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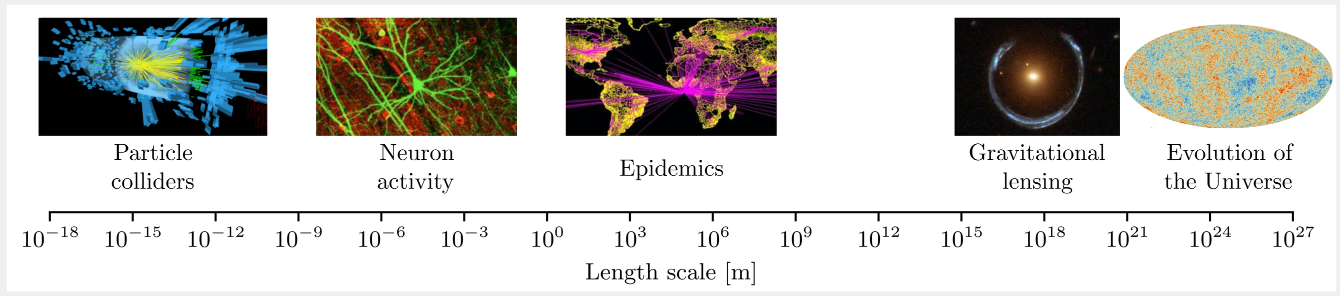
Mining gold: Improving simulation-based inference with latent information

Simulation-based inference

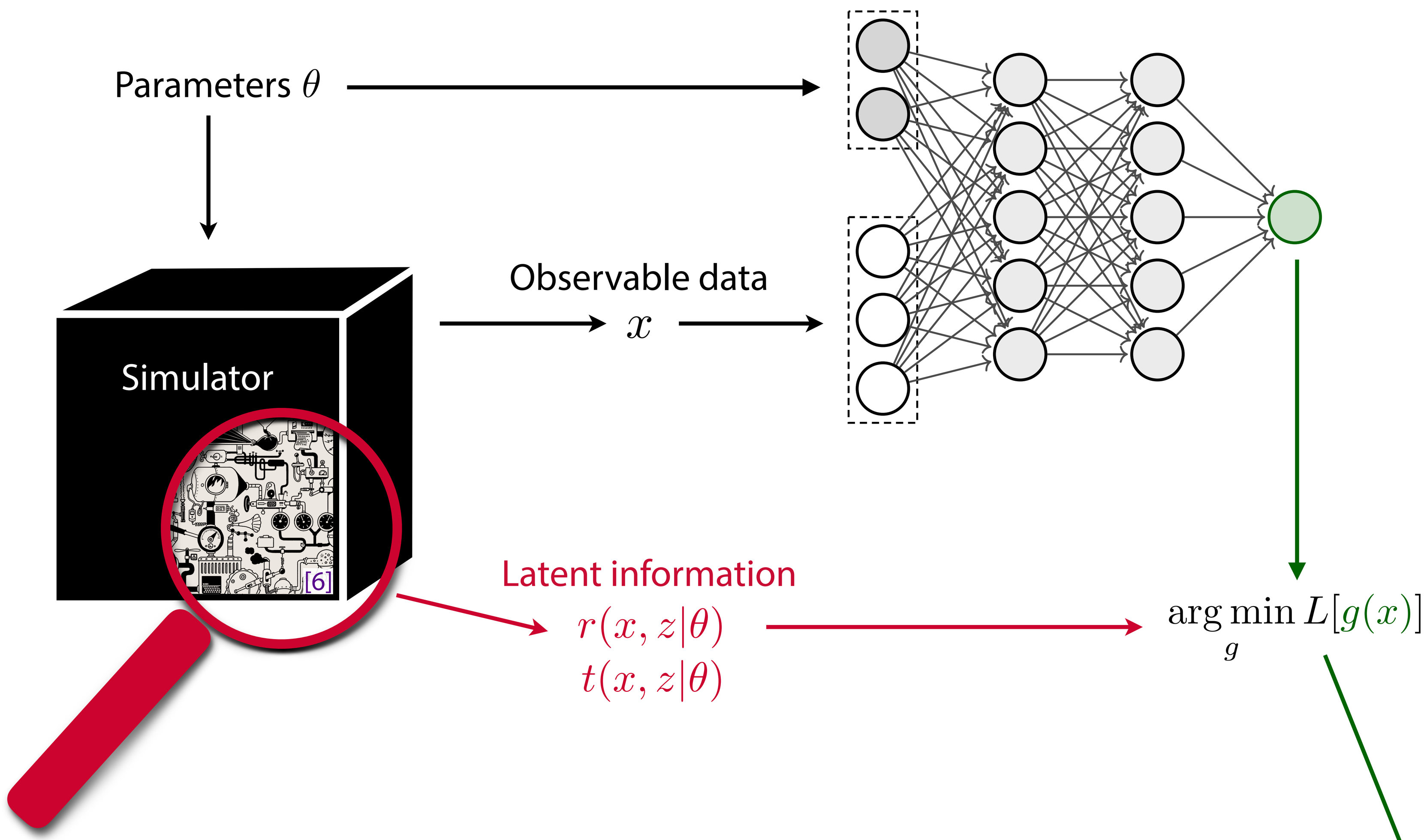
Kyle Cranmer, Johann Brehmer, Gilles Louppe: The frontier of simulation-based inference 1911.01429 | submitted to PNAS

