Modern machine learning methods in HEP

Lecture I — Introduction to Machine Learning

UCLouvain

4th Baltic School of High-Energy Physics

Ramon Winterhalder — UCLouvain

Why care about ML in physics?

Why ML in HEP?

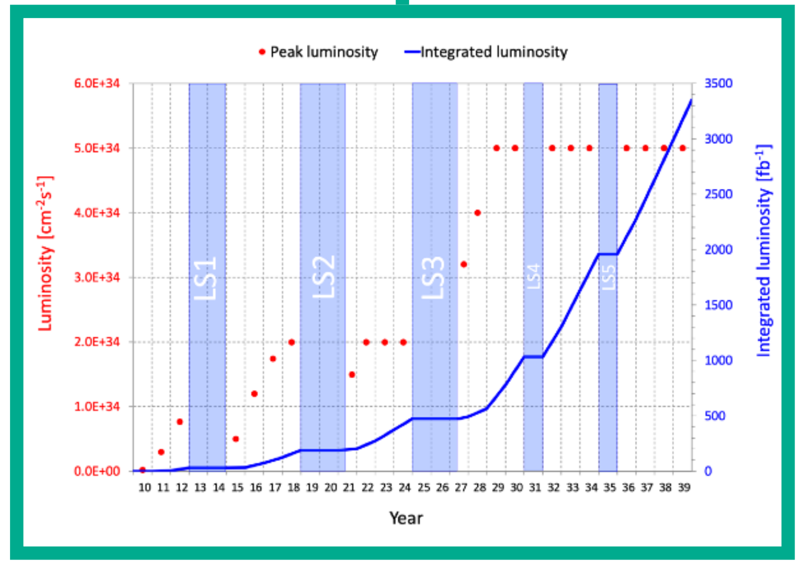
Data volume

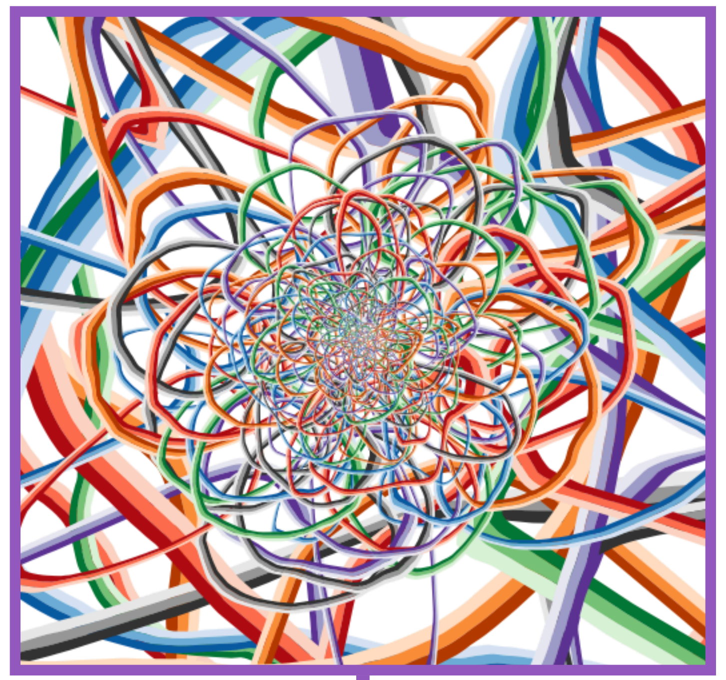
Large amounts of data

1. labeled (Simulation)
2. unlabeled (Detector)

ML wants lots of data

1





2

Complexity

High-dimensional & highly correlated data structure

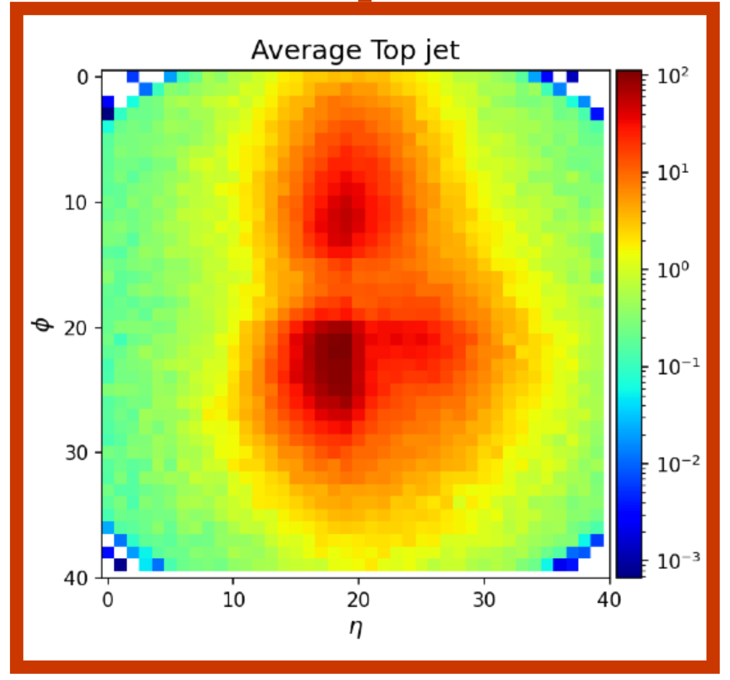
ML is expressive and flexible

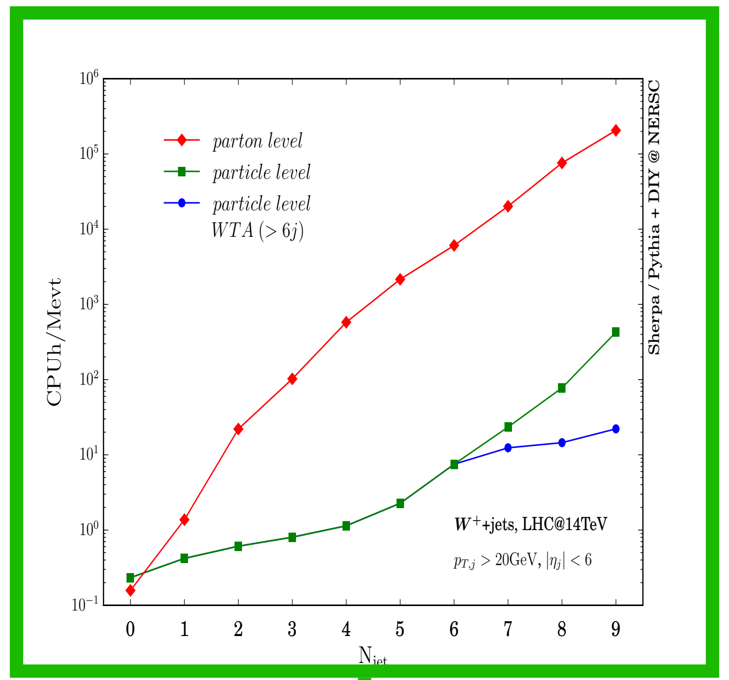
Signal detection

Rare and elusive signals among large backgrounds

ML has high accuracy and sensitivity

3





4

Computing Budget

Simulation & analysis is computationally expensive

ML is fast

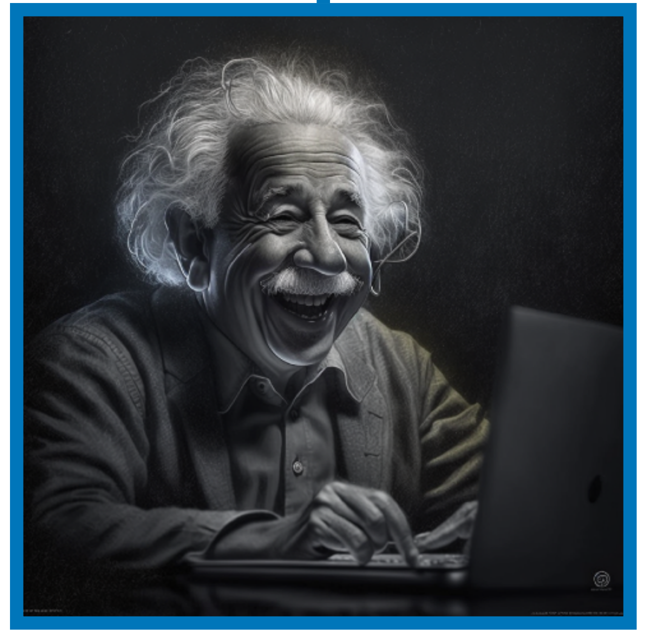
Increasing interest

> 150 paper/year

Future of HEP?

ML is fun!

5



LHC analysis (oversimplified)

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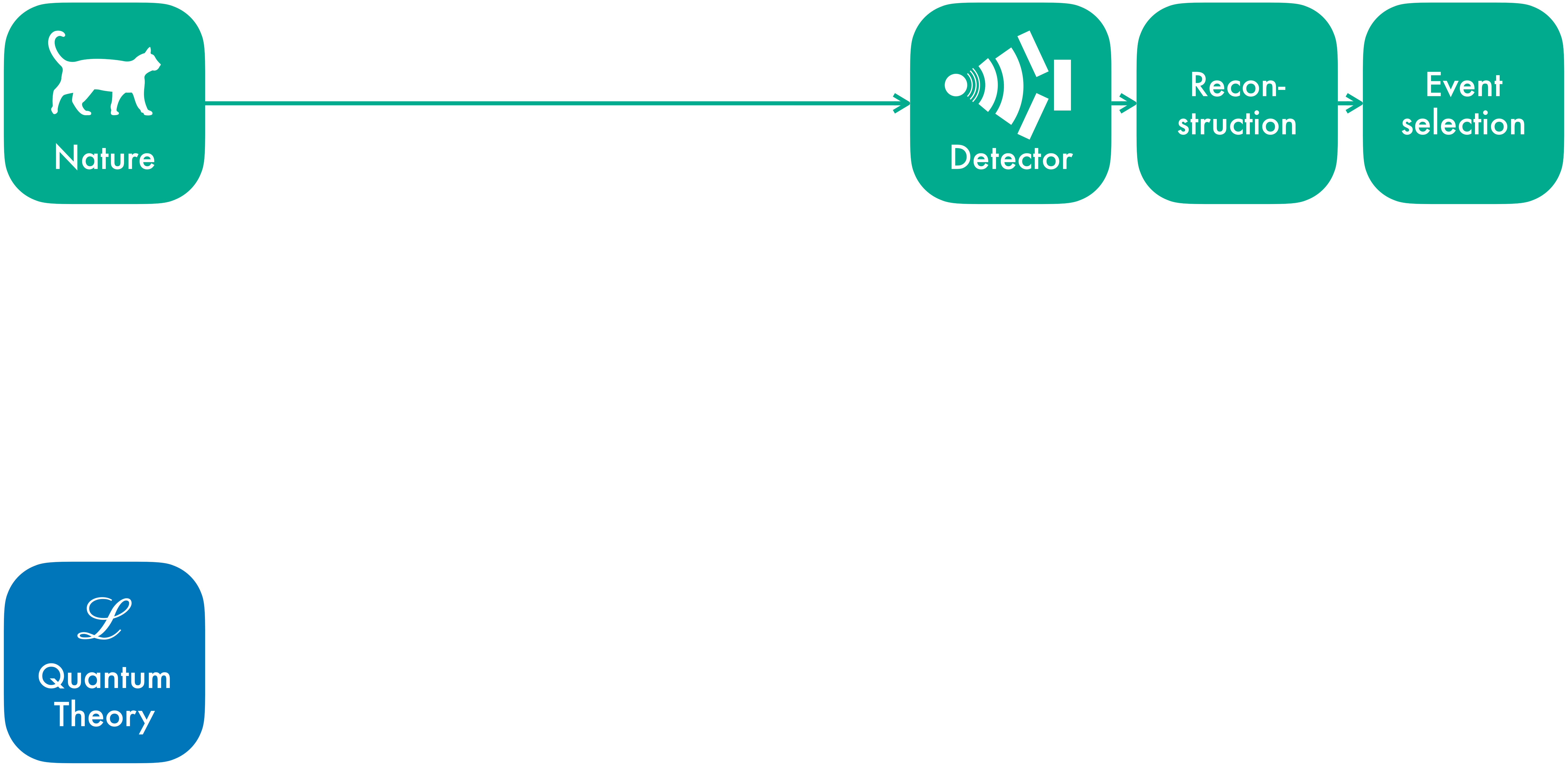

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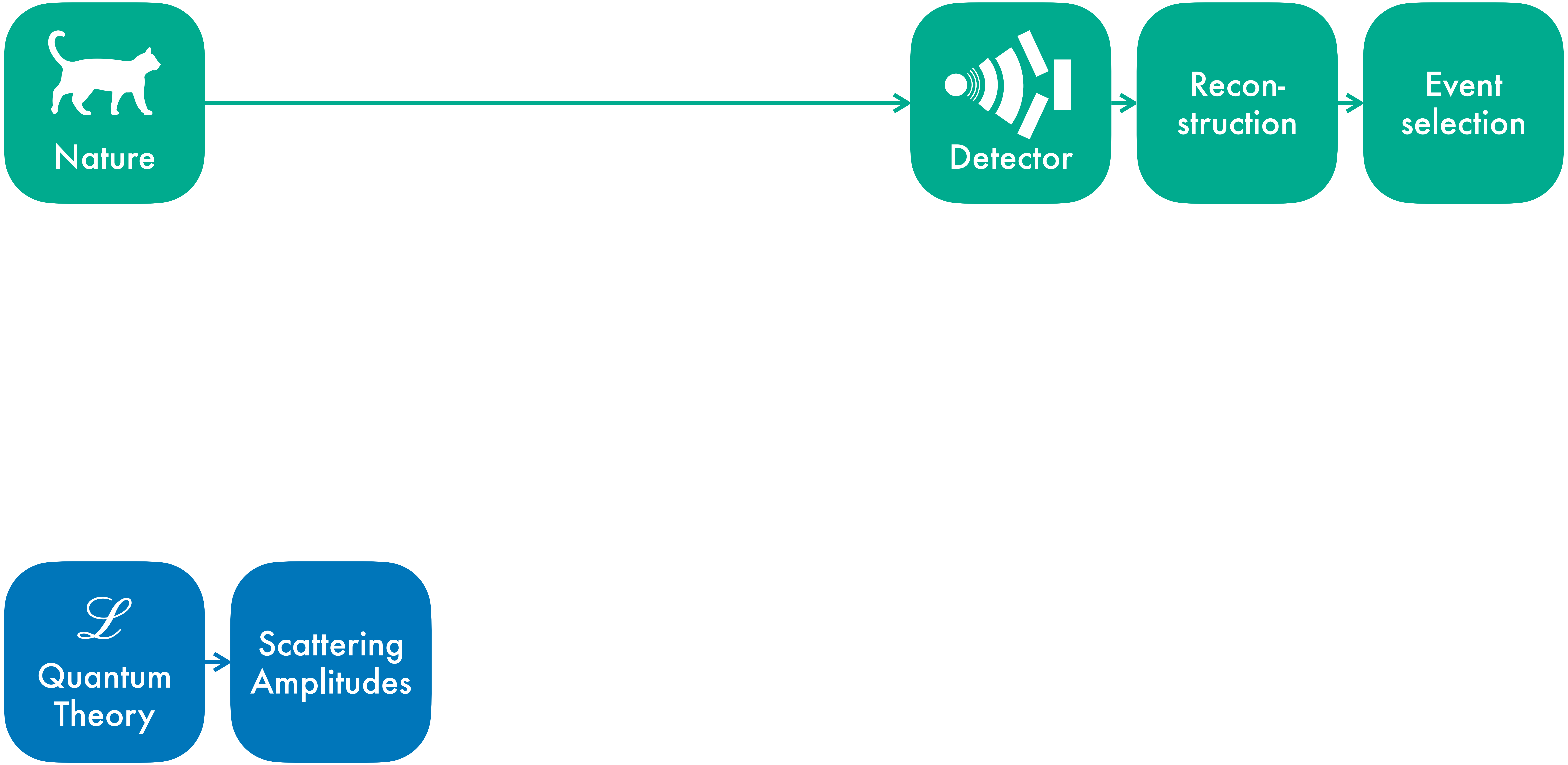

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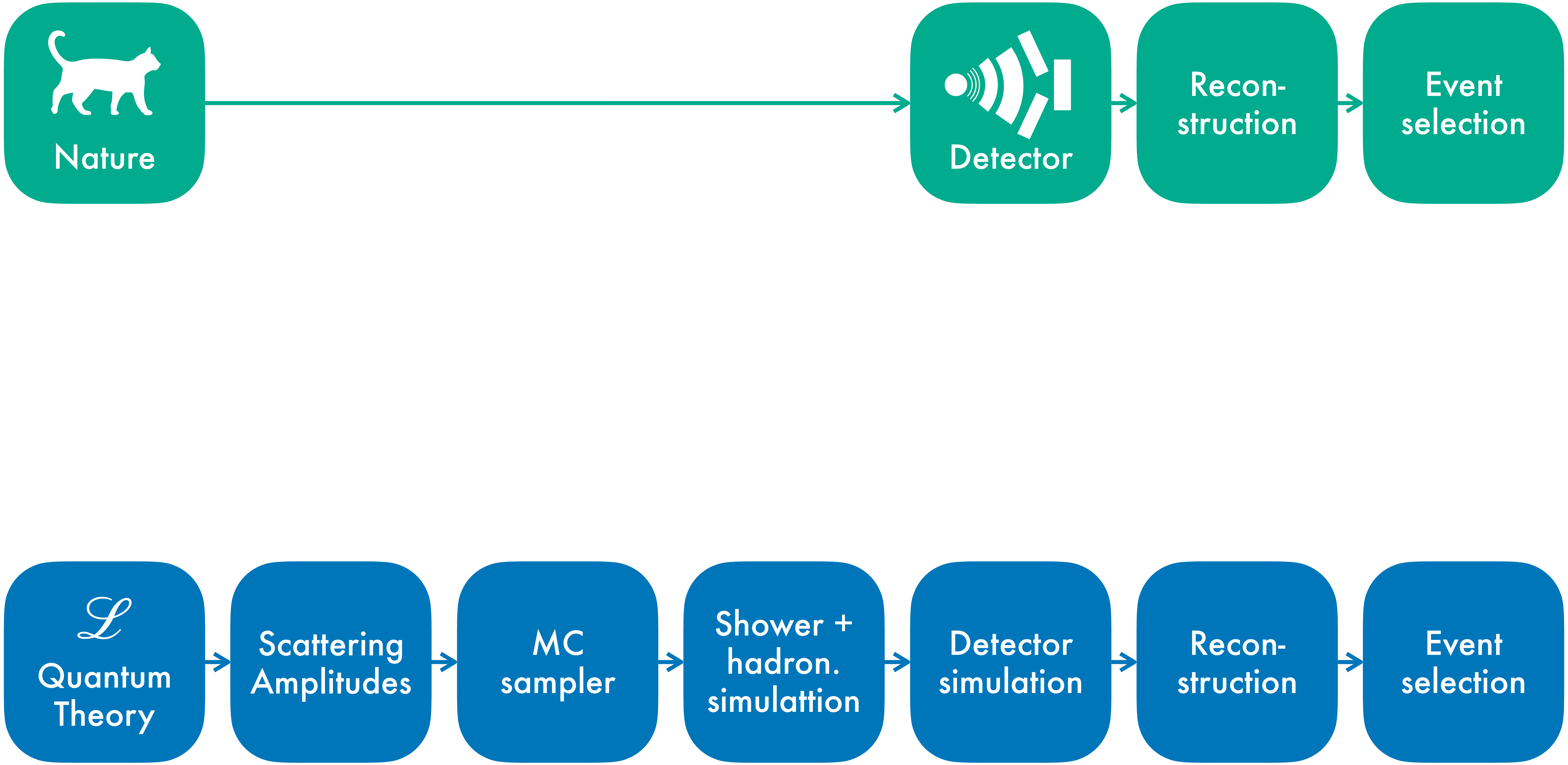

