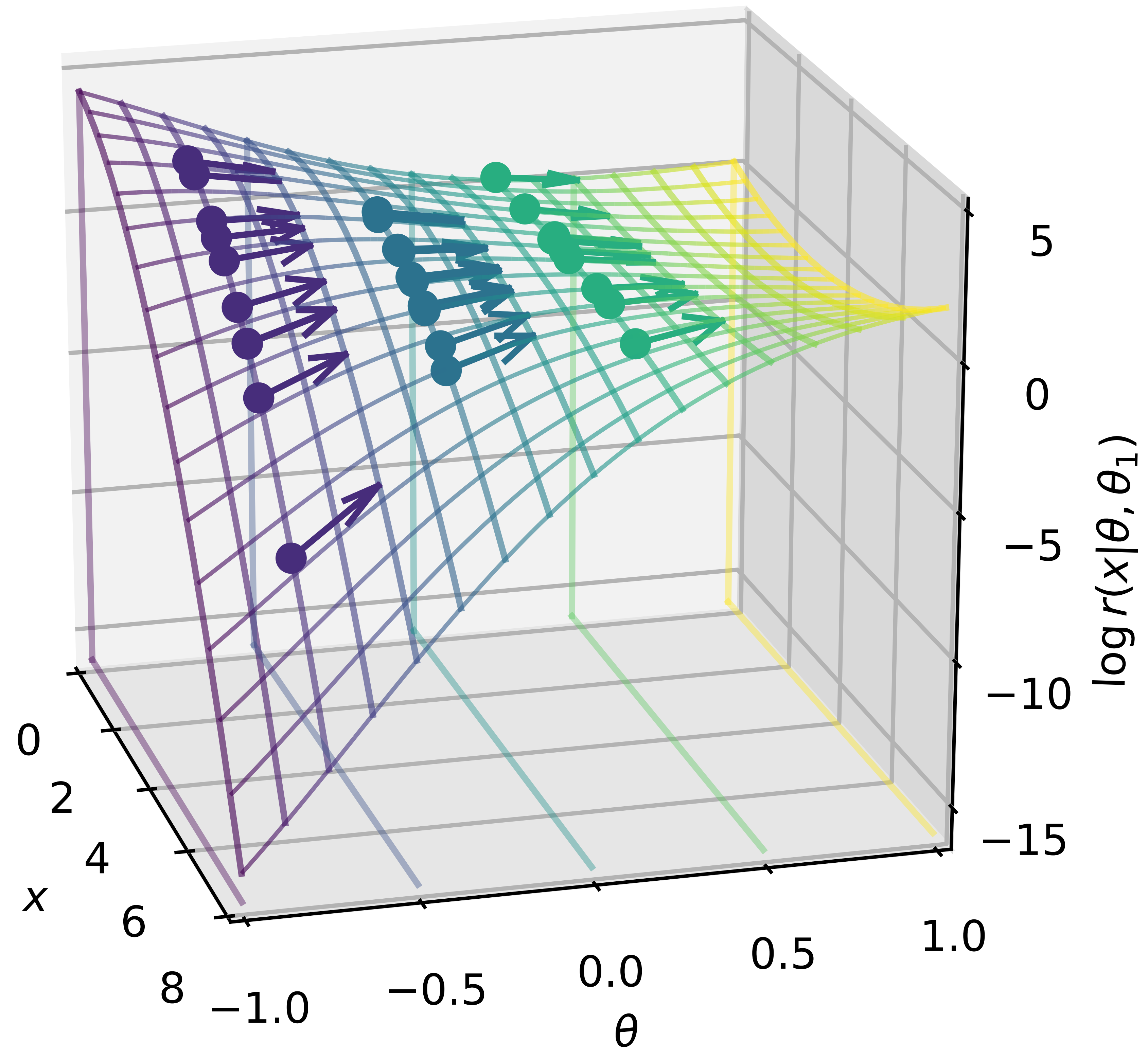
- If ratio estimator is differentiable, we can calculate the estimated score $\hat{t}(x|\theta_0) = \nabla_{\theta_0} \log \hat{r}(x|\theta_0, \theta_1)$
- Minimize combined loss function:

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

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



RASCAL combines three orthogonal pieces of information



A simpler variation:

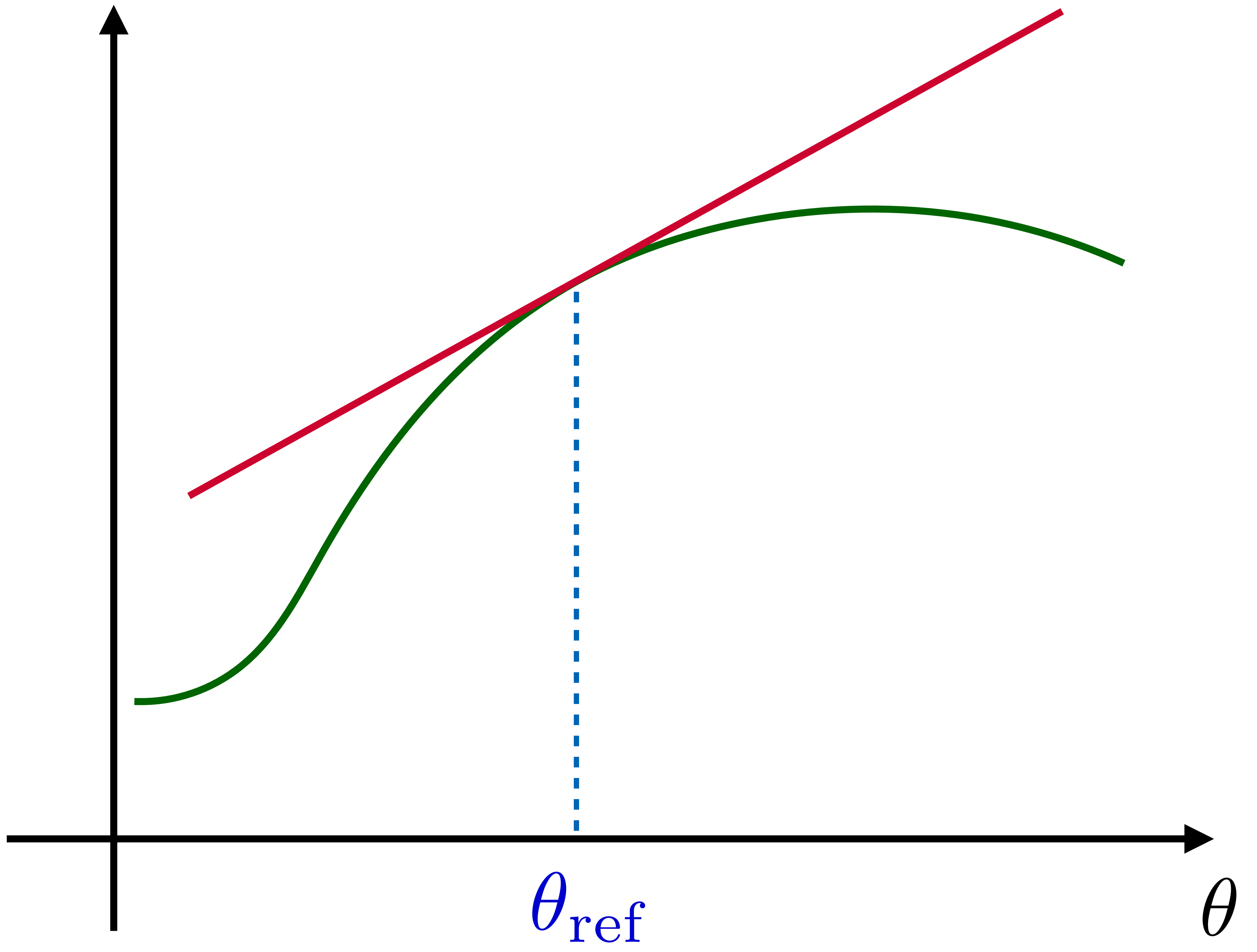
Learning optimal summary statistics

The local model

[see also J. Alsing, B. Wandelt 1712.00012;
J. Alsing, B. Wandelt. S. Freeney 1801.01497]

- Taylor expansion of $\log p(x|\theta)$ around θ_ref:

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



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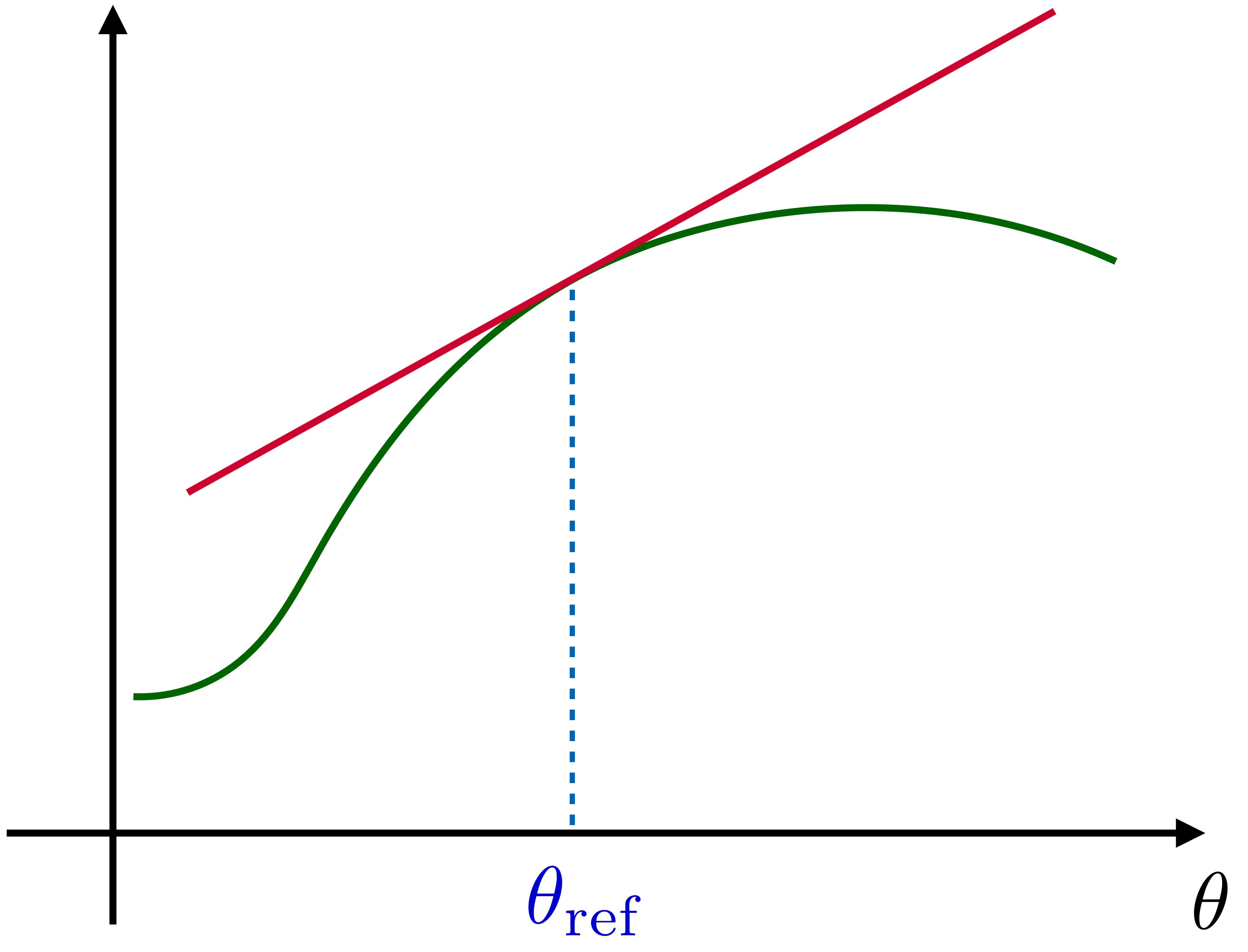
$$\begin{aligned}\log p(x|\theta) = &\log p(x|\theta_{\text{ref}}) \\ &+ \underbrace{\nabla_\theta \log p(x|\theta)\Big|_{\theta_{\text{ref}}}}_{\equiv t(x|\theta_{\text{ref}})} \cdot (\theta - \theta_{\text{ref}}) \\ &+ \mathcal{O}\left((\theta - \theta_{\text{ref}})^2\right)\end{aligned}$$

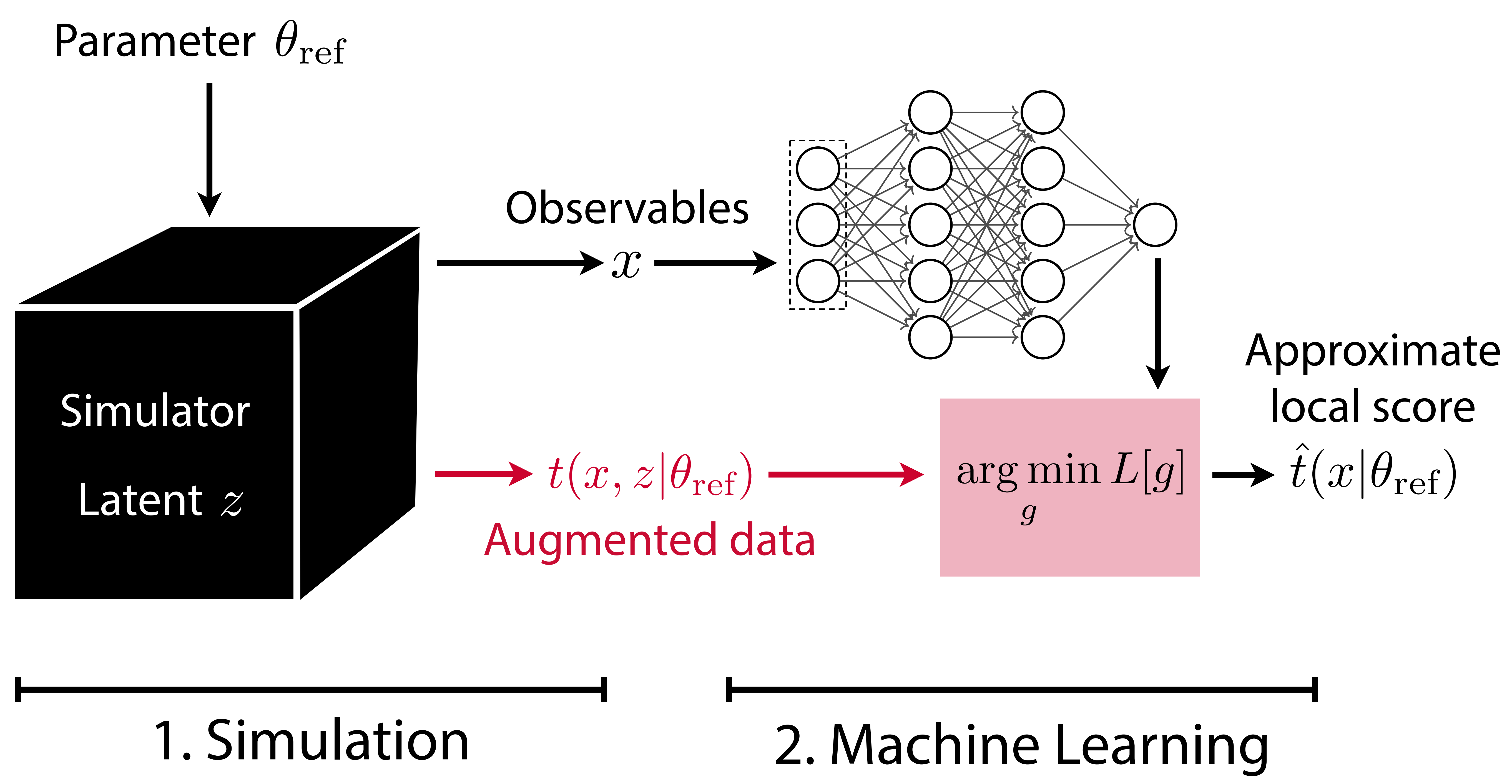


⇒ In the neighborhood of θ_{ref} (e.g. close to the SM), the score vector $t(x|\theta_{\text{ref}})$ is the sufficient statistics: it contains all information on θ

