Impressions PHYSTAT: Stats Meets ML

Lukas Heinrich, 12. Sept. 2024

Bayesian Methodologies with pyhf

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> Abstract. bayesian_pyhf is a Python package that allows for the parallel Bayesian and frequentist evaluation of multi-channel binned sta-

Profile Likelihoods in Cosmology: When, Why and How illustrated with Λ CDM, Massive Neutrinos and Dark Energy

> Laura Herold,¹,^{*} Elisa G. M. Ferreira,² and Lukas Heinrich³ ¹Department of Physics and Astronomy, Johns Hopkins University, 3400 North Charles Street, Baltimore, Maryland 21218, USA ²Kavli Institute for the Physics and Mathematics of the Universe (WPI),

My 5-D 14-Dimensional Outline

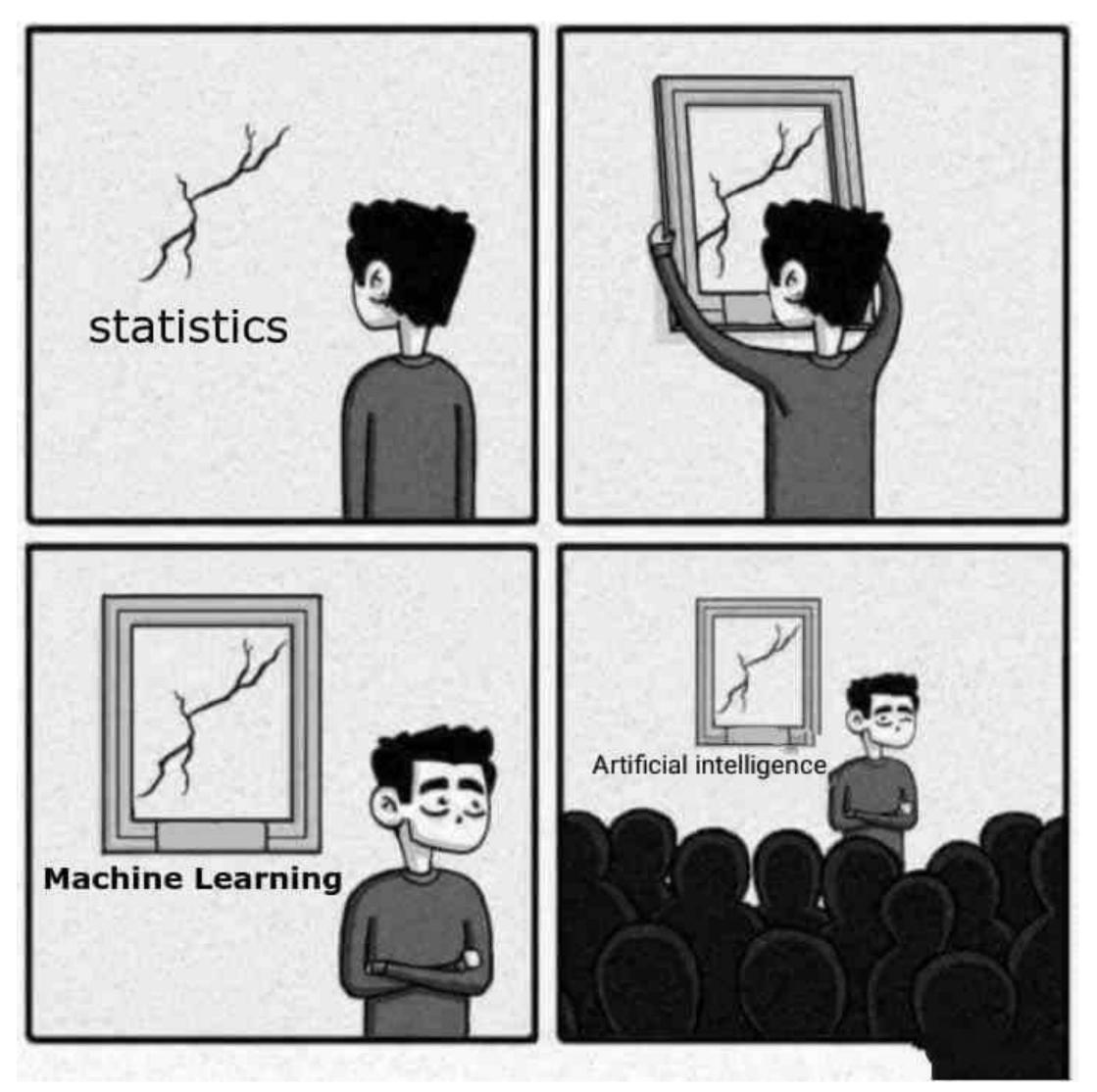


To deal with a 14-dimensional space, visualize a 3-D space and say 'fourteen' to yourself very loudly. Everyone does it.

— Geoffrey Hinton —

AZQUOTES

Stats Meets ML?



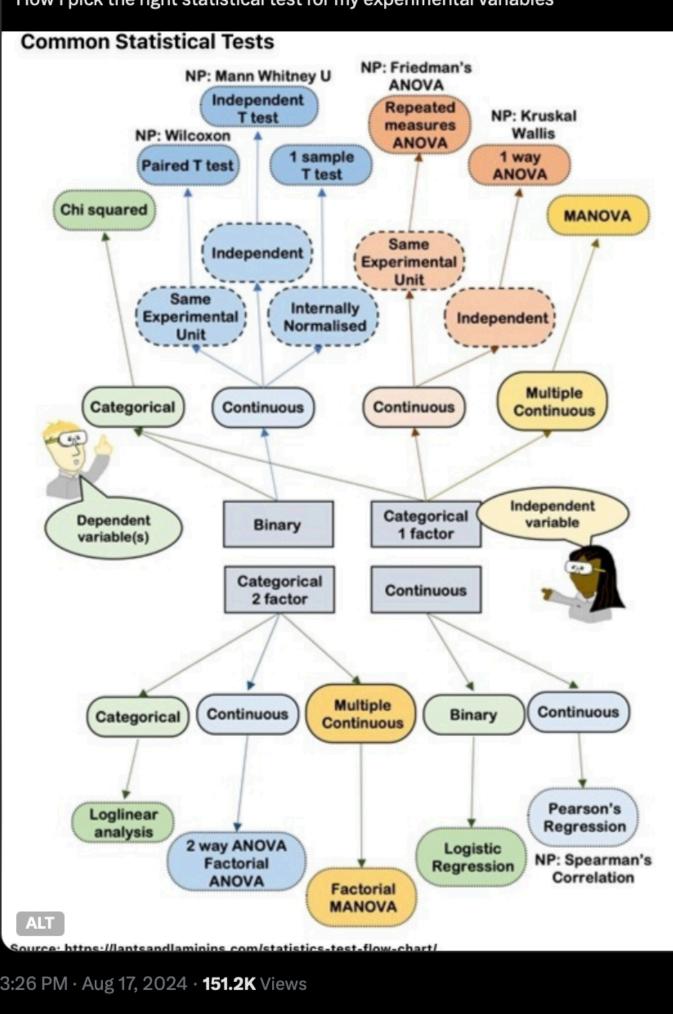
Stats Meets ML?

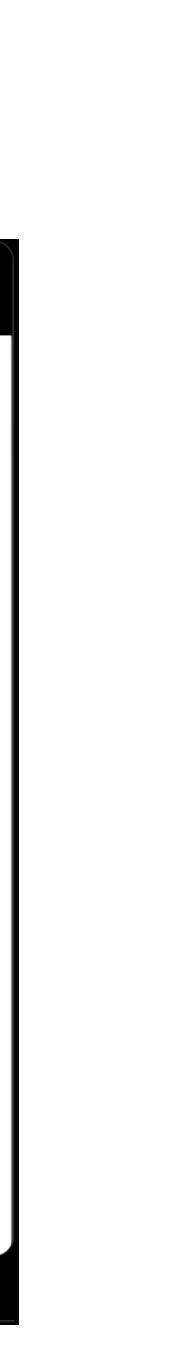
...



Whenever people say "statistics and machine learning are the same thing" just know that not a single person in machine learning knows (or cares about) any of this.

Prof Lennart Nacke, PhD 🤣 @acagamic · Aug 15 How I pick the right statistical test for my experimental variables

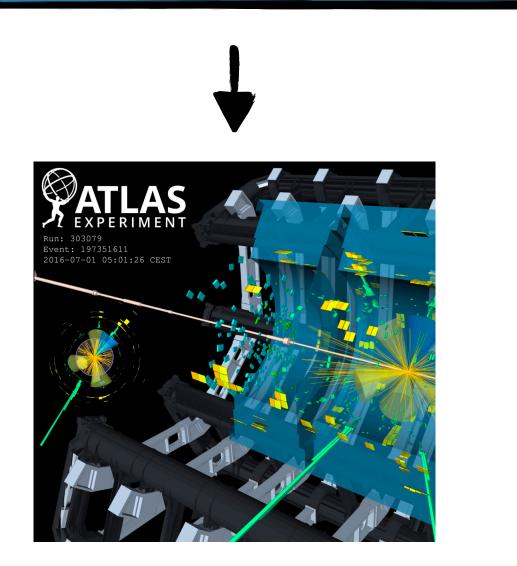




HEP (and others) & ML: deeply related

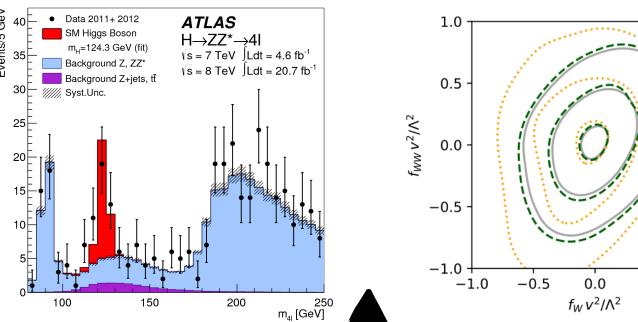
$$\begin{aligned} \mathcal{I} &= -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ &+ i \overline{\psi} \overline{\psi} \psi + h.c. \\ &+ \overline{\psi} \overline{\psi} \overline{\psi} \overline{\psi} + h.c. \\ &+ \overline{\psi} \overline{\psi} \overline{\psi} \overline{\psi} \overline{\psi} - V(\phi) \end{aligned}$$

generate low-level, high-dim data from high-level concepts

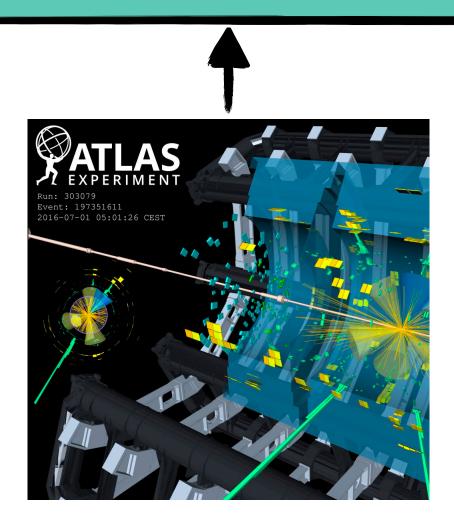


High-Level Concept





reconstruct high level concepts from low-level, high-dim data



0.5

1.0

HEP (and others) & ML: deeply related

street style photo of a woman selling pho at a Vietnamese street market, sunset, shot on fujifilm

generate low-level, high-dim data from high-level concepts

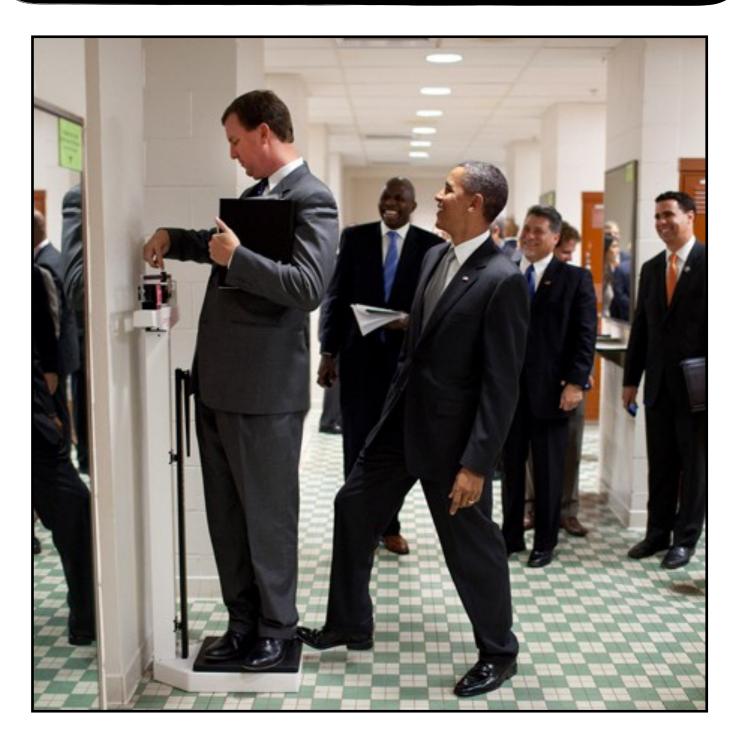


This is a picture of Barack Obama. His foot is positioned on the right side of the scale. The scale will show a higher weight.

High-Level Concept

Low-Level Data

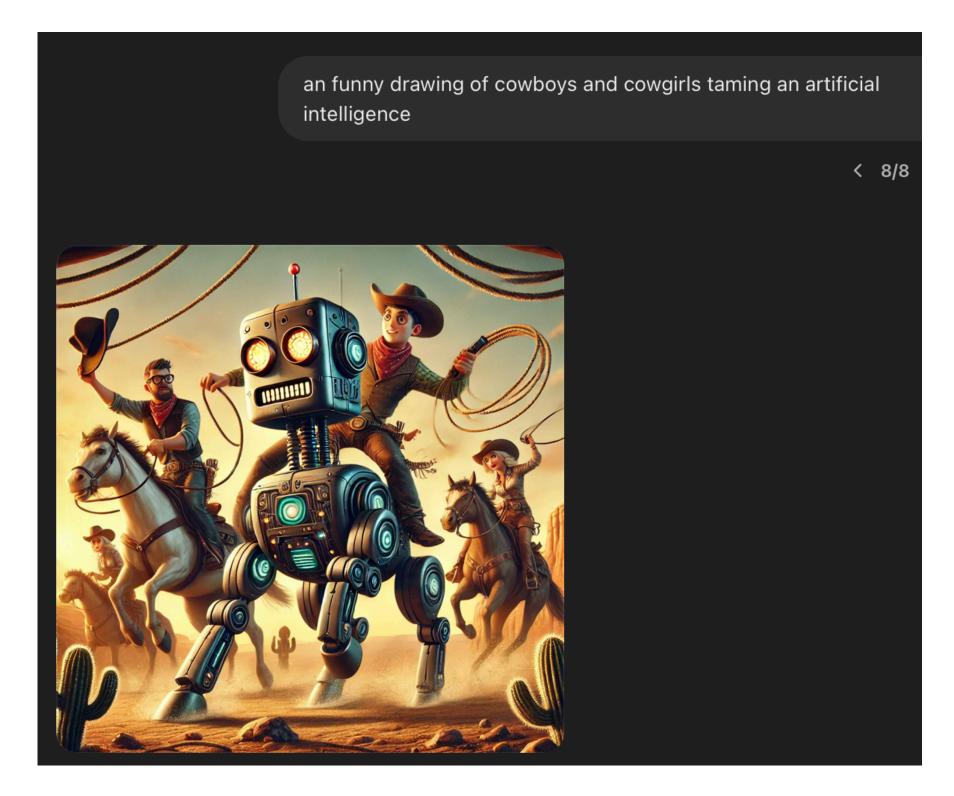
reconstruct high level concepts from low-level, high-dim data





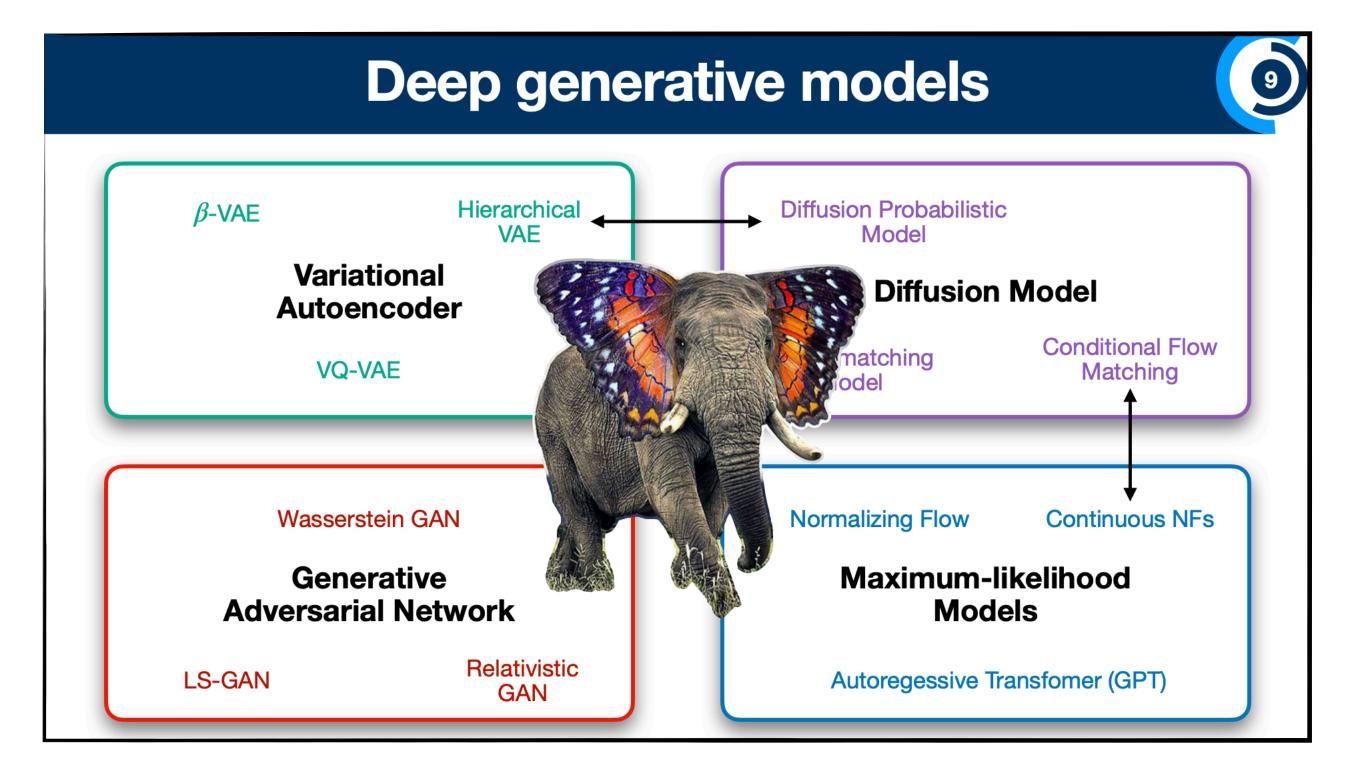
ML Wild West

A focus of the last years is to "to learn the technology" - build up



(Gregor)

- technical capability around this new set of "new numerical tools" (Tilman)
 - We have gotten very good at this



(Ramon)

ML: Eierlegende Wollmichsau?