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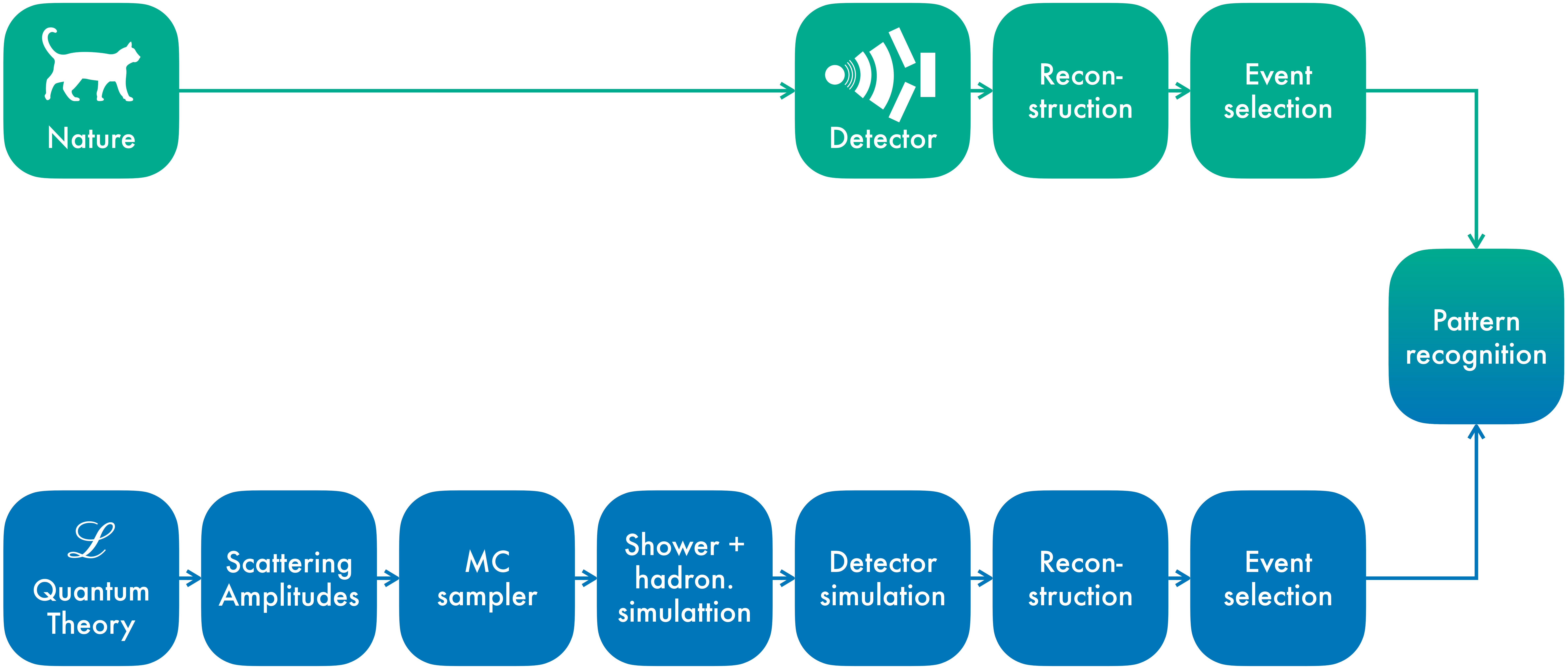

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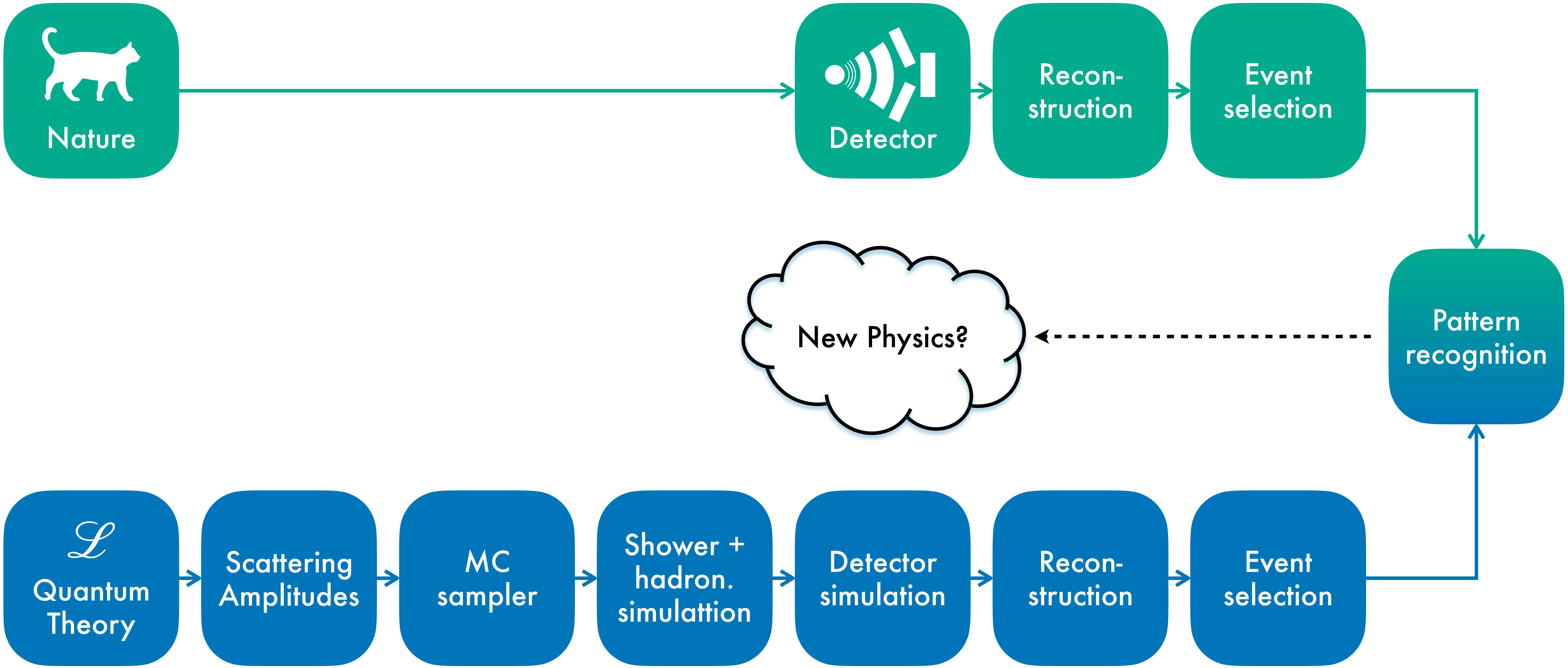

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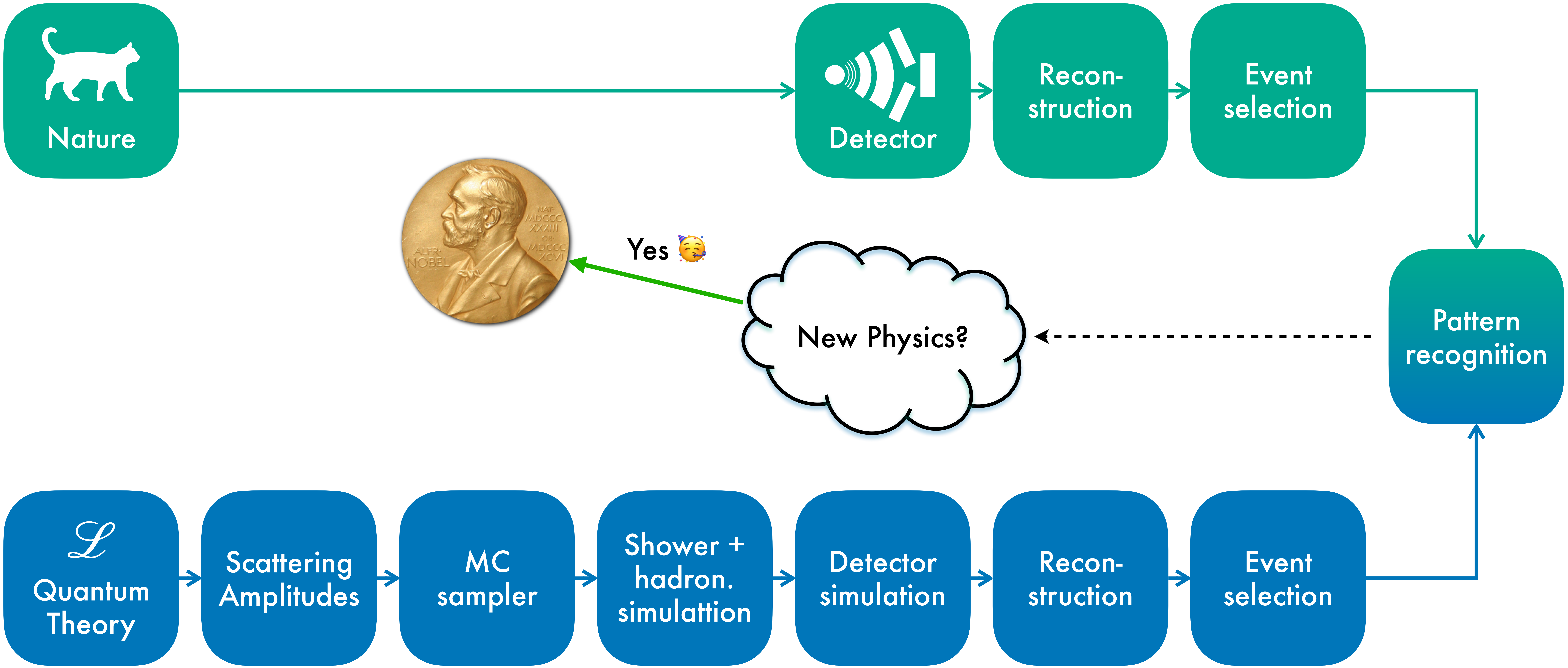

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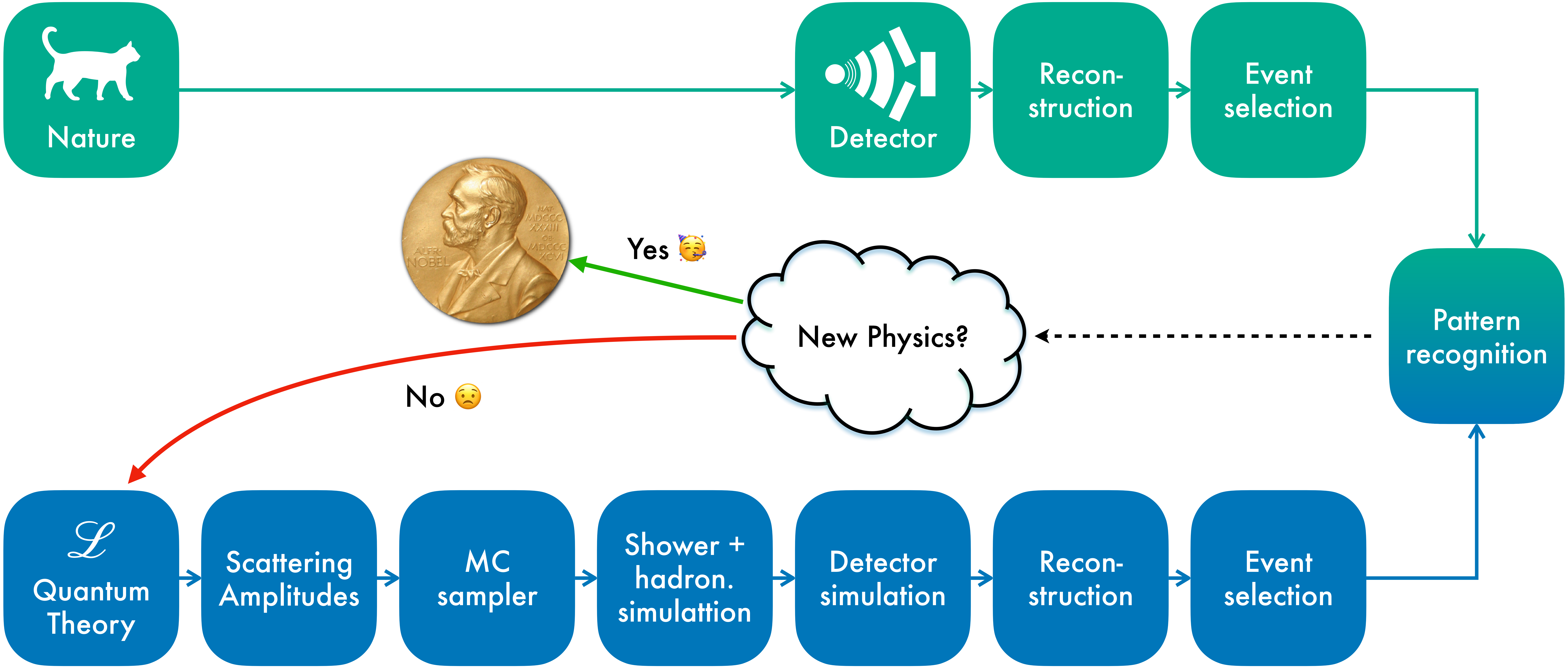