In this part of parameter space, knowing $t(x|\theta_{\text{ref}})$ is just as powerful as knowing the full function $\log p(x|\theta)$

$t(x|\theta_{\text{ref}})$ does not depend on θ — it's (locally) the most powerful observable

SALLY (Score approximates likelihood locally)



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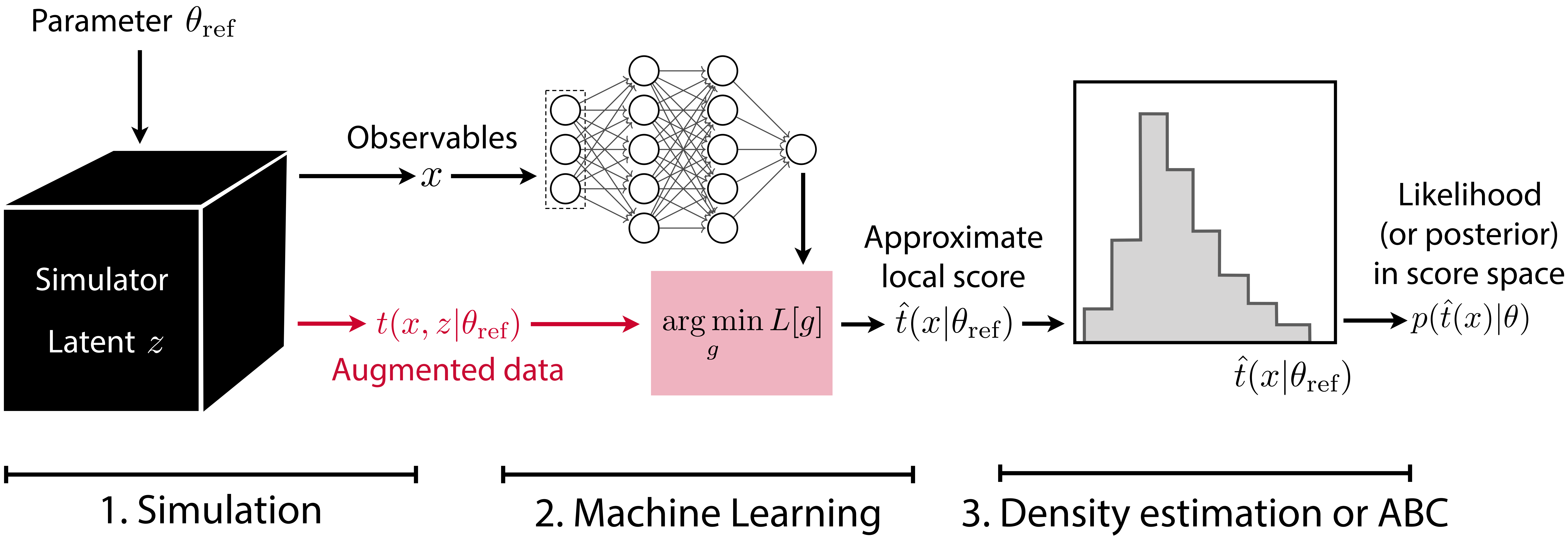

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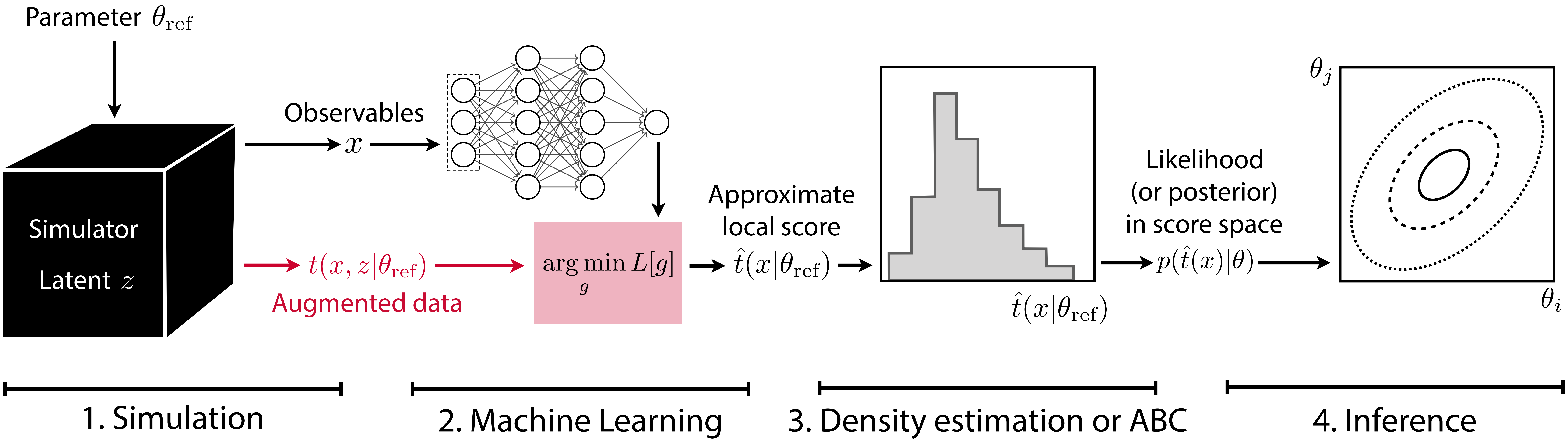

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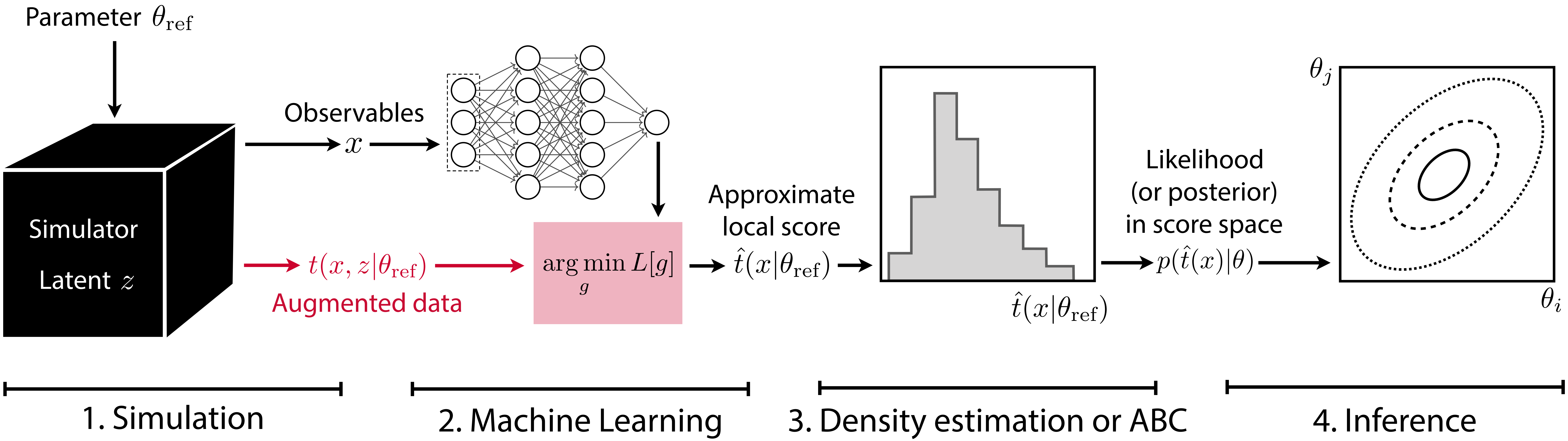

"The machine learning version of Optimal Observables":

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

A family of new inference techniques

Method	Simulate	Extract $r(x,z)$	Extract $t(x,z)$	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.	

Particle physics example

The legacy of the LHC

- LHC: so far, not so good at discovering unexpected new particles…
  but great at making Higgs bosons!

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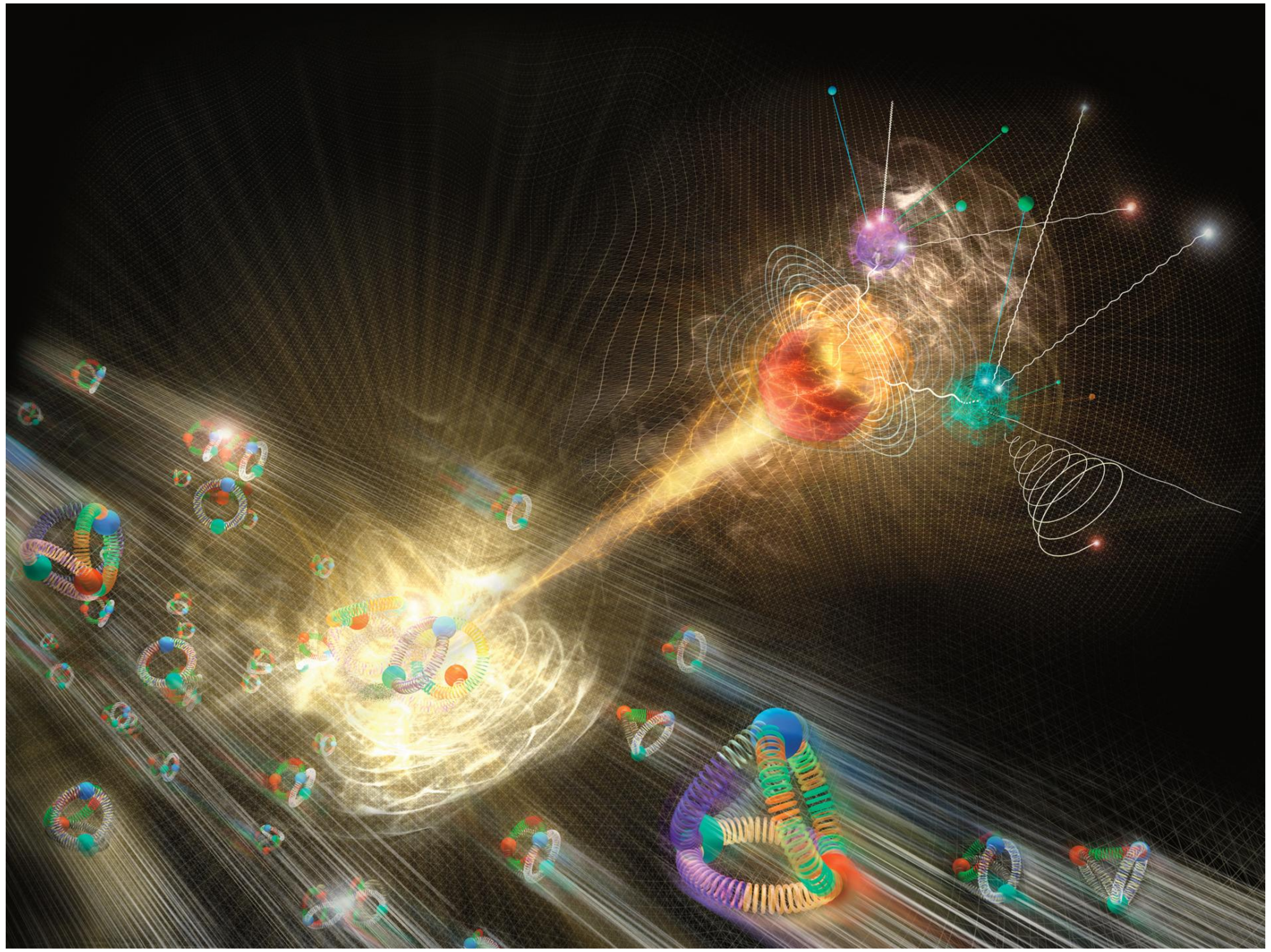

[National Geographic]

The legacy of the LHC

- LHC: so far, not so good at discovering unexpected new particles…
  but great at making Higgs bosons!

- Precision measurements of Higgs properties & electroweak interactions ~~might~~ will help us understand…
  - the hierarchy problem (why is gravity so weak?)
  - fermion masses (why is the electron so light?)
  - matter dominance (why are we?)
  - vacuum stability (why is anything like it is?)

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  - vacuum stability (why is anything like it is?)