\$

The "Eierlegende Wollmilchsau" (German for "egg-laying wool-milk-sow") is a humorous metaphor used to describe something that is supposed to do everything, typically in an exaggerated and impossible way. It represents a creature that lays eggs, produces wool, gives milk, and functions as a pig.

I'll create a whimsical and surreal image of this fictional creature combining elements of a pig, sheep (for wool), cow (for milk), and hen (for eggs), in a humorous and exaggerated style.

Generating this now!



Here is a whimsical representation of the "Eierlegende Wollmilchsau," capturing the fantastical nature of this humorous creature. Let me know if you'd like any changes!

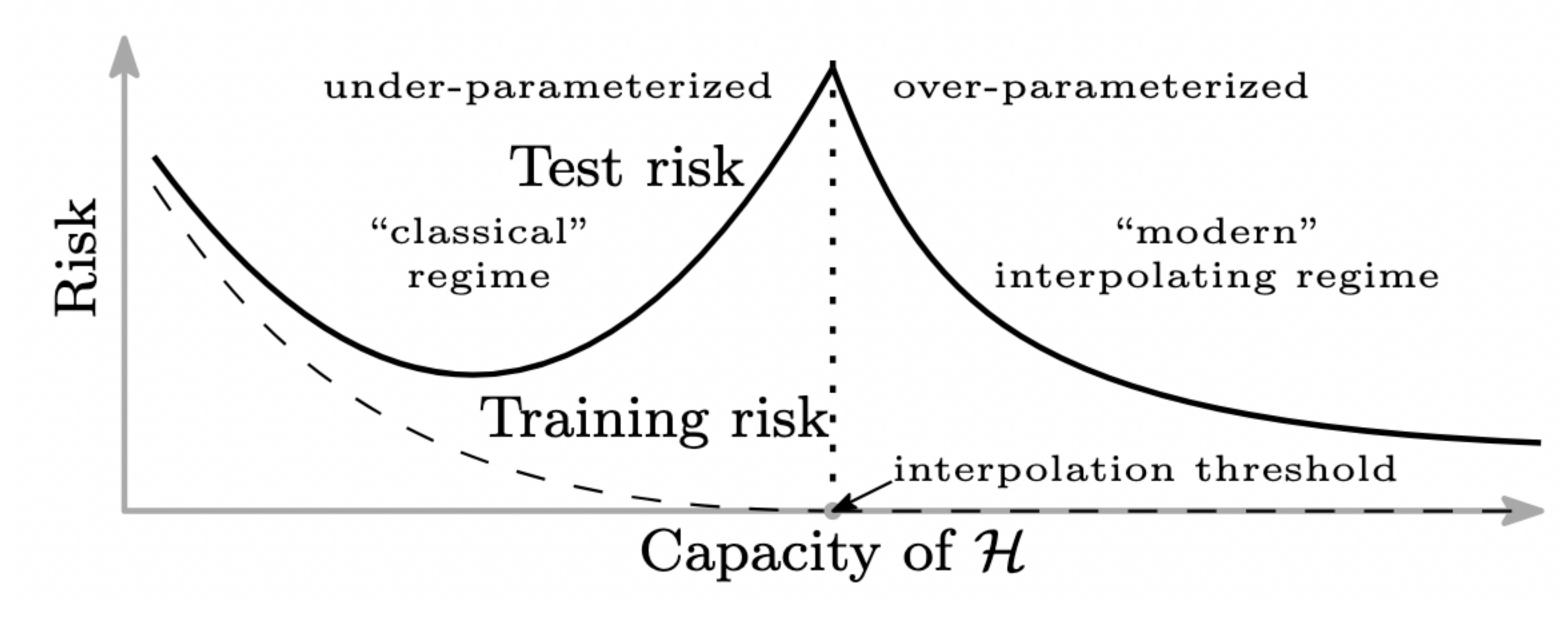
A picture of a Eierlegende Wollmichsau

(Ramon)

Where can a Statistical Point of View help?

ML is an extremely empirical science. In many ways it's successful because it ignored theory to some extent

help us tame ourselves.



- is this the Feldman-Cousins of ML? ;)

But once we tame this new technology maybe stats can in some ways

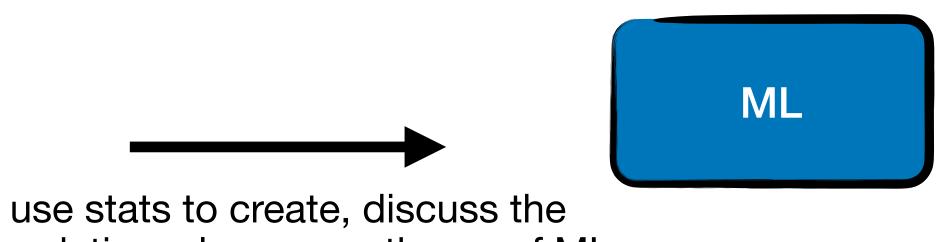
but e.g. interestingly, this just re-discovered some old statistics

(Pierre)

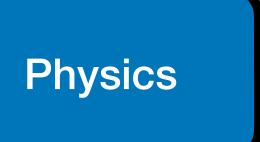


Statistics

Where is the Statistics ?



foundations, language, theory of ML



use ML to essentially implement the statistics workflow



Where is the Statistics ?

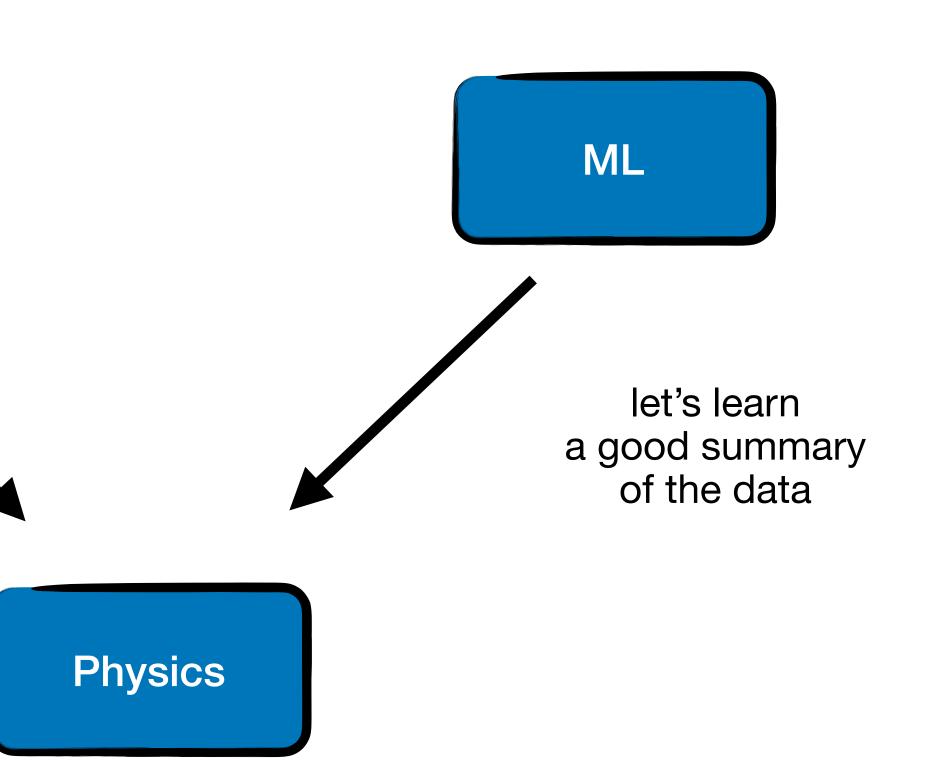




Statistics

hey physics, to do stats you need a good summary statistic

Where is the Statistics ?



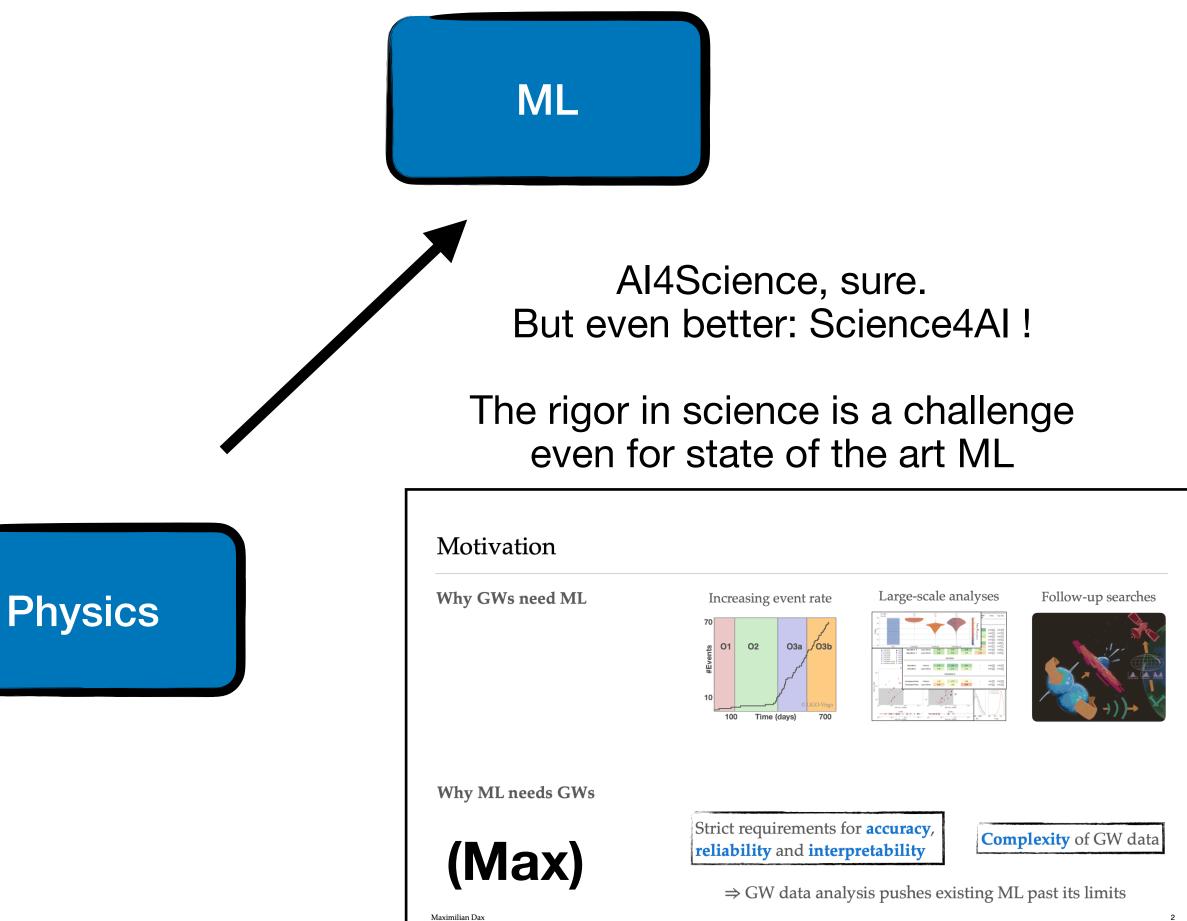
Where is the Statistics ?

Our Delusion of Grandeur (or not?)

Statistics

original PHYSTAT credo:

maybe our problems in limit-setting, are actually research problems in stats?





Anomaly Detection

Statistics can help bring clarity to how we frame ML use-cases where do we want statistical power?

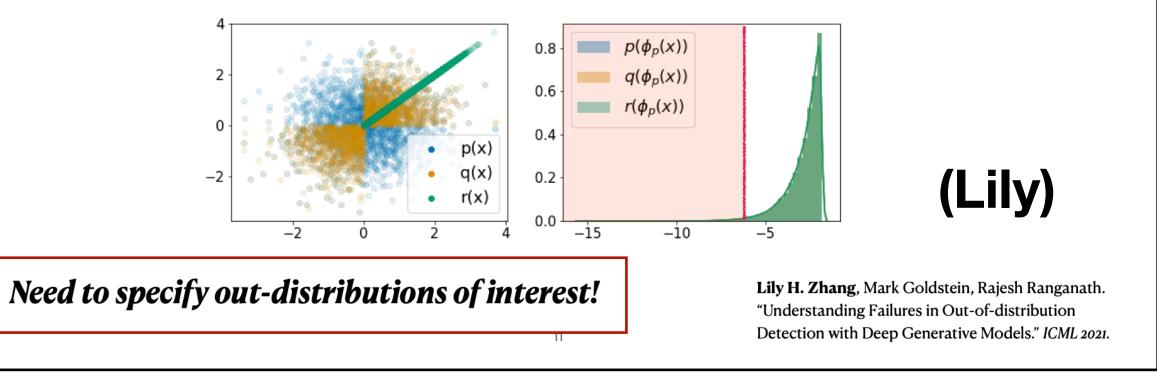


Proposition (informal): No method can guarantee performance better than random guessing without assumptions on the out-distributions.

This is the key in AD:

Are we ready to do it? If yes in what language?

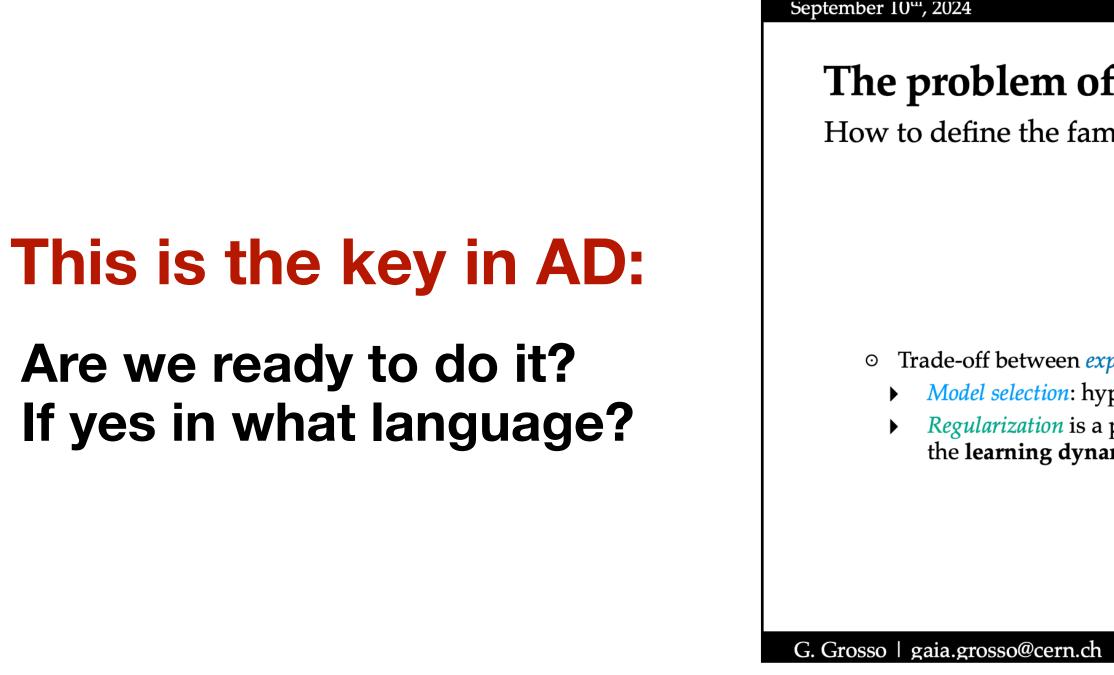
What's the right way to perform anomaly detection?



Ultimately goes back to what we learn in Stats Intro: there no universal most powerful test

Anomaly Detection

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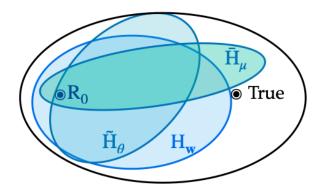


Challenge to Theorists: How do we specify theories we care about without specifying the Lagrangian? (History: GUT Theories \rightarrow Simplified Models \rightarrow ???)

The problem of *model selection*

How to define the family of universal approximants?

