Mining gold from implicit models to improve likelihood-free inference

Johann Brehmer[1], Gilles Louppe[2], Juan Pavez[3], and Kyle Cranmer[1]

[1]New York University, [2]University of Liège, [3]Federico Santa María Technical University

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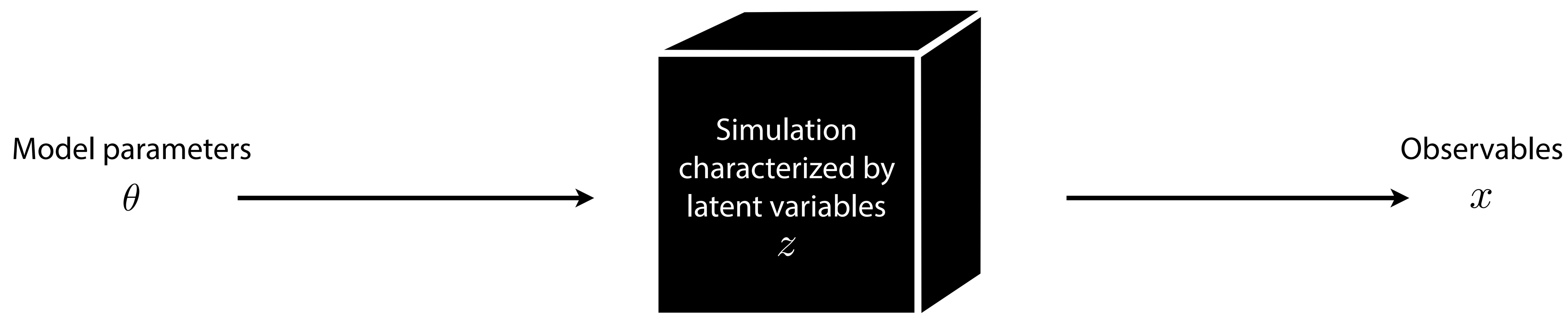
Simulator-based science

Many phenomena are best described by simulators:



Prediction: stochastic generative simulator can generate samples of observations $x \sim p(x|\theta)$

Inference: usually based on likelihood function $p(x|\theta) = \int \mathrm{d}z\; p(x,z|\theta)$.
But often the integral over the huge space of latent trajectories cannot be calculated!

The bottom line

The intractability of the likelihood function is a challenge for inference in many fields of science.

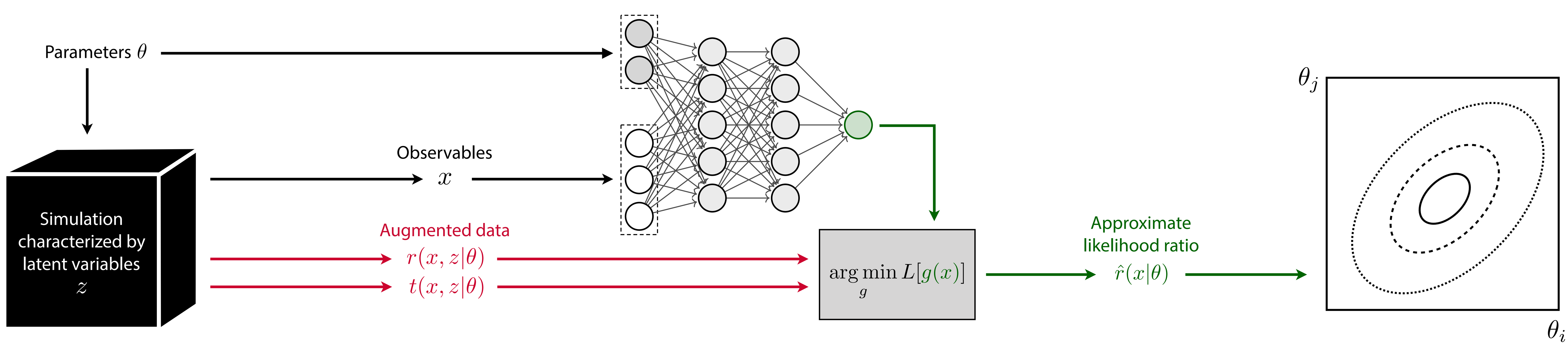
Established likelihood-free inference algorithms like Approximate Bayesian Computation [1] do not scale well to high-dimensional x. These methods generally only use that the simulator can generate samples of observables.

Here we develop a new approach:

- we point out that often additional information can be extracted from the simulator, and
- we develop new, more efficient inference techniques for this case.