- These measurements are difficult!
  - Many parameters
  - Many observables
  - Subtle kinematic effects
  - Intractable likelihood

Particle physics processes

Theory parameters
θ

Evolution

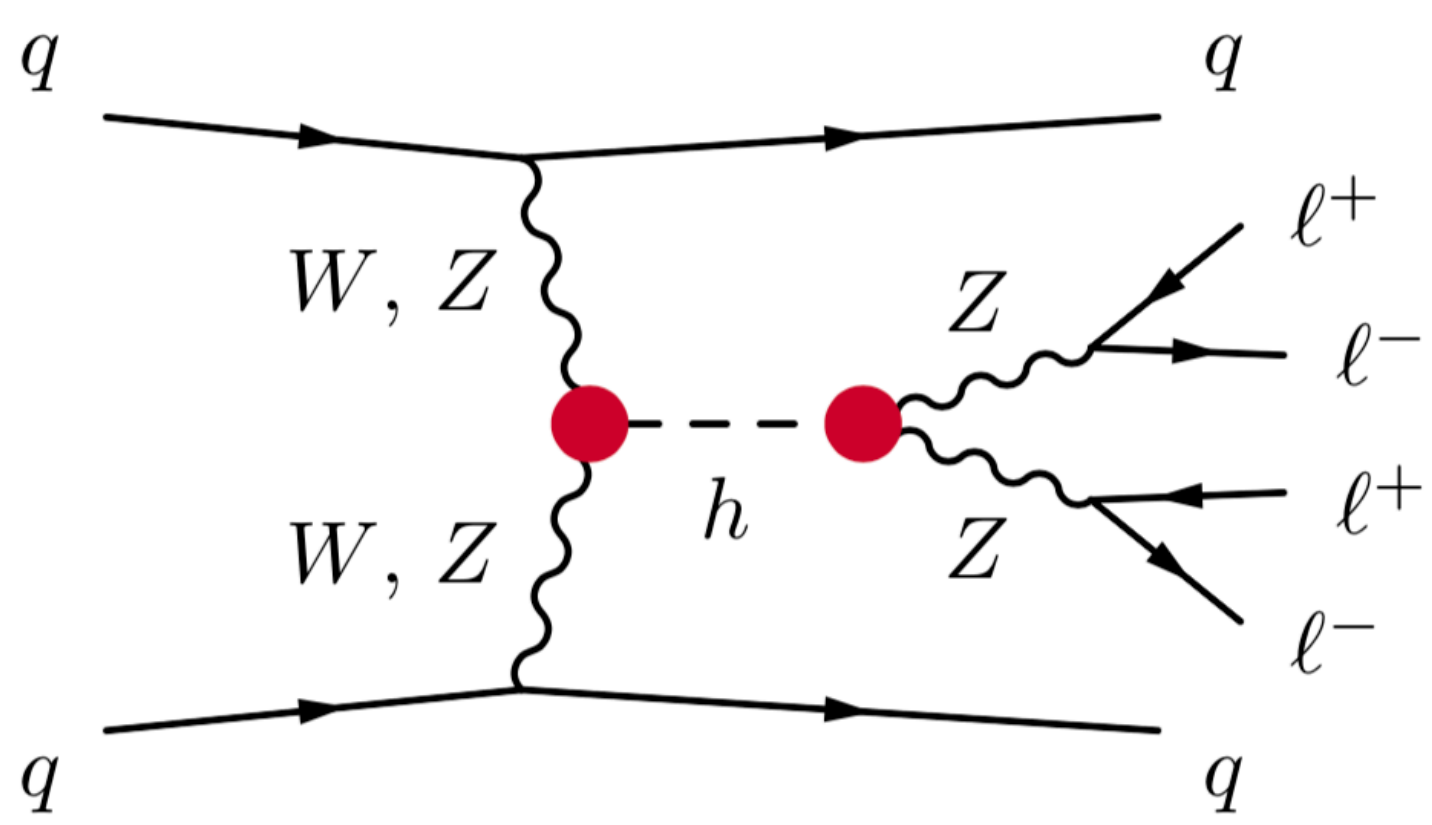
Particle physics processes

Latent variables

Parton-level momenta

Theory parameters

$$z_p \longleftarrow \theta$$



Evolution

Particle physics processes

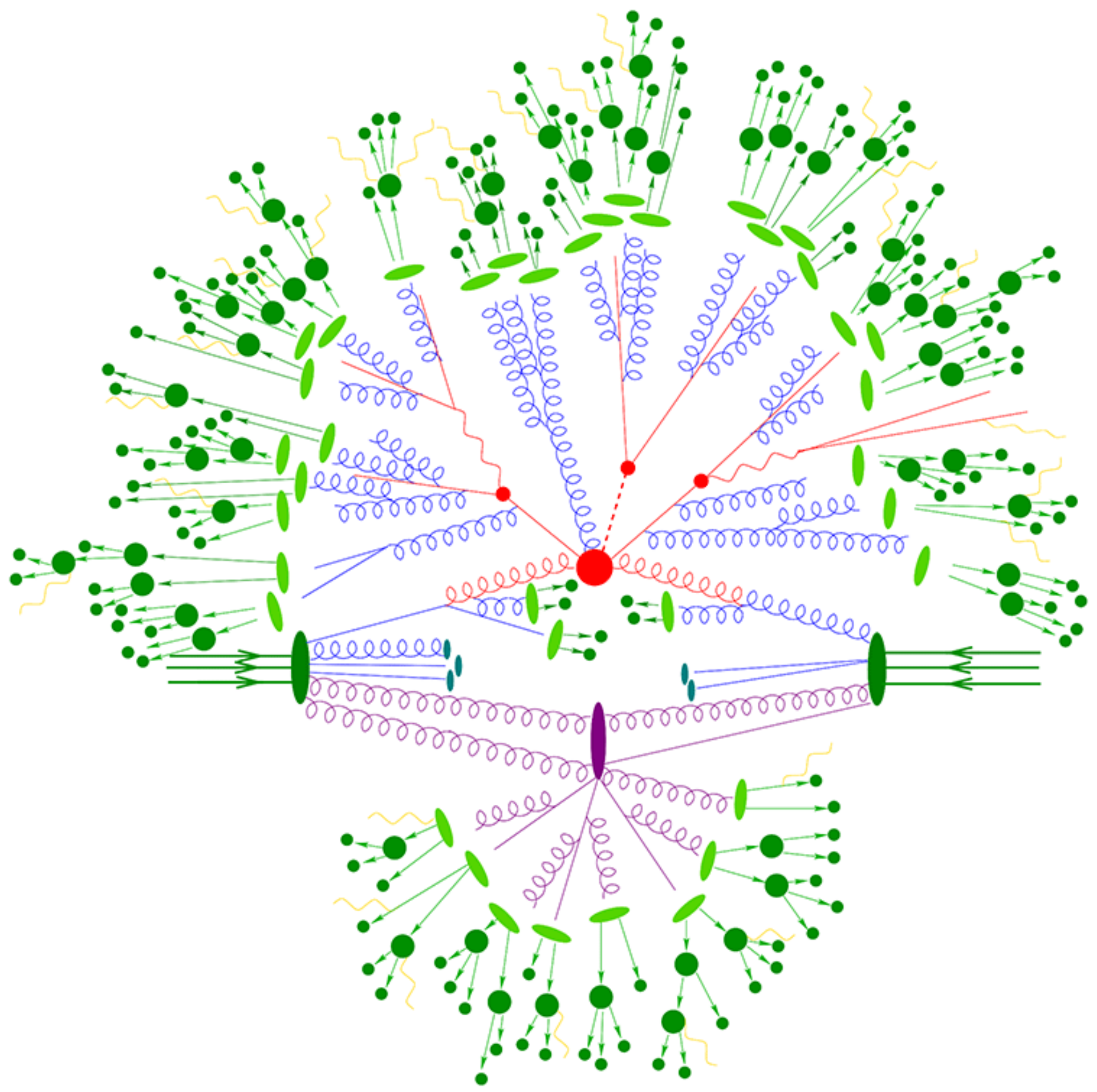
Latent variables

Shower splittings

Parton-level momenta

Theory parameters

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



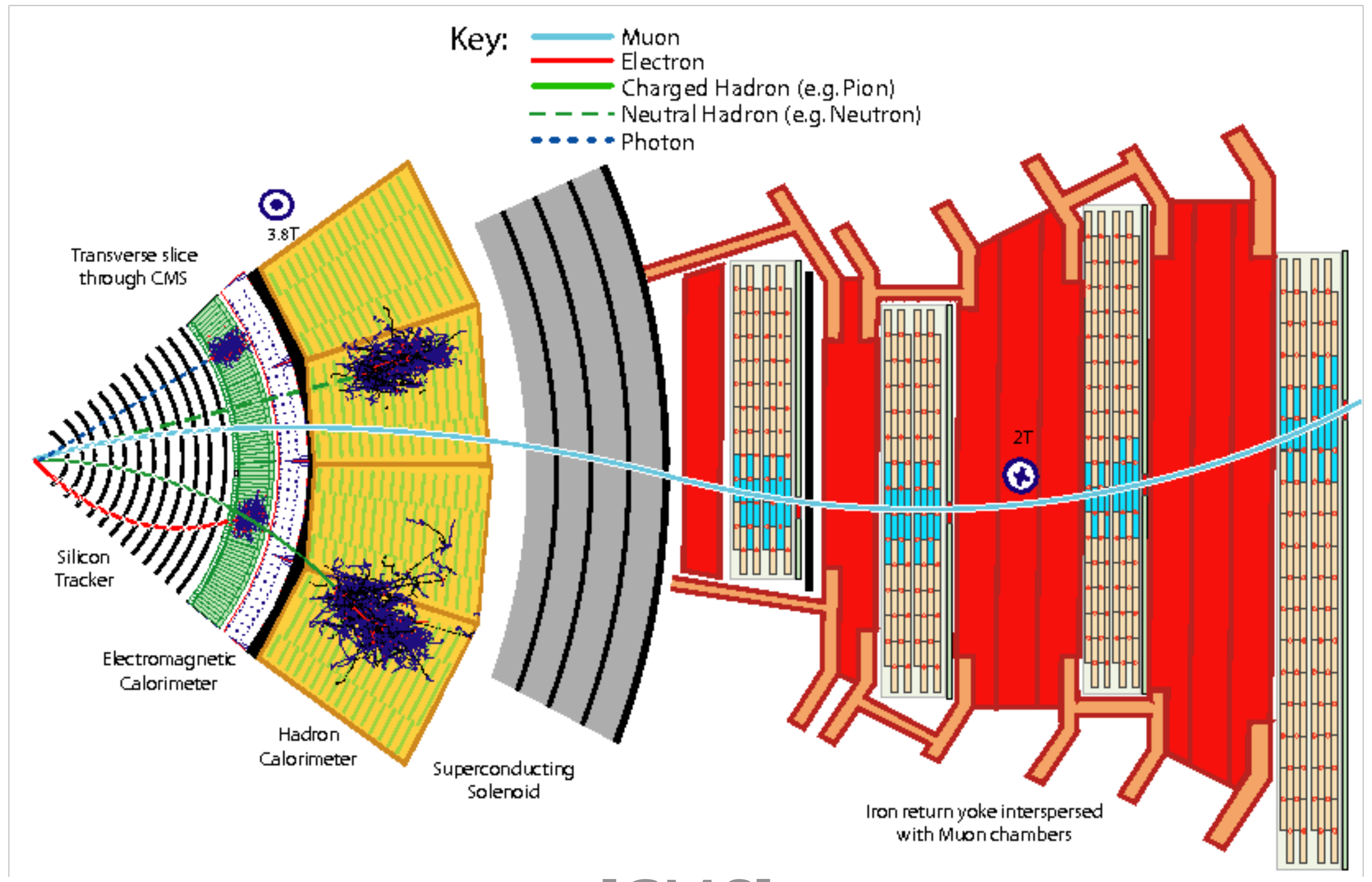
[F. Krauss]

Evolution

Particle physics processes

Latent variables

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



[CMS]

$\longleftarrow$

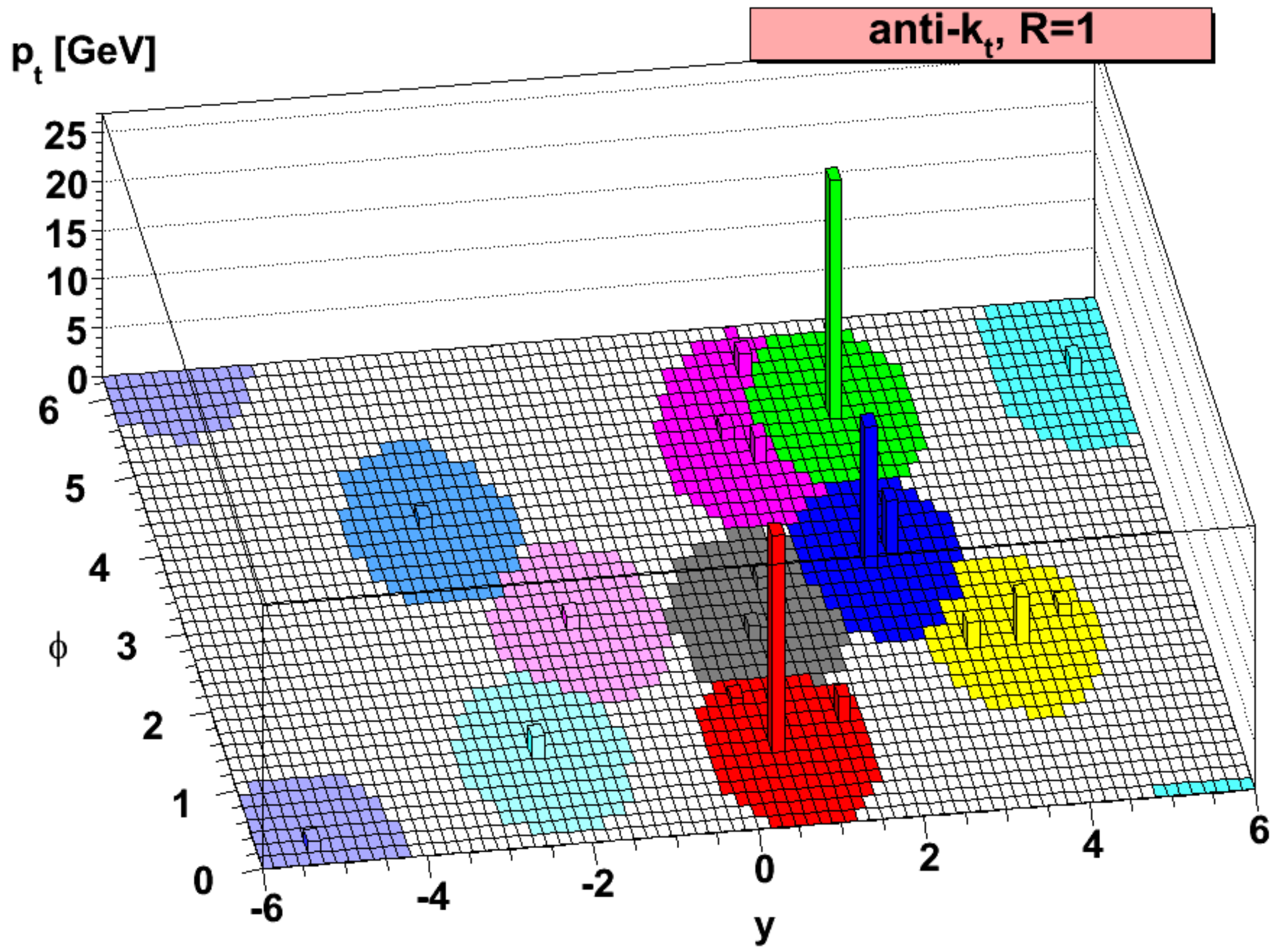
Evolution

Particle physics processes

Latent variables

Observables		Detector interactions	Shower splittings	Parton-level momenta	Theory parameters

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



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

Evolution

Particle physics processes

Latent variables

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

GEANT4
A SIMULATION TOOLKIT

MADGRAPH5_aMC@NLO

Prediction (simulation)