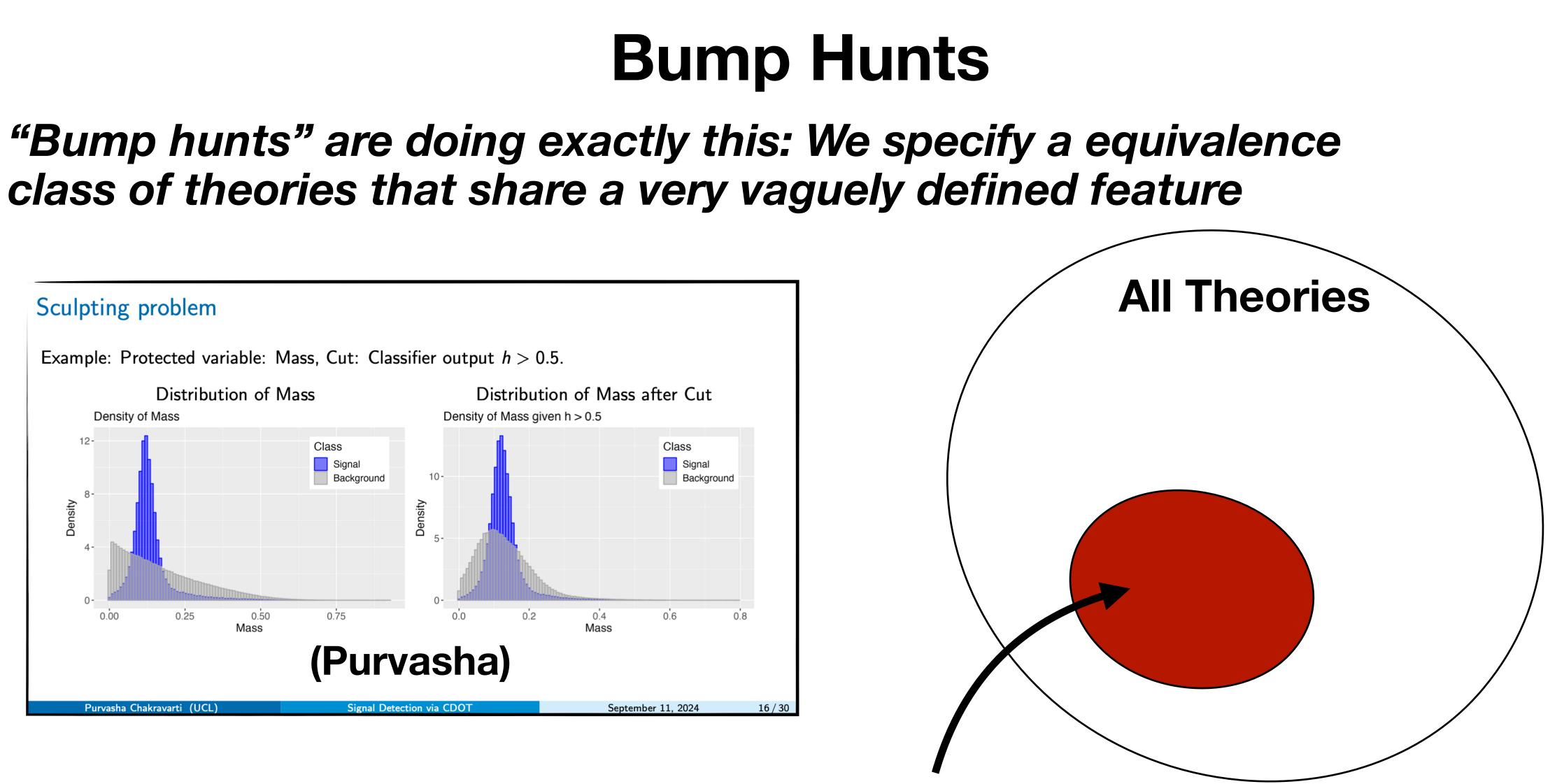
$$f(x, w) = \log\left[\frac{n(x \mid D)}{n(x \mid R)}\right]$$



Gala

- Trade-off between *expressivity* and *specificity* is required
 - *Model selection*: hyper-parameters choice poses hard constraints.
- *Regularization* is a powerful form of *inductive bias* (e.g. smoothness) affecting the learning dynamics

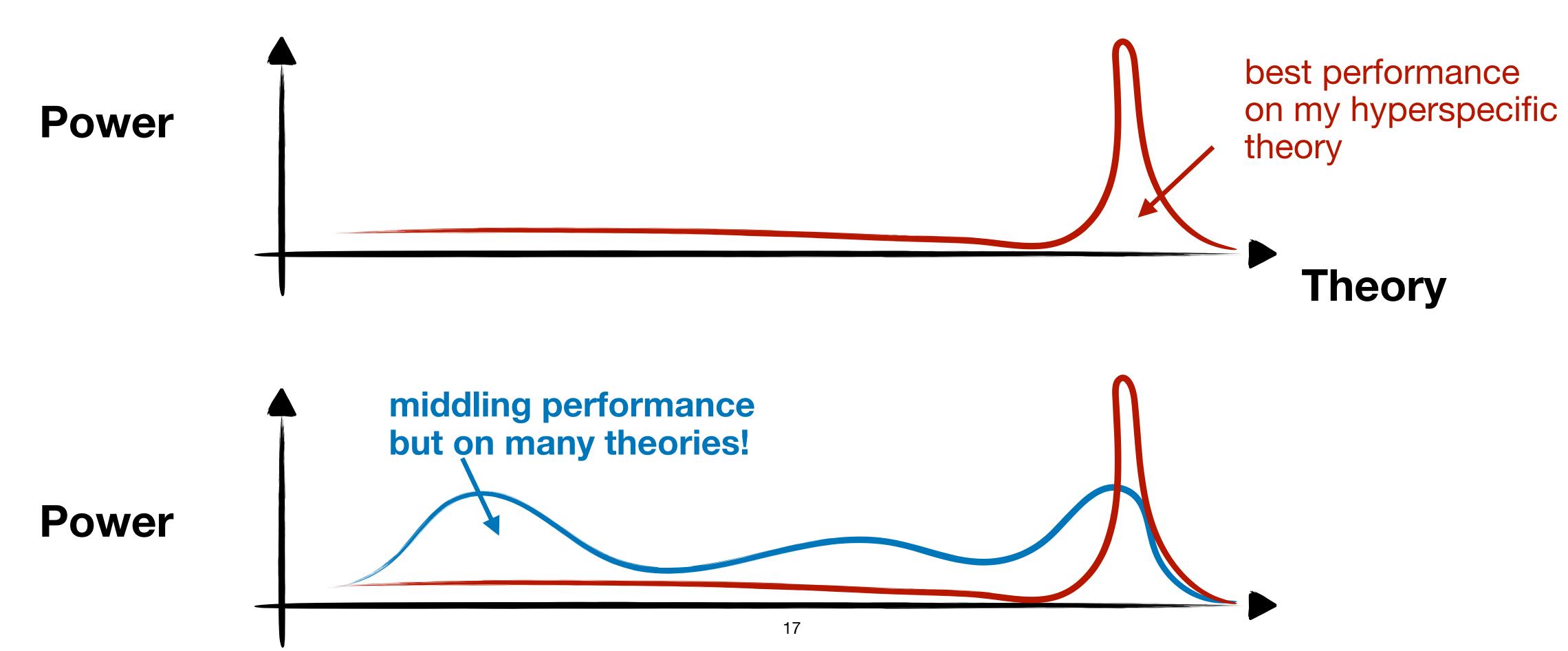
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Theories with a resonance at mass M (irrespective of the rest)

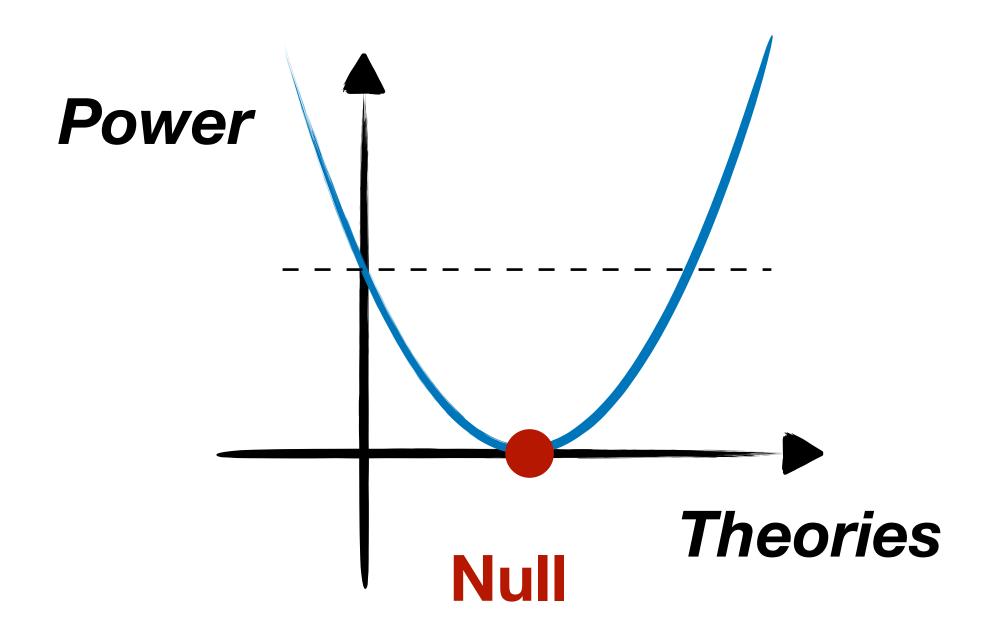
Anomaly Detection + Reinterpretation

The Story from Simplified Models Repeat: we give up power for any one specific theory: Effective in Multiple Testing Scenarios

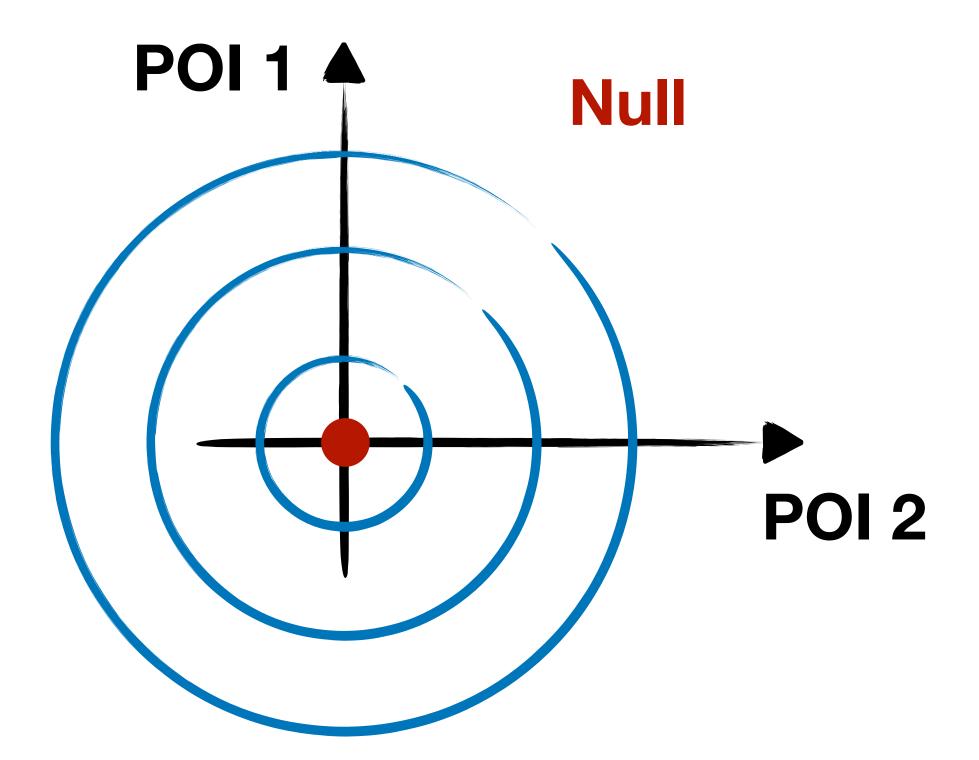


Reminder of Motivation of Profile L'hood

Profile Likelihood is designed to have ~ roughly equal power for all and we could make other once



alternatives that are "equally far away" from the null. It's a specific choice



Anomaly Detection

Statistics can help bring clarity to how we frame ML use-cases

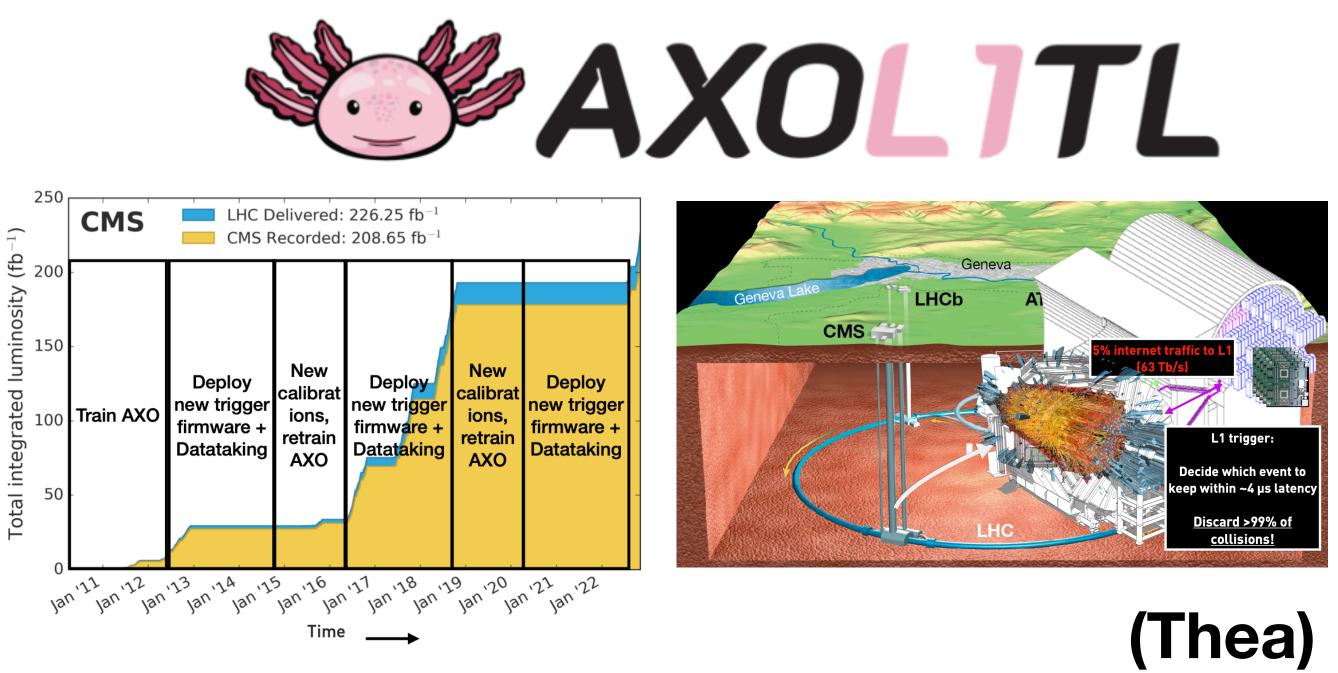
To me a useful experimentalist framing (and a Q I ask often)

You have 5 AD algorithms, but only **100 Hz of Bandwidth in the Trigger**

How do you decide which one to deploy?

If the answer involves any reference to performance on simulation, we essentially made a choice in theory space

Big jump in technical readiness in extreme environments:



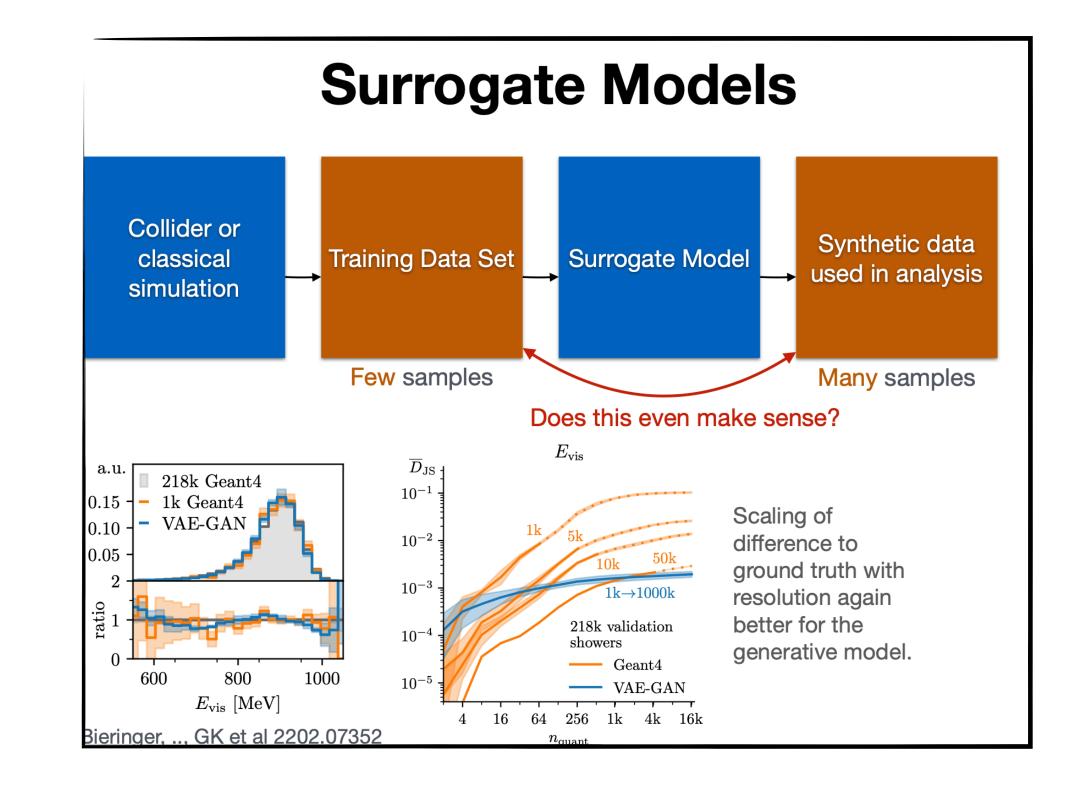
Confident we can implement any answer we come up with

Can you really create information out of nothing? No, so what's going on?

2. Generative models for many fast simulations from few full ones.

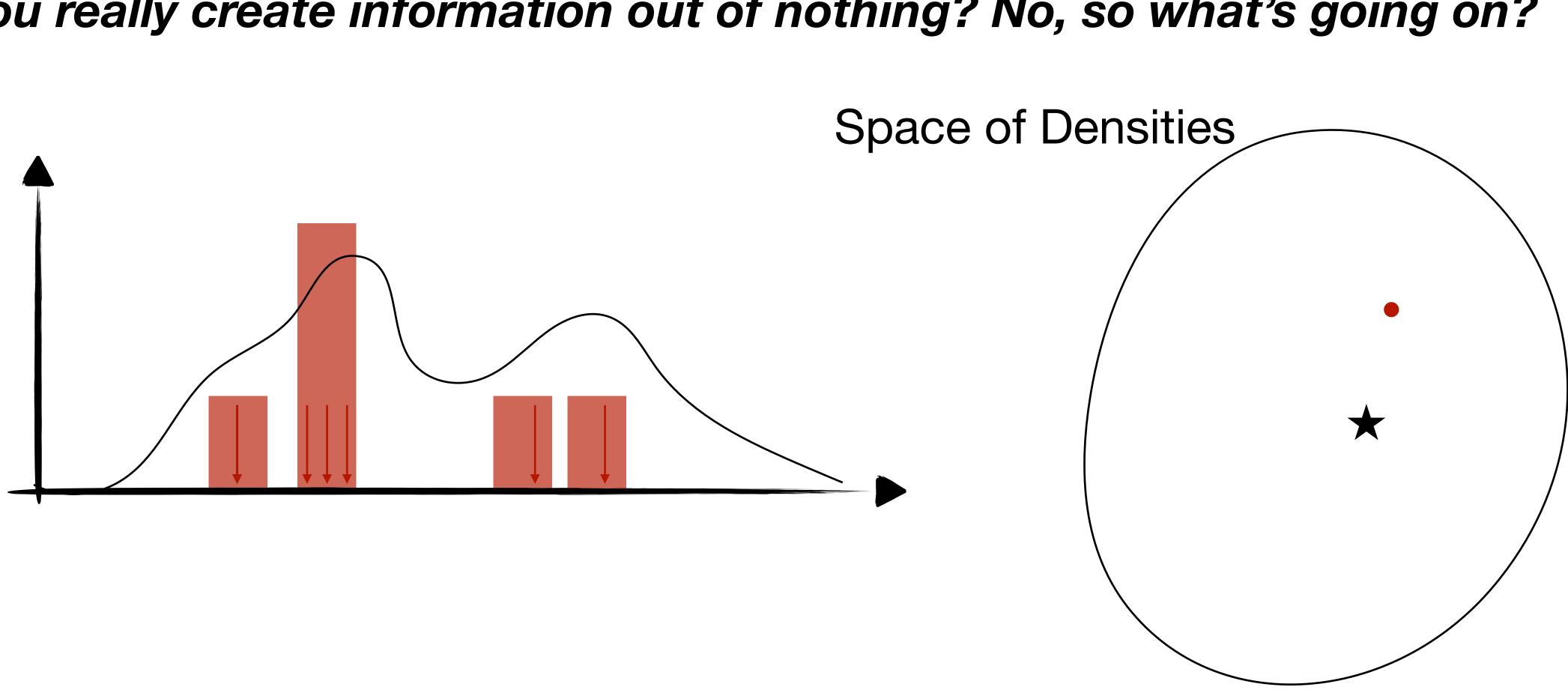
What do we gain by using ML to learn from a few fully simulated events how to generate a large number of events quickly?