- Phenomena across many scientific fields are described by complex simulators without a tractable likelihood function.
- Traditional likelihood-free inference methods like ABC [1] rely on low-dimensional summaries, losing information. New, amortized methods train neural networks (e.g. flows) as surrogates for likelihood [2-3] or posterior [4-5].
- Most methods treat the simulator as a black box. We show that we can reach into the simulator, extract information that characterizes the latent process, and use this information to train surrogates more efficiently. This is part of a broader movement towards the deep integration of autodiff and probabilitic programming elements into the simulator.



"Mining gold" from implicit models

Johann Brehmer, Gilles Louppe, Juan Pavez, Kyle Cranmer: Mining gold from implicit models to improve likelihood-free inference 1805.12244 | submitted to PNAS



1. We can extract more information from the simulator

In addition to the normal simulator input, the model parameters θ, and simulator output, the observables x, we can often extract two quantities from the simulator that characterize its latent process:

- the joint likelihood ratio $r(x,z|\theta) = \dfrac{p(x,z|\theta)}{p_{\mathrm{ref}}(x,z)}$
- the joint score $t(x,z|\theta) = \nabla_\theta \log p(x,z|\theta)$

They quantify how much more likely a particular execution of the simulator (with fixed latent variables z) becomes when changing the model parameters.

Strategies to open the black box

- Computation from existing simulator outputs based on domain knowledge
- Protocols like PPX [7]
- Simulators written as a probabilistic program [8]

2. This information can be used to train surrogates for the likelihood

The joint likelihood ratio and joint score can be used in several new loss functionals to train surrogates for the likelihood or likelihood ratio [see also 9].

For instance, we can train a normalizing flow with model density $\hat{p}(x|\theta)$ to learn the implicit likelihood $p(x|\theta)$ by minimizing