Particle physics processes

Latent variables

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

$$x \leftarrow z_d \leftarrow z_s \leftarrow z_p \leftarrow \theta$$

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

Inference

Particle physics processes

Latent variables

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

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

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

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

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

Inference

Mining gold from LHC simulations

Latent variables

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

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

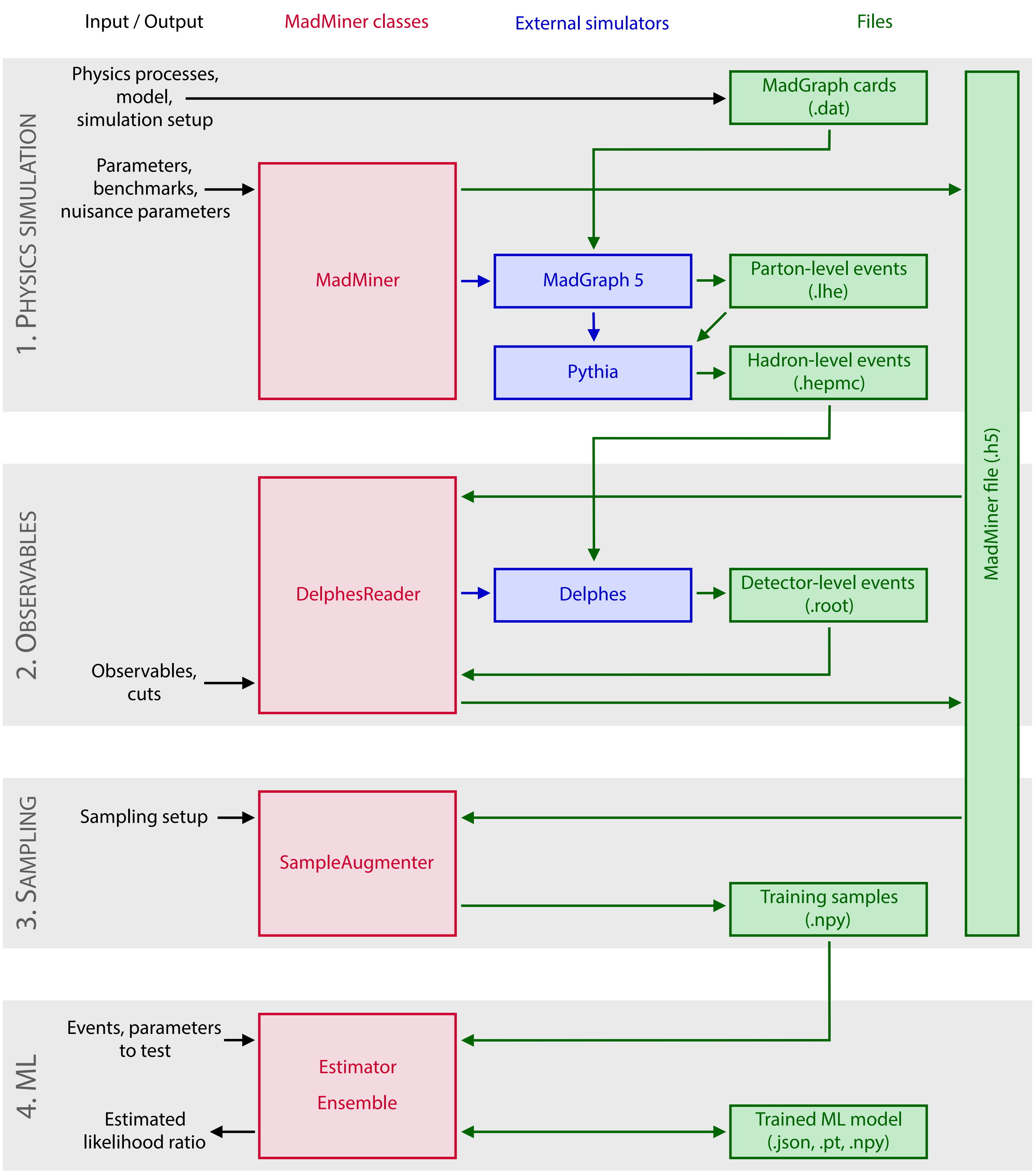
Parton-level likelihood is given by matrix element and can be evaluated!

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

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

Automization

We have developed MadMiner, which makes it straightforward to apply the new techniques to LHC problems

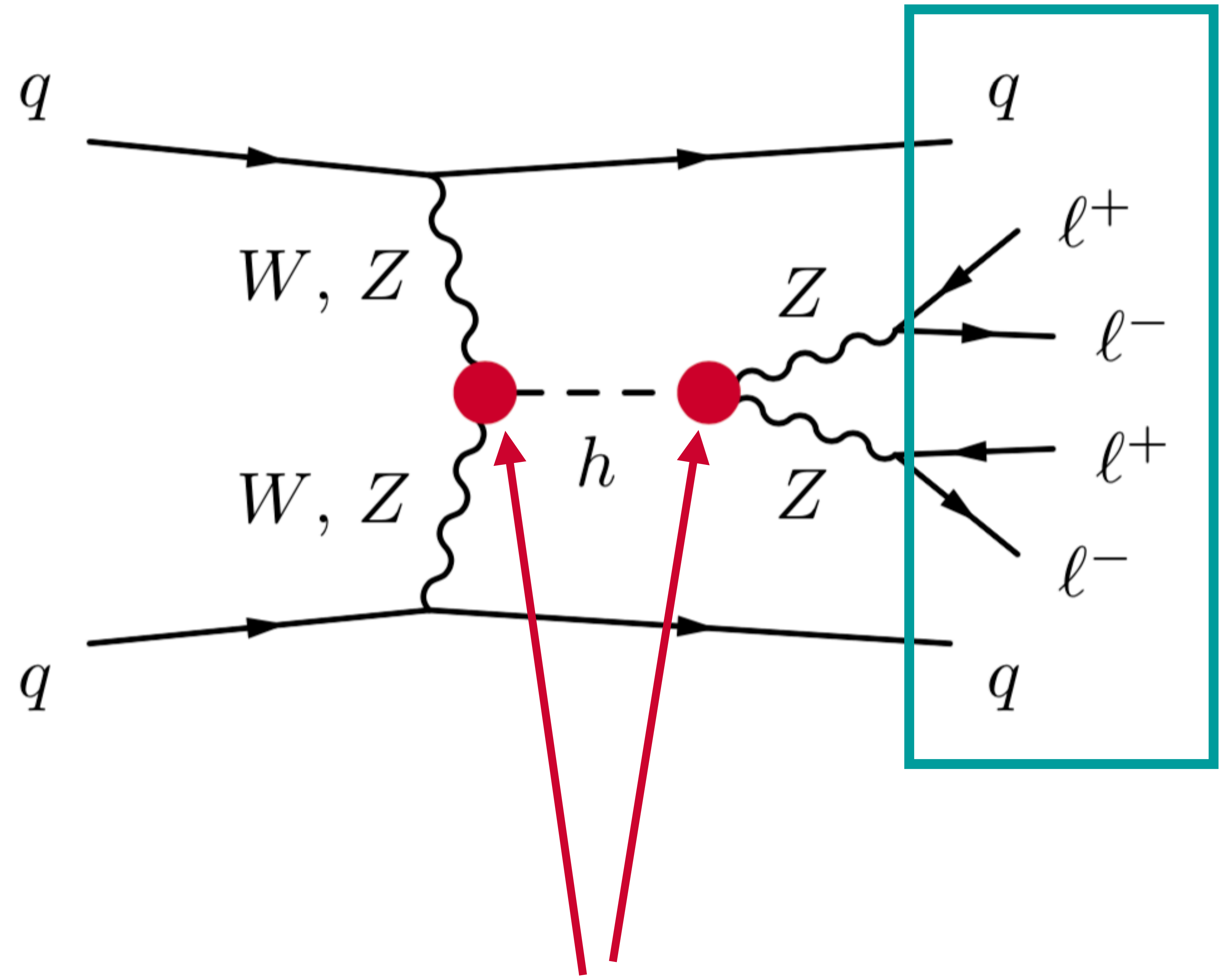


- "Mining gold" from LHC simulations — MadGraph, Pythia, Delphes…
- Likelihood / ratio / score / Fisher info estimation — RASCAL, SALLY & co
- Supports most aspects of real-life analyses:
  - Almost any theory model — UFO standard
  - Parameter morphing — for EFT-like situations
  - Hard process, shower, detector simulation — Currently only LO
  - Reducible + irreducible backgrounds
  - Systematic uncertainties — from PDF variation or scale variation
- Well-documented Python module

github.com/johannbrehmer/madminer   madminer.readthedocs.io   `pip install madminer`

Proof of concept: Higgs production in weak boson fusion

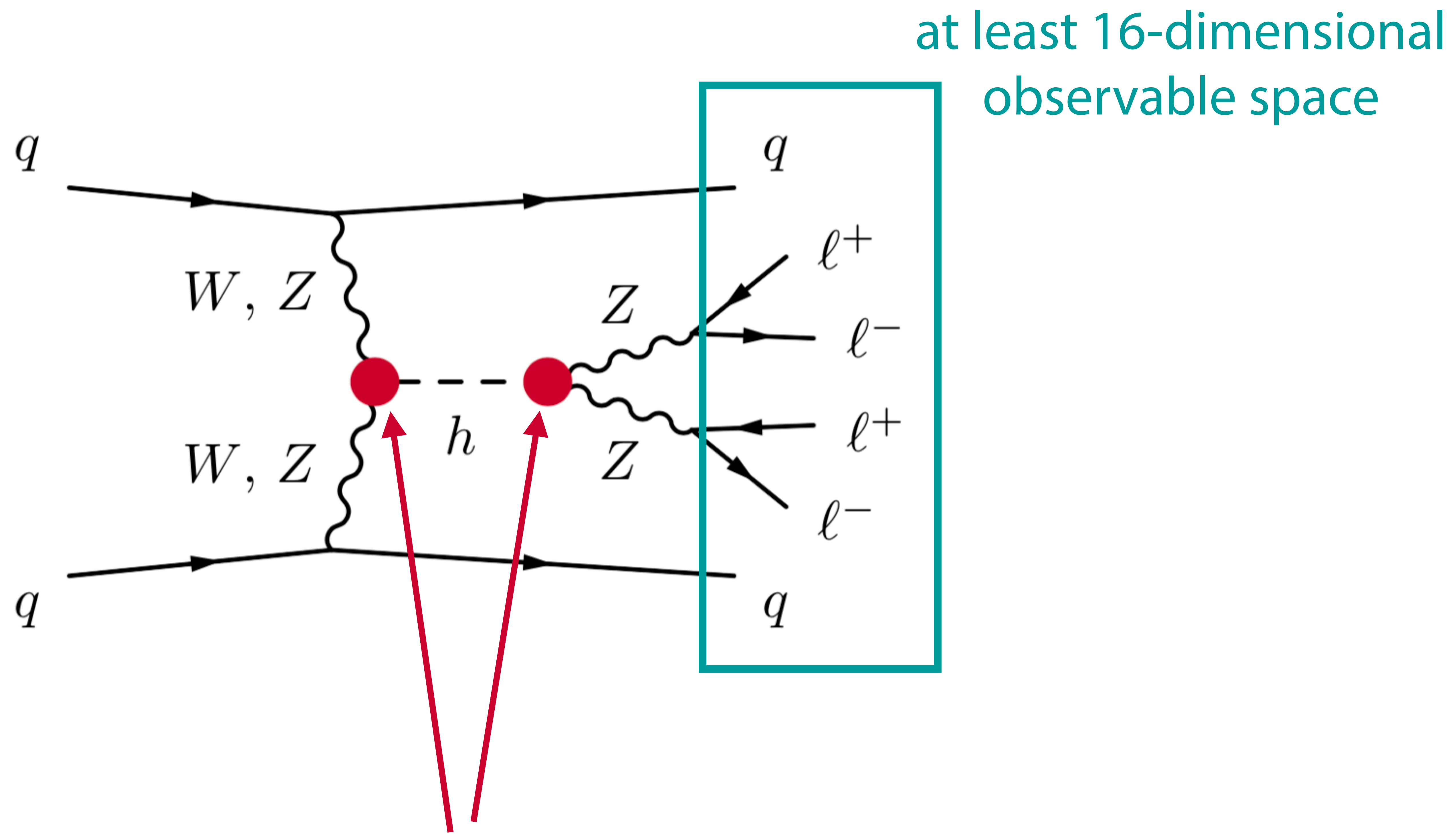
at least 16-dimensional
observable space



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

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

Proof of concept: Higgs production in weak boson fusion



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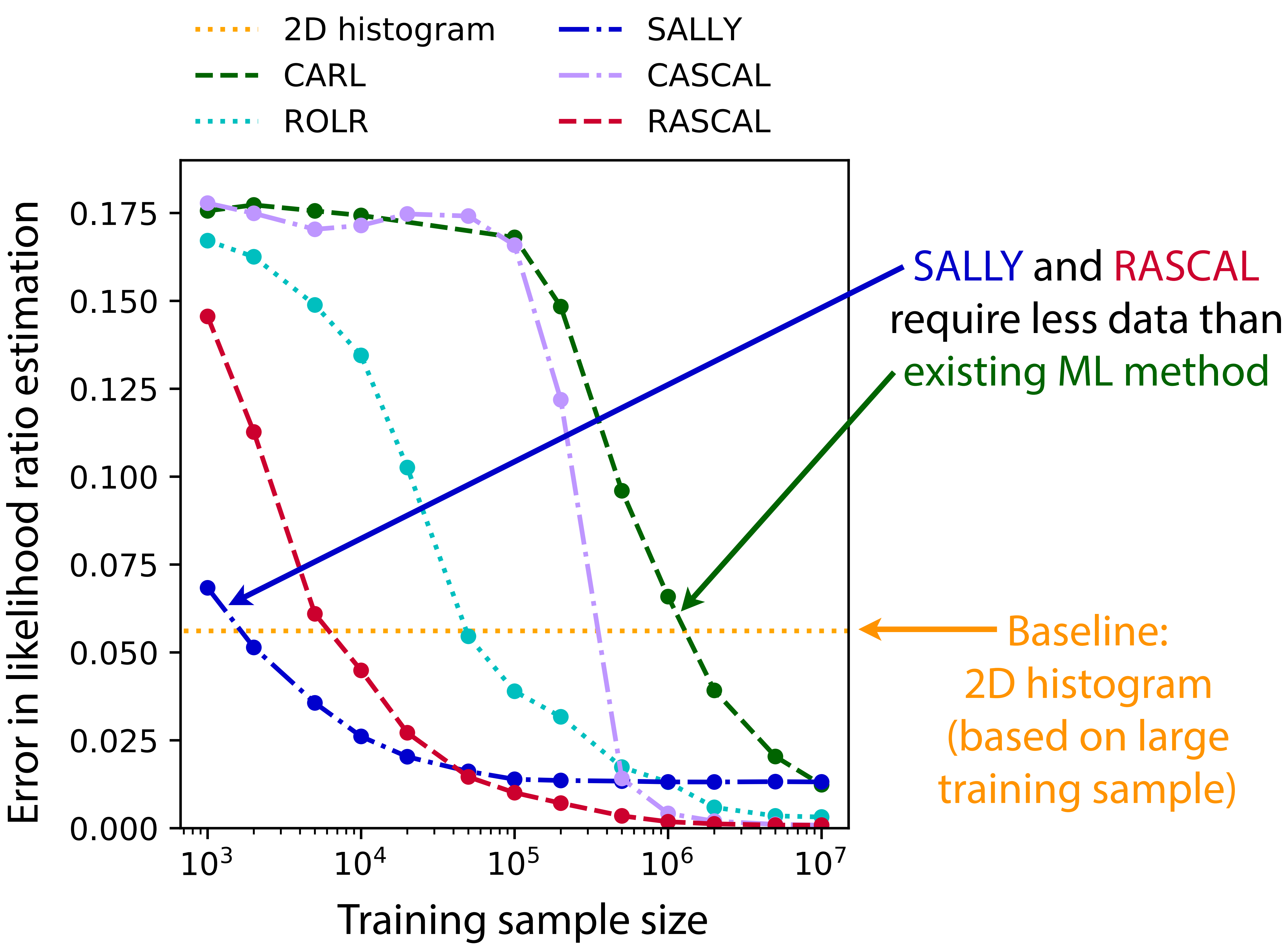
Goal: constrain the two EFT parameters