For example, we believe some (x,y) data should lie on a straight line and are interested in the gradient. With difficulty we do a full simulation of 4 (x,y) points. Our ML procedure learns from these 4 points how to generate new data, and produces 1000 new (x,y) pairs. The statistical uncertainty on the gradient is greatly reduces, but there is a large systematic related to the particular choice of the initial 4 points. Is there anything that we can useful we can learn from the larger sample? Are generative methods different from this in some subtle way?

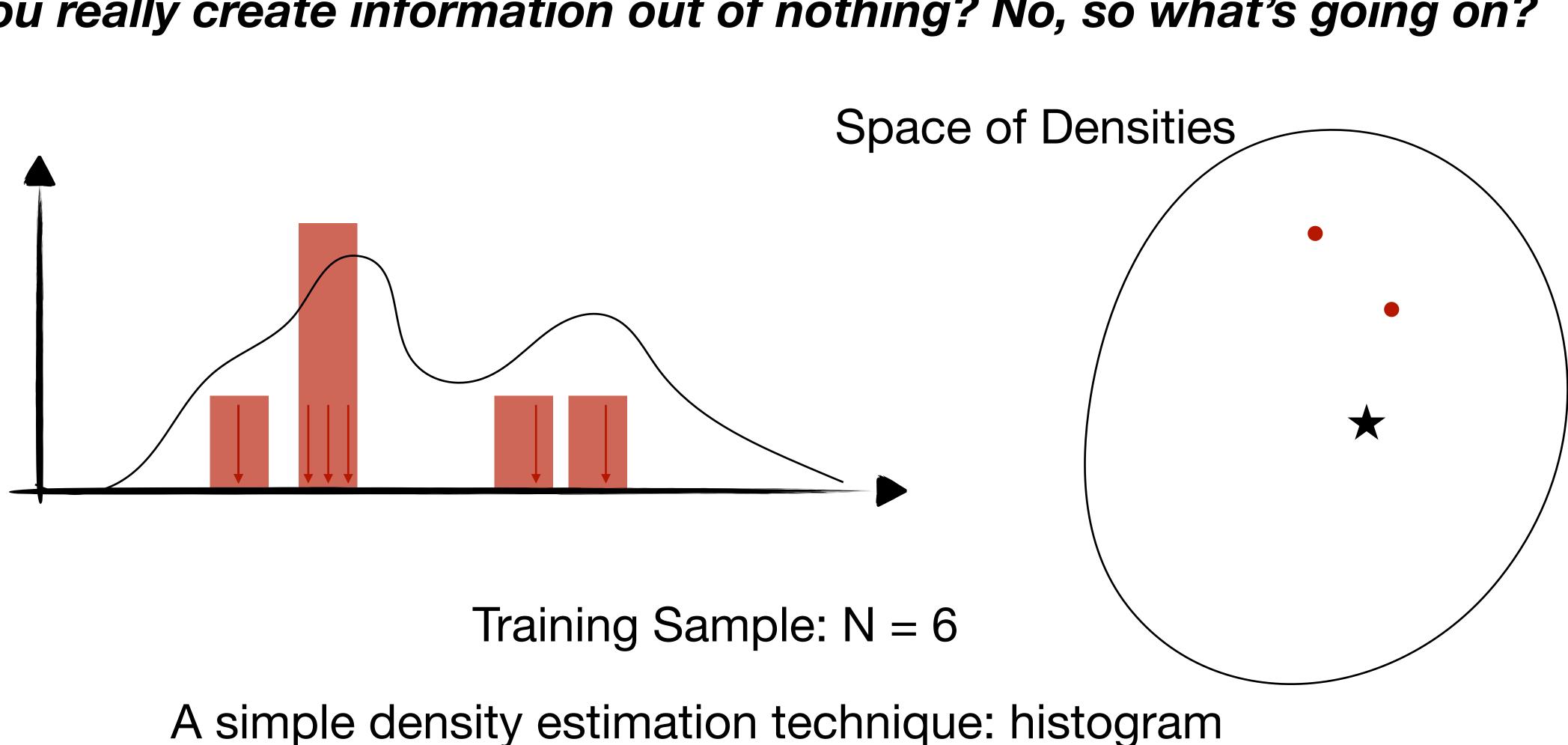




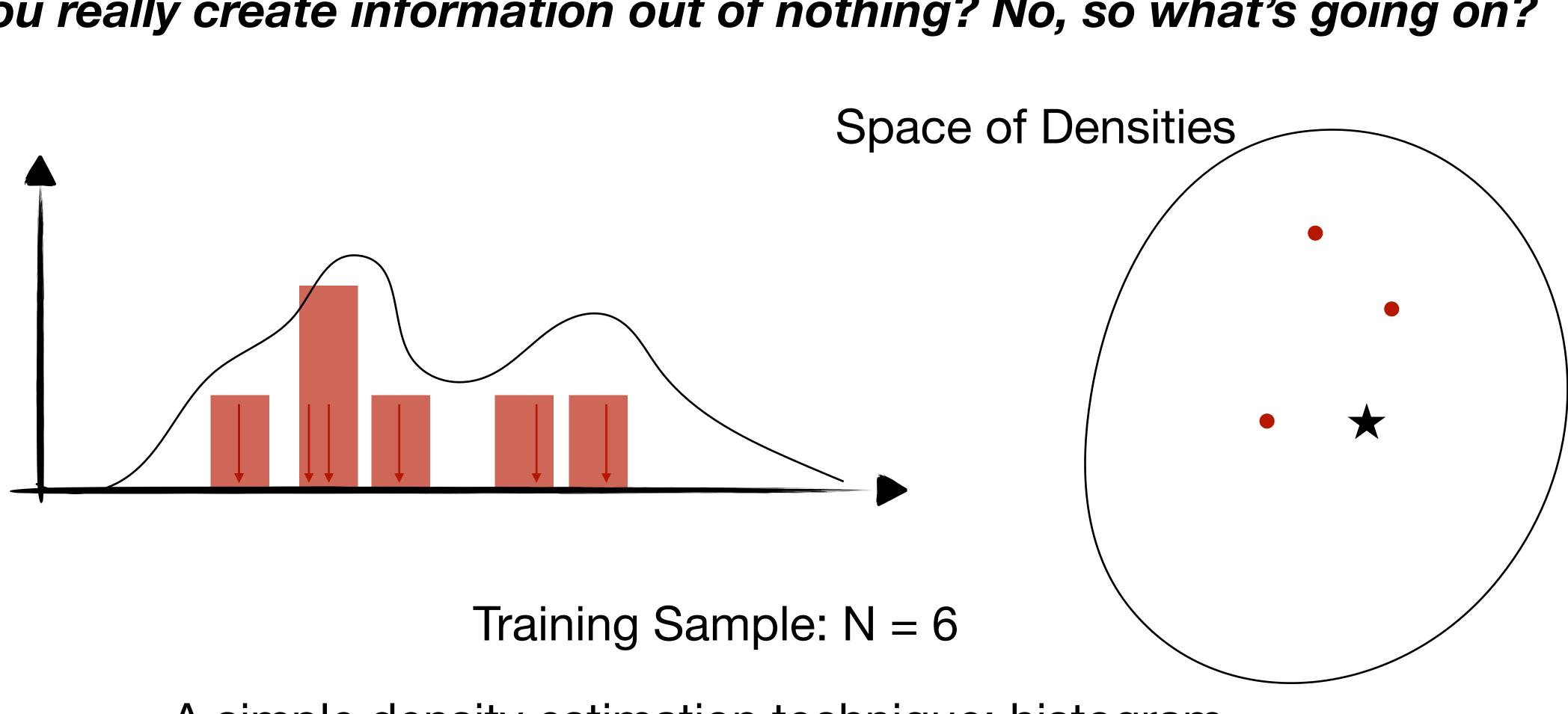
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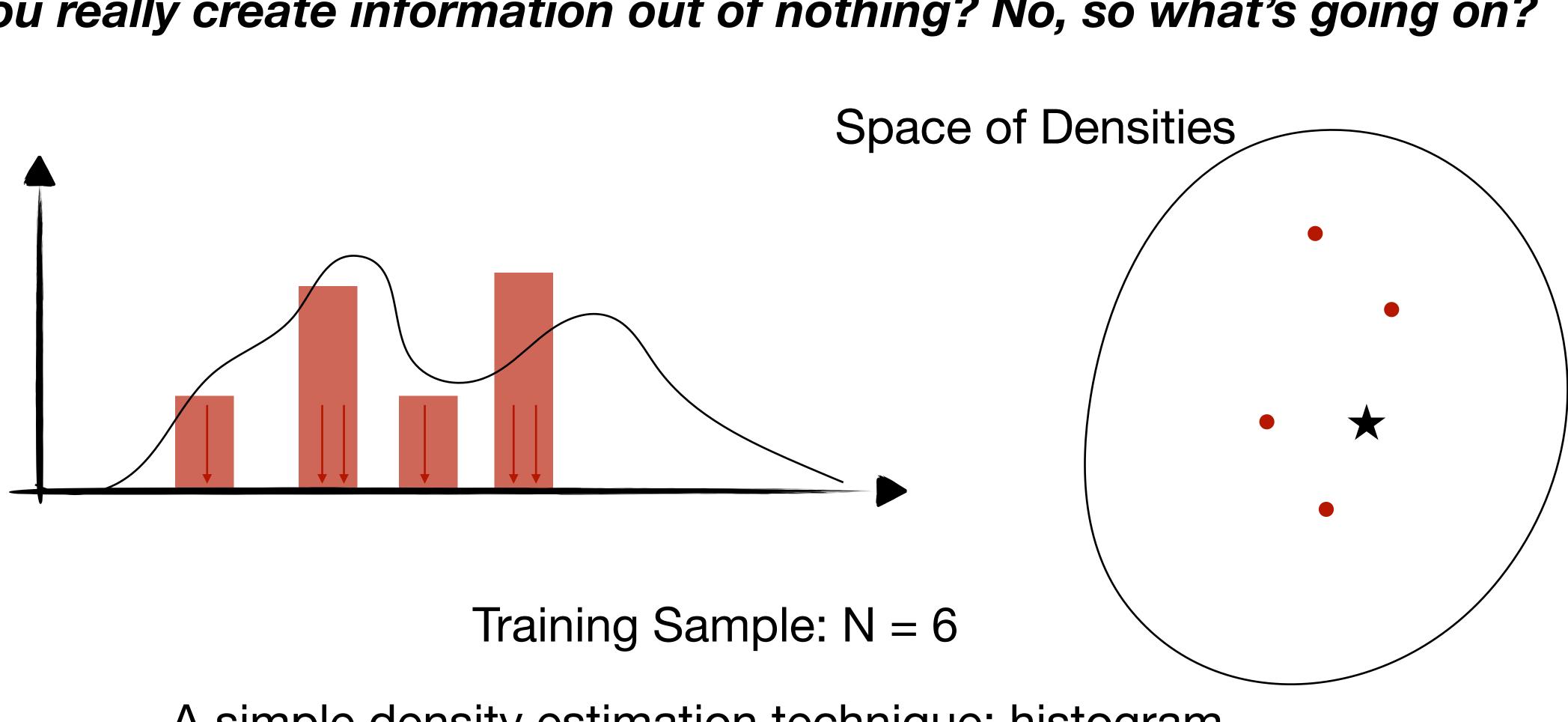


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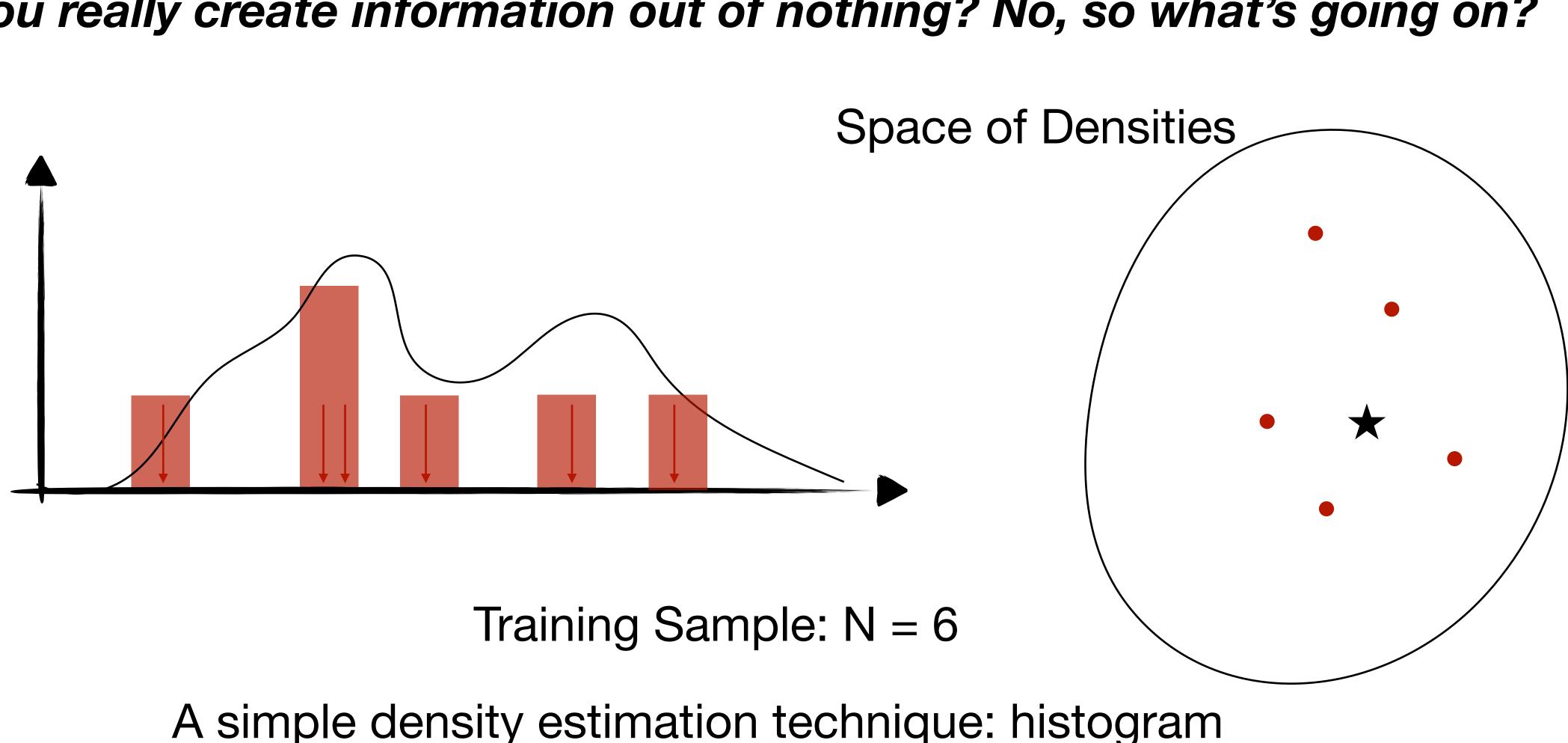
A simple density estimation technique: histogram

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A simple density estimation technique: histogram

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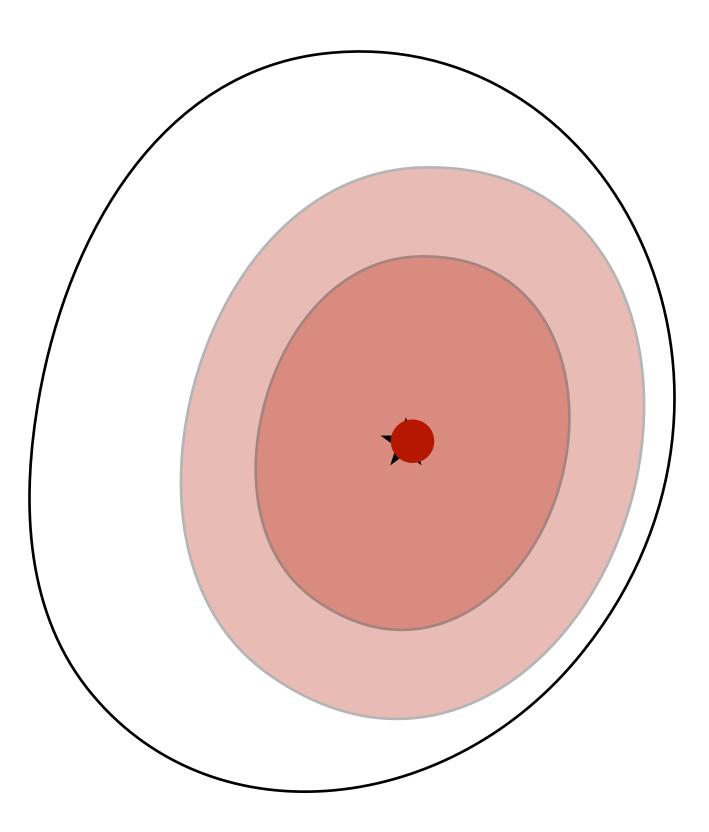


If we repeat this many times we can see how this density estimator fares

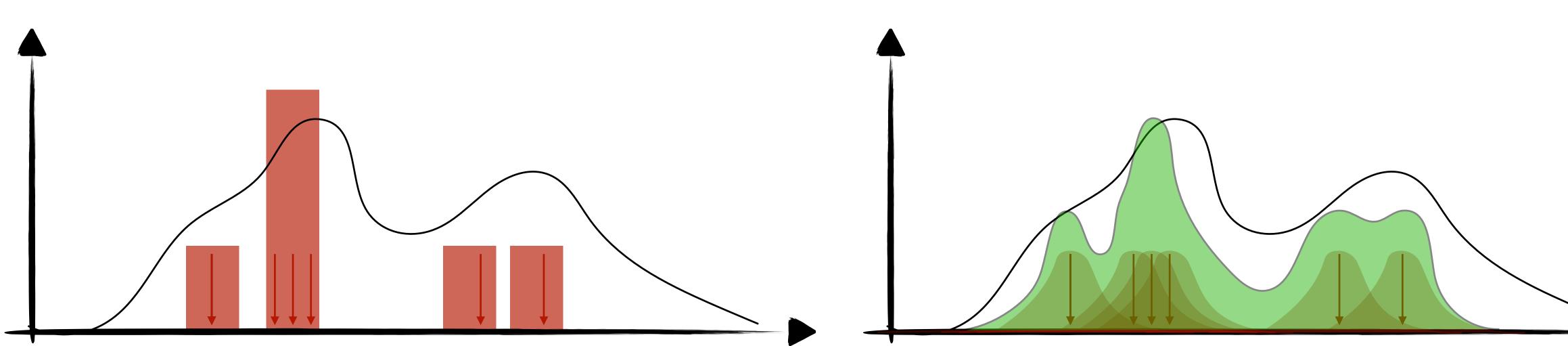
Unbiased: We sample from the real thing

High-Variance: with few samples, the estimate is all over the place from sampling variance

What we usually call "MC Stat Error"



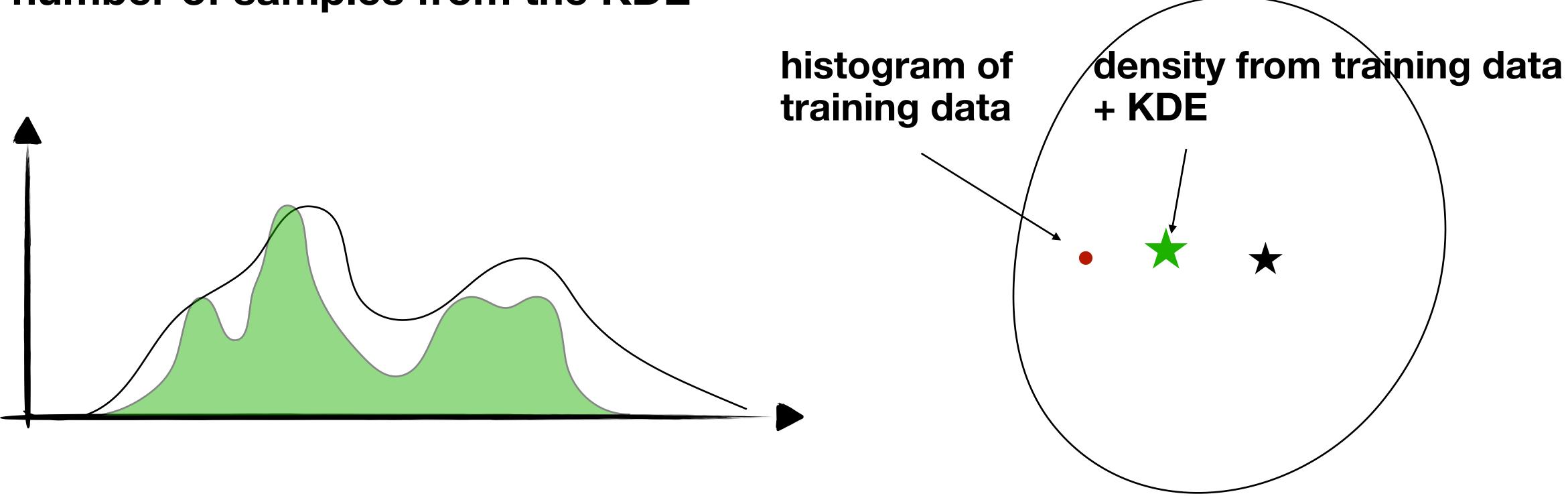
Nobody forces us to use mere histograms. A frequent idea that comes up: couldn't we do some other type of density estimate?