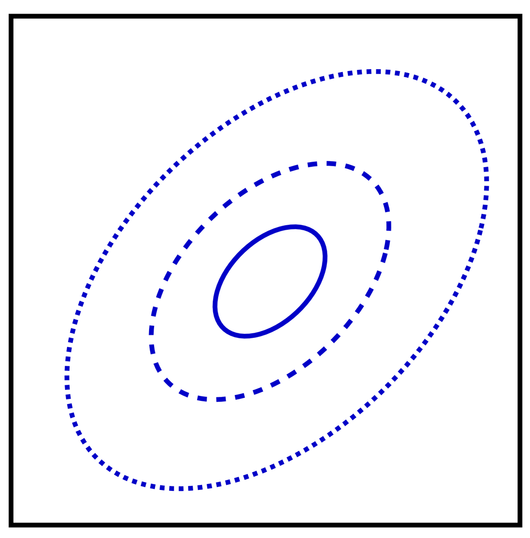
$$L[\hat{p}(x|\theta)] = \mathbb{E}_{\pi(\theta)} \mathbb{E}_{(x,z)\sim p(x,z|\theta)} \left\{ -\log \hat{p}(x|\theta) + \alpha \left| \nabla_\theta \log \hat{p}(x|\theta) - t(x,z|\theta) \right|^2 \right\}.$$

Why does this work?

The squared-error loss between $\nabla_\theta \log \hat{p}(x|\theta)$ and $t(x,z|\theta)$ is minimized by

$$\begin{aligned}\nabla_\theta \log \hat{p}^*(x|\theta) &= \mathbb{E}_{z\sim p(z|x,\theta)}[t(x,z|\theta)] = \int \mathrm{d}z \; p(z|x,\theta) \nabla_\theta \log p(x,z|\theta) \\ &= \int \mathrm{d}z \; \frac{p(x,z|\theta)}{p(x|\theta)} \frac{\nabla_\theta p(x,z|\theta)}{p(x,z|\theta)} = \int \mathrm{d}z \; \frac{\nabla_\theta p(x,z|\theta)}{p(x|\theta)} \\ &= \nabla_\theta \log p(x|\theta)\,.\end{aligned}$$

Surrogate for the likelihood $\hat{p}(x|\theta)$

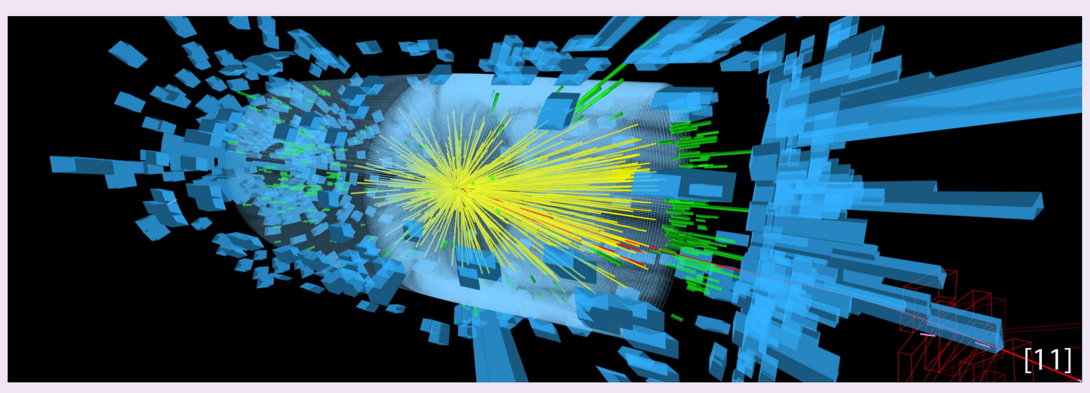


3. Inference with improved sample efficiency

A neural surrogate for the likelihood or likelihood ratio can be directly used for frequentist inference, or with MCMC or variational inference for Bayesian inference.