In first tests, this new class of methods is more sample-efficient and allows higher-fidelity inference. It is now being adapted to real-world problems in particle physics, cosmology, and epidemiology.

"Mining gold from the simulator": A new approach to simulator-based inference



1. Simulation

In addition to samples of observables x, we can often extract two quantities from the simulator that characterize the latent process:

- the joint likelihood ratio $r(x,z|\theta_0,\theta_1) = \dfrac{p(x,z|\theta_0)}{p(x,z|\theta_1)}$
- the joint score $t(x,z|\theta_0) = \nabla_\theta \log p(x,z|\theta)\Big|_{\theta_0}$

Both of these quantities can often be accumulated while the simulation runs forward through its control flow.

2. Machine Learning

The augmented data can be used to define a loss functional, for instance

$$L[g(x,\theta_0)] = \mathbb{E}_{\pi(\theta_0)}\left[\mathbb{E}_{p(x,z|\theta_1)}\Big(g(x,\theta_0) - r(x,z|\theta_0,\theta_1)\Big)^2 + \mathbb{E}_{p(x,z|\theta_0)}\Big(\nabla_{\theta_0}\log g(x,\theta_0) - t(x,z|\theta_0)\Big)^2\right]$$

(there is a family of loss functionals with similar properties). We then train a neural network $g(x,\theta_0)$ by minimizing $L[g(x,\theta_0)]$.

It can be shown that $\arg\min_g L[g(x,\theta_0)] = r(x|\theta_0,\theta_1) \equiv \dfrac{p(x|\theta_0)}{p(x|\theta_1)}$!

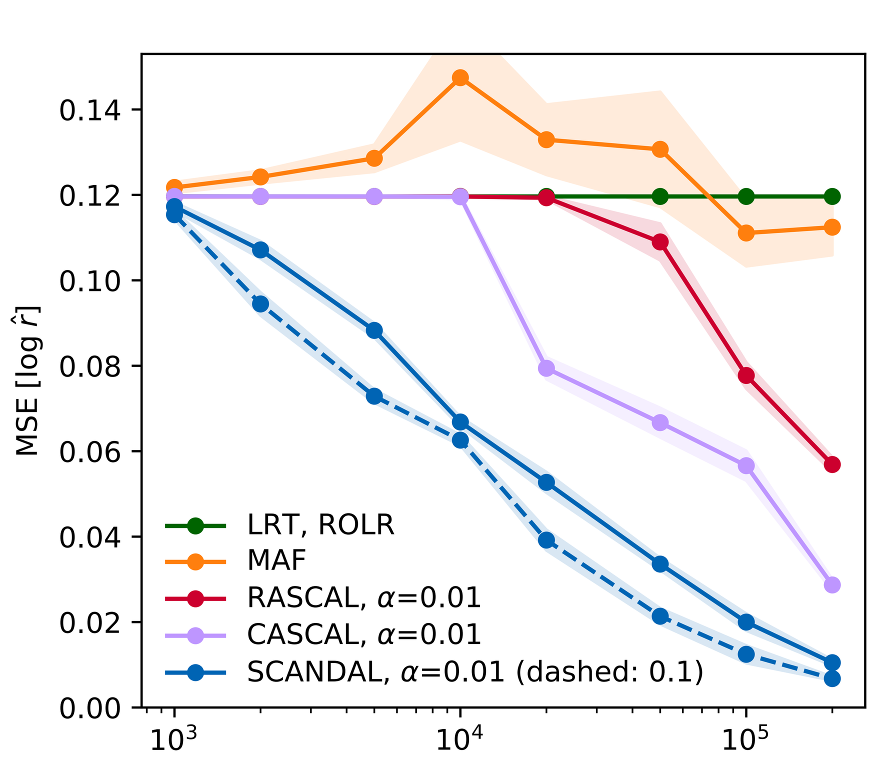
With enough training samples and an efficient optimizer, the network will thus approximate the (intractable) likelihood ratio!

3. Inference

Having trained a network to approximate the likelihood ratio for any parameters and observables, one can find the most likely parameters or set exclusion limits with standard frequentist or Bayesian methods.

Predator-prey dynamics

The Lotka-Volterra model describes the dynamics of a species of predators interacting with a species of prey. Four parameters set the rate of prey being born, predators dying, and predators eating prey.