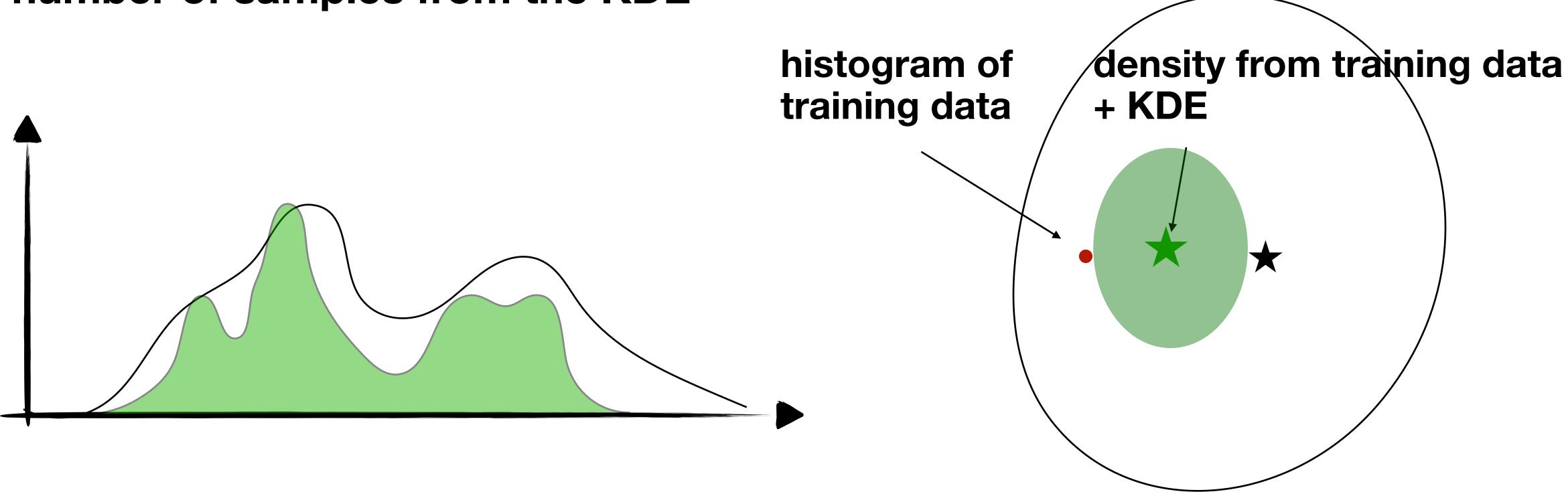
(like a pre-historic normalizing flow)

KDE of 6 samples: This is a density model and generative model!

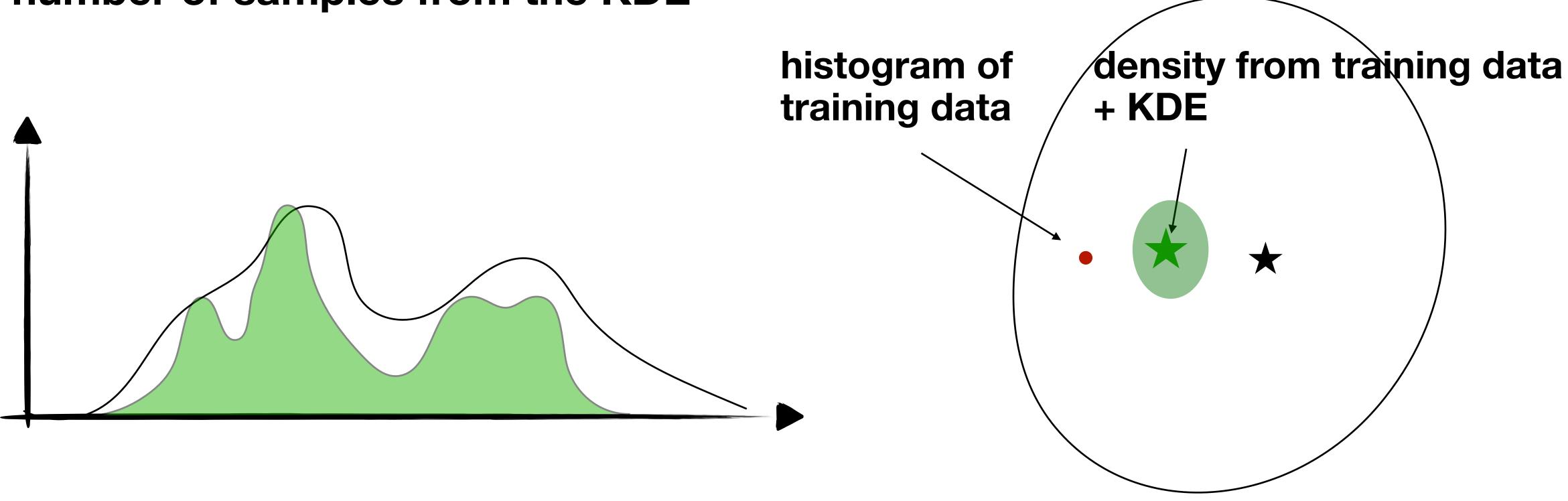
You can now sample quickly (call it "fast simulation") basically an infinite number of samples from the KDE



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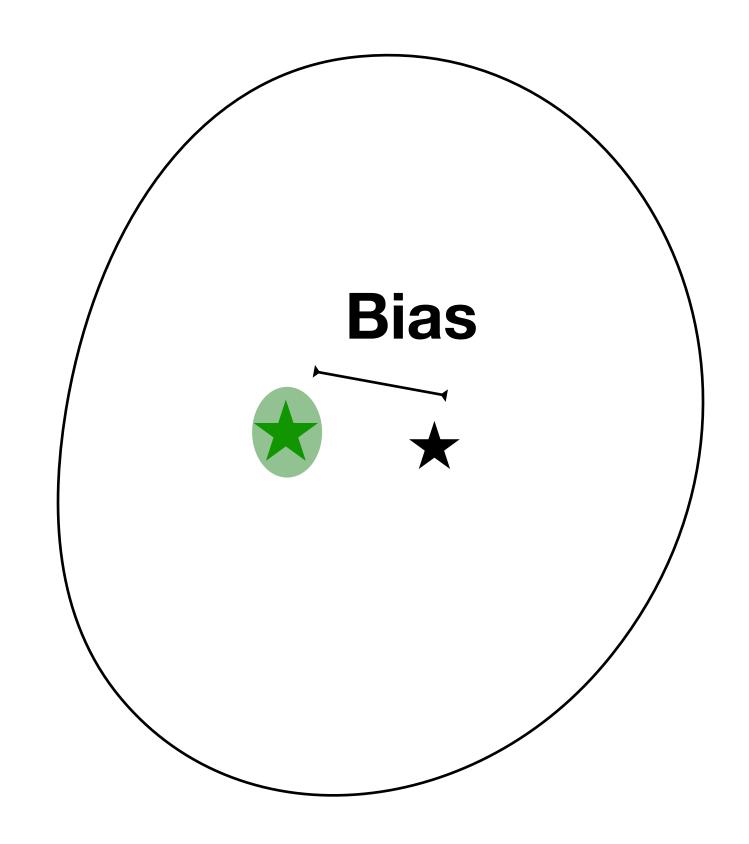
You can now sample quickly (call it "fast simulation") basically an infinite number of samples from the KDE



How do we characterize this estimator?

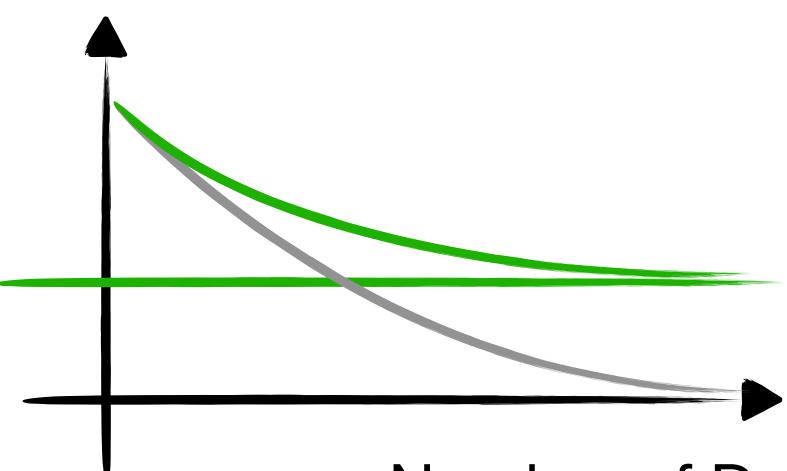
Biased: this depends basically depends on which training data + hyperparameters (bandwidth, etc)

Zero-Variance: if we can draw an infinite amount from this we can make it arbitrarily small



So how do the two compare?

sampling from Geant converges to true zero MSE



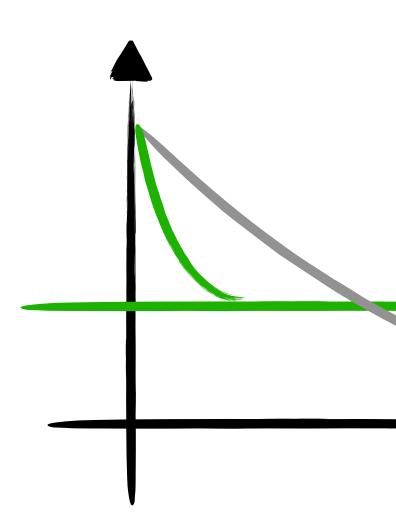
sampling from generative model converges to its inherent bias

Number of Drawn Samples



So how do the two compare?

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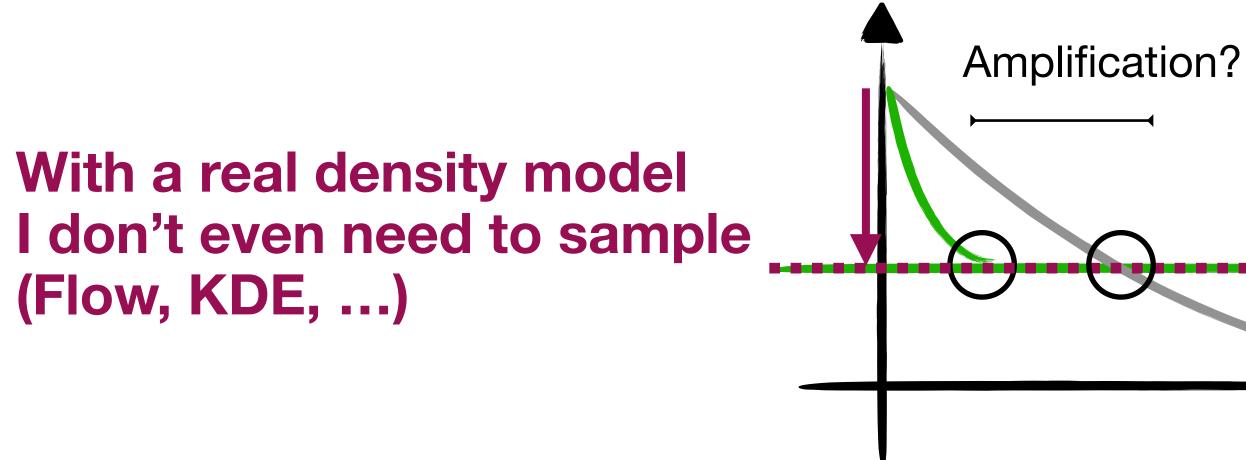
but this sampling is much faster! shrink time scale!





So how do the two compare?

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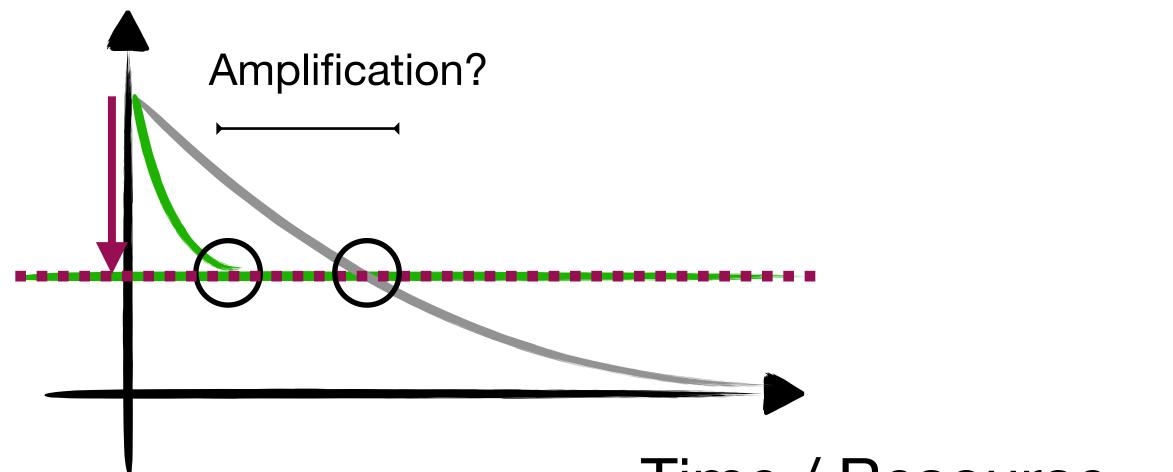
Time / Resource

You can reach same "MSE" in shorter (or zero) time...



In a way this just the bias-variance tradeoff. We trade off

- a zero-bias ~high-variance strategy (samples from G4 + naive histograms) biased, ~zero-variance strategy (density estimate trained on few samples e.g. KDE, Flows, GANs, ...)



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- a zero-bias ~high-variance strategy (samples from G4 + naive histograms) biased, ~zero-variance strategy (density estimate trained on few samples e.g. KDE, Flows, GANs, ...)

But it's a bit apples to oranges



biased, no-variance

Amplification only happens if you use a fancy density estimate on few samples to compare to a dumb density estimate with many samples

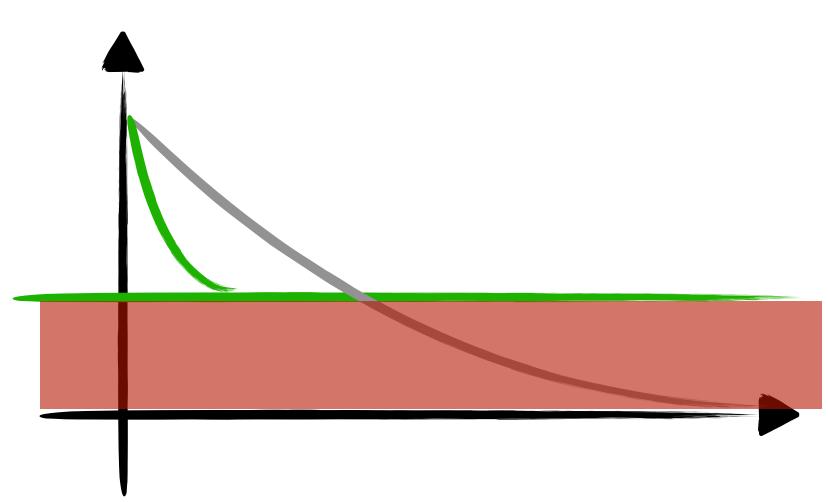


unbiased, high-variance



Amplification? This is a one-time gain. You can benefit from regularization once. But there is no general rule where 1 GenAl event $\approx 1/100$ Geant Event (i.e. if GenAl were 100x faster you would gain)

With a fixed generative model, you will never reach the true distribution no matter how many samples you draw. With Geant4 you will.