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

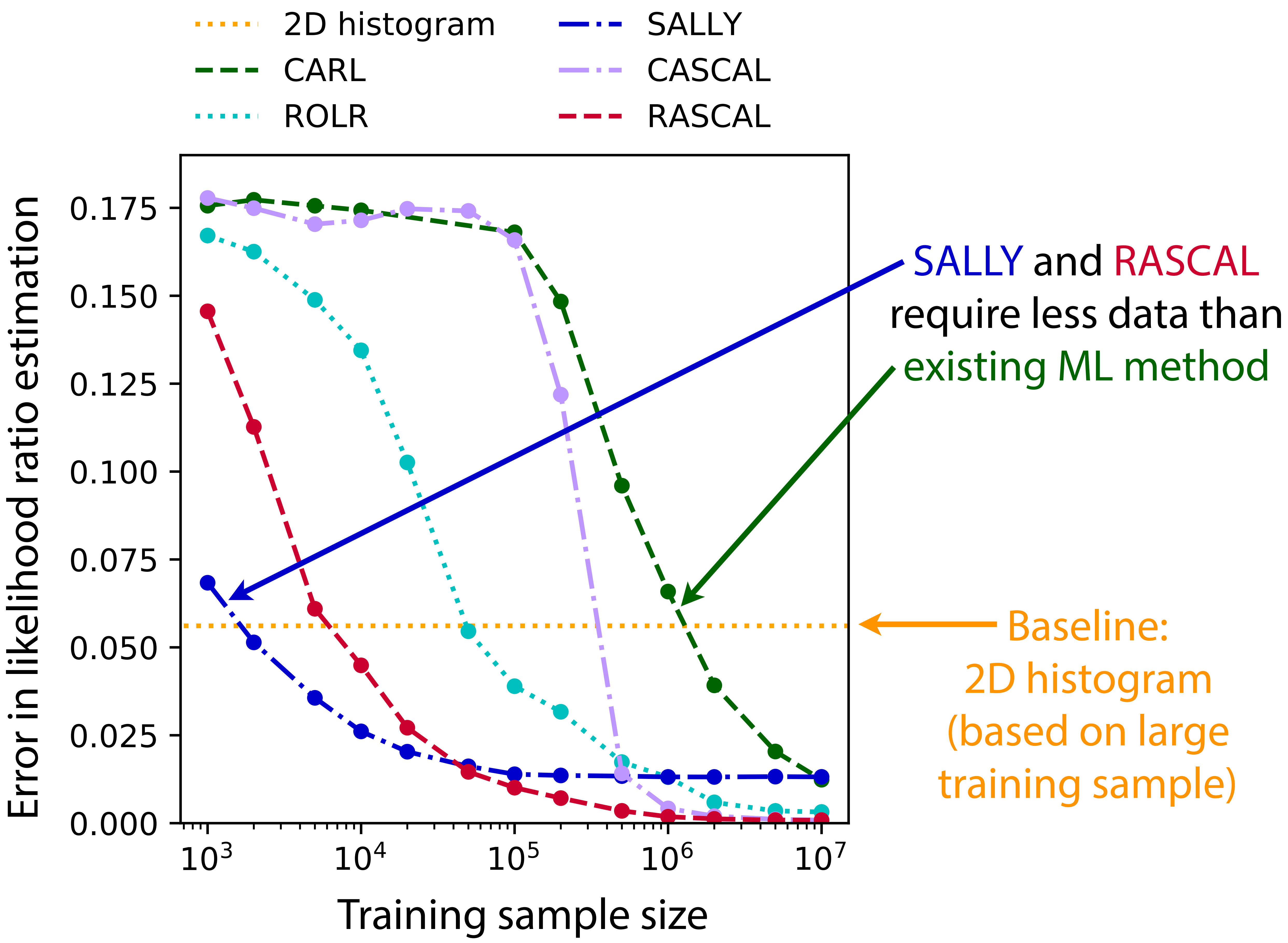
Two scenarios:

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

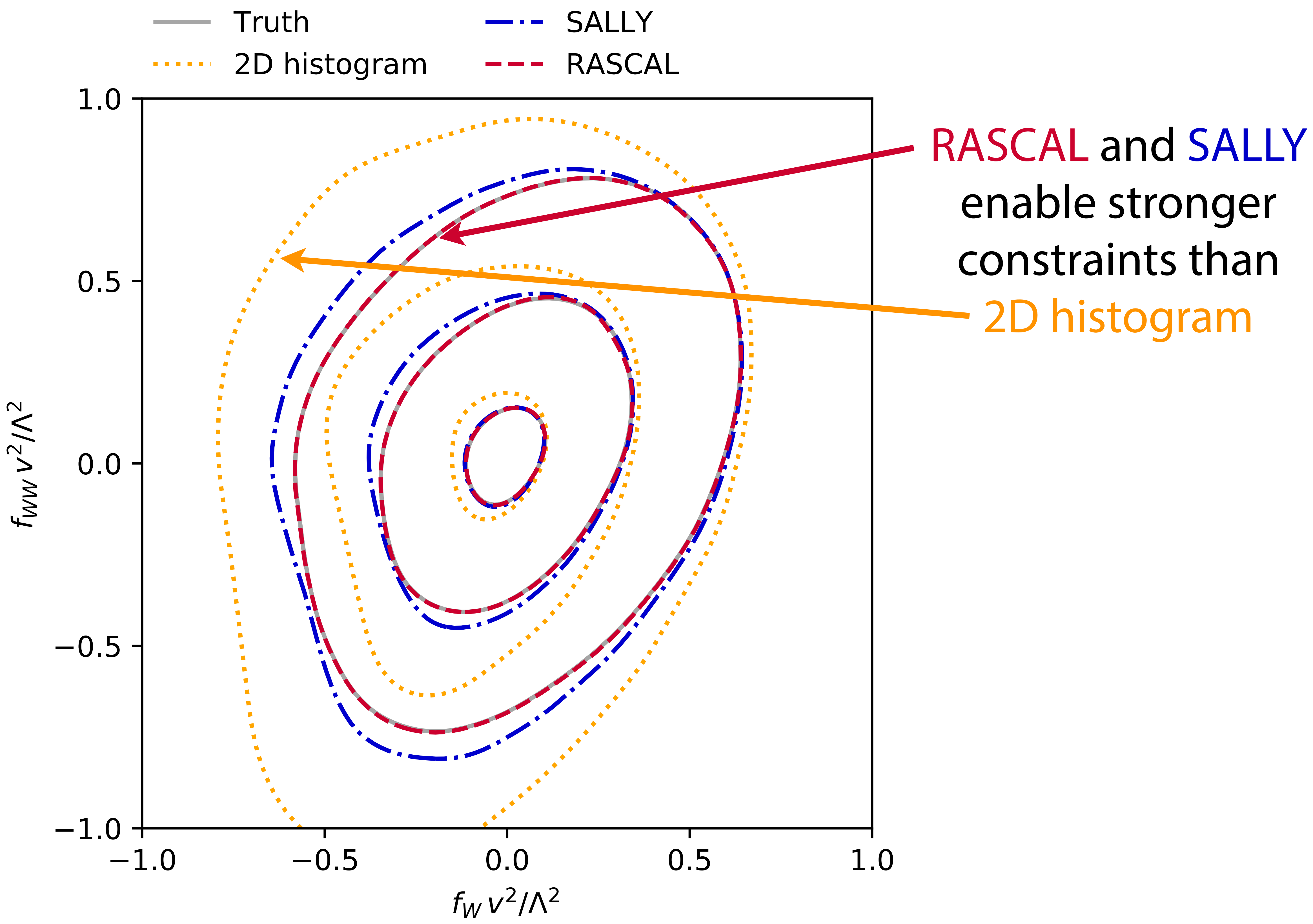
Stronger constraints with less training data



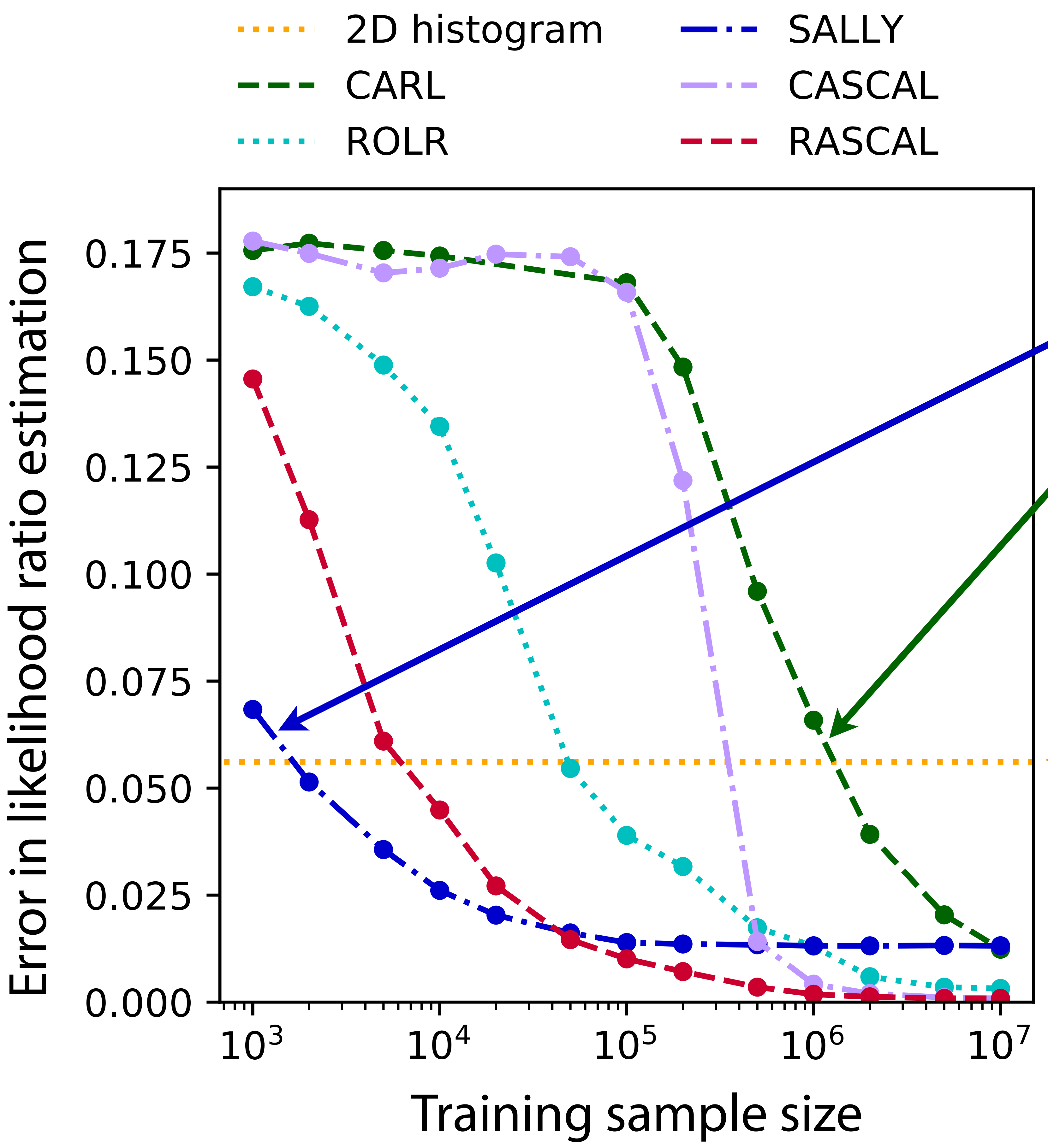
Stronger constraints with less training data



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



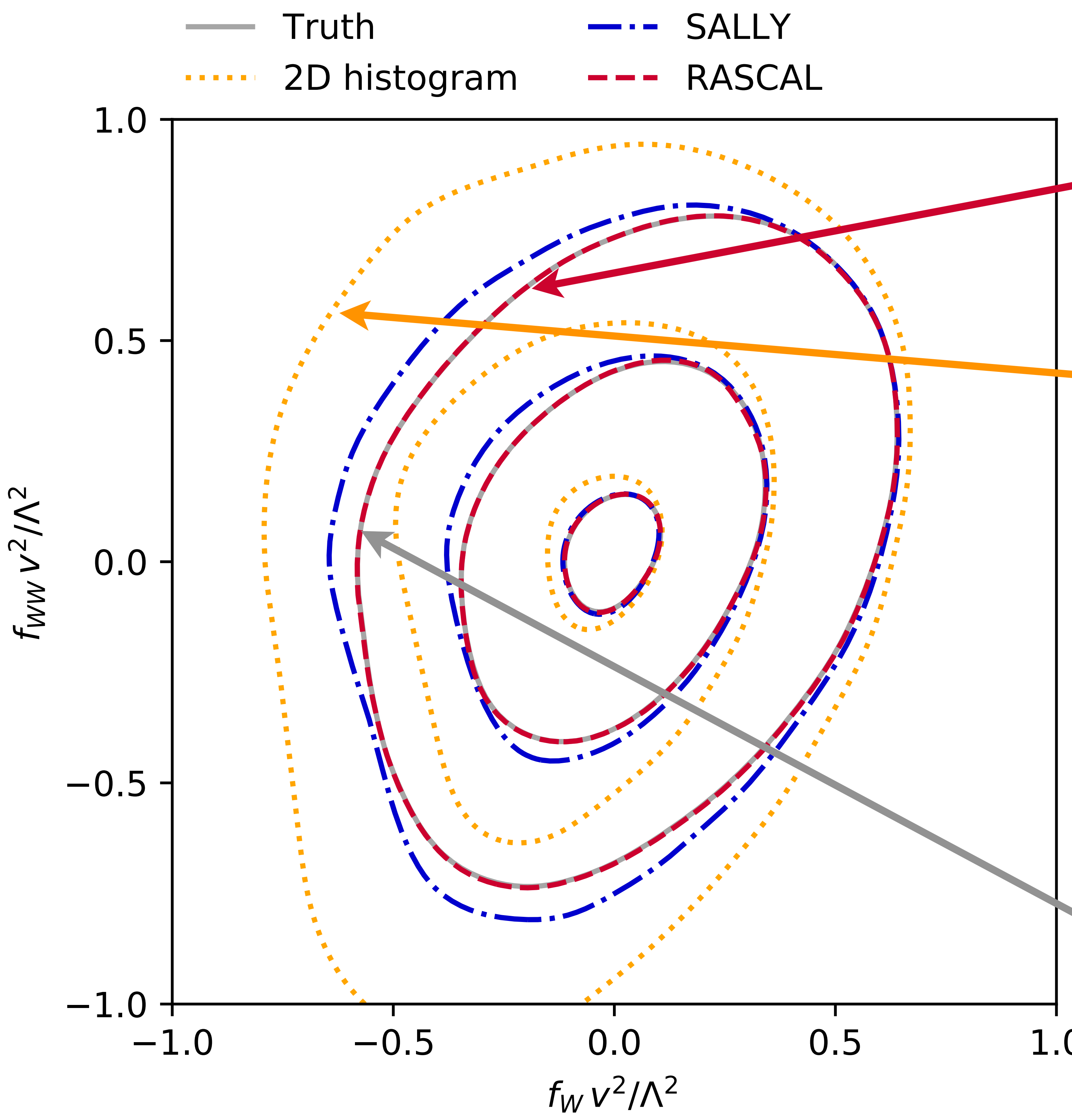
Stronger constraints with less training data