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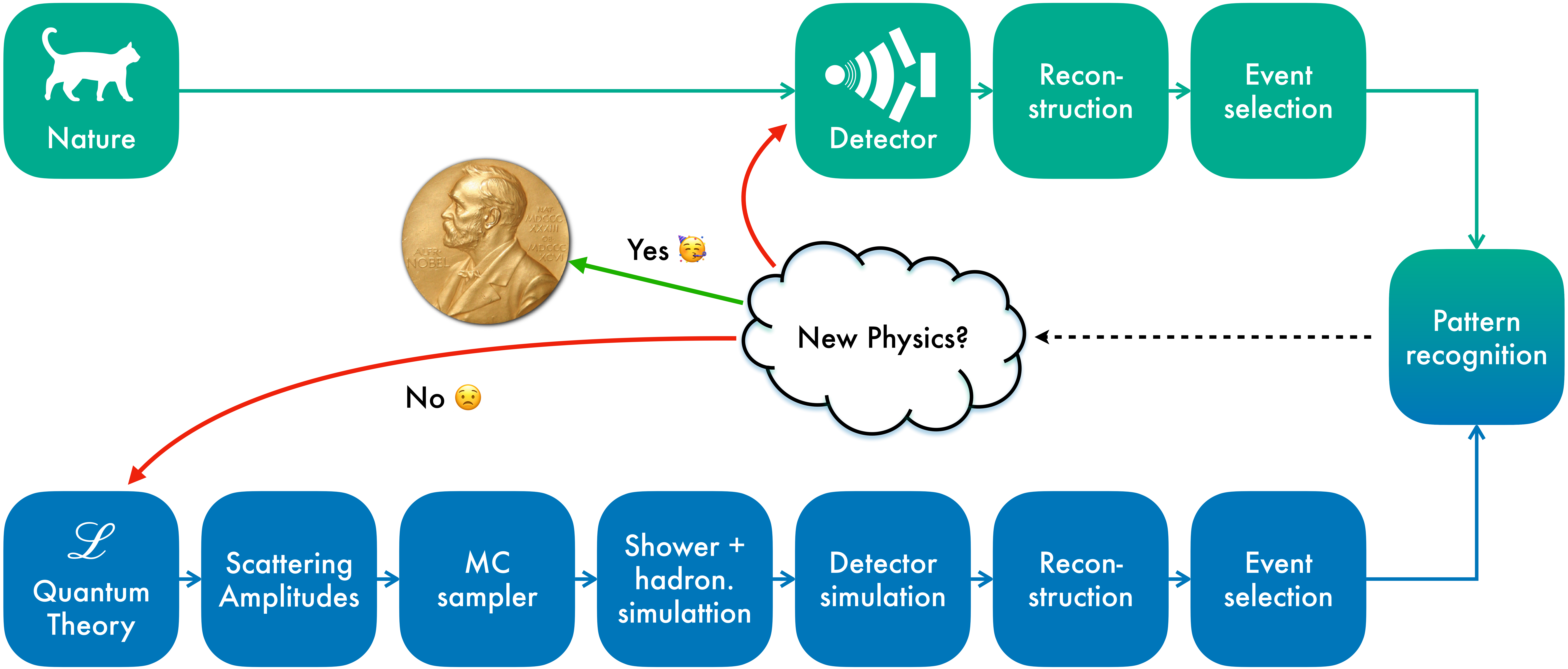
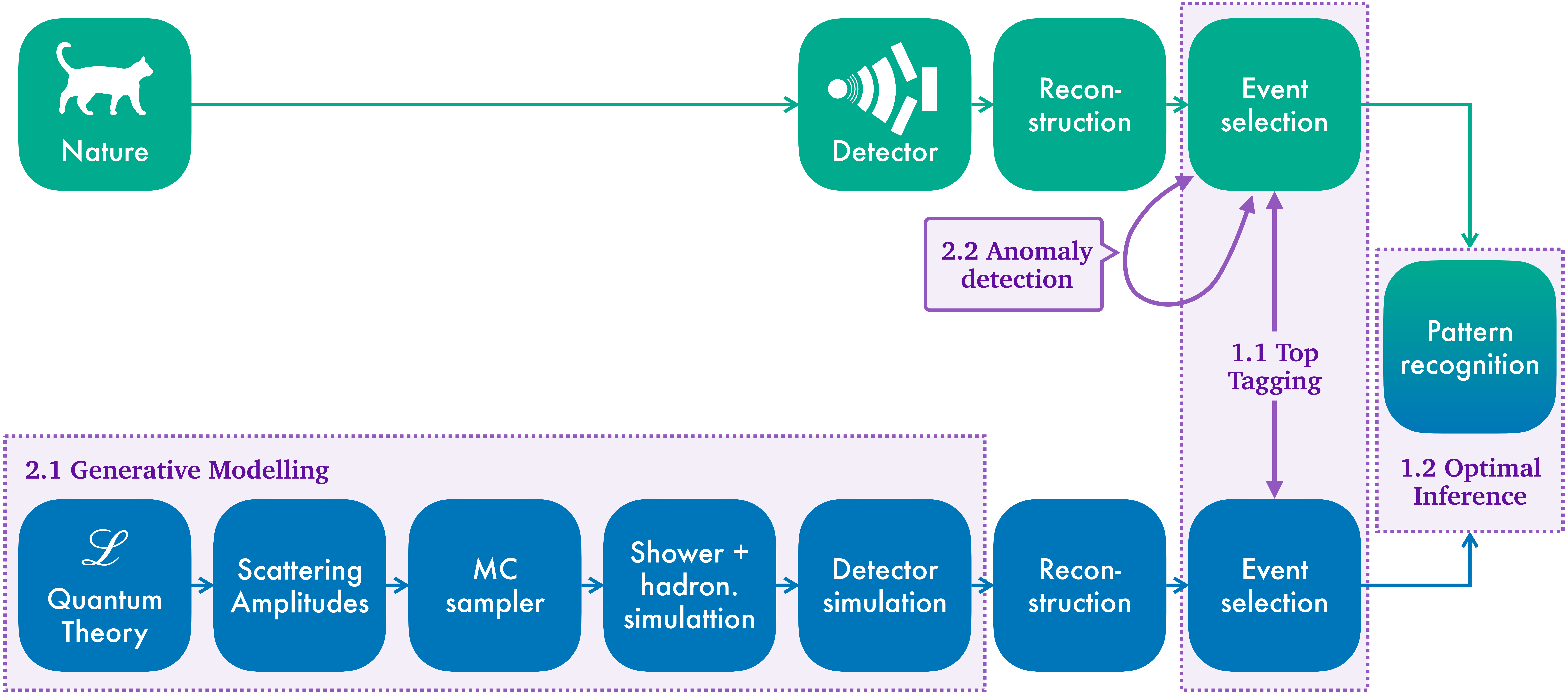
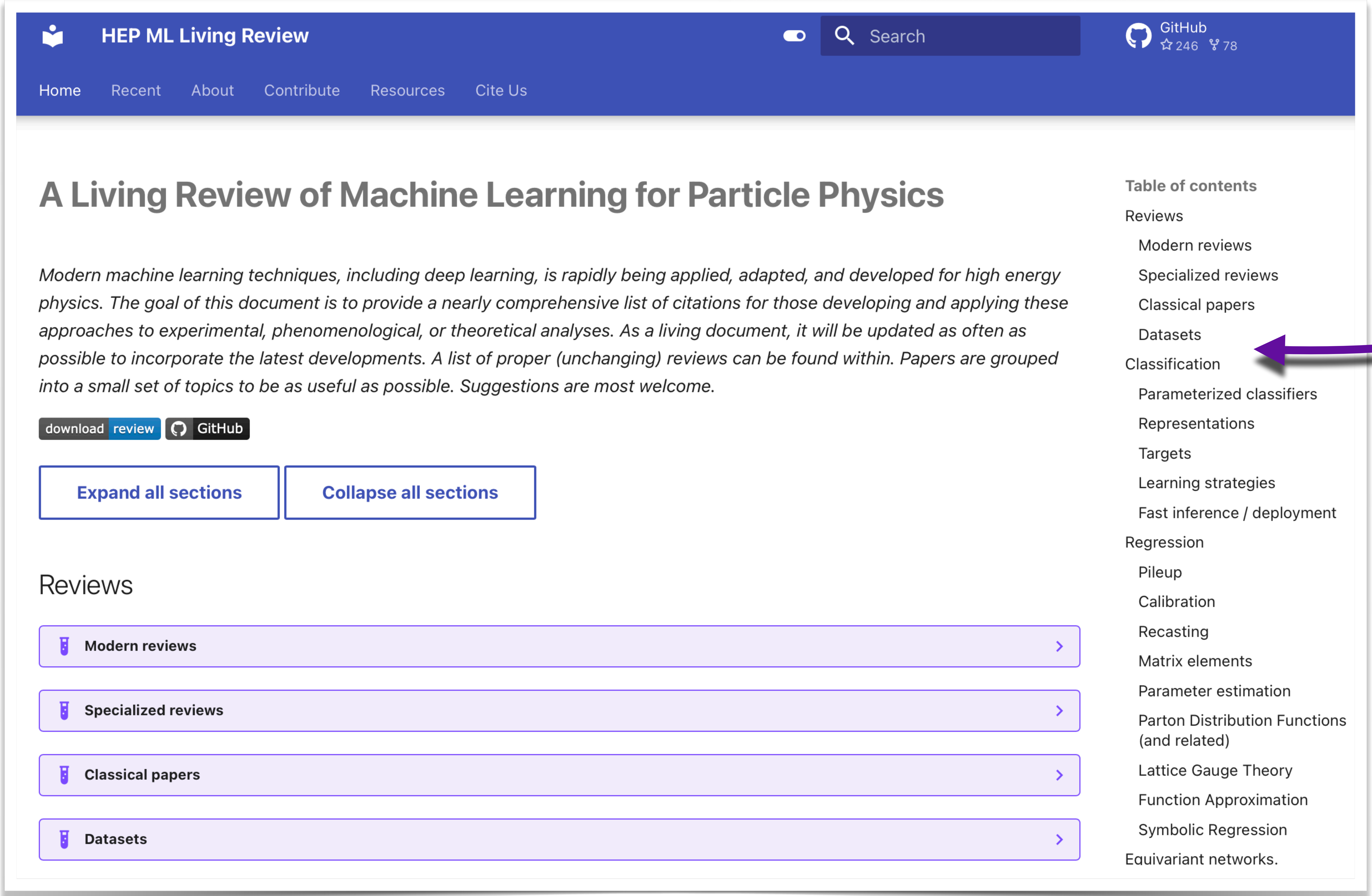


LHC analysis + ML



HEPML Living Review



- Check LivingReview for many **ML4HEP applications**

HEPML

Plan of attack

Today

1. Introduction to Machine Learning

- Basic concepts of machine learning
- Classification and Regression
- Example: **Top Tagging, MadMiner**

Lecture I (90min)

Friday

2. Generative Models for the LHC

- Normalizing flows
- CWoLA and Anomaly detection
- Examples: **MadNIS, CWoLA-Hunting,…**

Lecture II (90min)

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Part I

Introduction to Machine Learning

What is machine learning?

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Tom Mitchell

ML pioneer

"Machine learning (ML) is the study of computer algorithms that can improve automatically through experience and by the use of data"

Traditional approach

Input + Program = Output

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Machine learning

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"Machine learning (ML) is the study of computer **algorithms** that can **improve** **automatically** through **experience** and by the use of data"

1. **algorithm**: a method to perform a task of interest
2. **experience**: training data, which the algorithm can use to learn how to perform a task
3. **improve**: a way to measure the performance on the training data
4. **automatically**: a strategy to exploit the training data, without external input

What is machine learning?

"Machine learning is just statistics on steroids.
Lots and lots of steroids"

Ilya Sutskever

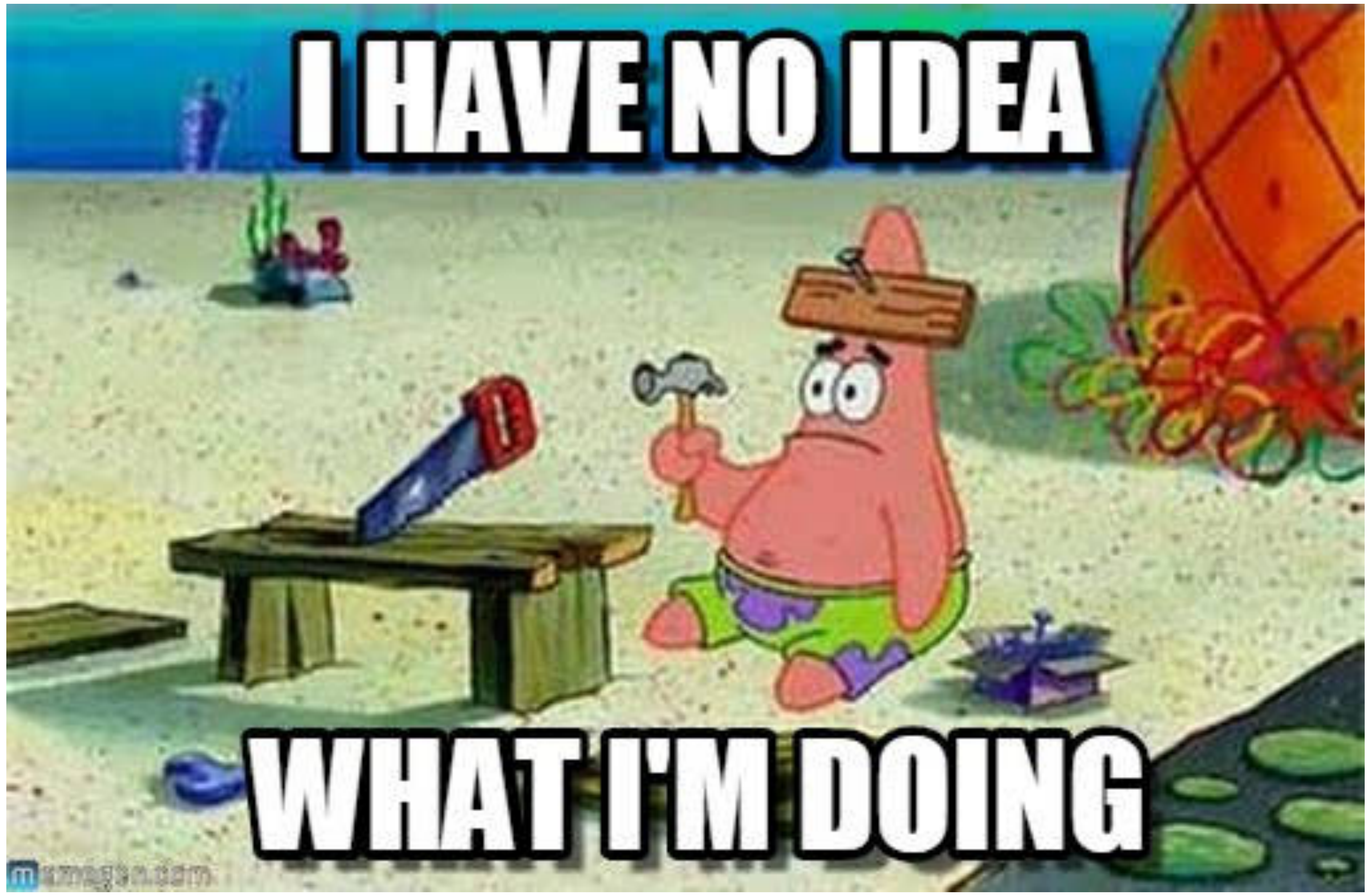
Co-founder of OpenAI

What is machine learning?

What if feels like… (sometimes)

Aim of the lectures:

Giving you the tools and ideas to use it right!



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Aim of the lectures:

Giving you the tools and ideas
to use it right!

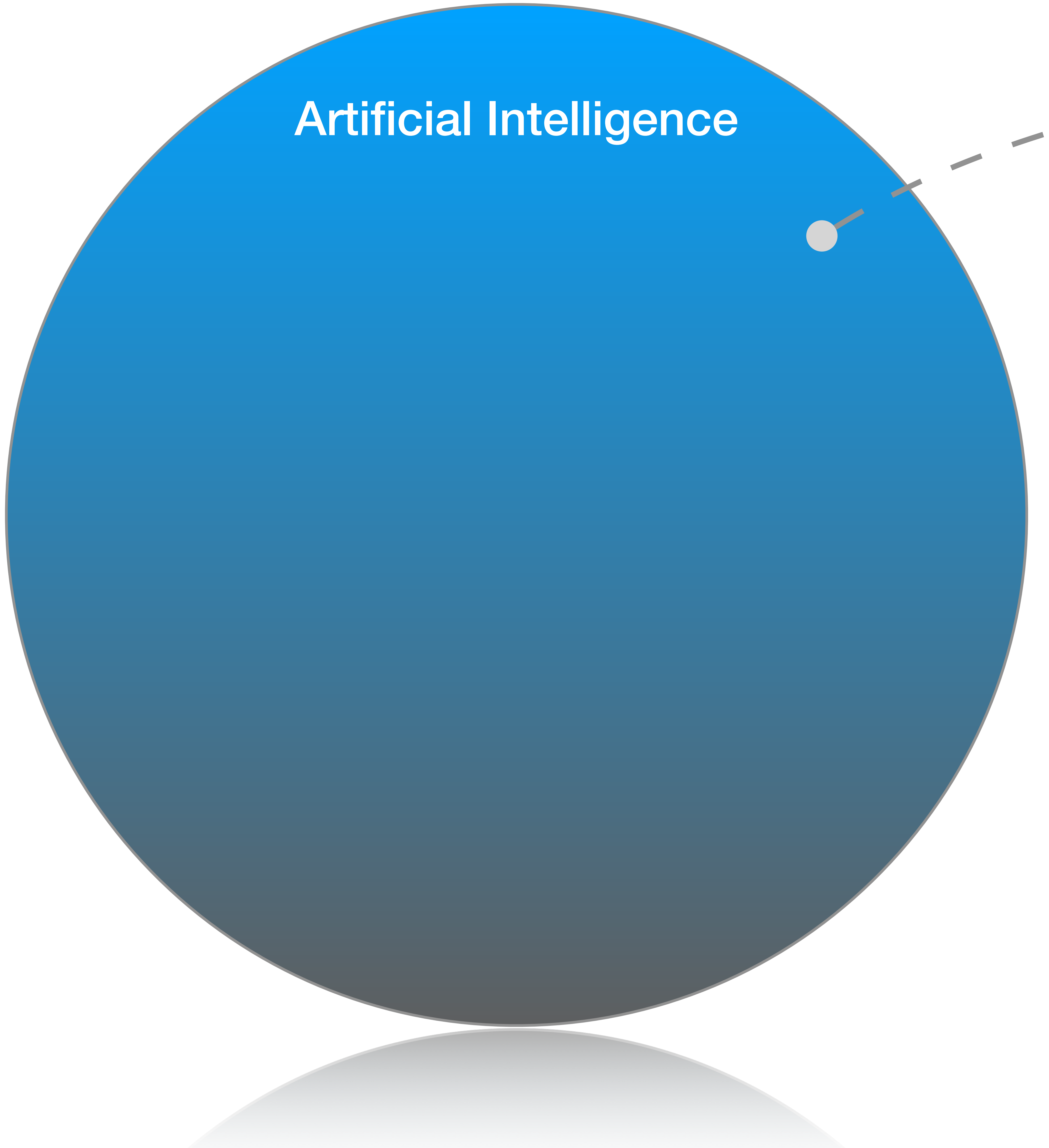
Be aware!

The core of machine learning is to find
structure in data - **no more no less!**

Thanks to machine-learning algorithms,
the robot apocalypse was short-lived.

What is deep learning?

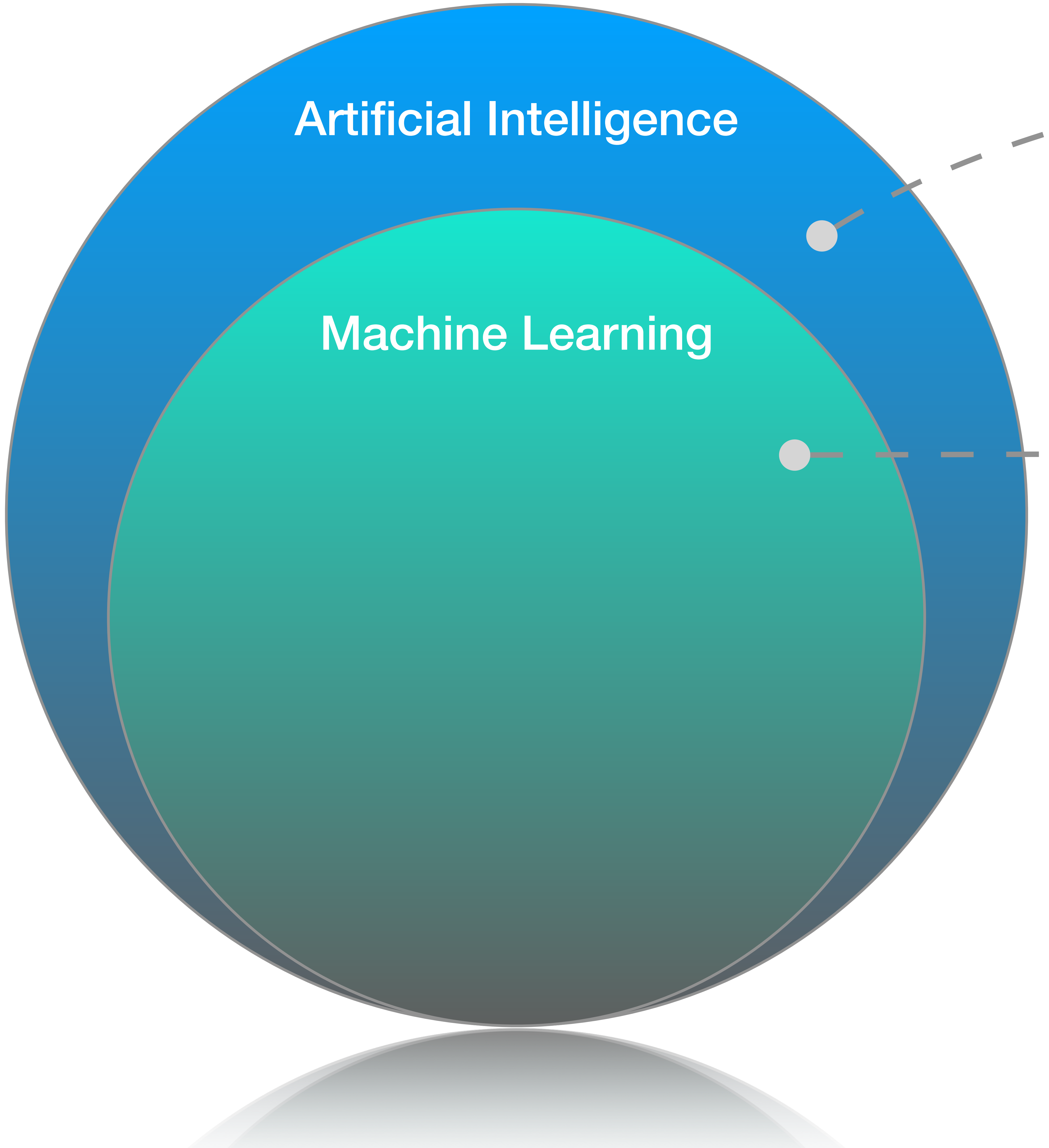
What is deep learning?



ARTIFICIAL INTELLIGENCE

A technique which enables machines to mimic human behaviour

What is deep learning?