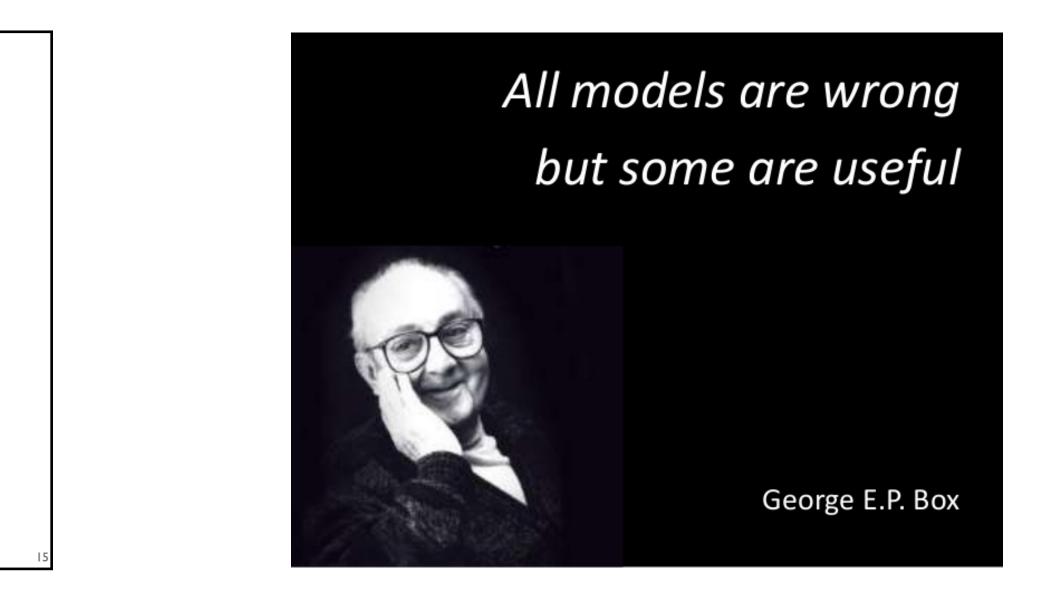
Interpretability & Control

Why might we want ML Or explainable, trustworthy, safe, robust, a	•	(Jesse)
Scientific Reasons:	Could be working in non-asymptotic regime Training data might be biased in some way Result could depend on poorly modeled features Limited ability to perform independent validation Need for compact symbolic expressions Desire to generalize away from specific context 	
Sociological Reasons:	Skeptical of algorithmic/statistical/com Need to explain decisions to external s Desire to manage risks from unforese 	stakeholders
All valid reasons, but sug	gest imperfect specification of	our initial goals!

It's a lot about retaining control in an uncertain world, when you don't trust the process

Not new: "Bayesian Workflow" / Iterative Model Building etc is a lot about understanding a system. If we'd trust the model / process we would just run MCMC and be done

We don't only want to tame us but also the networks - or "understand" them. But what are they learning??

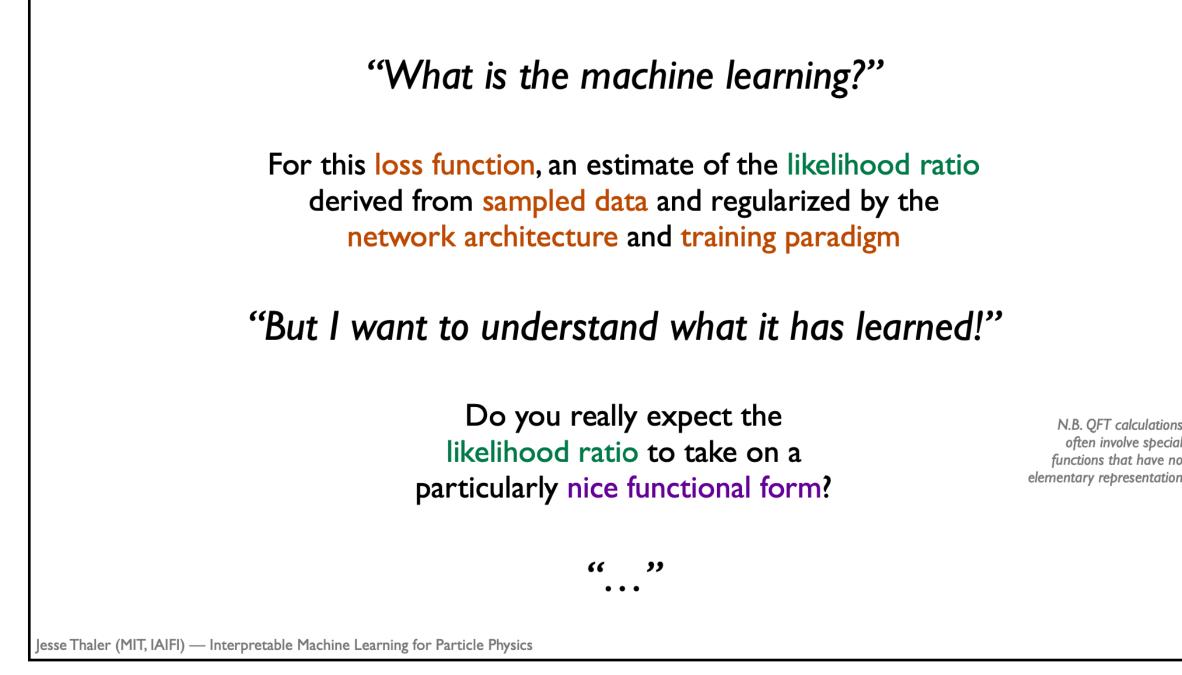




Interpretability & Control

Example: Likelihood-Ratio Estimation when you have a simulator you trust

When you trust the process & underlying tools we're fine w/o interpretability



39

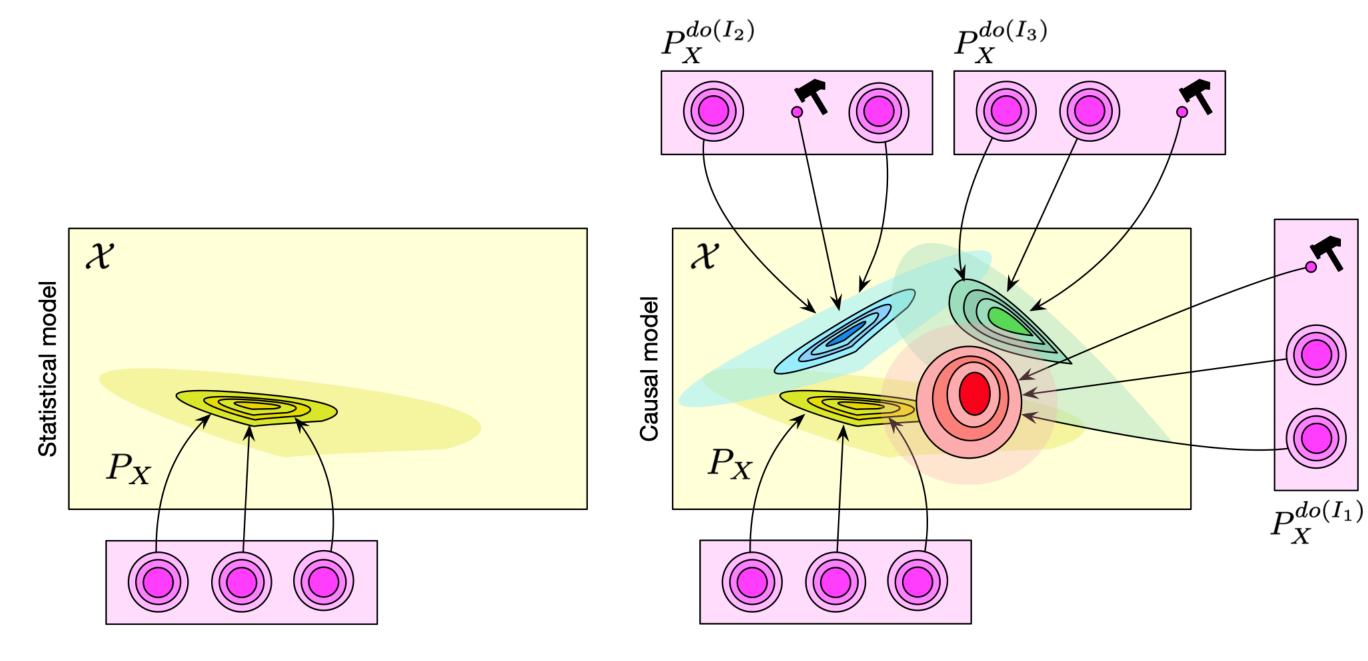




Performance under Intervention

What we do want to understand: how does ML react to distribution shift e.g. from interventions (Sherpa \rightarrow Herwig, etc)

A lot of literature (Causal Inference) that we don't use



2102.11107

Does a New Drug Improve Health Outcomes?

Causal Inference:

- Split subjects: treatment (A = 1) and control (A = 0) group.
- What if treatment group differs systematically from control group, e.g., in terms of *x*.

$$p_{\text{treatment}}(x) \stackrel{?}{=} p_{\text{control}}(x)$$

• Randomization is the gold standard, not always possible.

Propensity Scores:

HYSTAT 2024 - Statistics meets

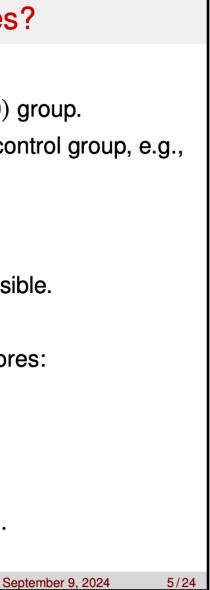
• Rosenbaum and Rubin (1983) define propensity scores:

$$e(x) = P(A = 1|x).$$

• Demonstrate that e(x) is a balancing score:

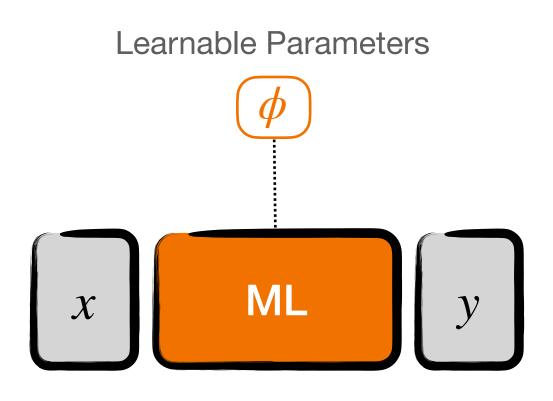
 $p_{\text{treatment}}(x|e(x)) = p_{\text{control}}(x|e(x)).$

(Maximilian)



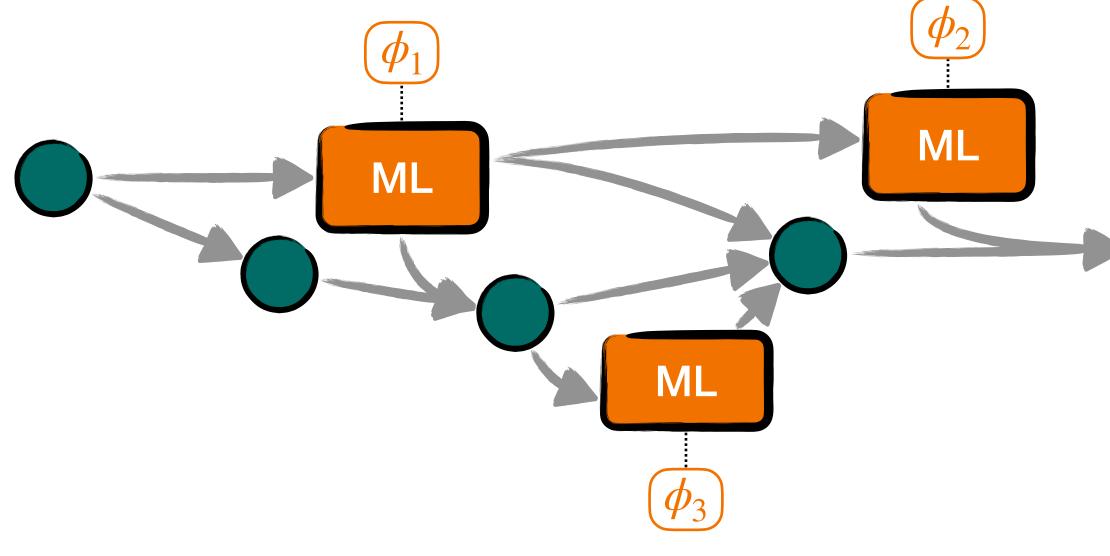
Inductive Bias: A Physicists' Love Affair

Two ways to think about it



 $f_{\phi}(r_x(g)x) = r_v(g)f_{\phi}(x)$

Statics (enforce symmetries etc)



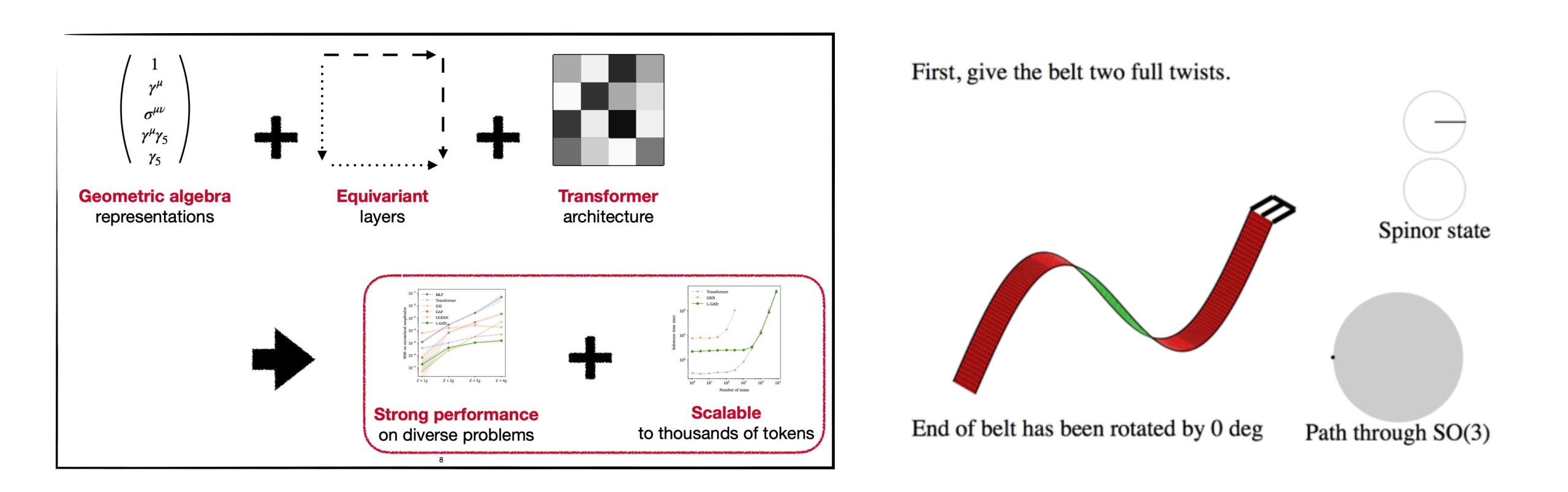
Physics Computation ML modules

41

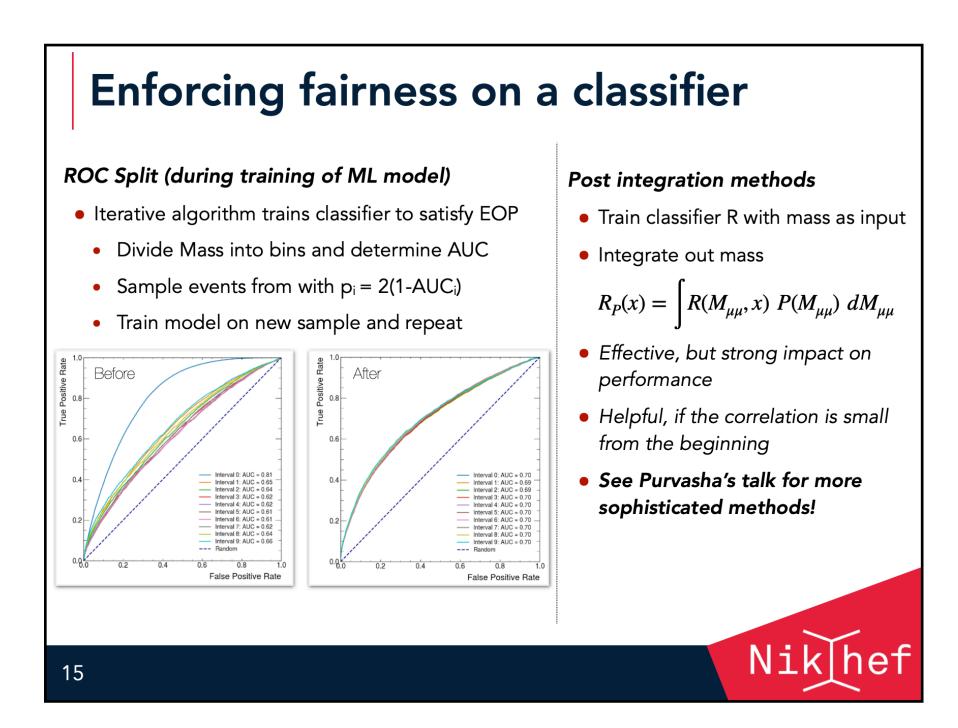
Dynamics mix physics + ML workflow, keep control over data flow



Inductive Bias: A Physicists' Love Affair

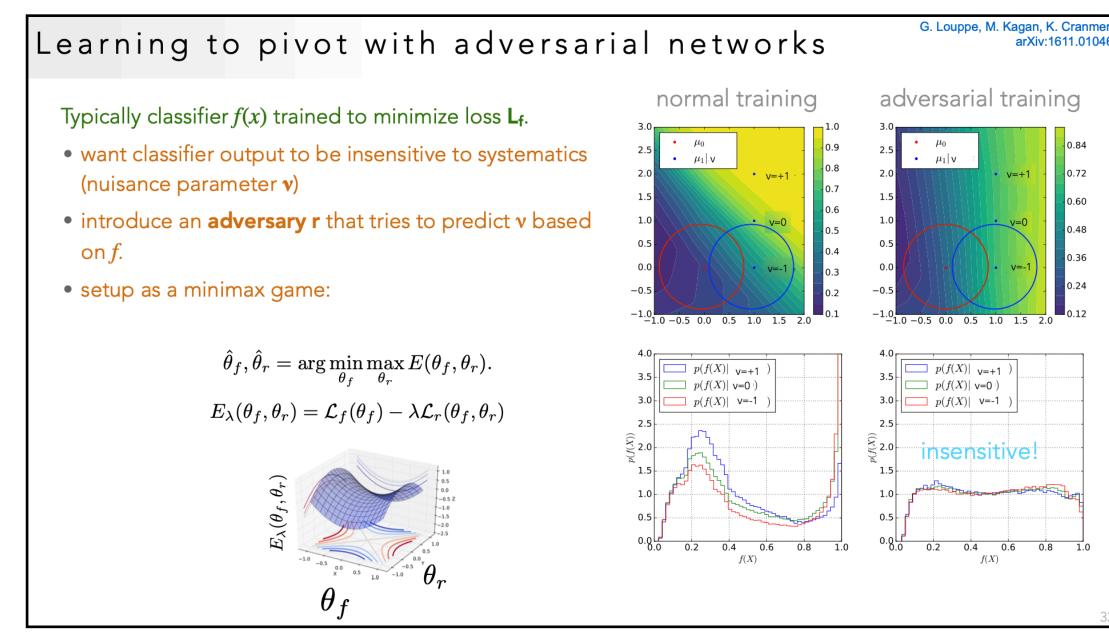


Another version of Control / Interpretability: Force Behavior onto ML



(Oliver)