SALLY and RASCAL require less data than existing ML method

Baseline: 2D histogram (based on large training sample)

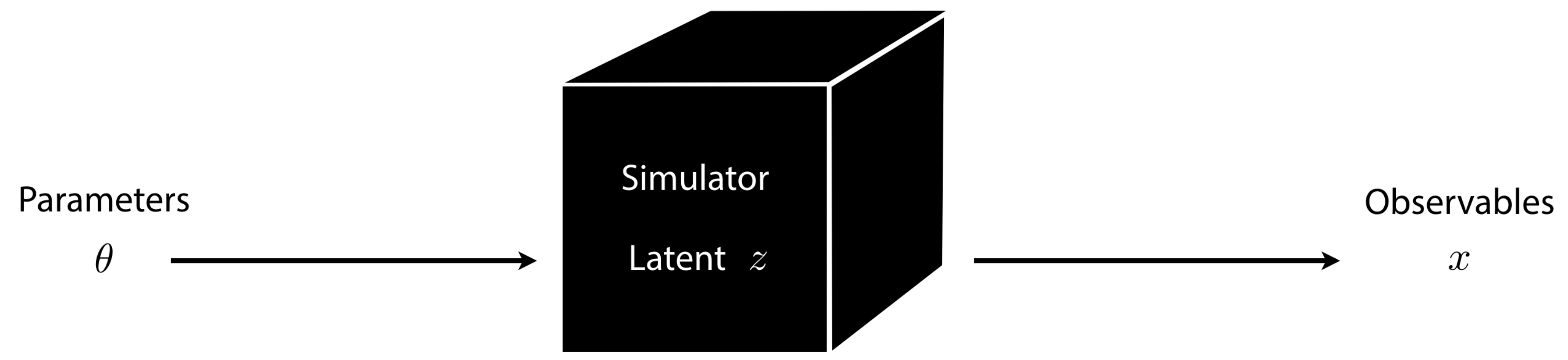
Expected exclusion limits at 68%, 95%, 99.7% CL



RASCAL and SALLY enable stronger constraints than 2D histogram

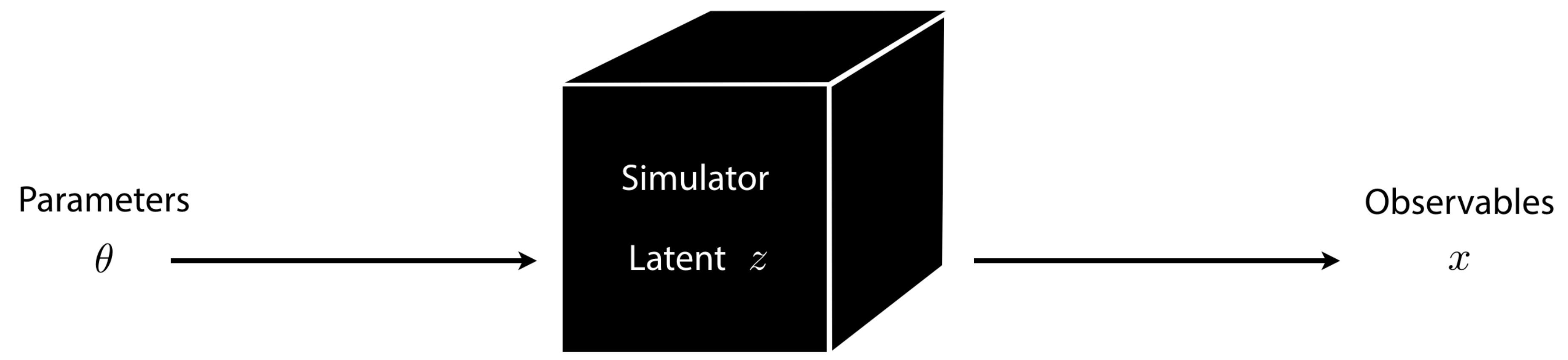
Limits from RASCAL indistinguishable from true likelihood

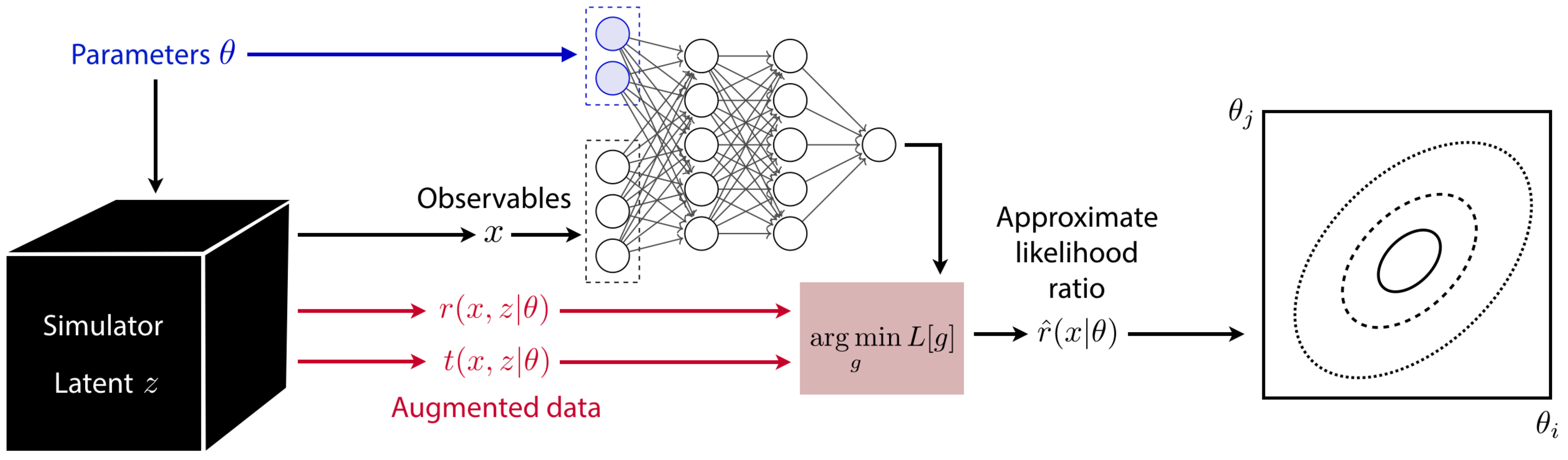
A new approach to simulator-based inference



- Many problems in modern science are based on simulations, “likelihood-free”

A new approach to simulator-based inference

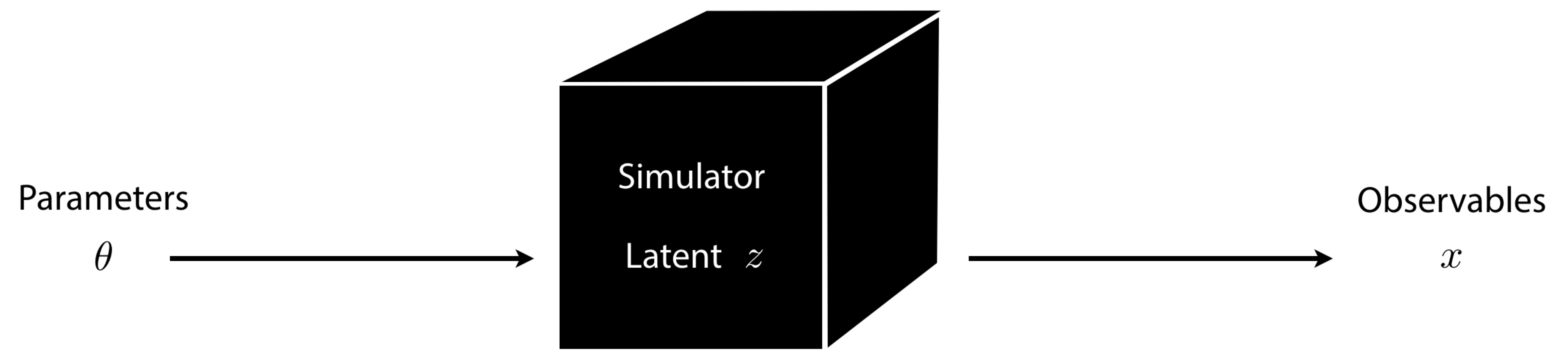


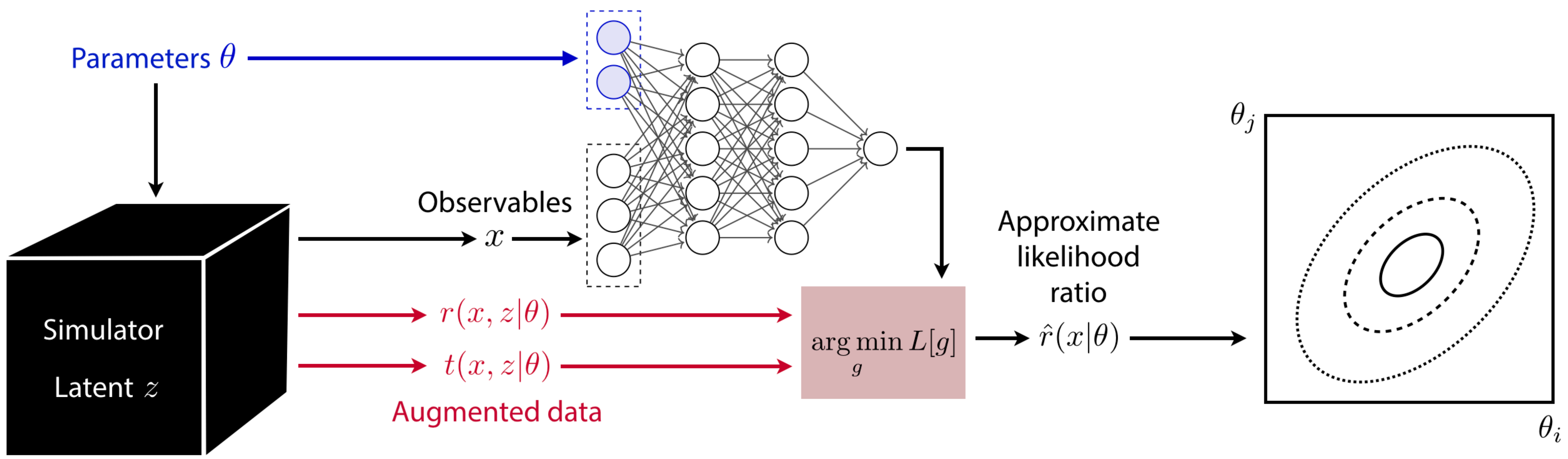


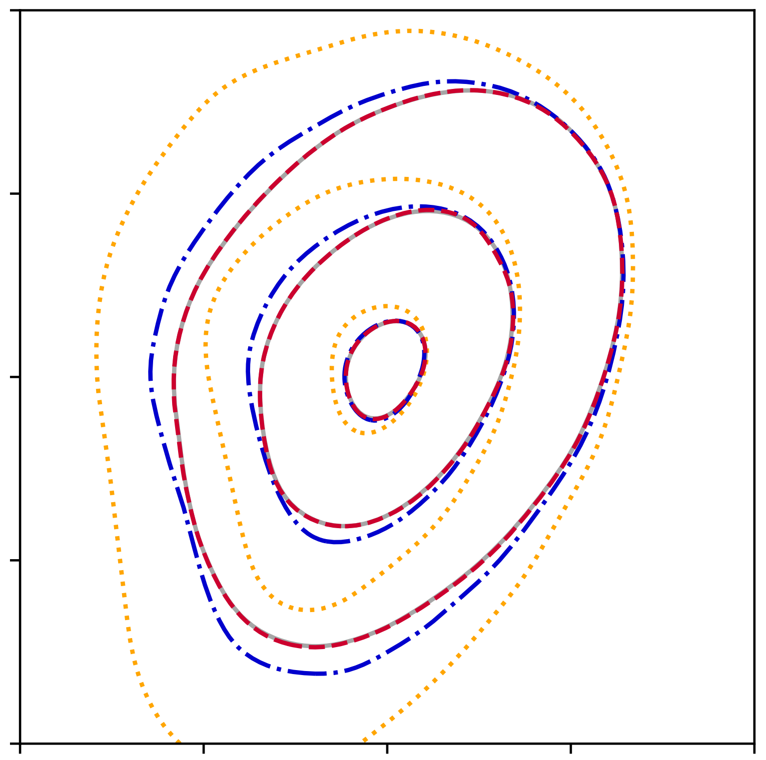
- Many problems in modern science are based on simulations, "likelihood-free"

- New inference techniques:
  Leverage insight into simulated process
  + power of machine learning

A new approach to simulator-based inference







- Many problems in modern science are based on simulations, "likelihood-free"
- New inference techniques:
  Leverage insight into simulated process
  + power of machine learning
- First application to LHC measurements:
  Stronger constraints with less simulations, automization with new tool MadMiner

References

Kyle Cranmer

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Juan Pavez

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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 [doi: 10.5281/zenodo.1489147]

Thanks to Kyle and Gilles for inspiring many slides!