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MACHINE LEARNING

Subset of AI technique which use statistical methods to enable machines to improve with experience

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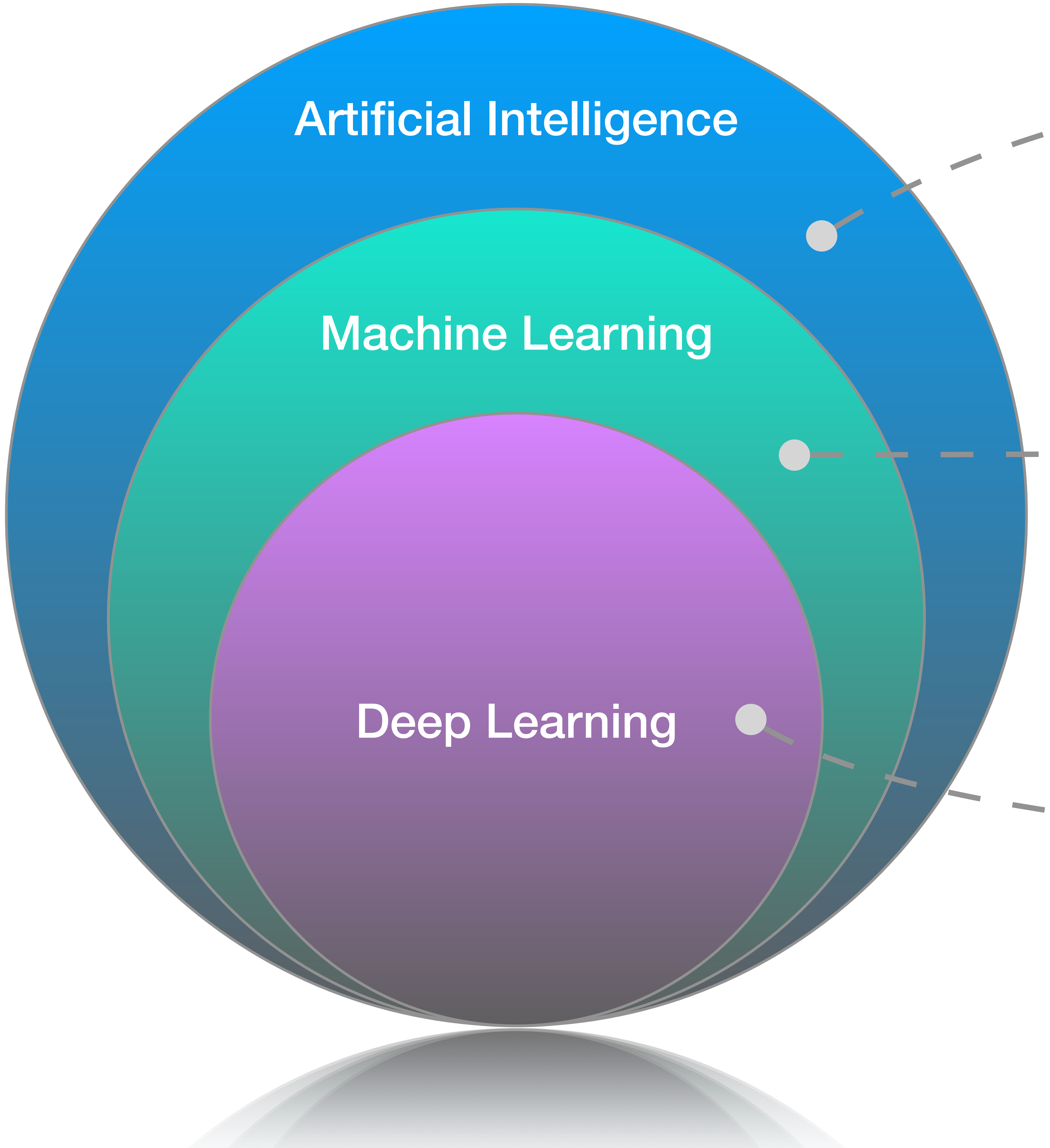

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MACHINE LEARNING

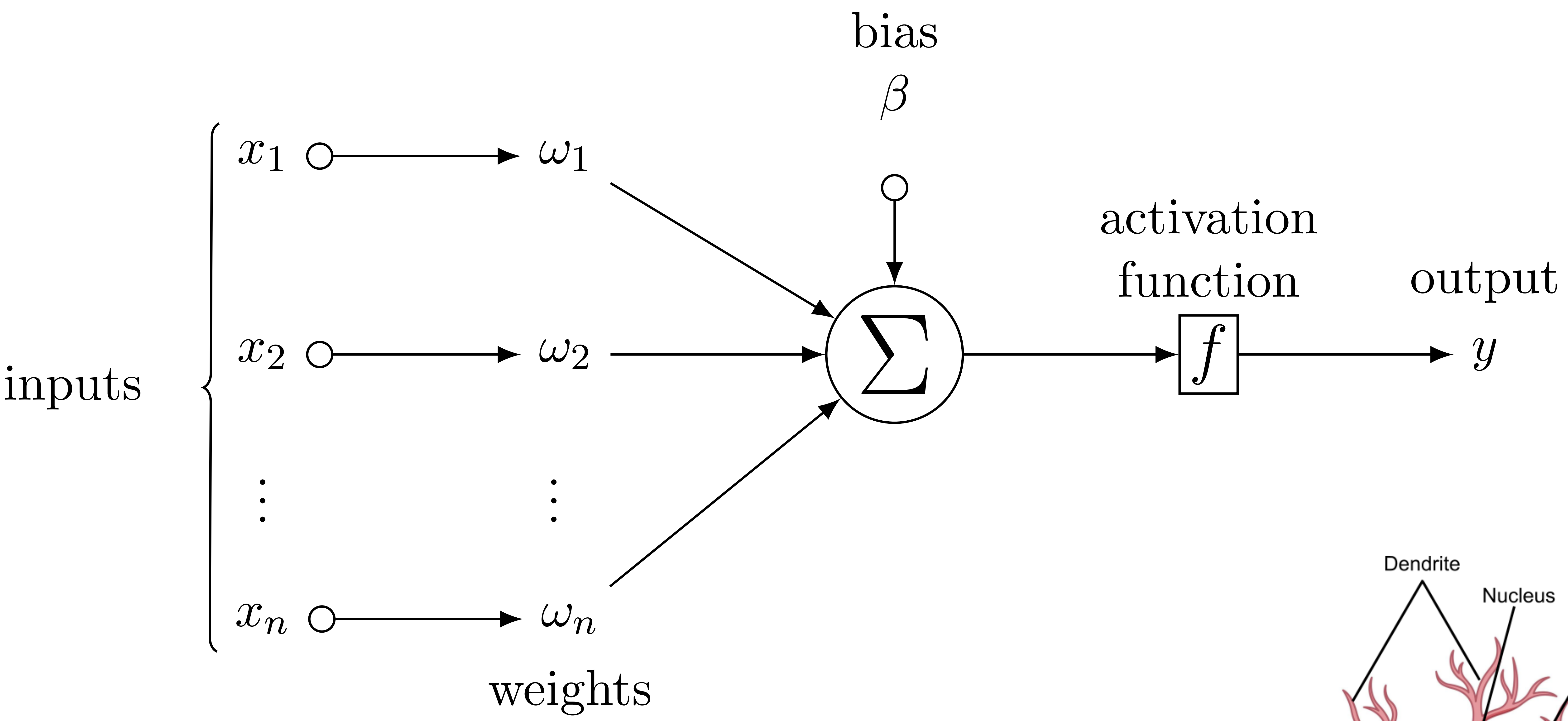
Subset of AI technique which use statistical methods to enable machines to improve with experience

DEEP LEARNING

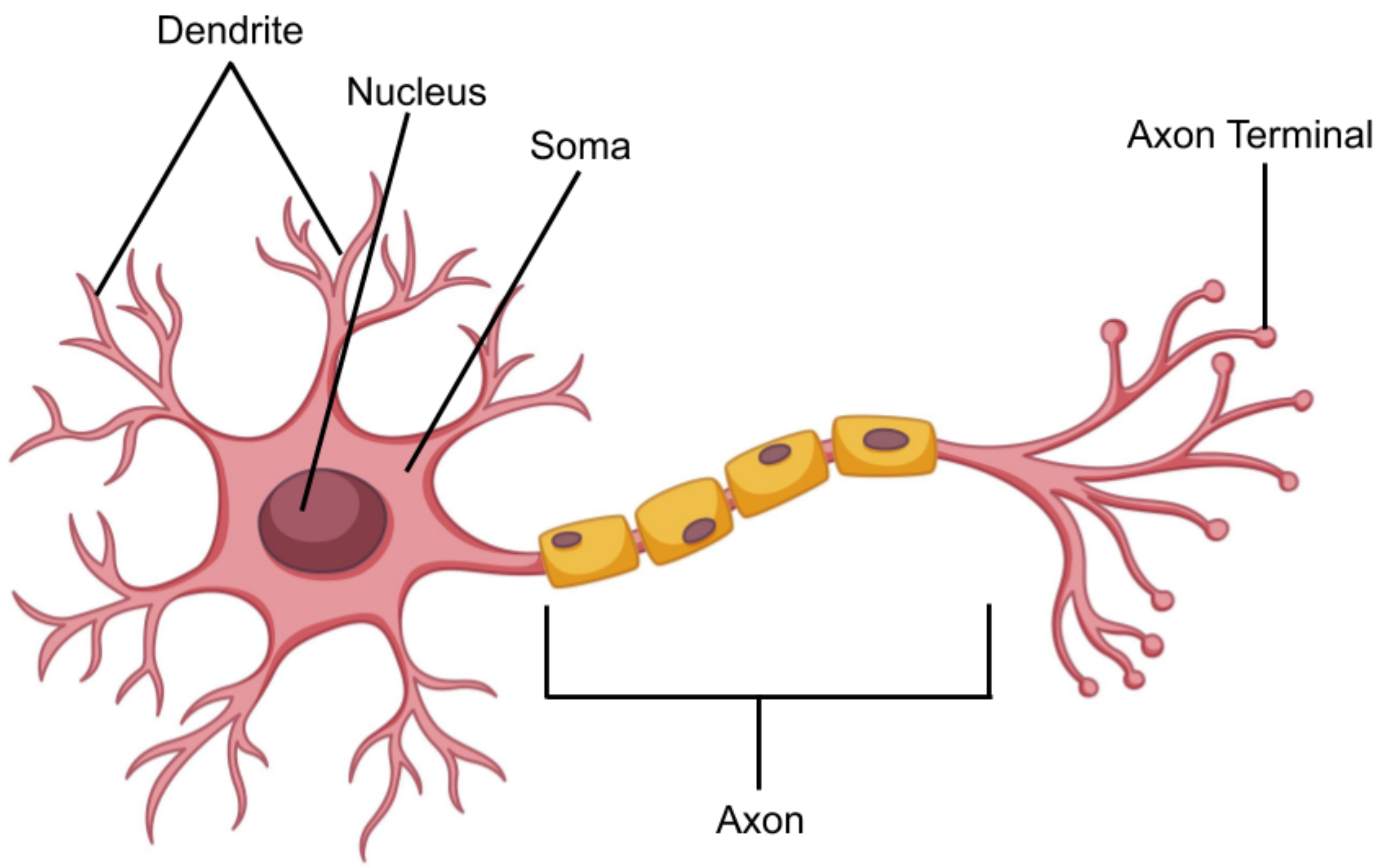
Subset of ML which make the computation of neural networks feasible

What are neural networks?

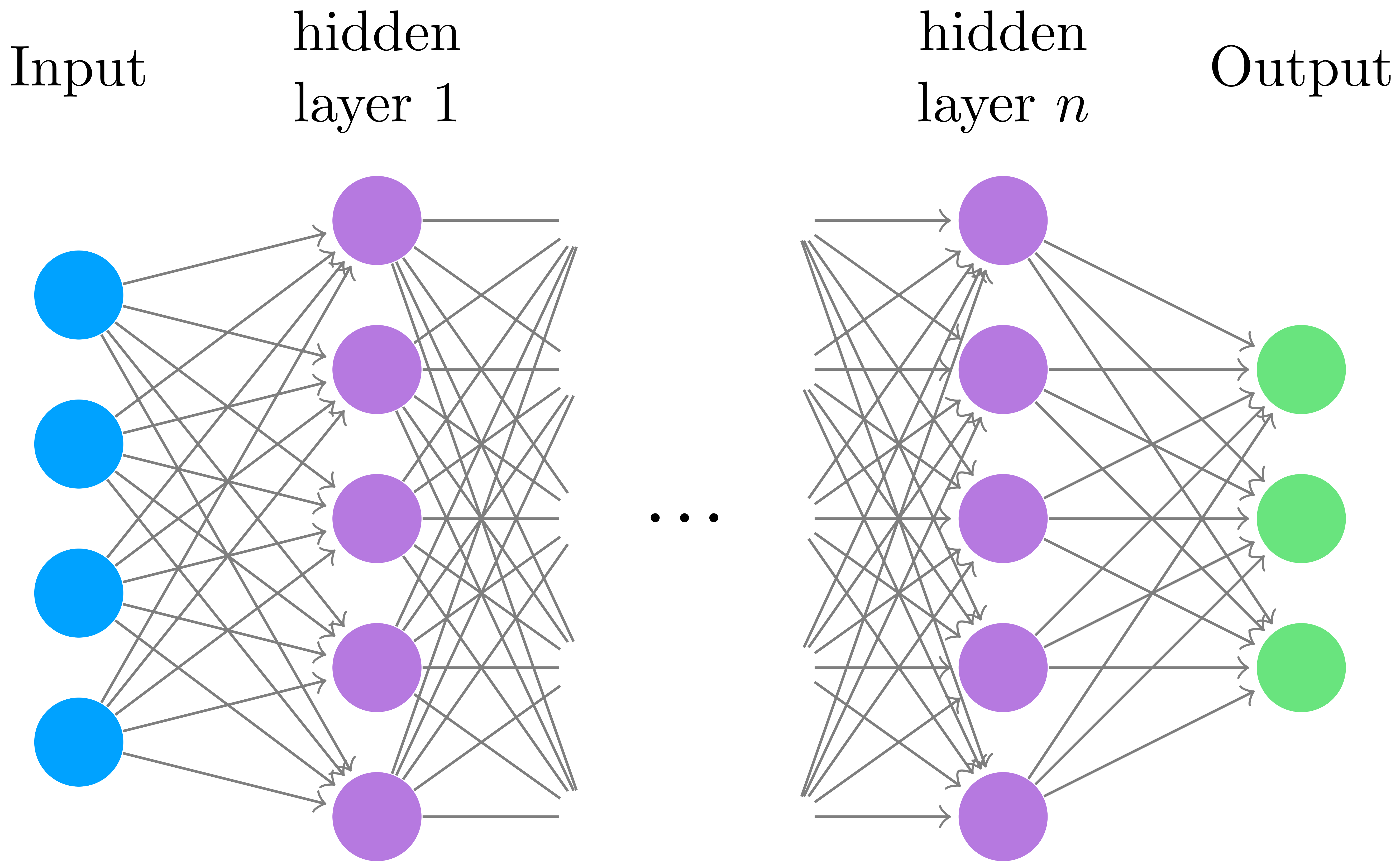
Components of artificial neurons



$$y = f\left(\sum_{i=1}^{n} \omega_i x_i + \beta_i\right)$$



Deep neural network



$$y_j = f_j\left(\sum_m \omega_{jm}^{(n+1)} g_m^{(n)}\left(\cdots\left(\sum_i \omega_{kl}^{(2)} g_l^{(1)}\left(\sum_i \omega_{li}^{(1)} x_i + \beta_l^{(1)}\right) + \beta_k^{(2)}\right)\cdots\right) + \beta_j^{(n+1)}\right)$$

Training objective and optimization

Performance measure

In order to train the neural network, we need a **training objective** or **loss function**:

$$\mathscr{L}_{\text{tot}} = \sum_{i}^{N} \mathscr{L}(f_\omega(x_i), y_i)$$

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Backpropagation

$$\nabla_\omega \mathscr{L}(f_\omega(x), y) = \frac{\mathrm{d}\mathscr{L}(f_\omega(x), y)}{\mathrm{d}\omega} = \sum_{ij} \frac{\partial \mathscr{L}}{\partial f_{j,\omega}} \cdot \frac{\partial f_{j,\omega}}{\partial \omega_i} \stackrel{!}{=} 0$$

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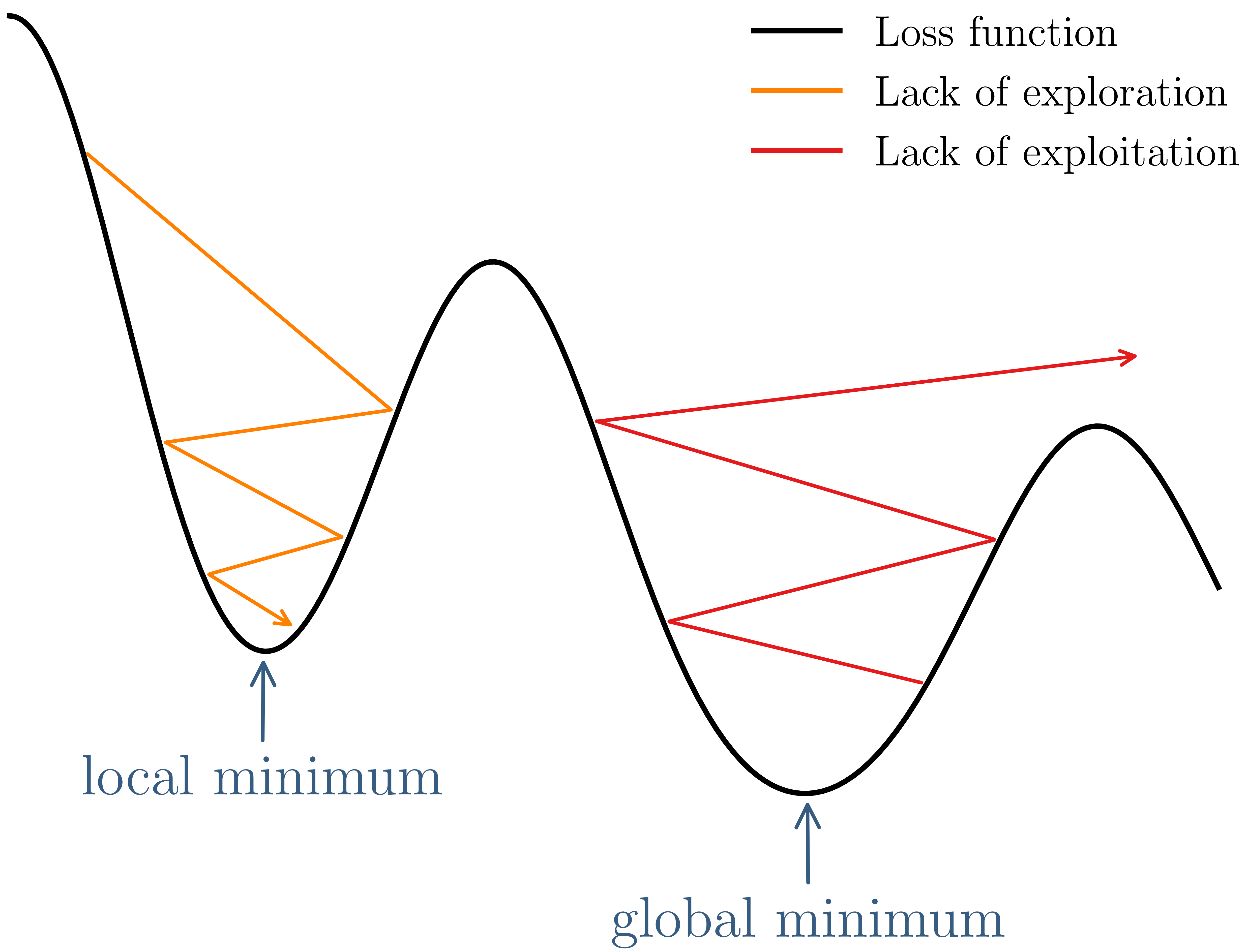
Stochastic gradient descent

$$\omega_{t+1} = \omega_t - \eta \nabla_{\omega_t} \mathcal{L}_b(\omega), \qquad \text{with} \quad \mathcal{L}_b(\omega) = \sum_i^b \mathcal{L}(f_\omega(x_i), y_i)$$