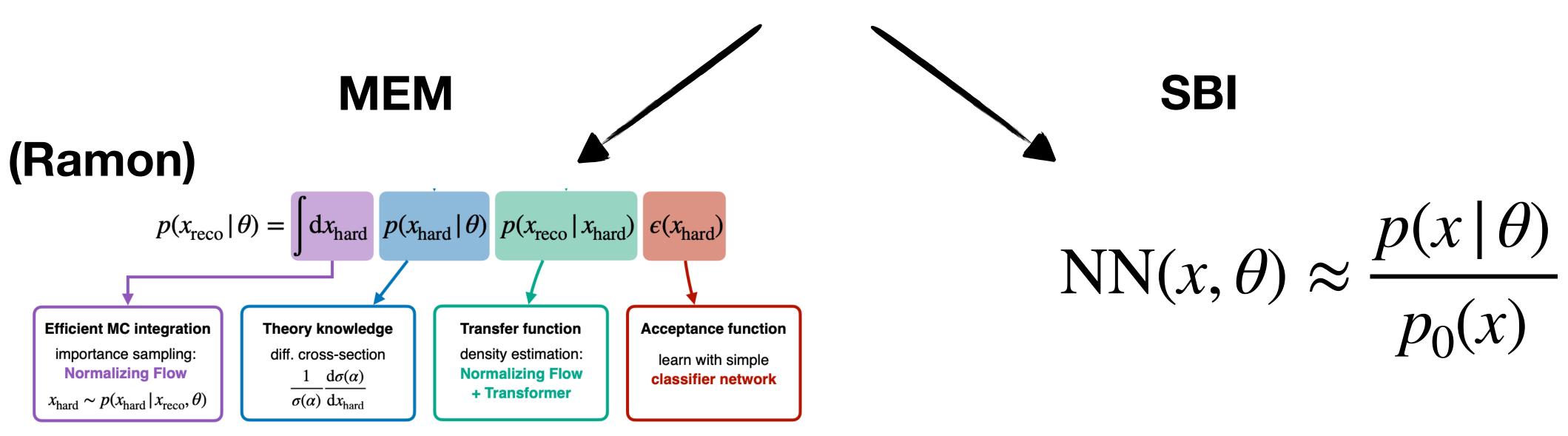
Soft Symmetries



(Kyle)



Dynamics: Control over the Data Flow



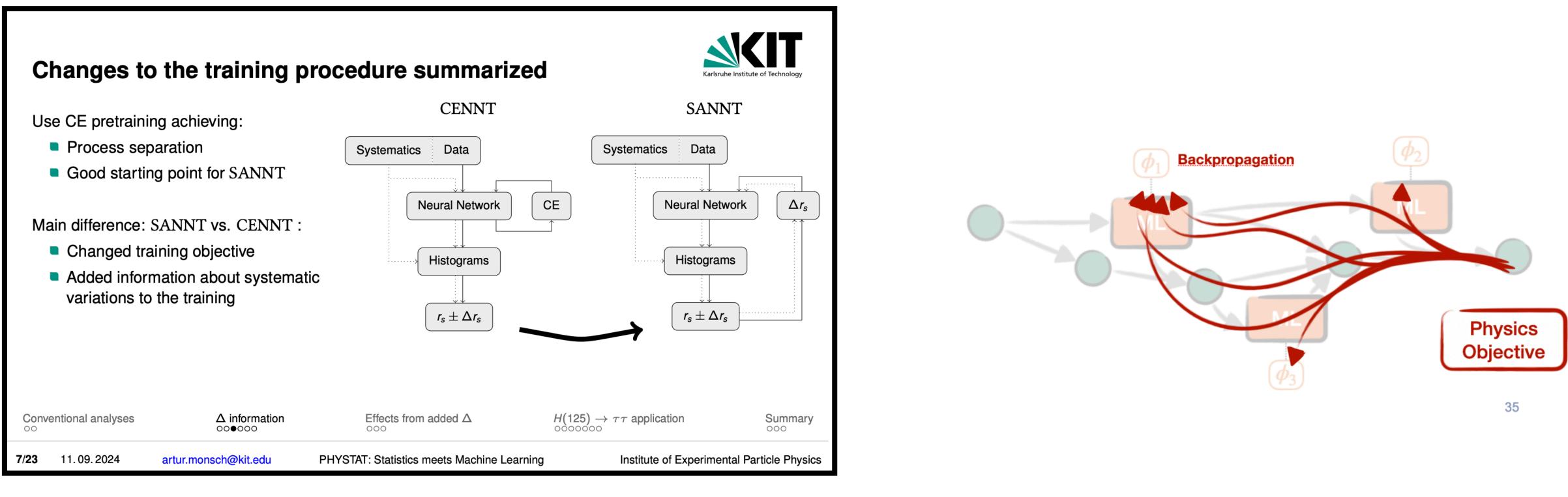
A lot of ML tied together by domain knowledge

why should you ever do MEM after we got SBI? \rightarrow maybe to have a fuzzy feeling of control \rightarrow to separately debug each piece \rightarrow the fuzzy feeling is very expensive - how much do we care?

Two ways to do optimal observables

Extreme Version of Dynamics

end-to-end gradient based optimization: SANNT, neos, Inferno,



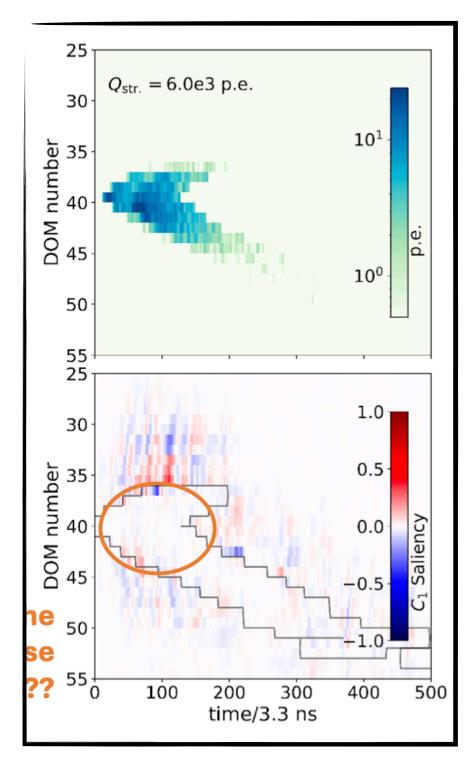
Interesting parallel to foundation models: pretrain a initial analysis w/o systematics, finetune later e2e in-situ w/ full physics context

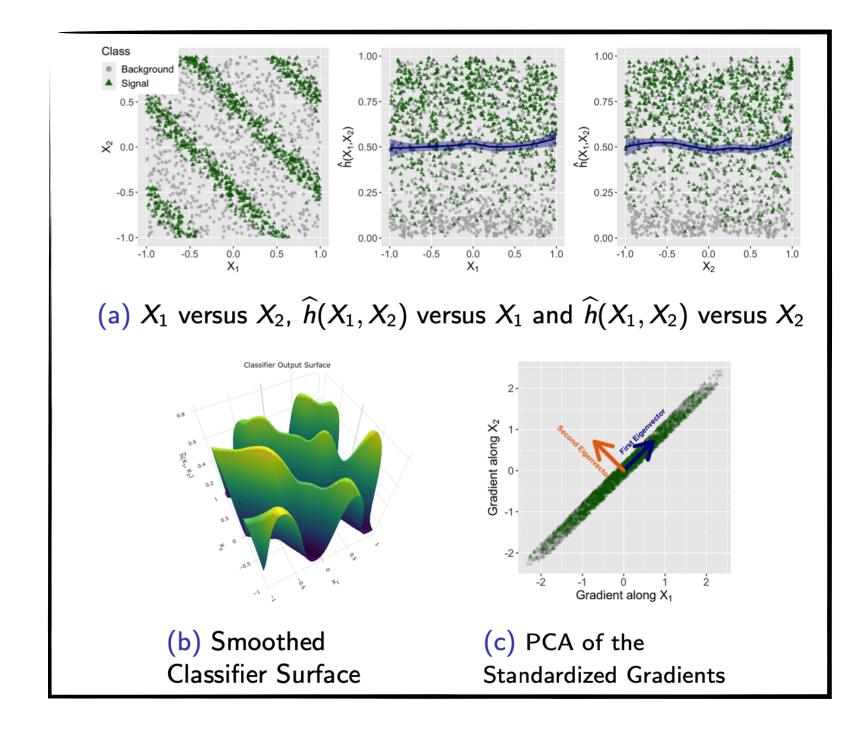


Intuitive & Interpretable is what you are used to

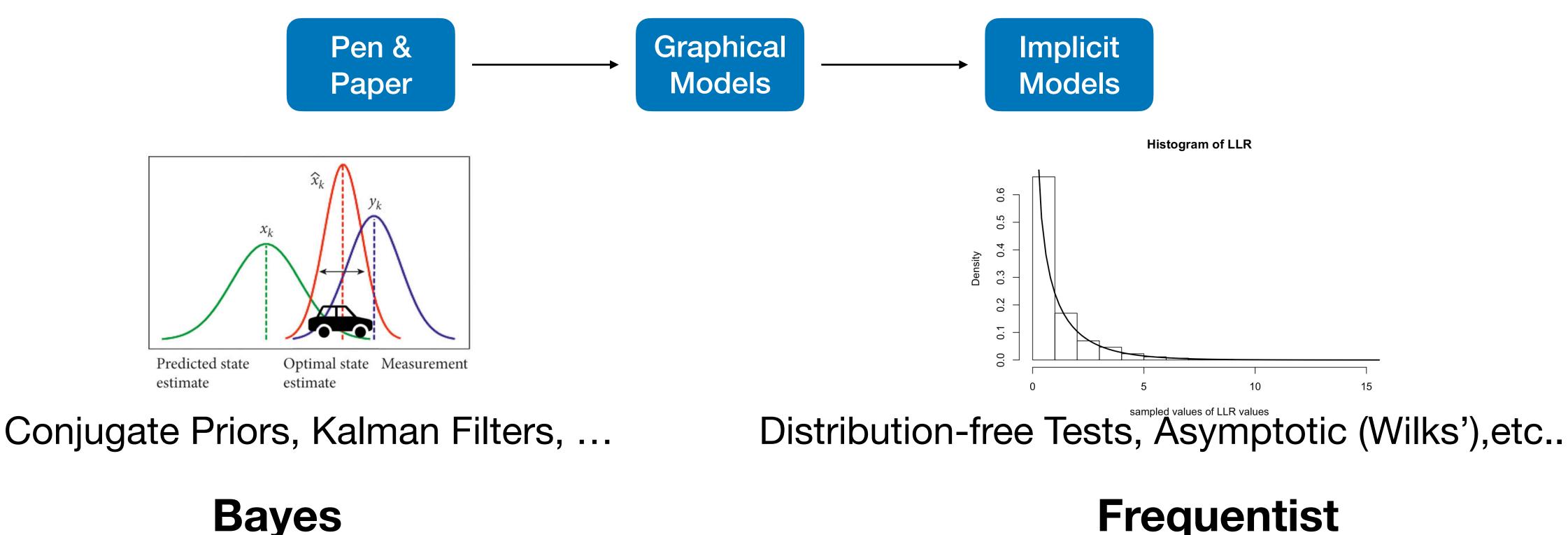


(Tobias, Mikael, Philipp, Pierre, etc)





many different fields that are driven by data, irrespective of the details



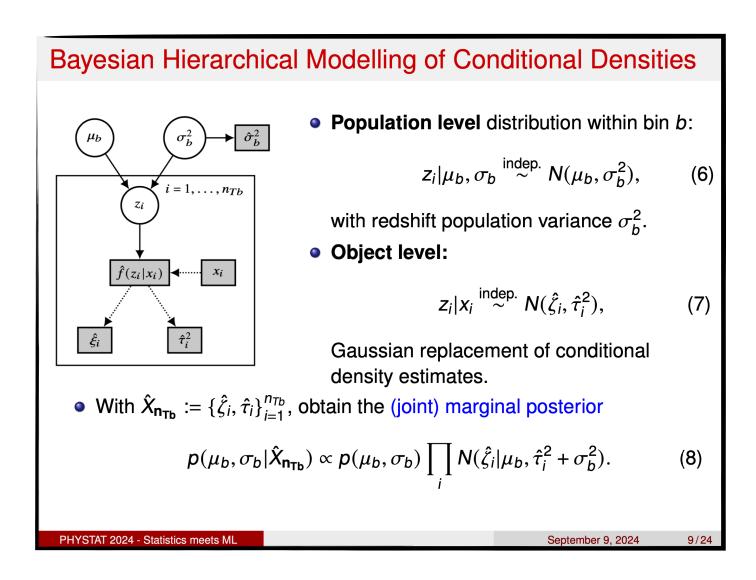
- Statistics always had a nice quality: a common language to tie together
 - **Version 1: "Pen & Paper" Statistics**



many different fields that are driven by data, irrespective of the details

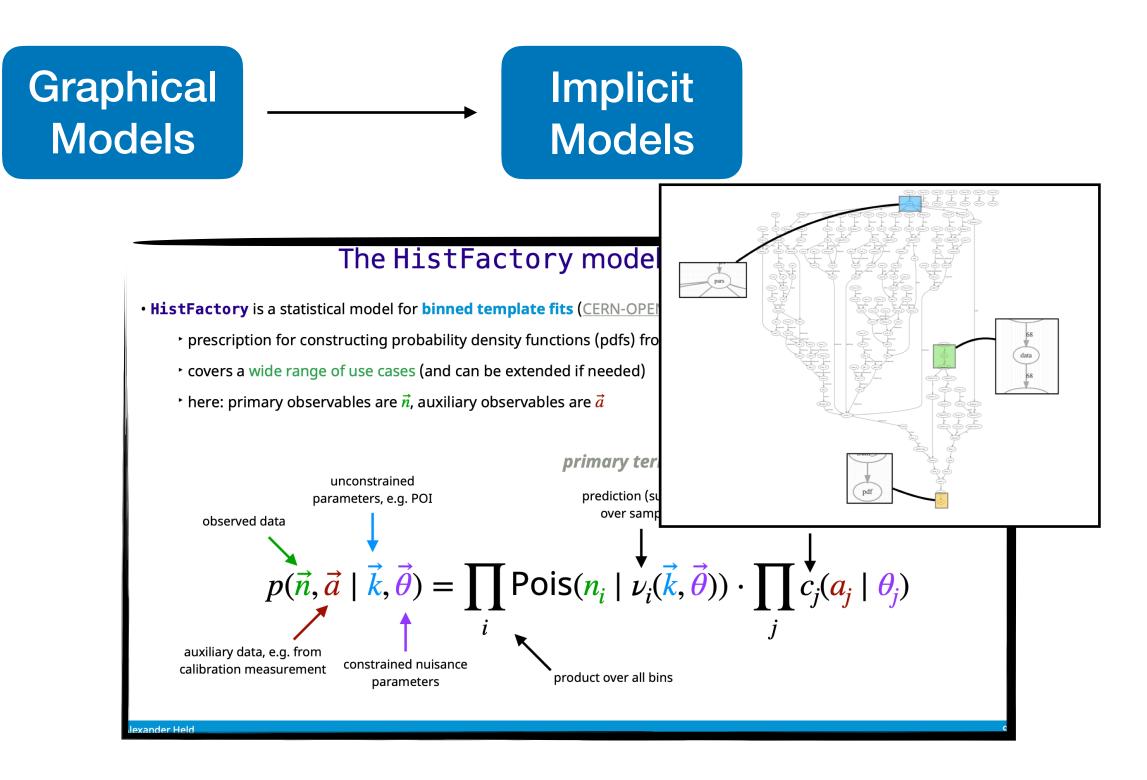
Version 2: Principled, Heavy Compute Stats

Pen & Paper



(Maximilian)