Bonus material

Variational calculus

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

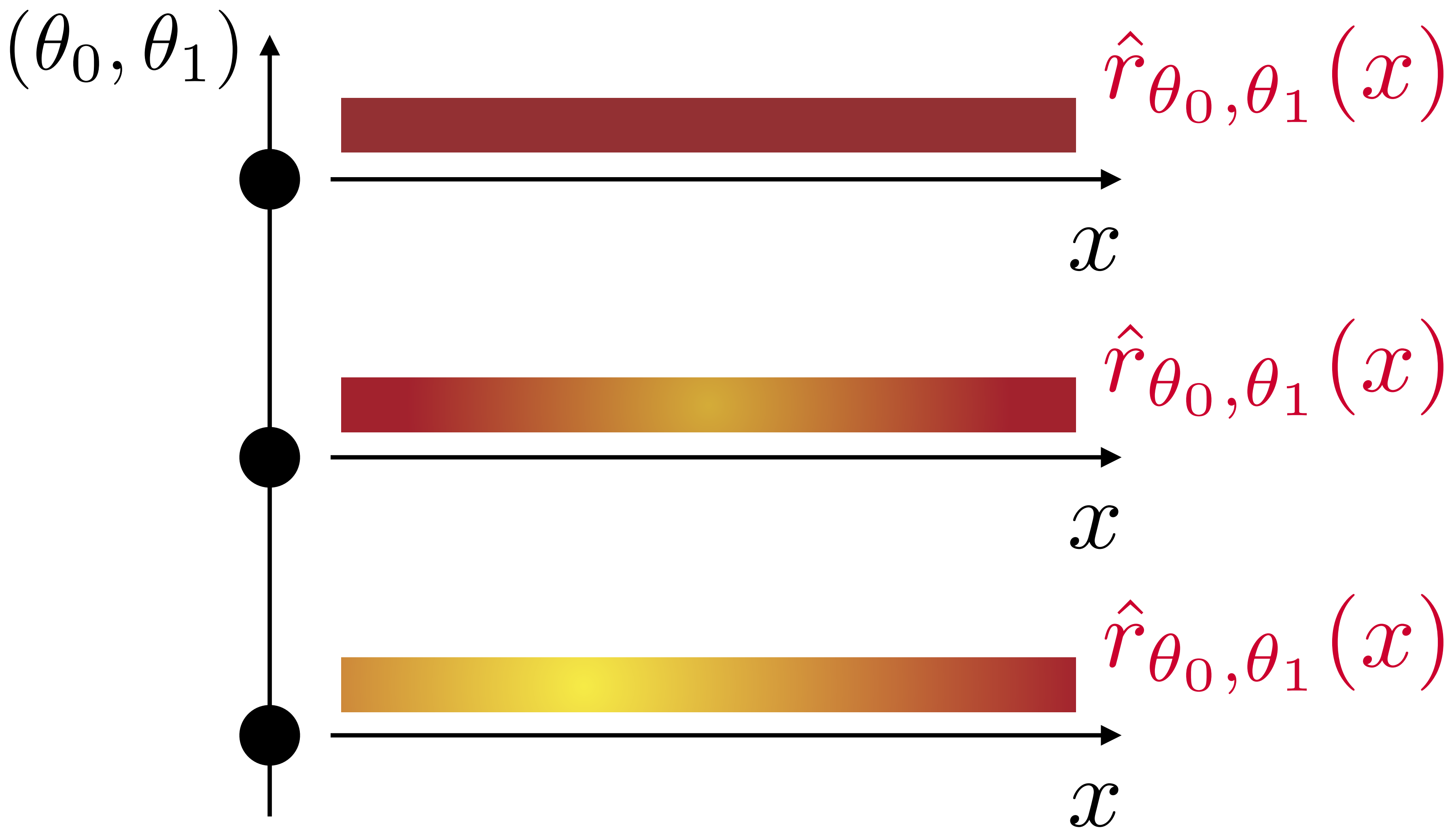
$$
0 = \left.\frac{\delta F}{\delta \hat{g}}\right|_{g^*} = 2\hat{g} \underbrace{\int \mathrm{d}z\; p(x, z|\theta)}_{= p(x|\theta)} - 2 \int \mathrm{d}z\; p(x, z|\theta)\, g(x, z)
$$

$$
g^*(x) = \frac{1}{p(x|\theta)} \int \mathrm{d}z\; p(x, z|\theta)\, g(x, z)
$$

Two types of likelihood ratio estimators

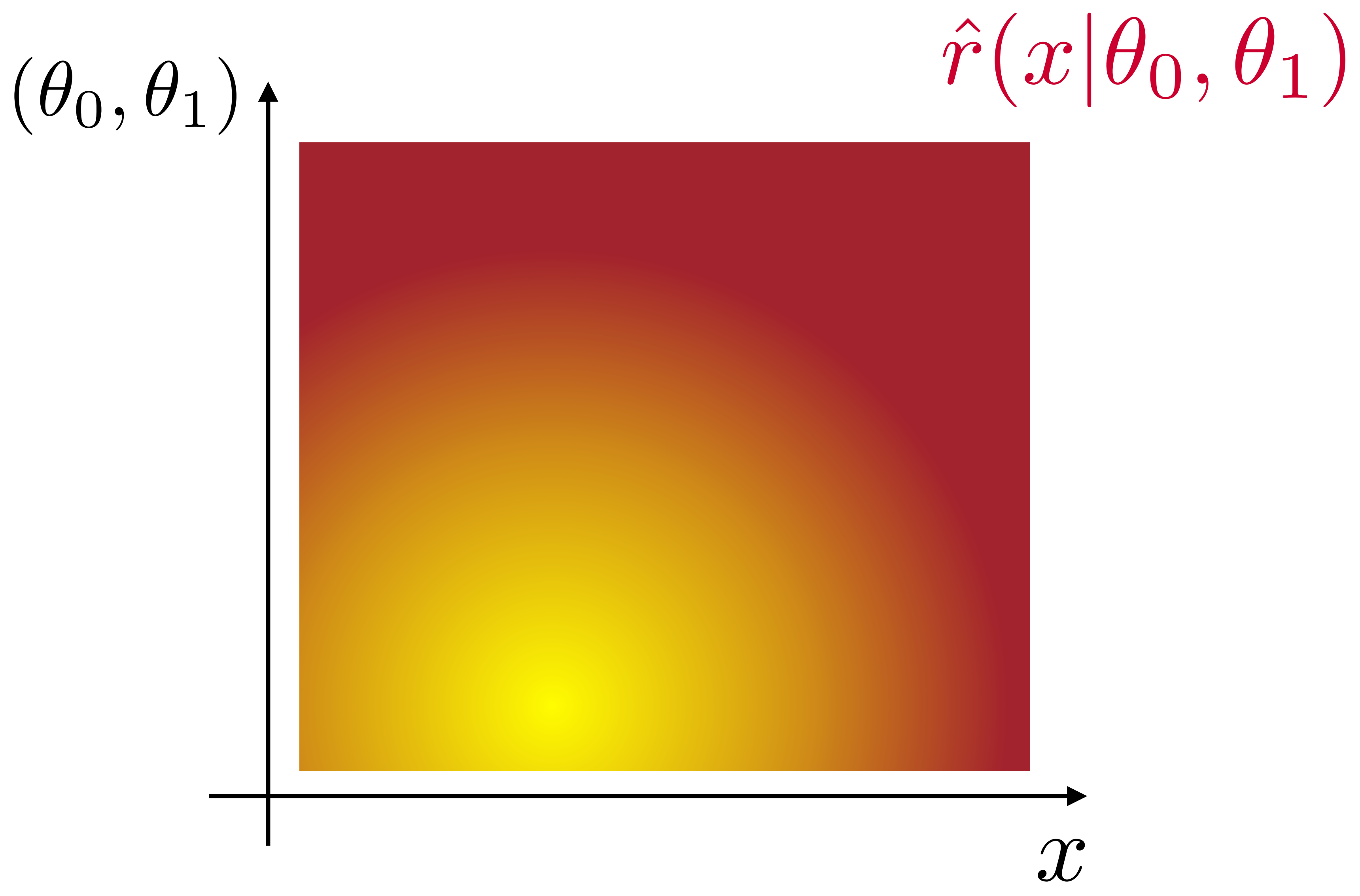
A) Point by point:

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

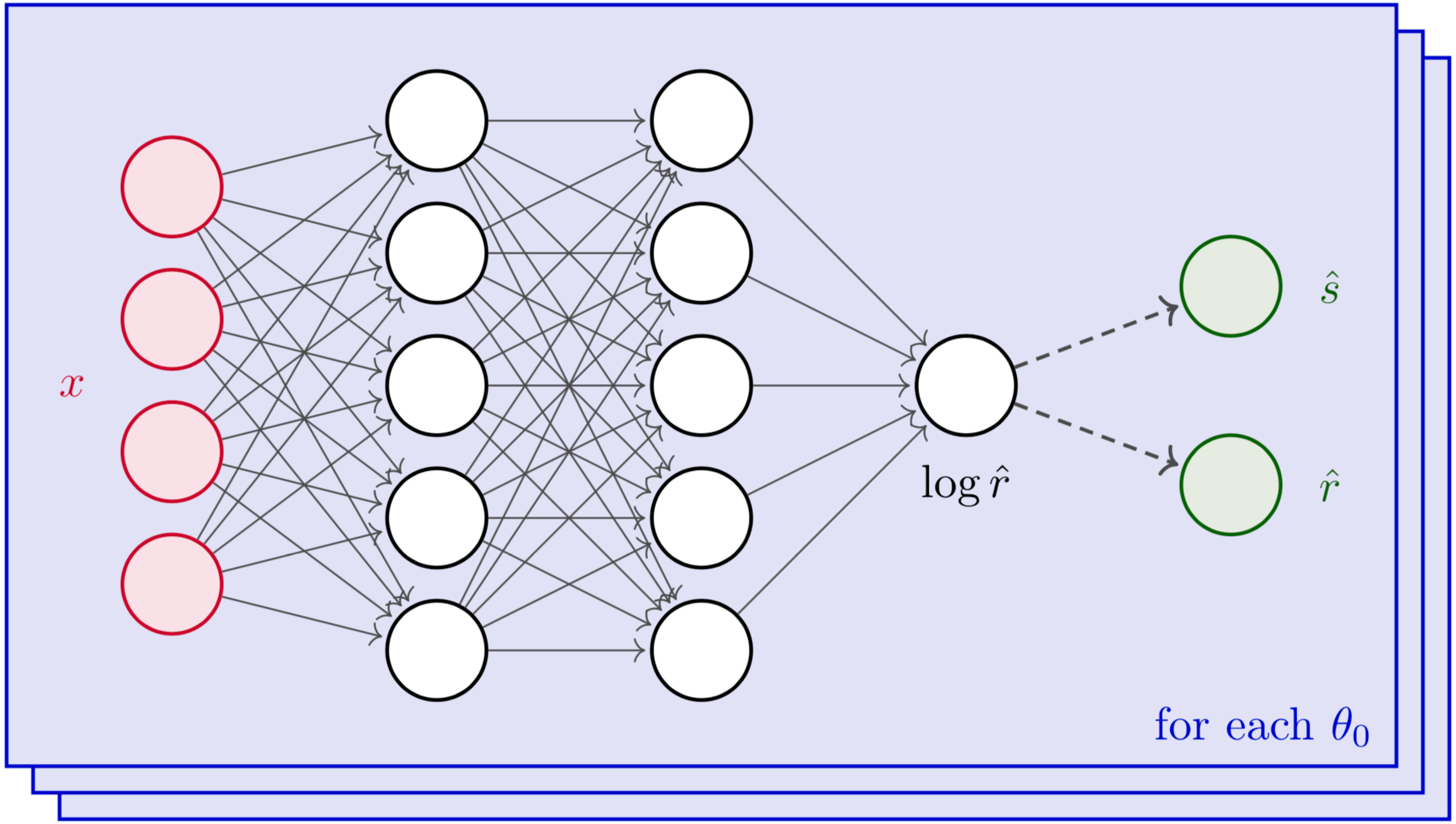


B) Parameterized: [P. Baldi et al. 1506.02169]

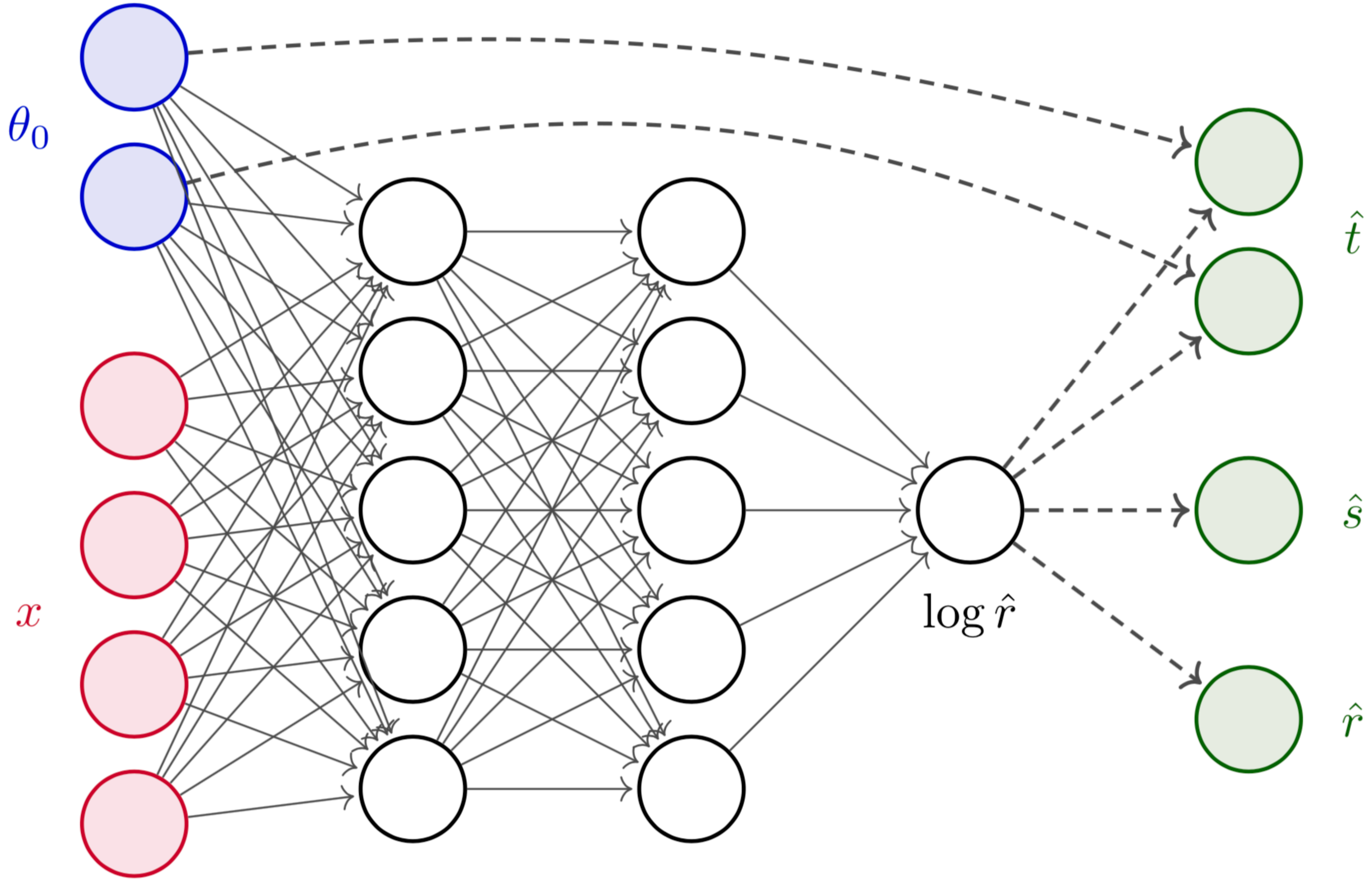
- create one estimator $\hat{r}(x|\theta_0, \theta_1)$ that is a function of θ_0 and θ_1
- no further interpolation necessary
- "borrows information" from close points