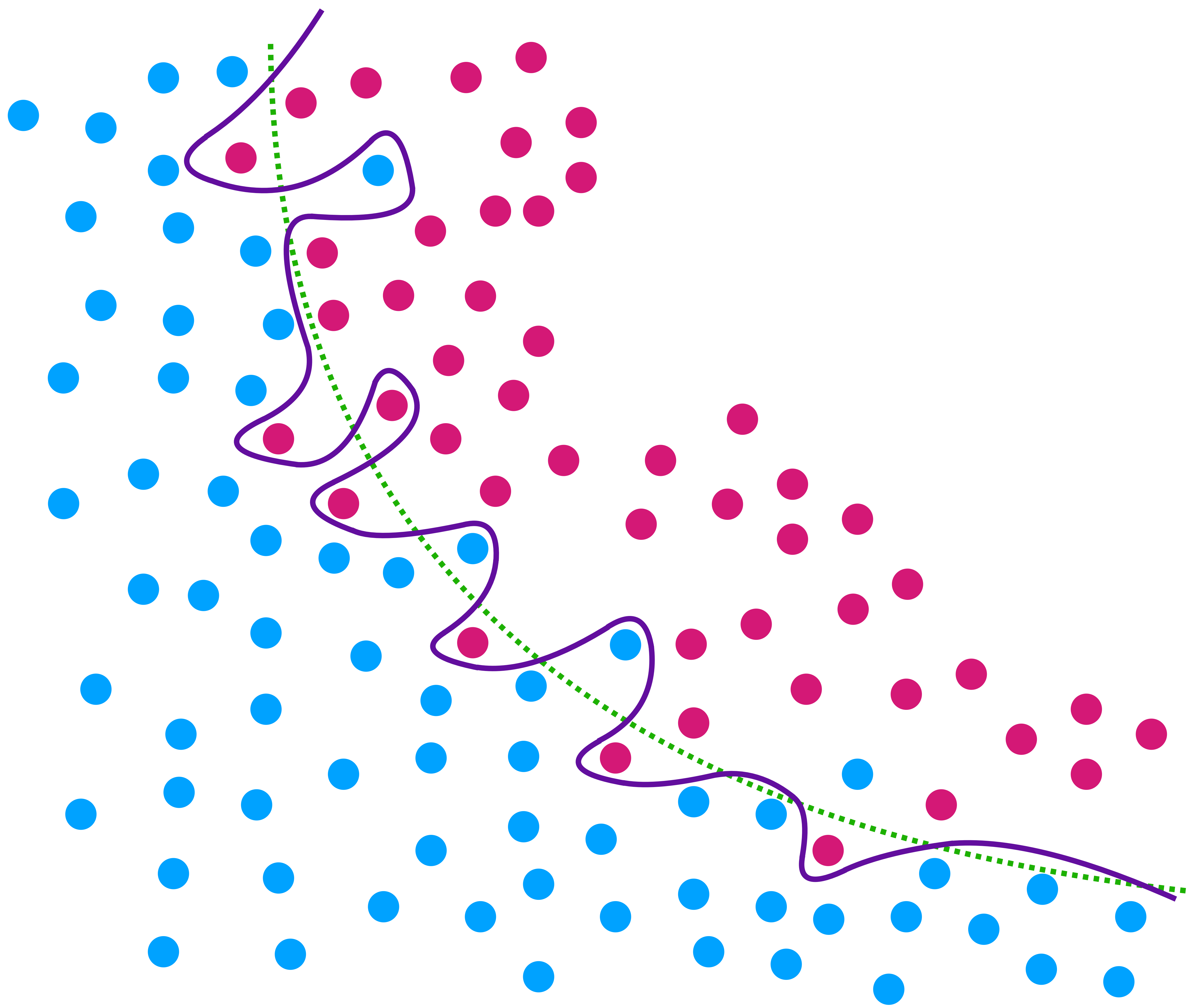

3.75
3.6
2.8
MINIMA
MINIMA
0.15
0.16
MODE CONNECTIVITY
OPTIMA OF COMPLEX LOSS FUNCTIONS CONNECTED BY SIMPLE CURVES OVER
WHICH TRAINING AND TEST ACCURACY ARE NEARLY CONSTANT
BASED ON THE PAPER BY TIMUR GARIPOV, PAVEL IZMAILOV, DMITRII PODOPRIKHIN, DMITRY VETROV, ANDREW GORDON WILSON
VISUALIZATION & ANALYSIS IS A COLLABORATION BETWEEN TIMUR GARIPOV, PAVEL IZMAILOV AND JAVIER IDEAMI@LOSSLANDSCAPE.COM
NeurIPS 2018, ARXIV:1802.10026 | LOSSLANDSCAPE.COM
LOSS (TRAIN MODE)
REAL DATA, RESNET-20 NO-SKIP,
CIFAR10, SGD-MOM, BS=128
WD=3e-4, MOM=0.9
BN, TRAIN MOD, 90K PTS
LOG SCALED (ORIG LOSS NUMS)

Optimizer and loss landscape

Finding the global minimum in a sea of local minima



Overfitting und regularization



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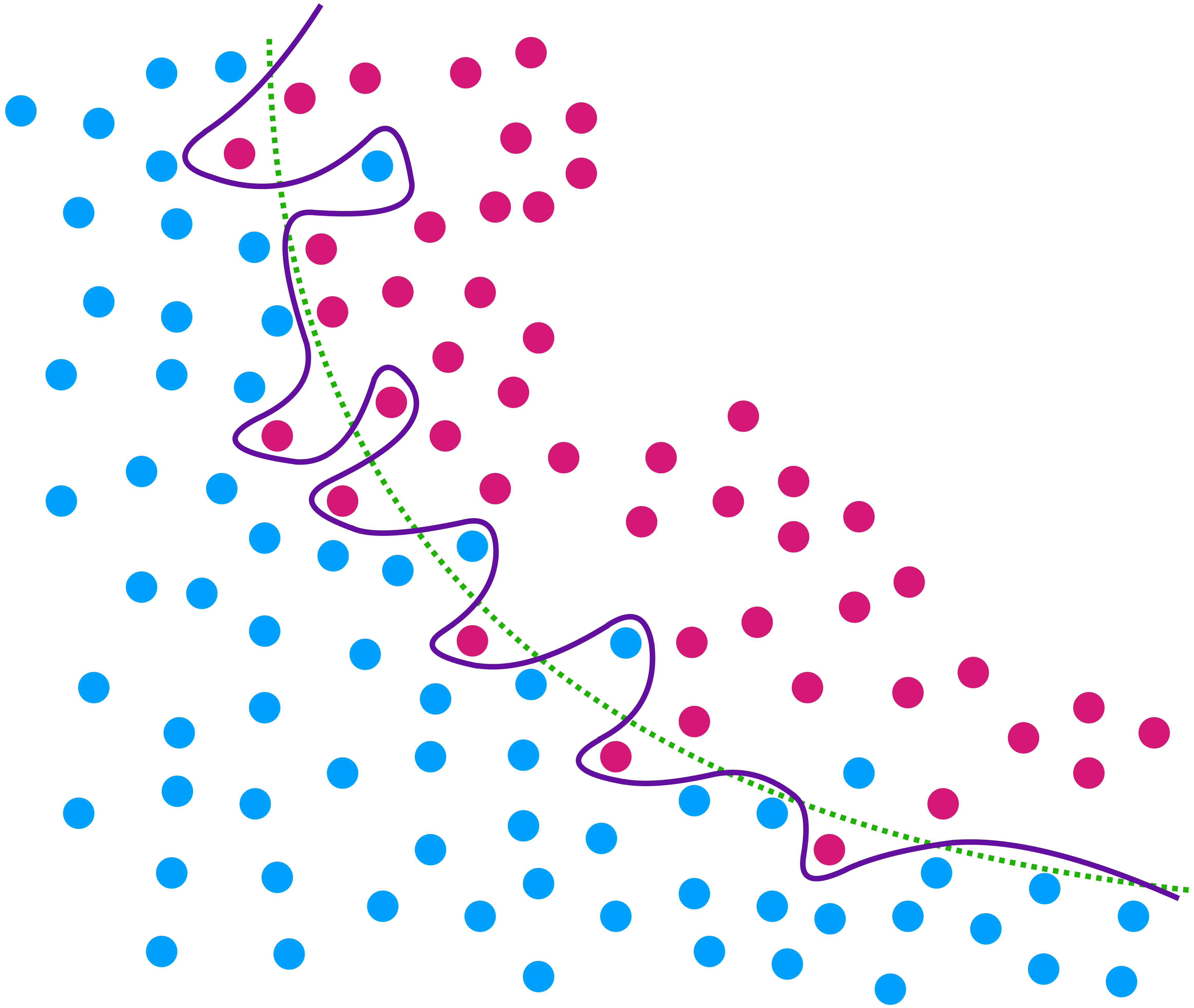
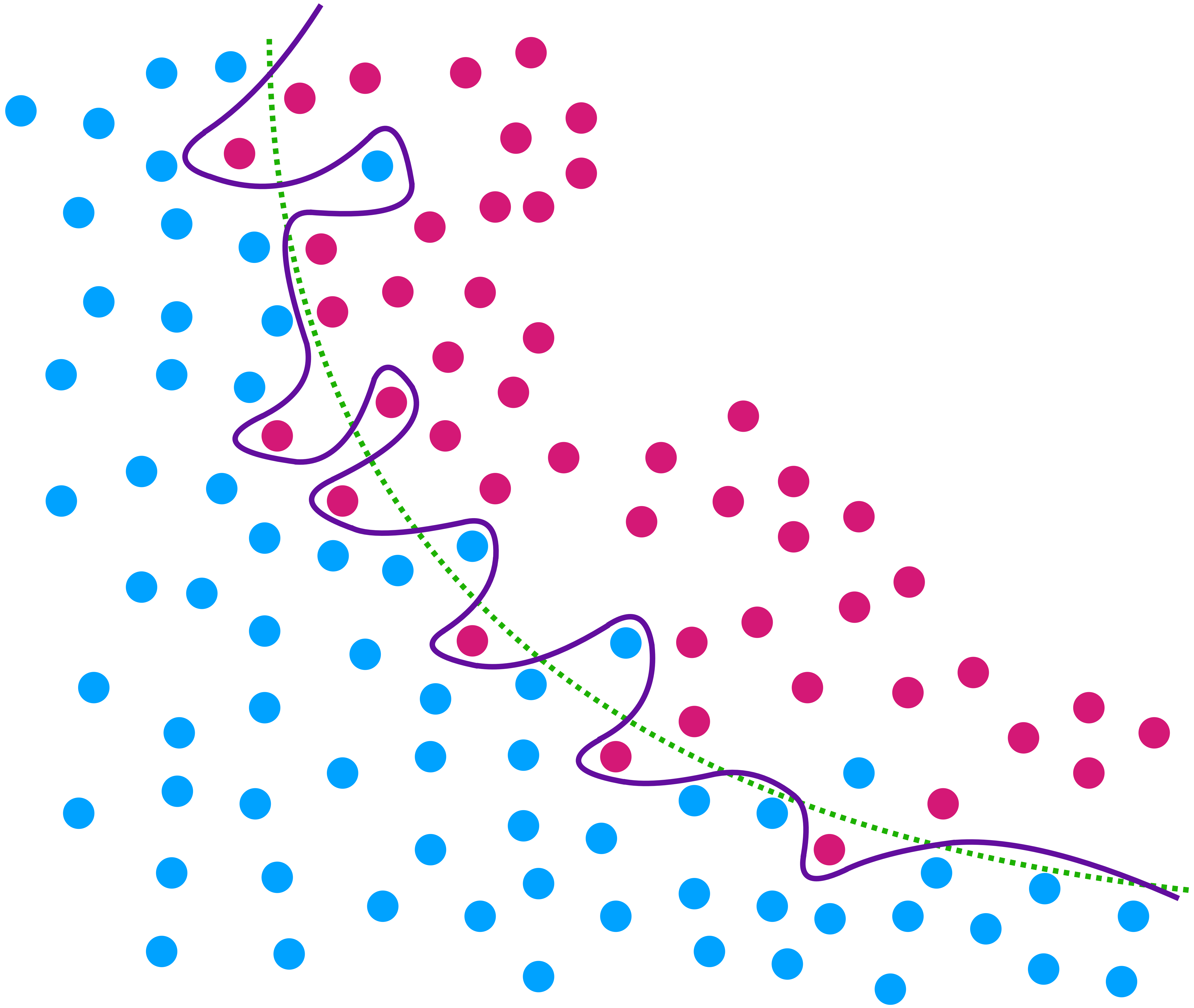


Identify

- Test/validation set:
  independent samples for testing/ validation

Overfitting und regularization



Identify

- Test/validation set:
  independent samples for testing/ validation

Regularization

- L1 & L2 Regularization: penalty term in the loss function
- Dropout: randomly sets the inputs to some nodes to zero

How to choose the loss function?

Fits and interpolations

Approximate function

$$f_\omega(x) \approx f(x)$$

Maximize probability for fit output

$$p(x\,|\,\omega) = \prod_j \frac{1}{\sqrt{2\pi\sigma_j}} \exp\left(-\frac{|f_j - f_\omega(x_j)\,|^2}{2\sigma_j}\right)$$

$$\Rightarrow \quad \log p(x\,|\,\omega) = -\sum_j \frac{|f_j - f_\omega(x_j)\,|^2}{2\sigma_j} + \text{const}$$

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Minimize negative log-likelihood

Loss function of the fit

$$\mathscr{L}_{\text{fit}} = \sum_j \frac{\mathscr{L}_j}{N} = \sum_j \frac{|f_j - f_\omega(x_j)\,|^2}{2\sigma_j N}$$

Regression in Machine Learning

Loss function in fits

$$\mathscr{L}_{\text{fit}} = \frac{1}{N}\sum_j \mathscr{L}_j = \frac{1}{N}\sum_j \frac{|f_j - f_\omega(x_j)|^2}{2\sigma_j}$$

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if error σ_j unknown
or same for all

Typical ML Regression loss

$$\mathscr{L} = \frac{1}{2\sigma N}\sum_j |f_j - f_\omega(x_j)|^2 \equiv \frac{1}{2\sigma}\text{MSE}$$

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Preprocessing of the training data

$$f_j \to \log f_j \qquad f_j \to f_j - \langle f_j \rangle \qquad f_j \to \frac{f_j}{\langle f_j \rangle} \cdots$$

Regression in Machine Learning

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Mean-absolute error

$$\mathscr{L}_{\text{MAE}} = \frac{1}{N}\sum_j |f_j - f_\omega(x_j)|$$

What about Classification?

Approximate data probability

$$\boxed{p_\omega(x) \approx p_{\text{data}}(x)}$$

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IX. *On the Problem of the most Efficient Tests of Statistical Hypotheses.*

By J. NEYMAN, *Nencki Institute, Soc. Sci. Lit. Varsoviensis, and Lecturer at the Central College of Agriculture, Warsaw, and* E. S. PEARSON, *Department of Applied Statistics, University College, London.*

(*Communicated by* K. PEARSON, *F.R.S.*)

(Received August 31, 1932.—Read November 10, 1932.)

ratio of the two likelihoods is the **most powerful** test statistic

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Optimal test statistic

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Kullback-Leibler divergence

$$D_{\text{KL}}(p_{\text{data}} | p_\omega) = \left\langle \log \frac{p_{\text{data}}(x)}{p_\omega(x)} \right\rangle_{p_{\text{data}}} = \int \mathrm{d}x\, p_{\text{data}}(x) \log \frac{p_{\text{data}}(x)}{p_\omega(x)}$$

Classification loss function

Classification loss

$$\mathscr{L}_{\text{class}} = \sum_{j=S,B} D_{\text{KL}}(p_{\text{data},j} | p_{\omega,,j})$$
$$= -\sum_{\{x\}} \left[p_{\text{data},S} \log p_{\omega,S} + p_{\text{data},B} \log p_{\omega,B}\right] + \text{const}$$

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$\downarrow$ Using $p_B = 1 - p_S$

Binary cross-entropy loss

$$\mathscr{L}_{\text{BCE}} = -\sum_{\{x\}} \left[p_{\text{data},S} \log p_{\omega,S} + (1 - p_{\text{data},S}) \log(1 - p_{\omega,S}) \right]$$

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Generalization (multi-class)

$$\mathscr{L}_{\text{CE}} = -\sum_{j \in C_i} p_{\text{data},j} \log p_{\omega,j}$$

Useful libraries + algorithms

- **scikit-learn:** For most of the “basic” algorithms like Linear Regression and Boosted Decision Trees. Also useful for preprocessing, model combination, etc.