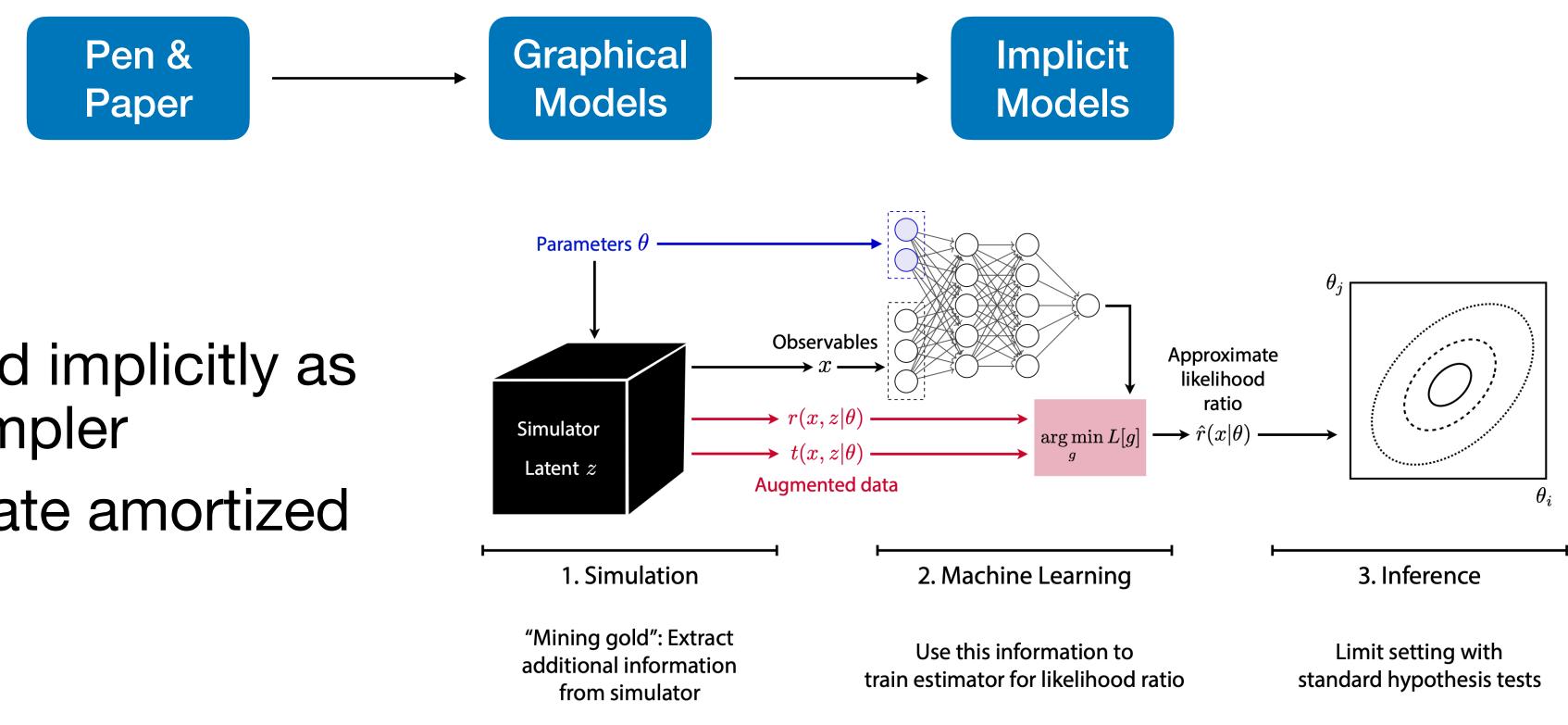
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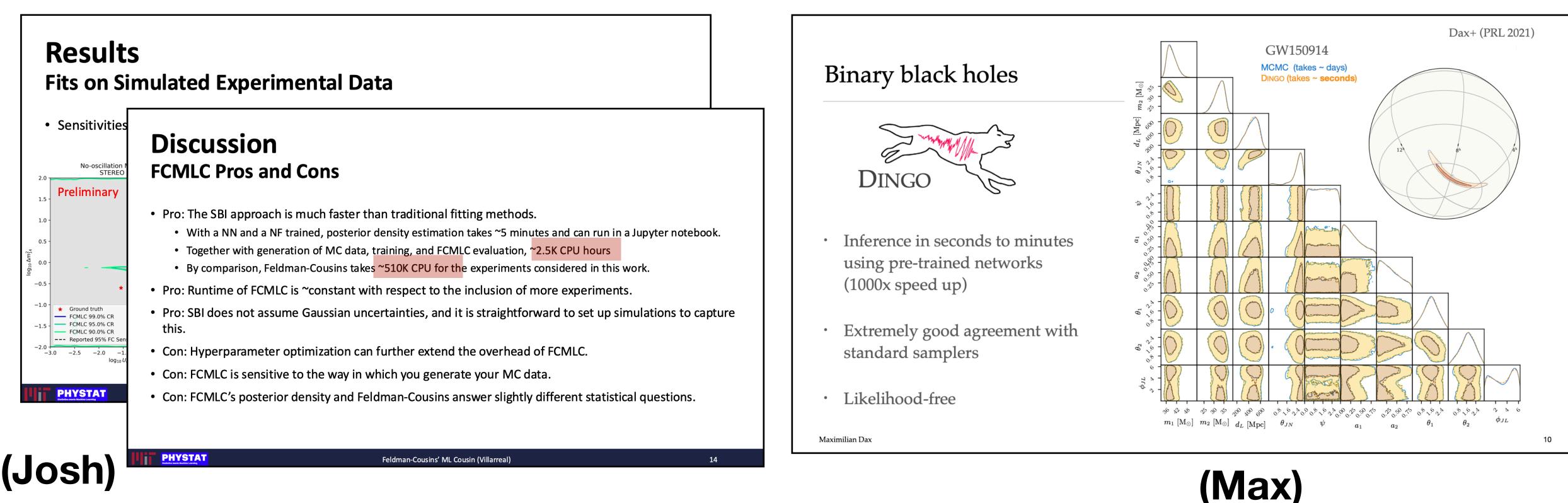
Version 3: Implicit Models aka Simulation-based Inference



- Model is defined implicitly as a black box sampler
- Fast, approximate amortized Interence

- Statistics always had a nice quality: a common language to tie together

Simulation-Based Inference (also see Gilles' Talk)

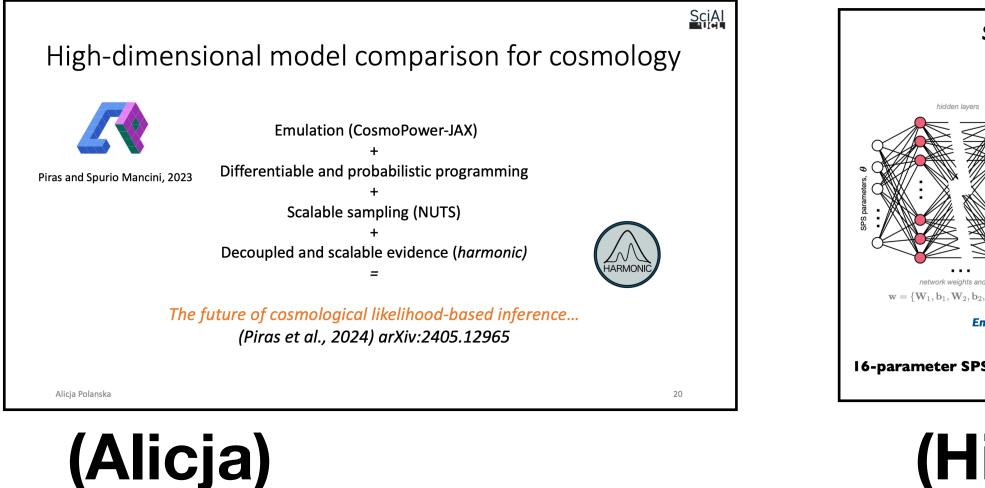


Not better, but much much faster. Interesting Observation:

SBI useful even in not likelihood-free settings, just as a fast amortized inference \rightarrow are there principled ways to do L'hood-full SBI? (Gradients, L'hood, etc..)

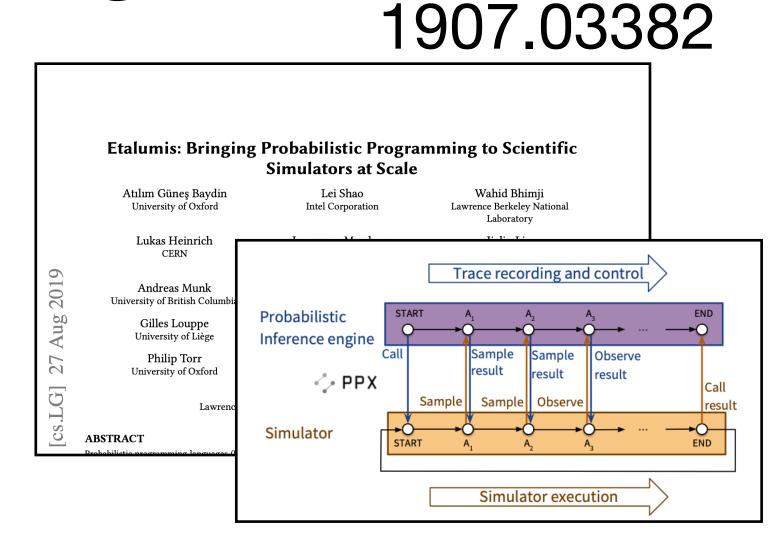
Tooling, Tooling Tooling

Differentiable & Probabilistic Programming bridge the gap between "black box" simulators and graphical models



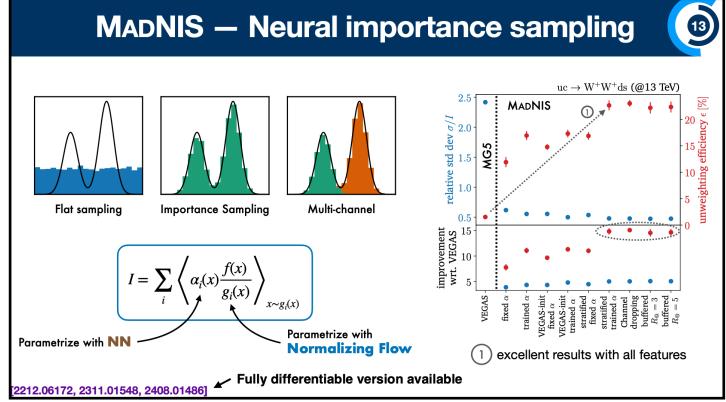
(Hiranya)

PYRO Deep Universal Probabilistic Programming



Speeding things up with neural emulators $\mathbf{w} = \{\mathbf{W}_1, \mathbf{b}_1, \mathbf{W}_2, \mathbf{b}_2, \dots, \mathbf{W}_n, \mathbf{b}_n\}$

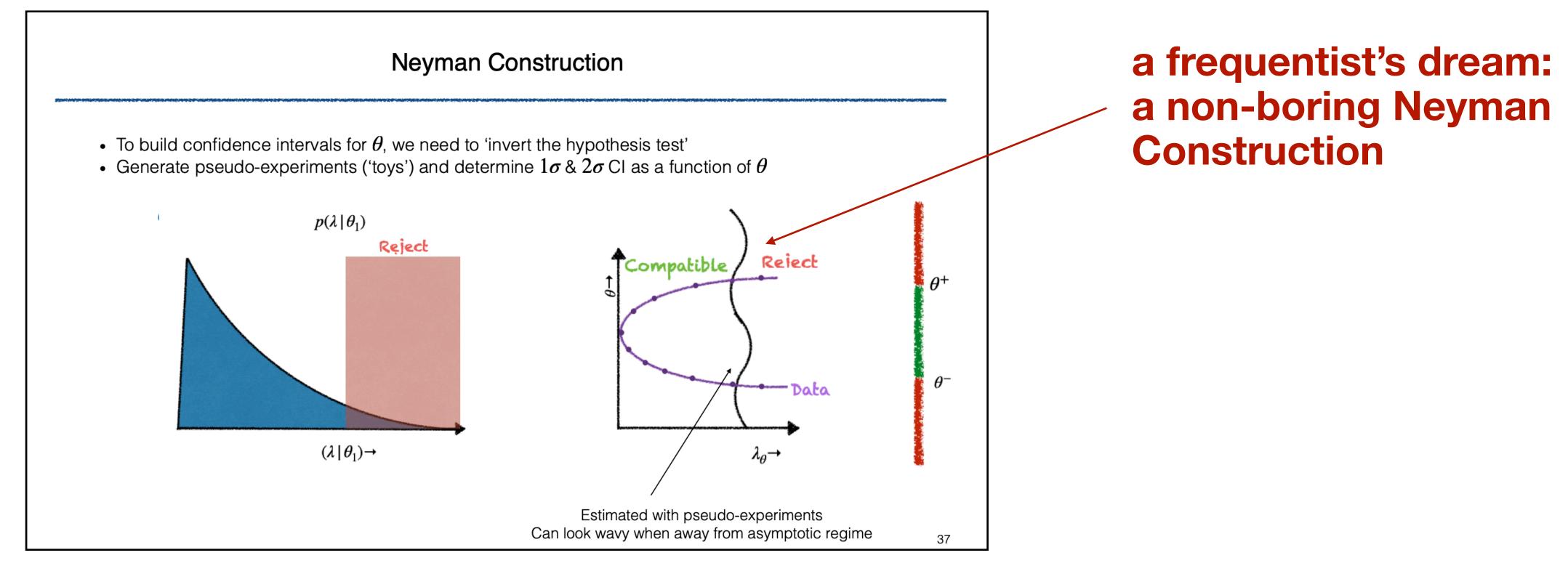
I6-parameter SPS model | sub-percent accuracy | factors x 10^4 speed-up | differentiable Alsing, Peiris, Leja, Hahn, Tojeiro, Mortlock, Leistedt, Johnson, Conroy (APJS, 2020



(Ramon)

Slowly, but surely: we are actually doing this in HEP. Step change soon?

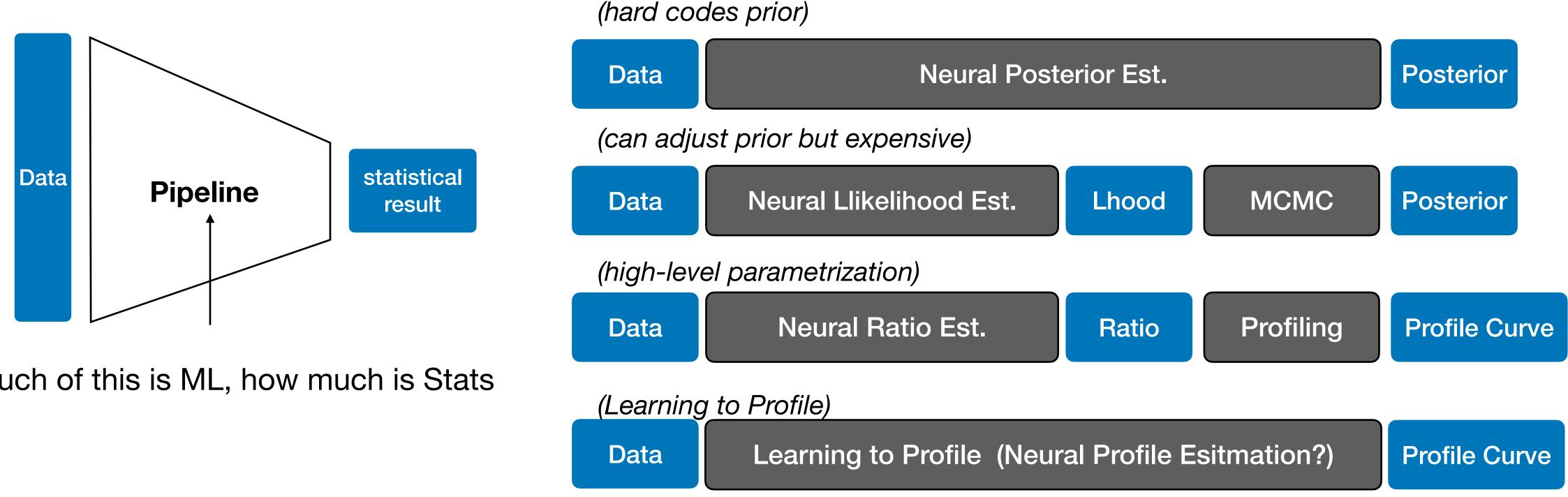
#SBI analyses at LHC: $0 \rightarrow 1$. How will we ensure $1 \rightarrow N$ is easier?







How much Statistics can we cram into ML Statistics: Data \rightarrow Insight



how much of this is ML, how much is Stats

How much do we trust the process? Where, how many inspectable intermediate steps do we want?

Getting Rid of the Simulator: Unfolding

Reminder that HEP is always also a social enterprise. Core question: what's the format. ML allows is to go beyond histograms and into full phasespace but in which direction? If folding becomes trivial, what does this mean?

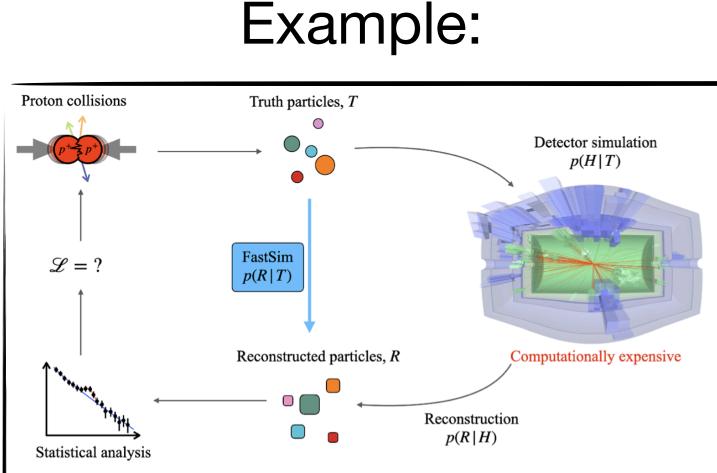
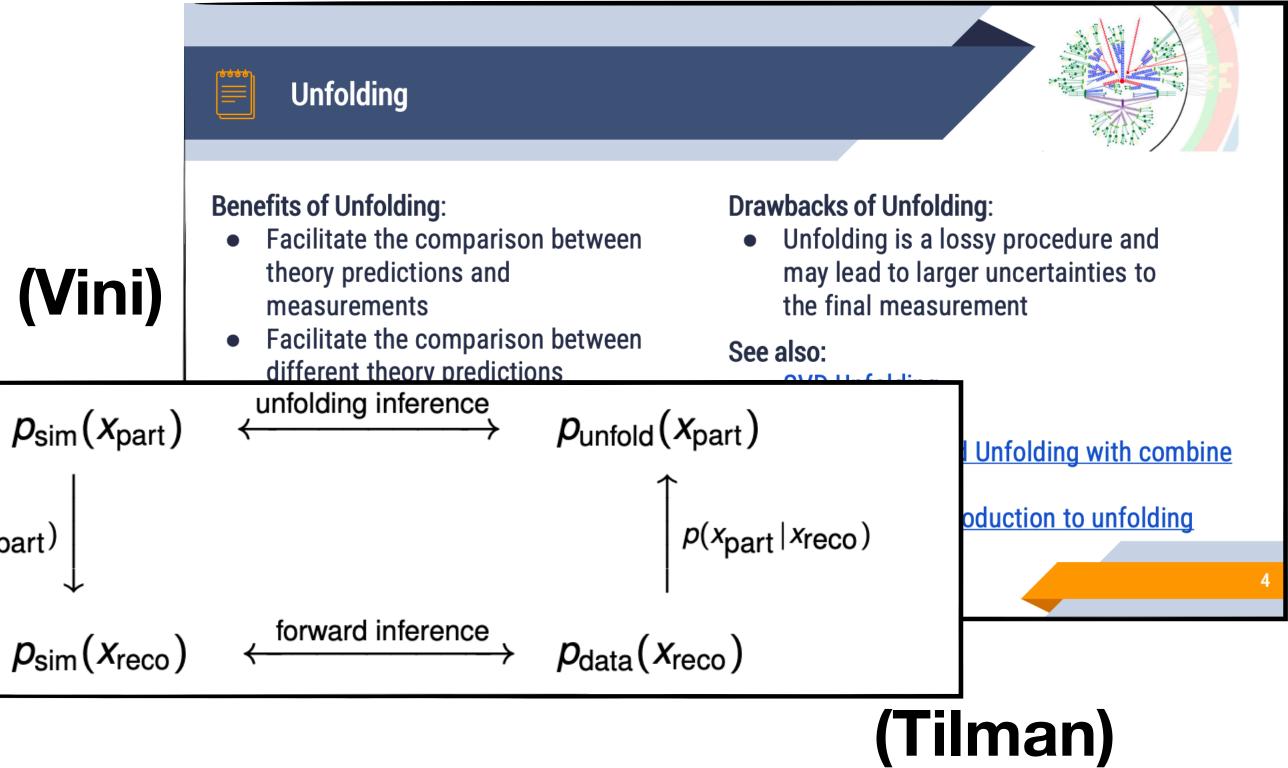


Figure 1. Classical simulation pipeline in particle physics: collision simulation generates truth particles *T*, detector simulation produces high-dimensional signals *H*, and reconstruction algorithm recovers truth input from detector readout as reconstructed particles *R*. Proposed fast simulation skips detector simulation and reconstruction, directly obtaining reconstructed particles from the truth.

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 $p(x_{reco} | x_{part})$



Summary

We're very good at learning new ML methods and finding a way to move them closer to production

Classic Statistics can give us guidance towards *what's possible in principle*

Interpretability is largely about trusting a process & convincing ourselves

Domain Knowledge helps until it doesn't (bitter lesson?)

SBI as a 3rd-wave of statistical methodology / common language between sciences