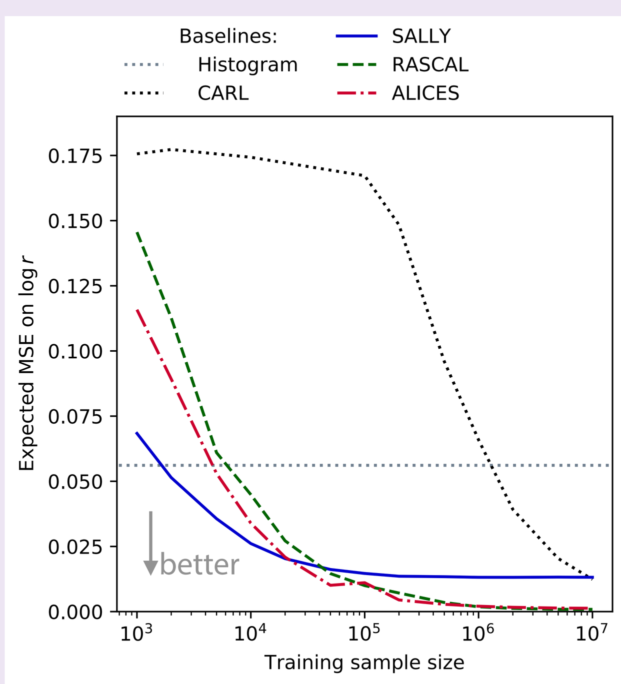
Using the latent information improves the sample efficiency of the surrogate model and ultimately the quality of inference.

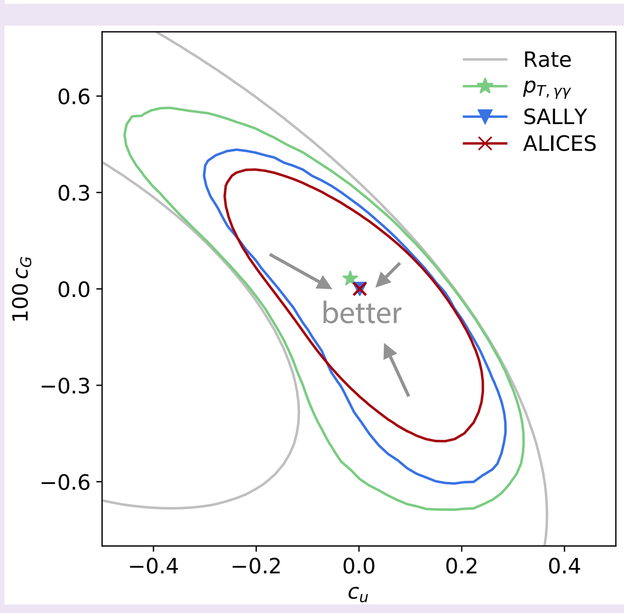
Hunting new physics at particle colliders



The LHC experiments collide protons close to the speed of light in maybe the most complicated machine ever built by humans, probing the laws of Nature at length scales down to 10^{-17} m.

We have automated the new inference techniques for these processes in the MadMiner library and studied many signatures [see also 11]. Compared to the industry standard, we find a dramatically improved sample efficiency (top right) and increased sensitivity to new physics (bottom right).