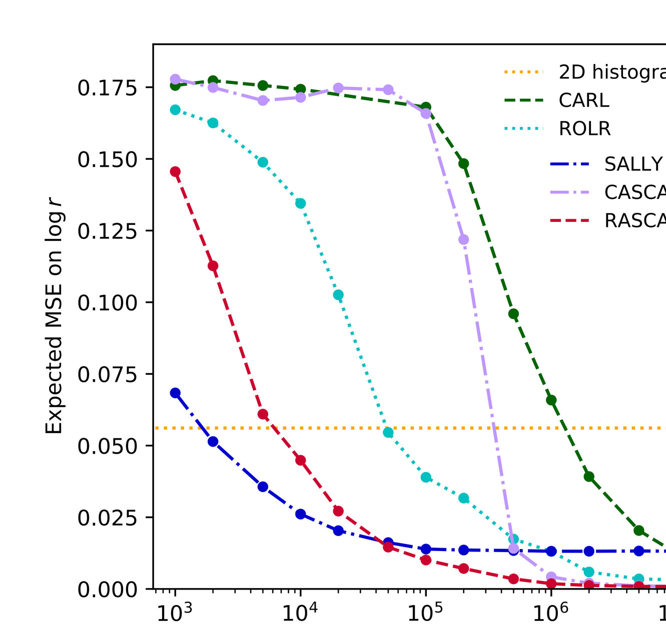
Our goal is to estimate likelihood ratios between close parameter points given observed evolutions of the two animal species.

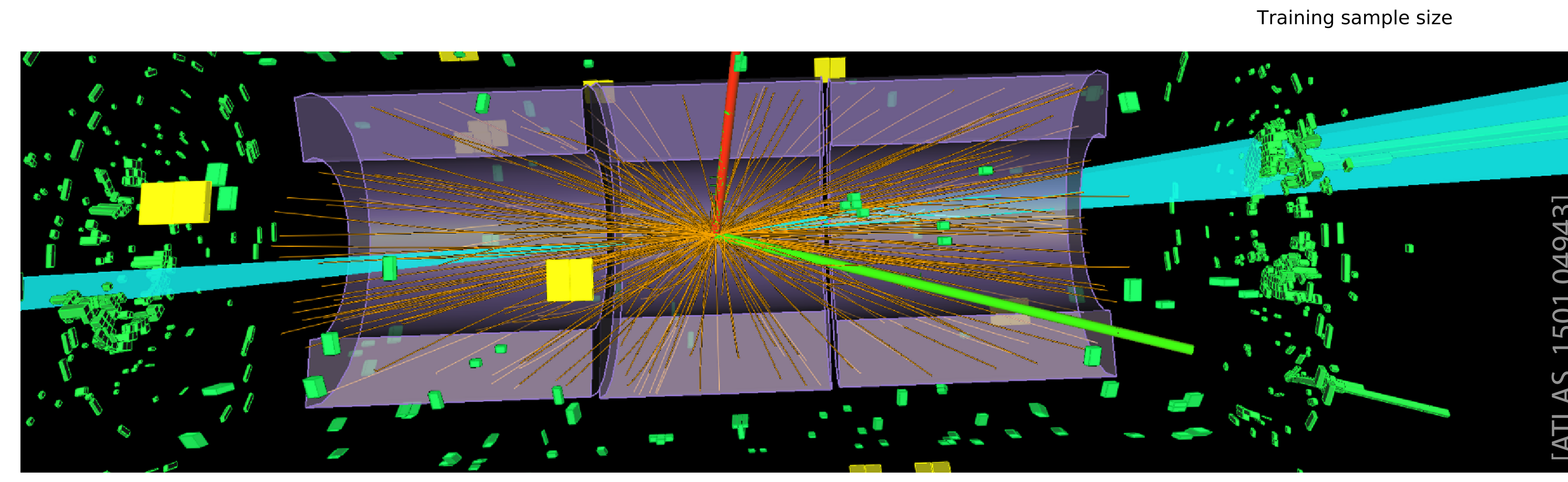
Left: Our new methods (including SCANDAL) learn more efficiently from few training samples than existing methods [2, 3].

Particle physics

We simulate the production of a Higgs boson at the Large Hadron Collider experiments. For each collision, 42 observables are measured, and we try to infer the value of two parameters that characterize the effect of "new physics" on these interactions.

Right: Our new techniques (including SALLY, RASCAL) require substantially less training samples than established methods [2], and allow us to measure the parameters with higher precision.





[1] D. Rubin, Ann. Statist. 12 (4), p. 1151, 1984
[2] K. Cranmer, J. Pavez, G. Louppe [1506.02169]
[3] G. Papamakarios, I. Murray, T. Pavlakou, NIPS 2017 [1705.07057]

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