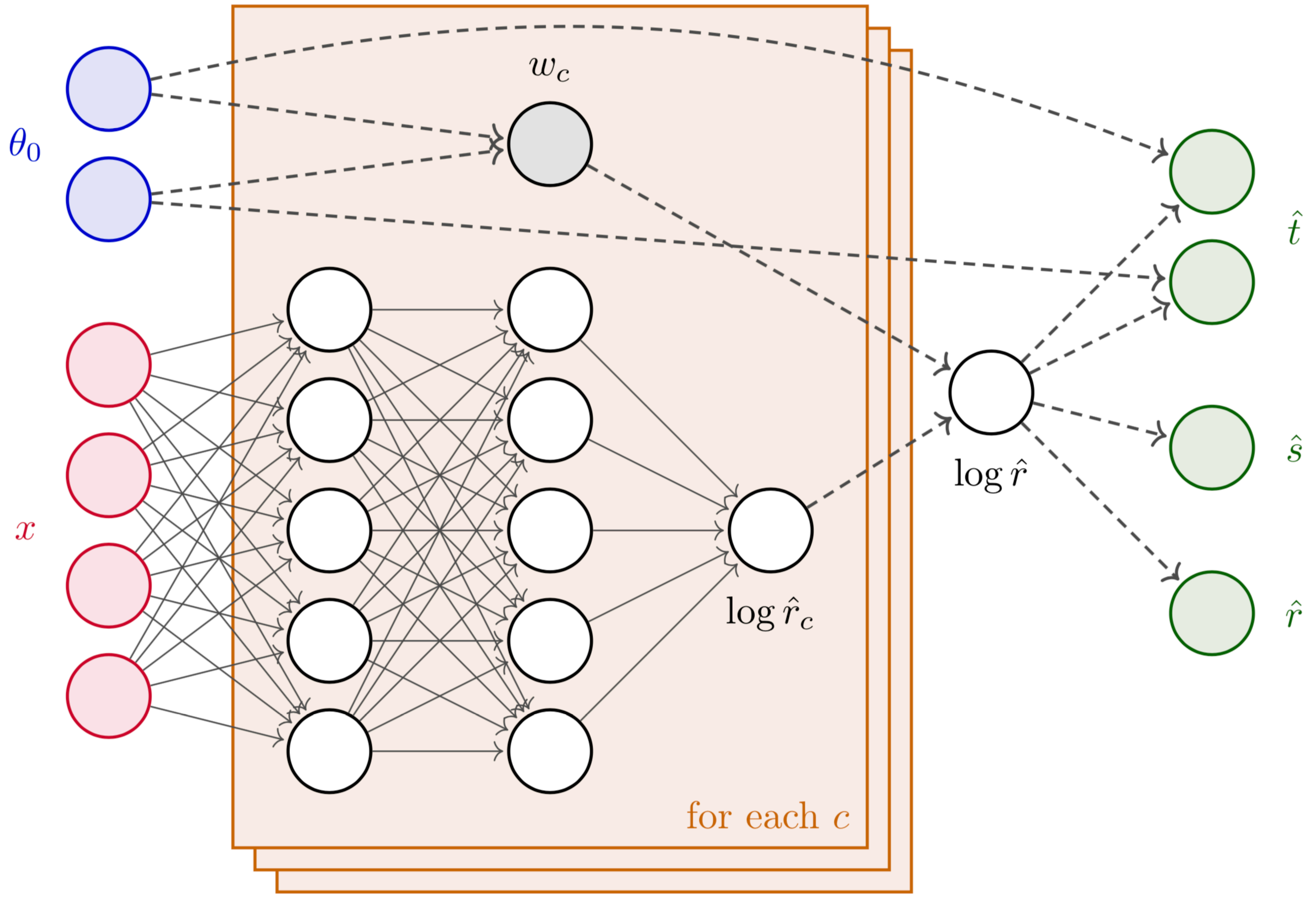
Point by point



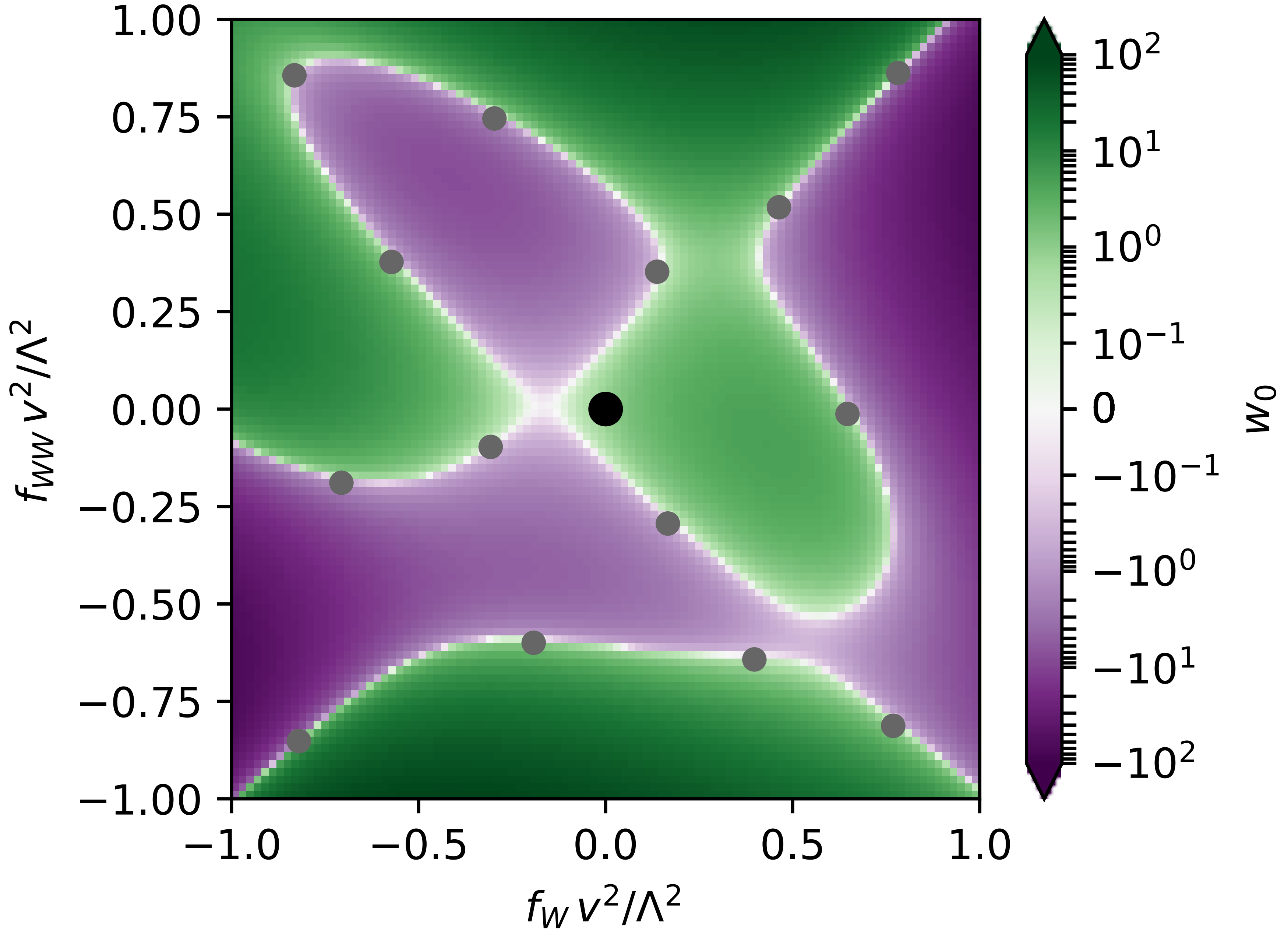
(Agnostic) parameterized estimators



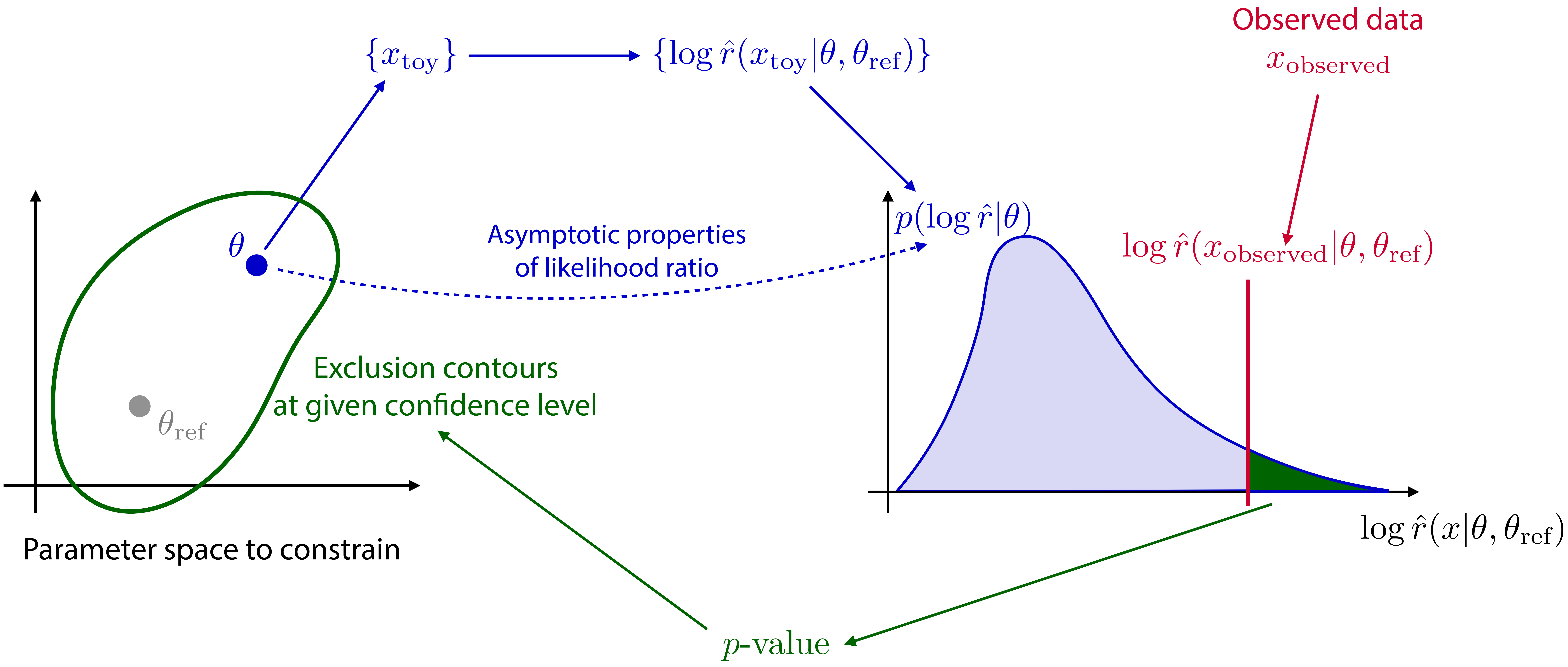
Morphing-aware parameterized estimators



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



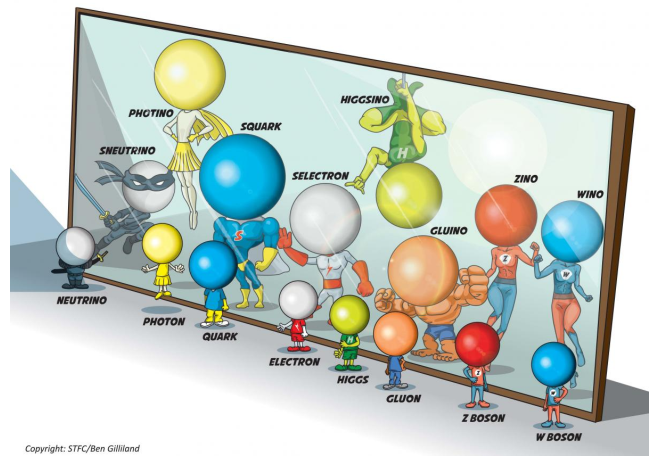
Limit setting (frequentist)



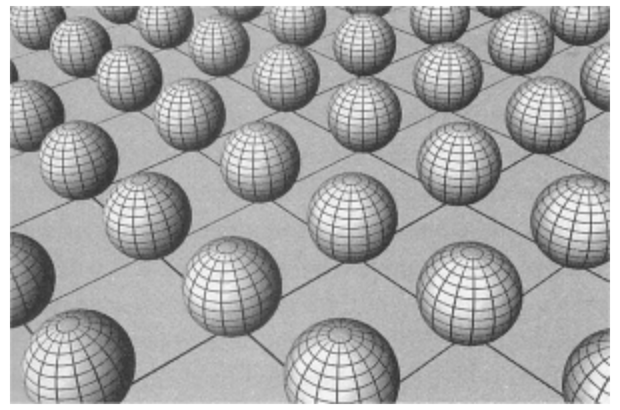
Effective field theory

Energy

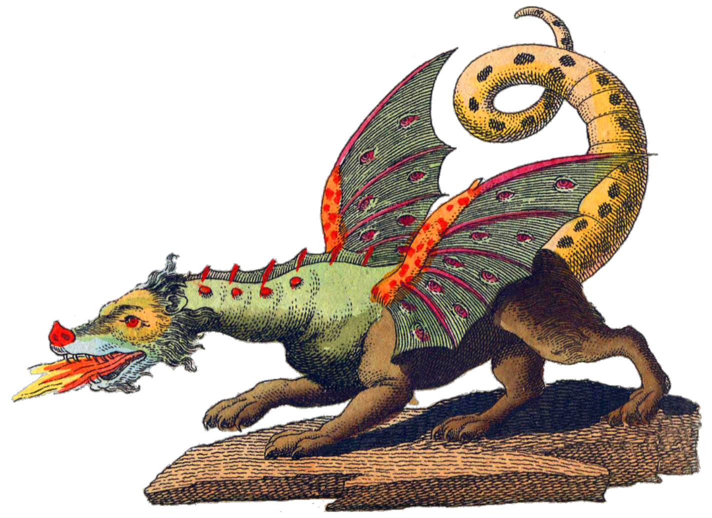
Λ



Supersymmetry?



Extra dimensions?



Dragons?

Composite Higgs?

…

Matching

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

Effective field theory

Measurements

$E \ll \Lambda$

LHC Higgs

Other LHC measurements

LEP

Flavour

…

Detector effects