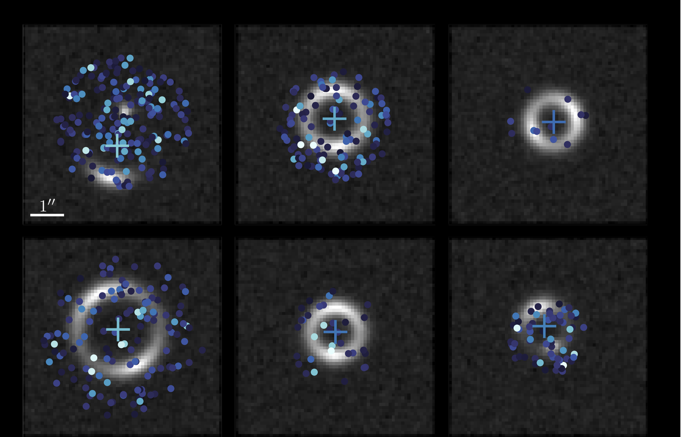


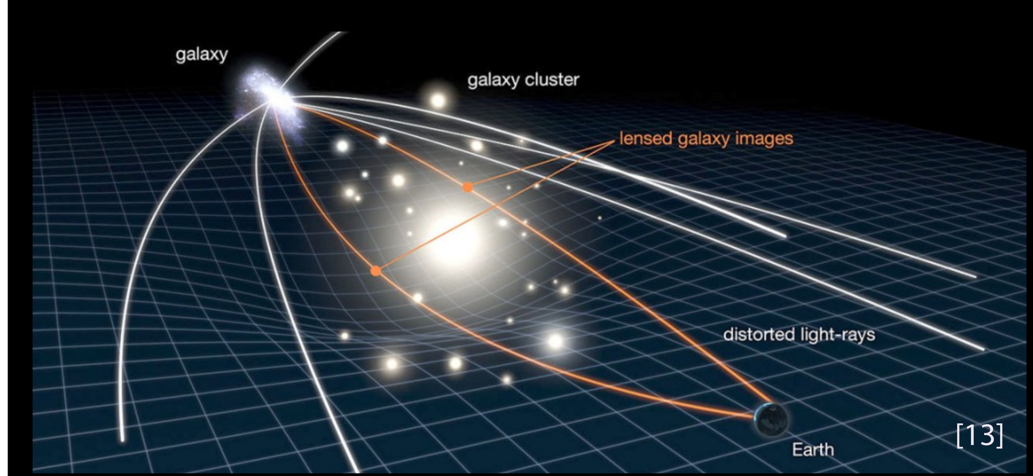
Johann Brehmer, Kyle Cranmer, Gilles Louppe, Juan Pavez: Constraining Effective Field Theories with Machine Learning 1805.00013 | Physical Review Letters

Johann Brehmer, Felix Kling, Irina Espejo, Kyle Cranmer: MadMiner: Machine learning-based inference for particle physics 1907.10621 | Submitted to Computing and Software for Big Science

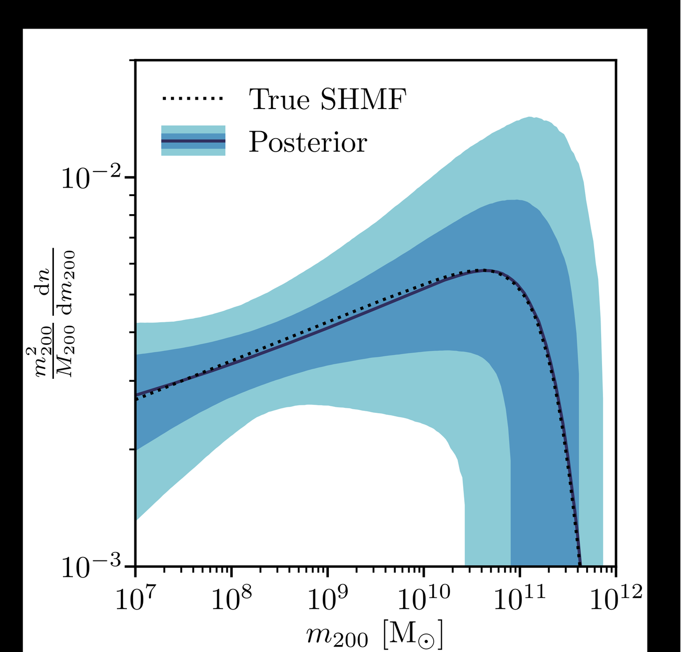
Dark Matter substructure from gravitational lensing

The same inference methods can be applied to systems spanning 10^{20} m: In gravitational lensing, light emitted from a background galaxy is bent by the gravitational field of another galaxy [12]. Its observation offers us the rare chance to search for clumps of Dark Matter, but the signals in the images are subtle.





We have built a simulator and implemented a "gold-mining" inference technique. On a synthetic data set (top right), this lets us successfully determine the distribution of Dark Matter substructure (bottom right).



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[11] Image source: CDS
[12] A. Einstein 1915
[13] Image source: NASA/ESA