- **XGBoost, LightGBM, CatBoost:** For optimized tree-based models

- **TensorFlow, PyTorch, Jax:** For deep learning models

The Landscape of Machine Learning

Machine Learning
Supervised Learning
Classification
Point Clouds [2102.05073]
PELICAN [2211.00454]
Energy Flow Networks [1810.05165]
Landscape of Top tagger [1902.09914]
Bayesian Tagger [1904.10004]
Regression
MadMiner [1907.10621,…]
NNPDF [2109.02653]
Matrix Elements [2206.14831]
Symbolic regression [2109.10414]
Reinforcement Learning
Flavor structure [2304.14176]
Simplifying Polylogs [2206.04115]
String vacua & landscape [1903.11616, 2111.11466]
Model Building [2103.04759]
Analytic continuation [2112.13011]
Unsupervised Learning
Clustering
Jet Clustering [2008.06064]
3D Pixel Clustering [2007.03083]
Anomaly Detection
Normalized AE [2206.14225]
CATHODE [2109.00546]
CWoLA Hunting [1902.02634]
(R-)ANODE [2001.04990,…]
Generative Models
NF
Precision Generation [2110.13632]
MEM [2210.00019]
MADNIS [2212.06172,..]
CaloFlow I-IV [2106.05285,…]
ELSA [2305.07696]
VAE
OTUS [2101.08944]
Jet Simulation [2203.00520]
Diffusion Models
PC-JeDi [2303.05376]
FPCD [2304.01266]
DDPM & CFM [2305.10475]
GAN
EPiC-GAN [2301.08128]
How to GAN [1907.03764]
CaloGAN [1712.10321]
Transformer
JetGPT [2305.10475]


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MEM [2210.00019]
MADNIS [2212.06172,..]
CaloFlow I-IV [2106.05285,…]
ELSA [2305.07696]
Diffusion Models
PC-JeDi [2303.05376]
FPCD [2304.01266]
DDPM & CFM [2305.10475]
GAN
EPiC-GAN [2301.08128]
How to GAN [1907.03764]
CaloGAN [1712.10321]
Transformer
JetGPT [2305.10475]
Clustering
Jet Clustering [2008.06064]
3D Pixel Clustering [2007.03083]
Anomaly Detection
Normalized AE [2206.14225]
CATHODE [2109.00546]
CWoLA Hunting [1902.02634]
(R-)ANODE [2001.04990,…]
Reinforcement Learning
Flavor structure [2304.14176]
Simplifying Polylogs [2206.04115]
String vacua & landscape [1903.11616, 2111.11466]
Model Building [2103.04759]
Analytic continuation [2112.13011]

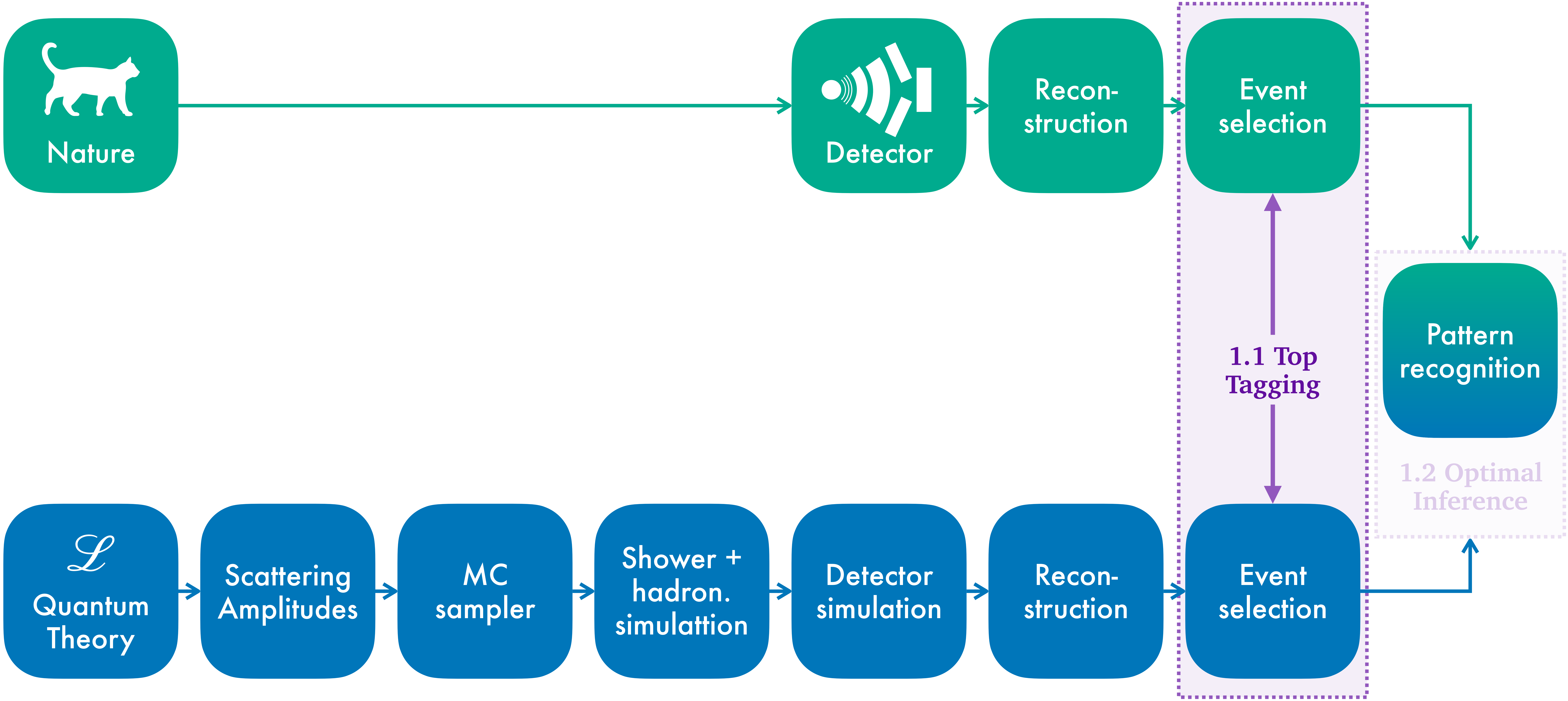
Break & Questions

3 Minutes

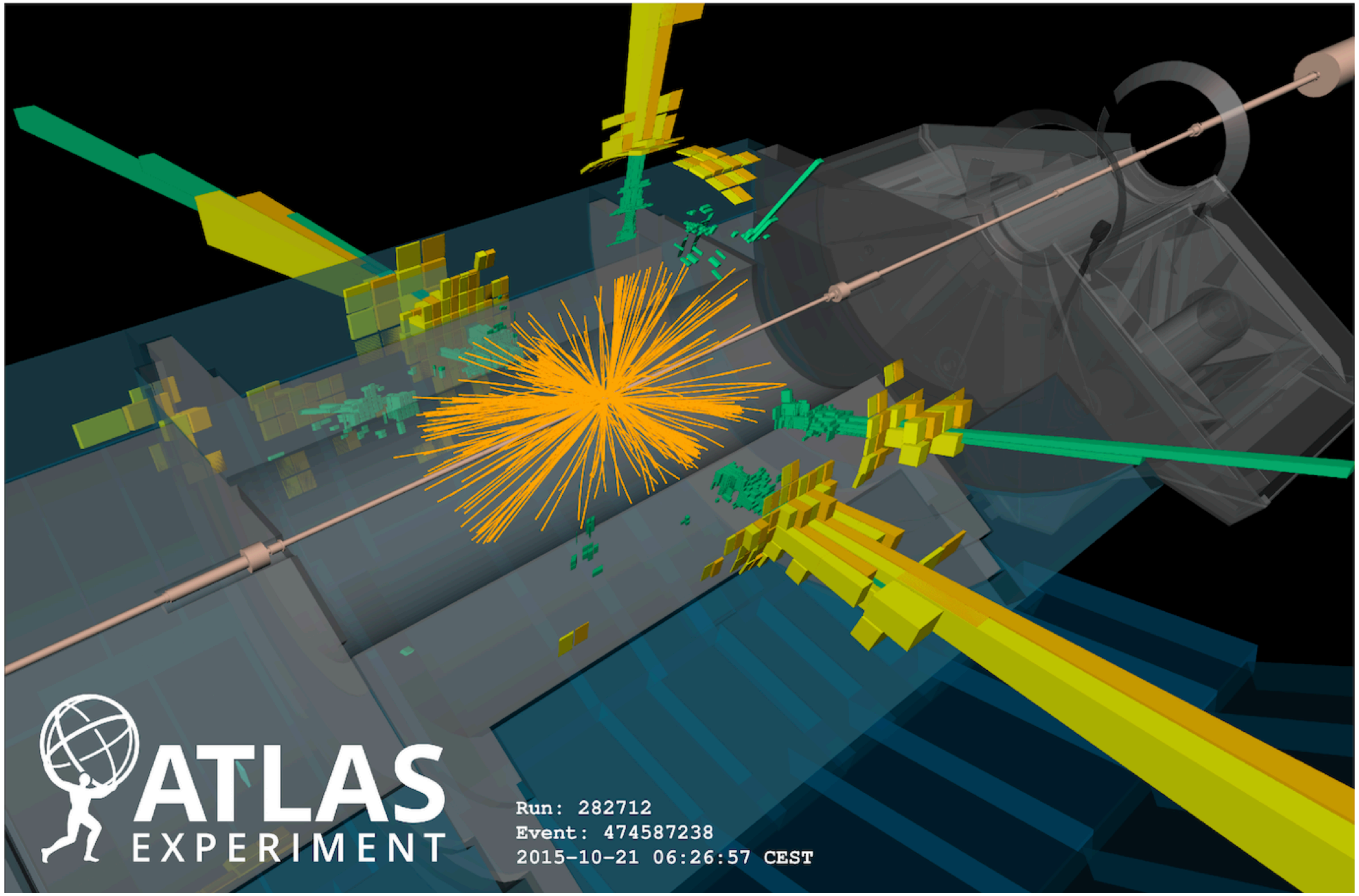
Example I

Classification with Top Tagging

LHC analysis + ML

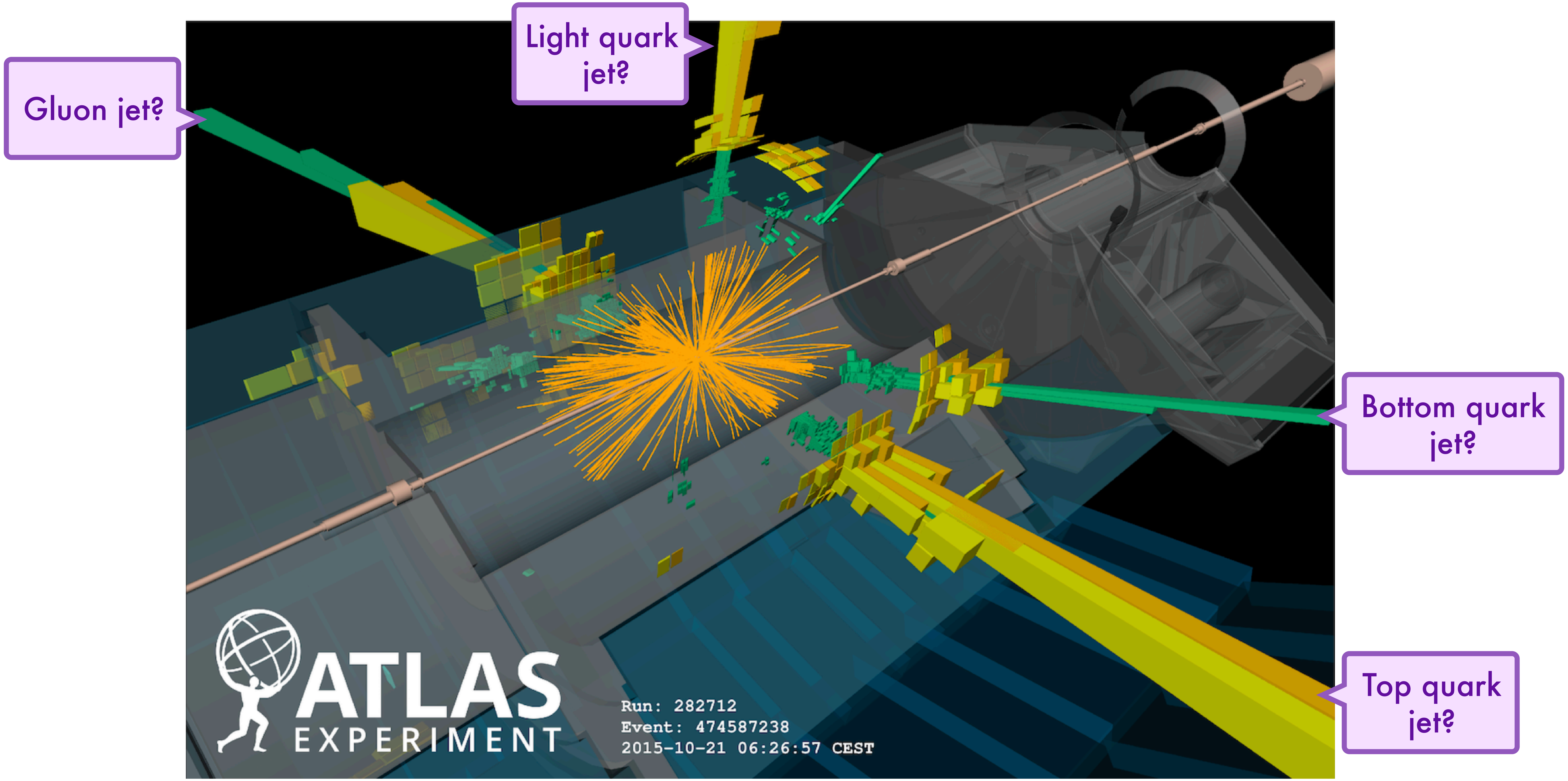


What is jet tagging?



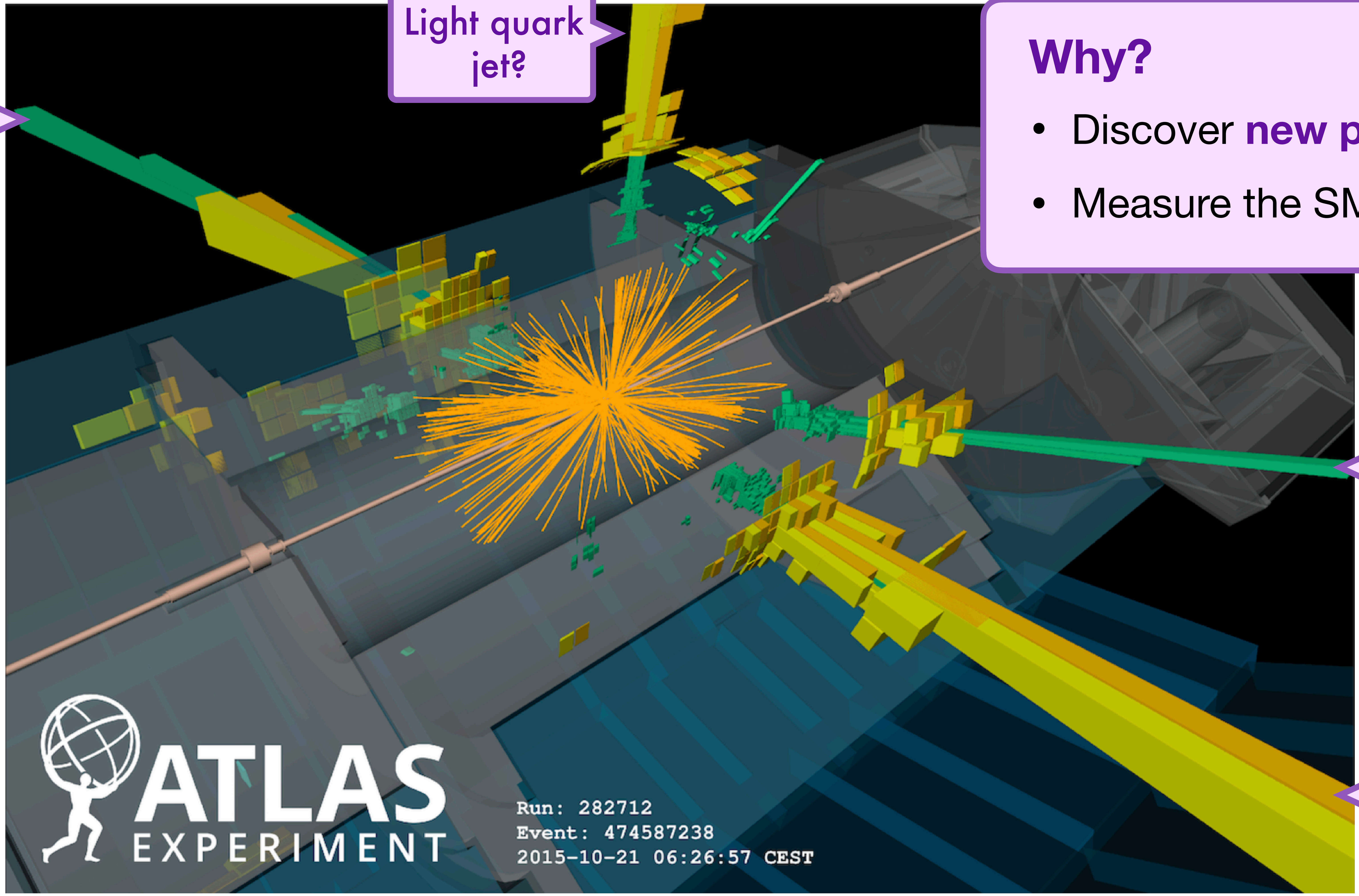
A jet is **collimated shower** of particles in the collider

What is jet tagging?



We want to know **which particle** produced the jet!

What is jet tagging?



Gluon jet?

Light quark jet?

Bottom quark jet?

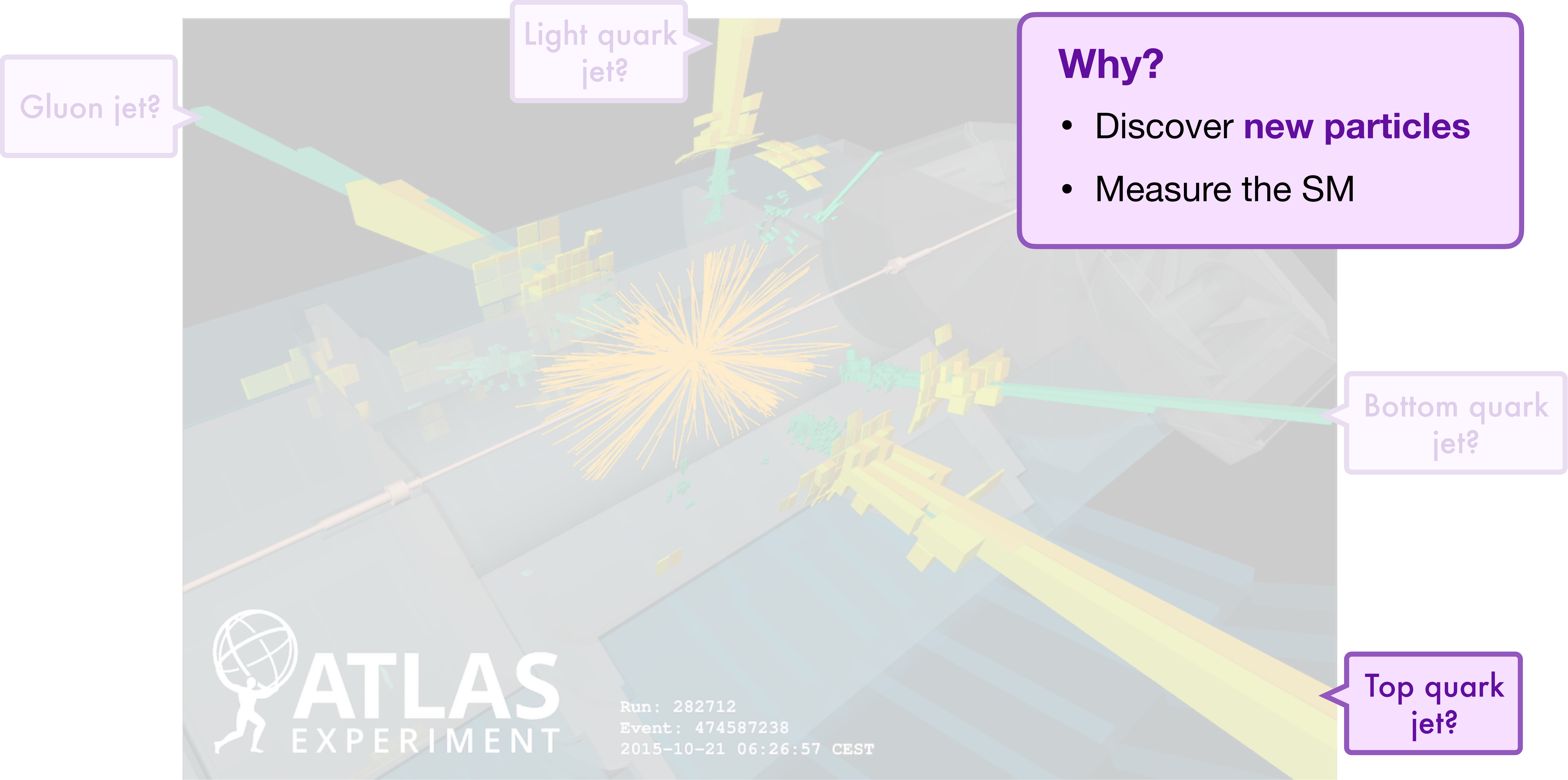
Top quark jet?

Why?

- Discover **new particles**
- Measure the SM

We want to know **which particle** produced the jet!

What is jet tagging?

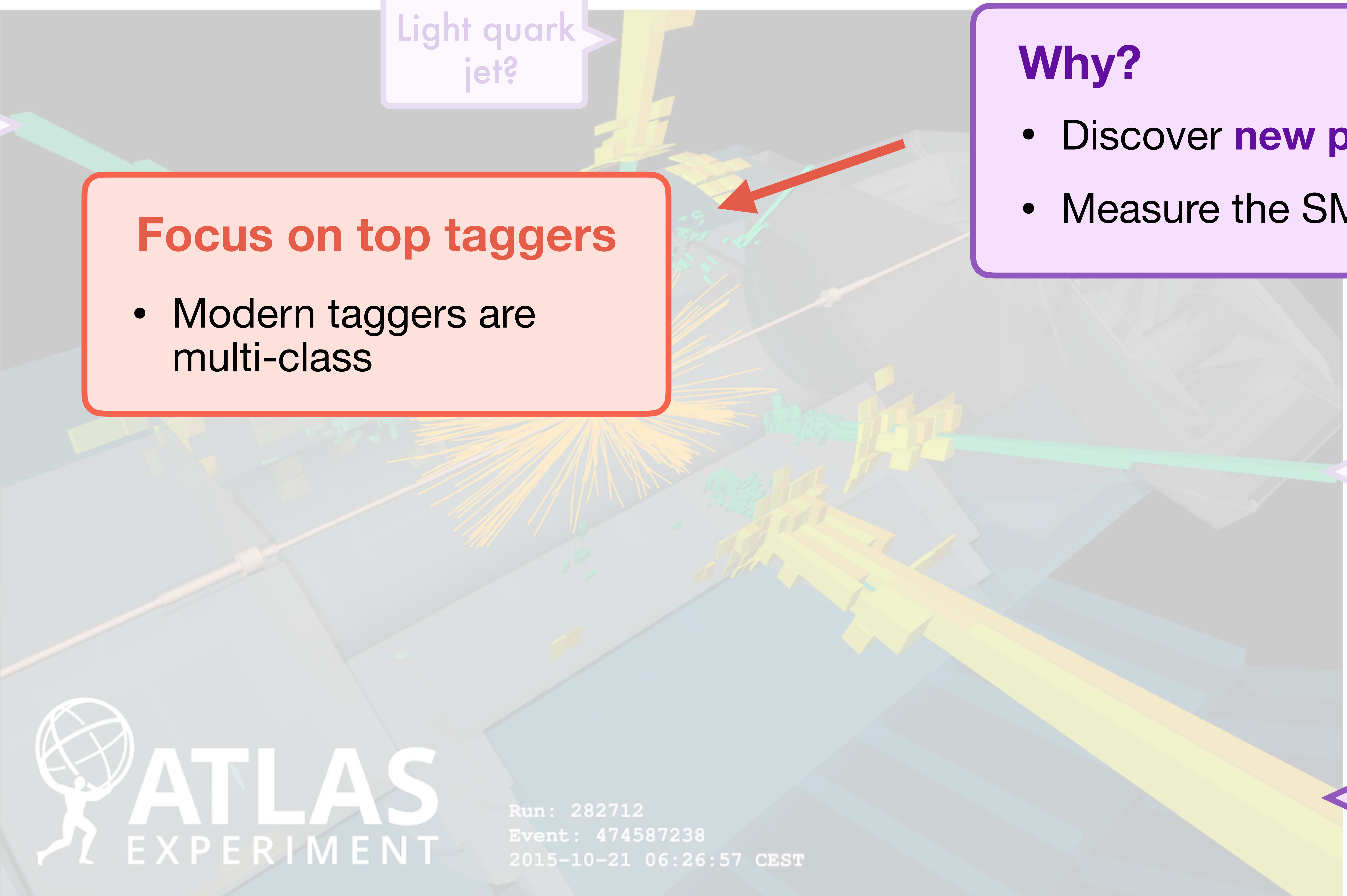


Why?

- Discover **new particles**
- Measure the SM

We want to know **which particle** produced the jet!

What is jet tagging?



Focus on top taggers

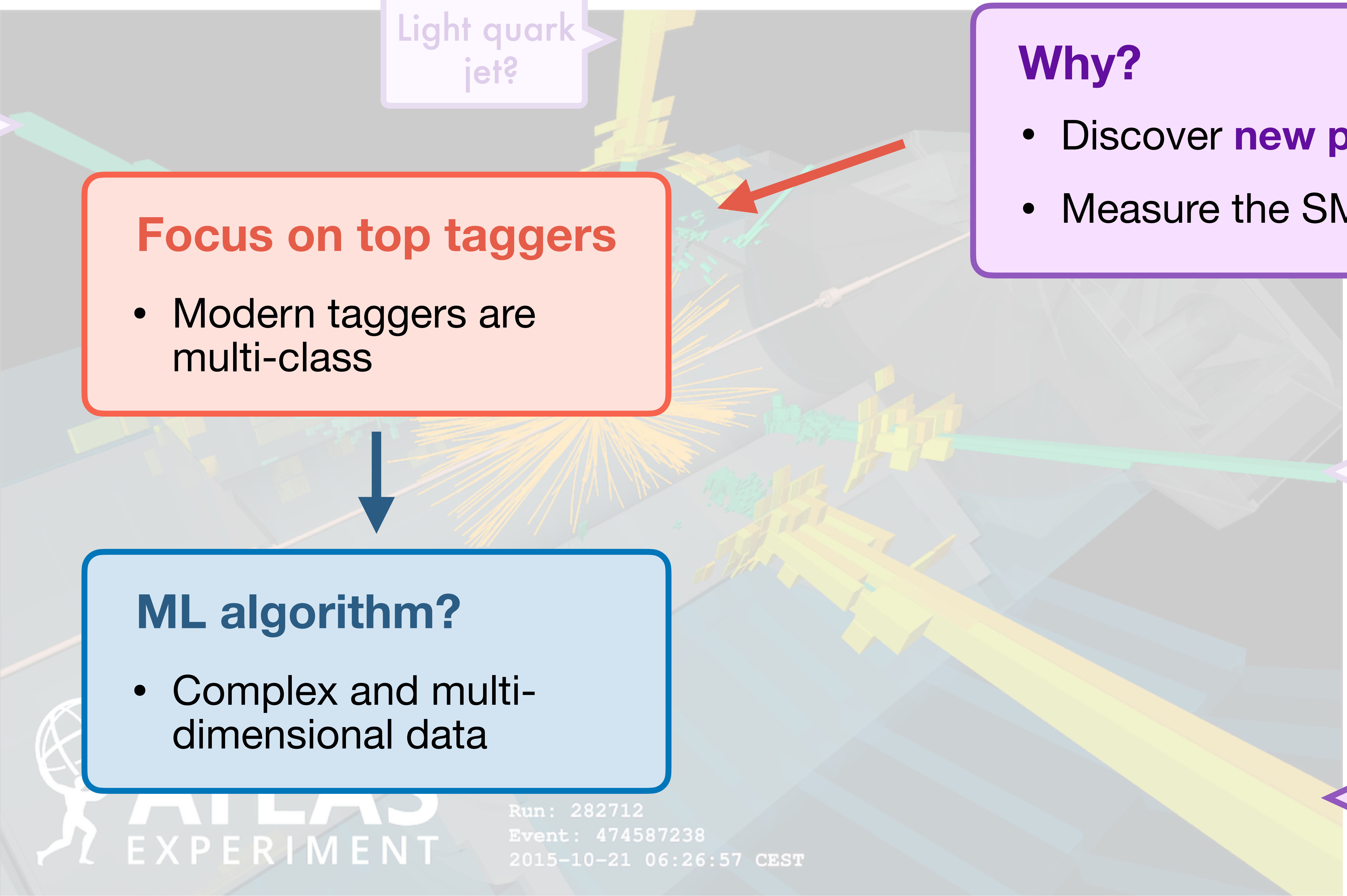
- Modern taggers are multi-class

Why?

- Discover **new particles**
- Measure the SM

We want to know **which particle** produced the jet!

What is jet tagging?



Gluon jet?

Light quark jet?

Bottom quark jet?

Top quark jet?

Why?

- Discover **new particles**
- Measure the SM

Focus on top taggers

- Modern taggers are multi-class

ML algorithm?

- Complex and multi-dimensional data

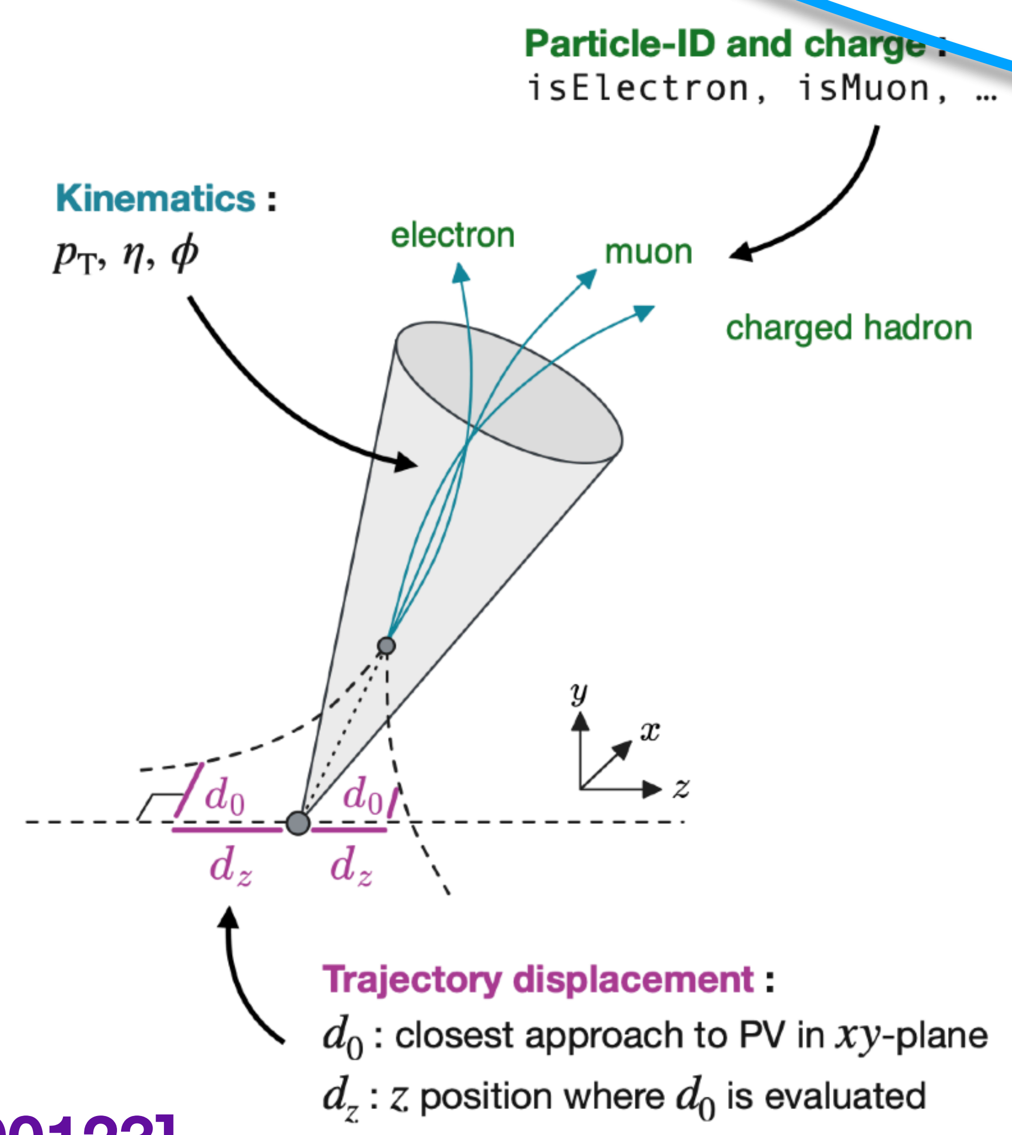
We want to know **which particle** produced the jet!

What is jet tagging?

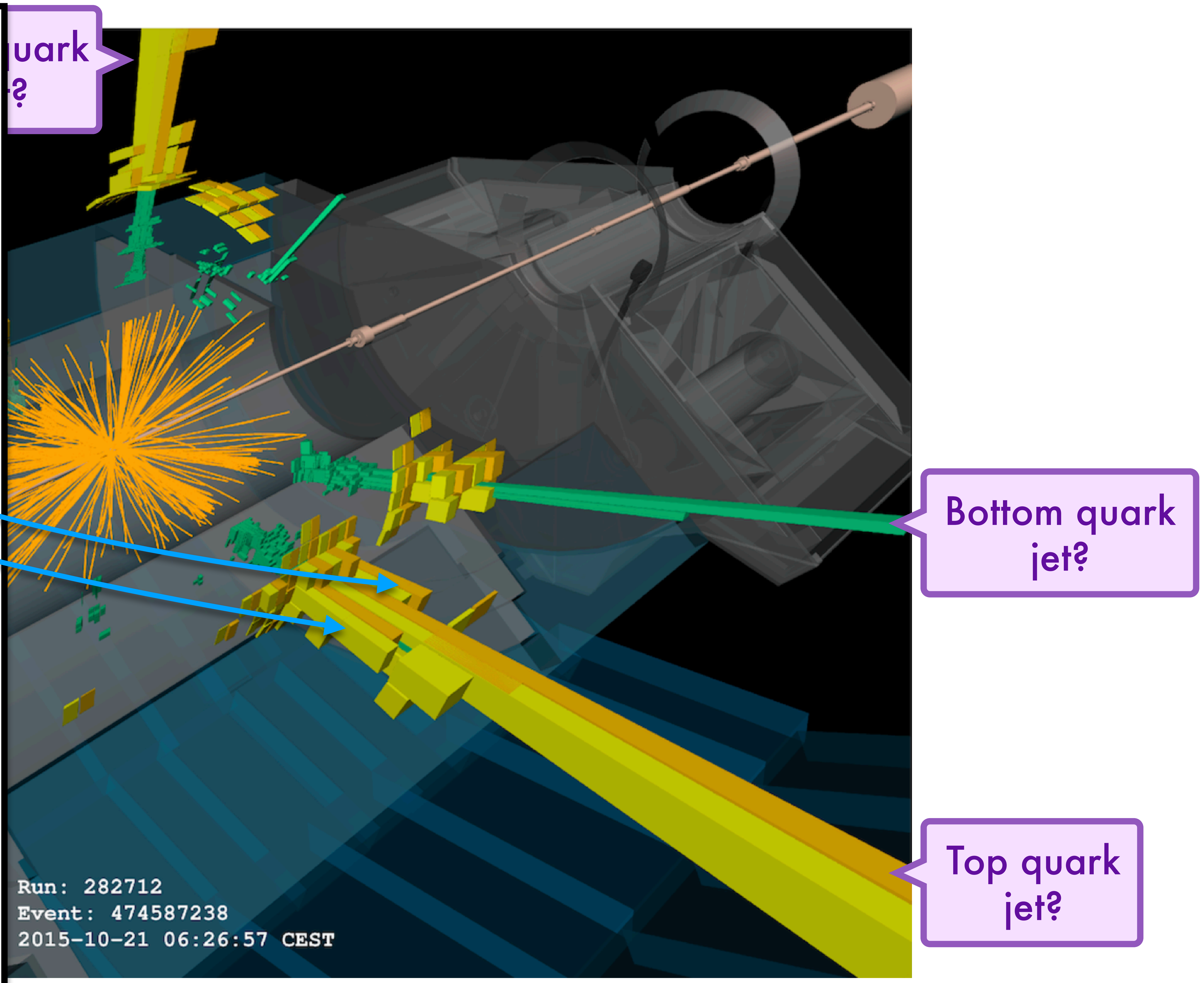
Data most naturally as **point cloud**

Each **input** (jet, event,…)
is a **set of k-dimensional vectors**
(individual particles, hits,…)

$$J_i = \{\vec{p}_1, \ldots, \vec{p}_n\}$$



[2312.00123]



Landscape Dataset

- Open dataset for the devolopment of better tagging algorithms for particle physics

- 2 million simulated examples

- Perfect class labels:
  S=top jet or B=light quark/gluon jet

- Input: momentum sorted list of 200 particles/jets with 3 features/particle
  (p_x, p_y, p_z)


SciPost Physics Submission

The Machine Learning Landscape of Top Taggers

G. Kasieczka (ed)[1], T. Plehn (ed)[2], A. Butter[2], K. Cranmer[3], D. Debnath[4], B. M. Dillon[5], M. Fairbairn[6], D. A. Faroughy[5], W. Fedorko[7], C. Gay[7], L. Gouskos[8], J. F. Kamenik[5,9], P. T. Komiske[10], S. Leiss[1], A. Lister[7], S. Macaluso[3,4], E. M. Metodiev[10], L. Moore[11], B. Nachman,[12,13], K. Nordström[14,15], J. Pearkes[7], H. Qu[8], Y. Rath[16], M. Rieger[16], D. Shih[4], J. M. Thompson[2], and S. Varma[6]

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4 NHECT, Dept. of Physics and Astronomy, Rutgers, The State University of NJ, USA
5 Jozef Stefan Institute, Ljubljana, Slovenia
6 Theoretical Particle Physics and Cosmology, King's College London, United Kingdom
7 Department of Physics and Astronomy, The University of British Columbia, Canada
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10 Center for Theoretical Physics, MIT, Cambridge, USA
11 CP3, Universitéxx Catholique de Louvain, Louvain-la-Neuve, Belgium
12 Physics Division, Lawrence Berkeley National Laboratory, Berkeley, USA
13 Simons Inst. for the Theory of Computing, University of California, Berkeley, USA
14 National Institute for Subatomic Physics (NIKHEF), Amsterdam, Netherlands
15 LPTHE, CNRS & Sorbonne Université, Paris, France
16 III. Physics Institute A, RWTH Aachen University, Germany

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plehn@uni-heidelberg.de

July 24, 2019

arXiv:1902.09914v3 [hep-ph] 23 Jul 2019

Abstract

Based on the established task of identifying boosted, hadronically decaying top quarks, we compare a wide range of modern machine learning approaches. Unlike most established methods they rely on low-level input, for instance calorimeter output. While their network architectures are vastly different, their performance is comparatively similar. In general, we find that these new approaches are extremely powerful and great fun.

[1902.09914]

Landscape Dataset

- Open d
  of bette
  for parti
- 2 millio
- Perfect
  S=top j
- Input: m
  200 par
  3 featur
  (p_x, p_y, p_z)

SciPost Physics Submission

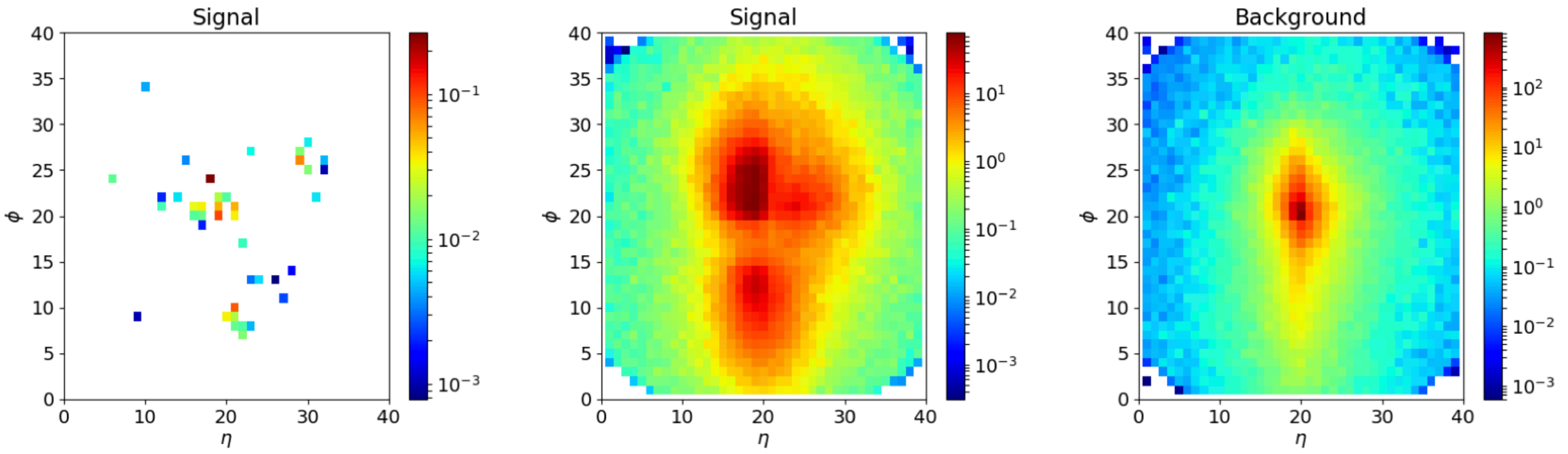


Figure 1: Left: typical single jet image in the rapidity vs azimuthal angle plane for the top signal after pre-processing. Center and right: signal and background images averaged over 10,000 individual images.

[1902.09914]

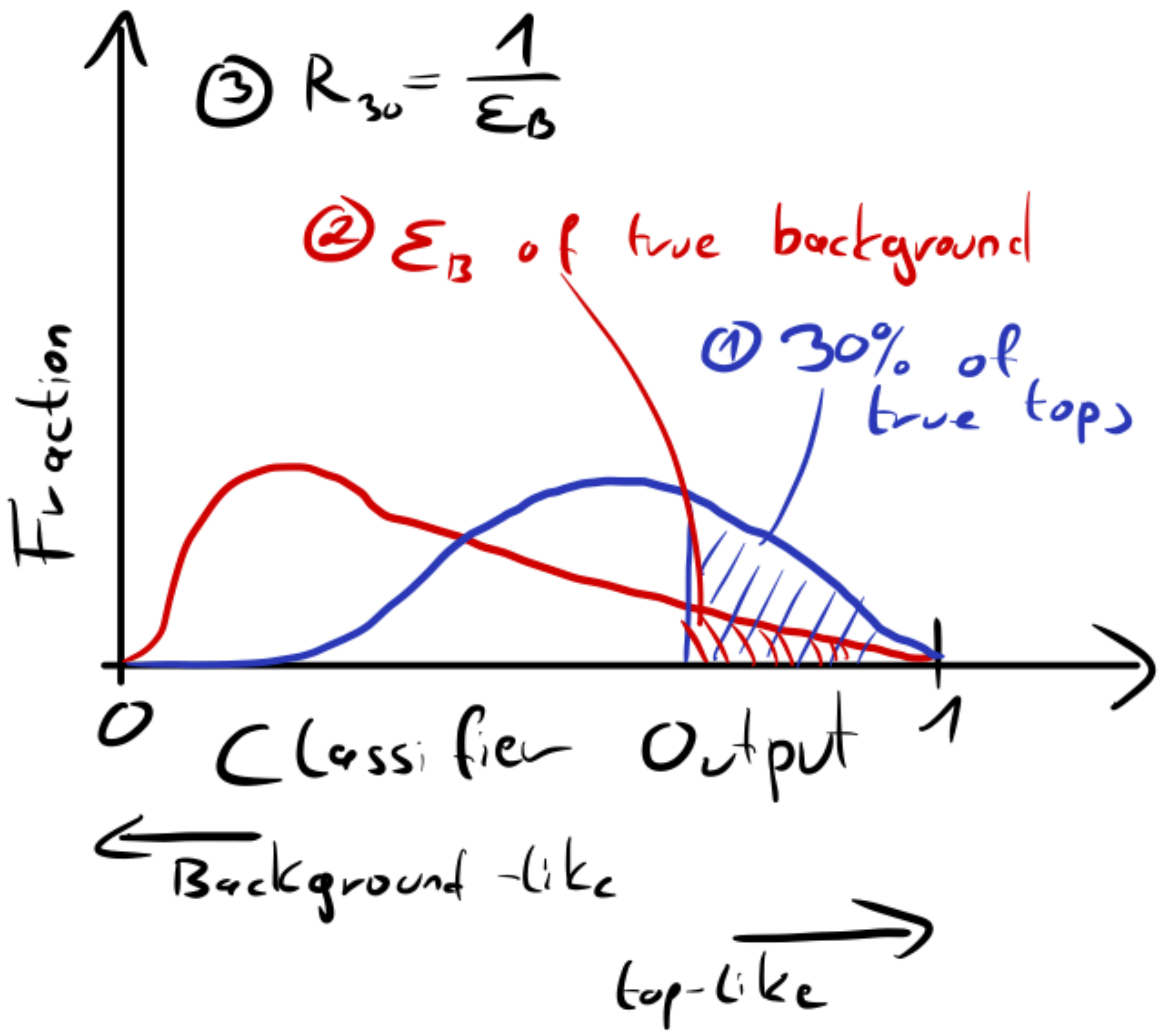
Based on the established task of identifying boosted, hadronically decaying top quarks, we compare a wide range of modern machine learning approaches. Unlike most established methods they rely on low-level input, for instance calorimeter output. While their network architectures are vastly different, their performance is comparatively similar. In general, we find that these new approaches are extremely powerful and great fun.

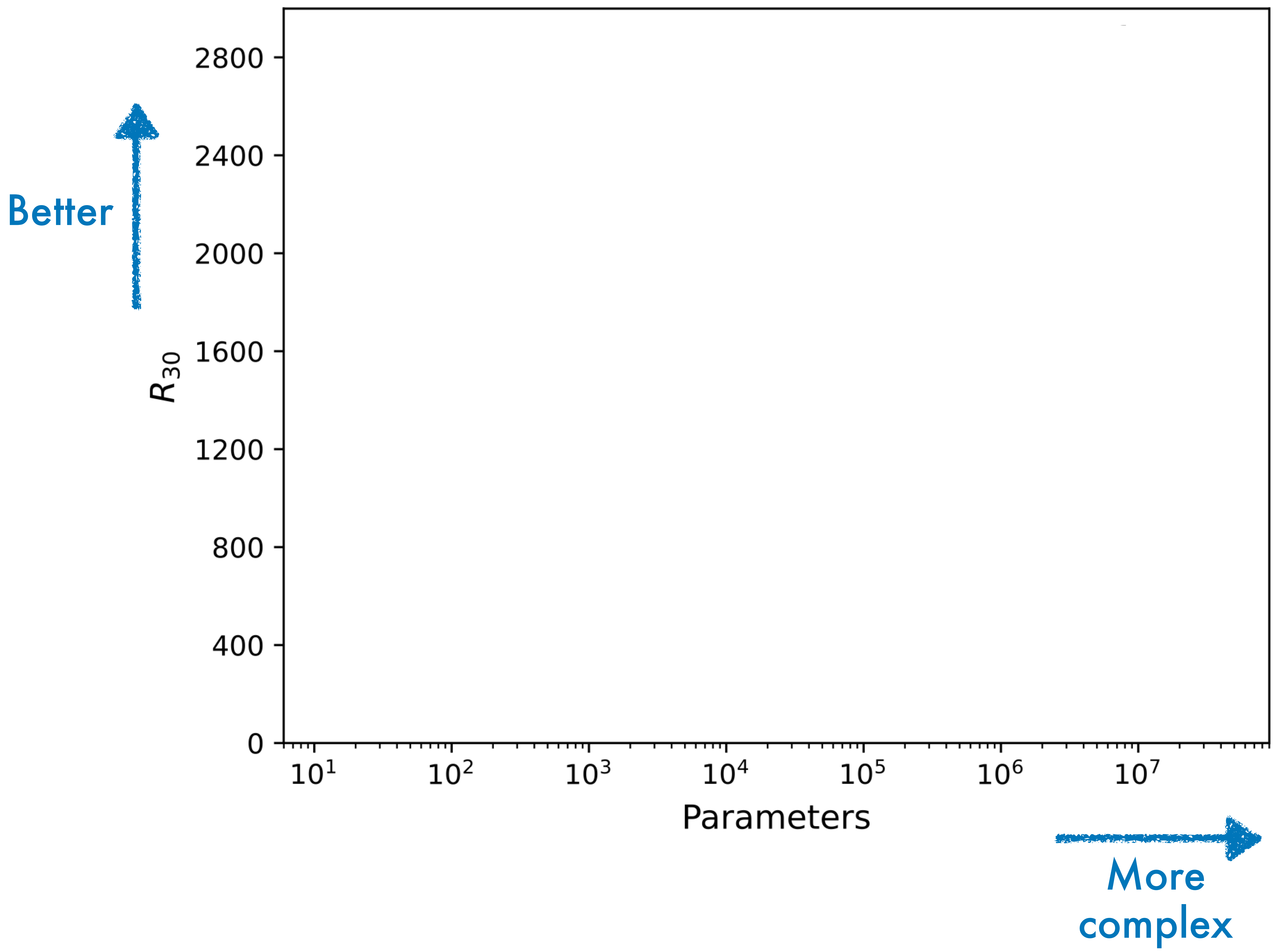
[1902.09914]

Evaluation metrics and results

Cut so that **30%** of top quarks pass selection:

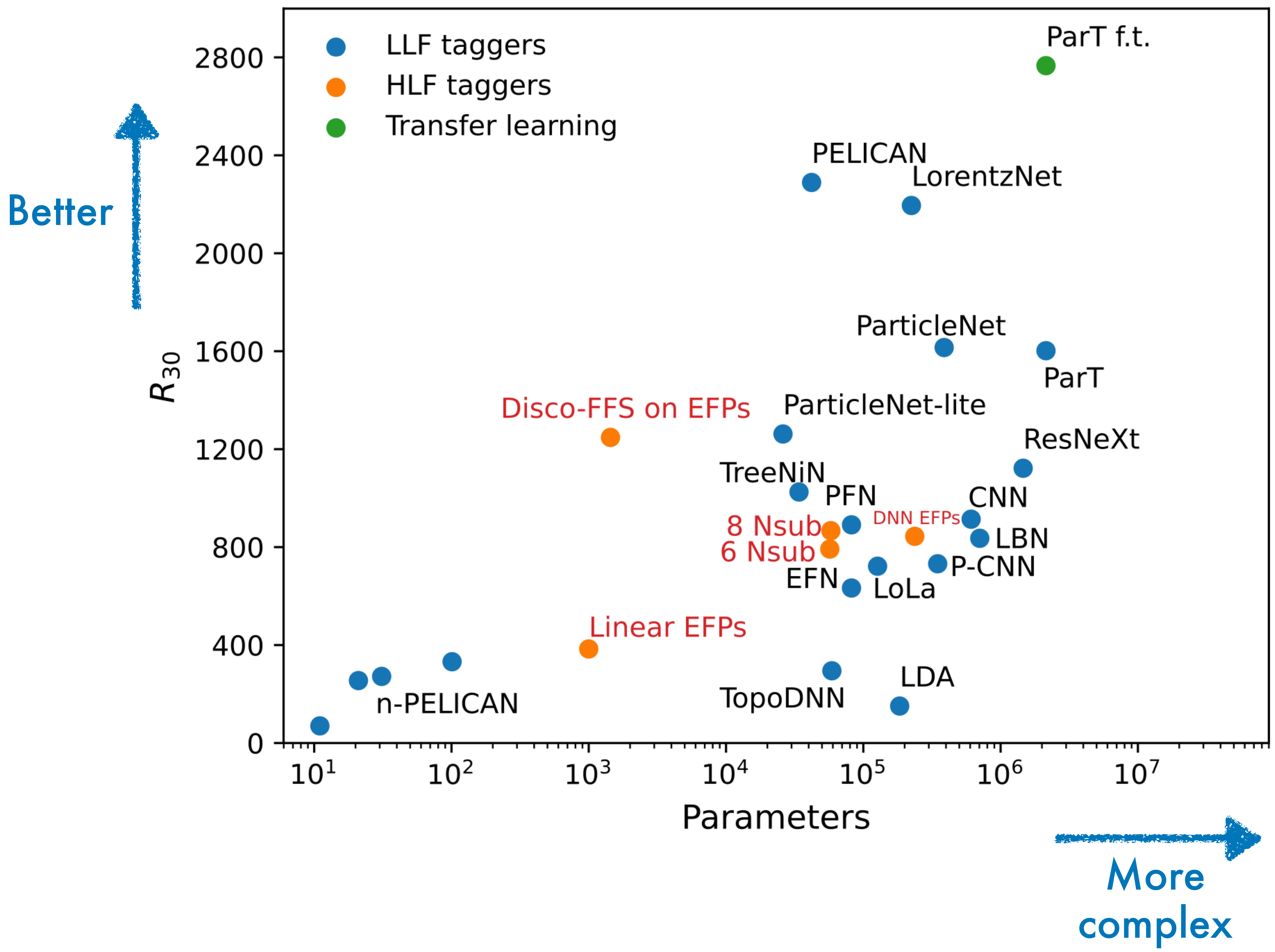
R_{30} is the inverse of the number of background jets that also pass





Evaluation metrics and results

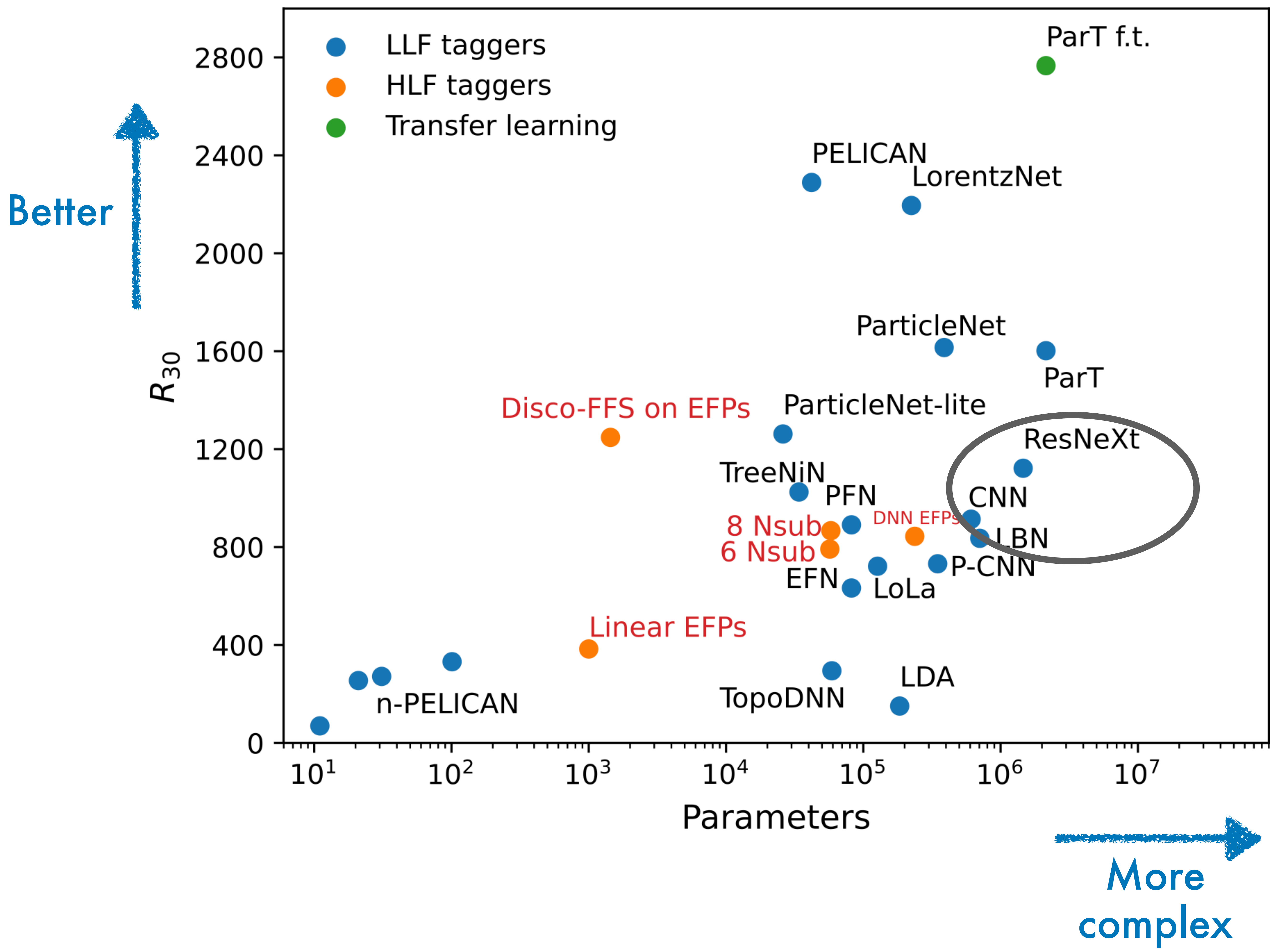
[2212.00046] + G. Kasieczka



Evaluation metrics and results

- **Jets as images**
  [1701.08784, 1803.00107]

[2212.00046] + G. Kasieczka

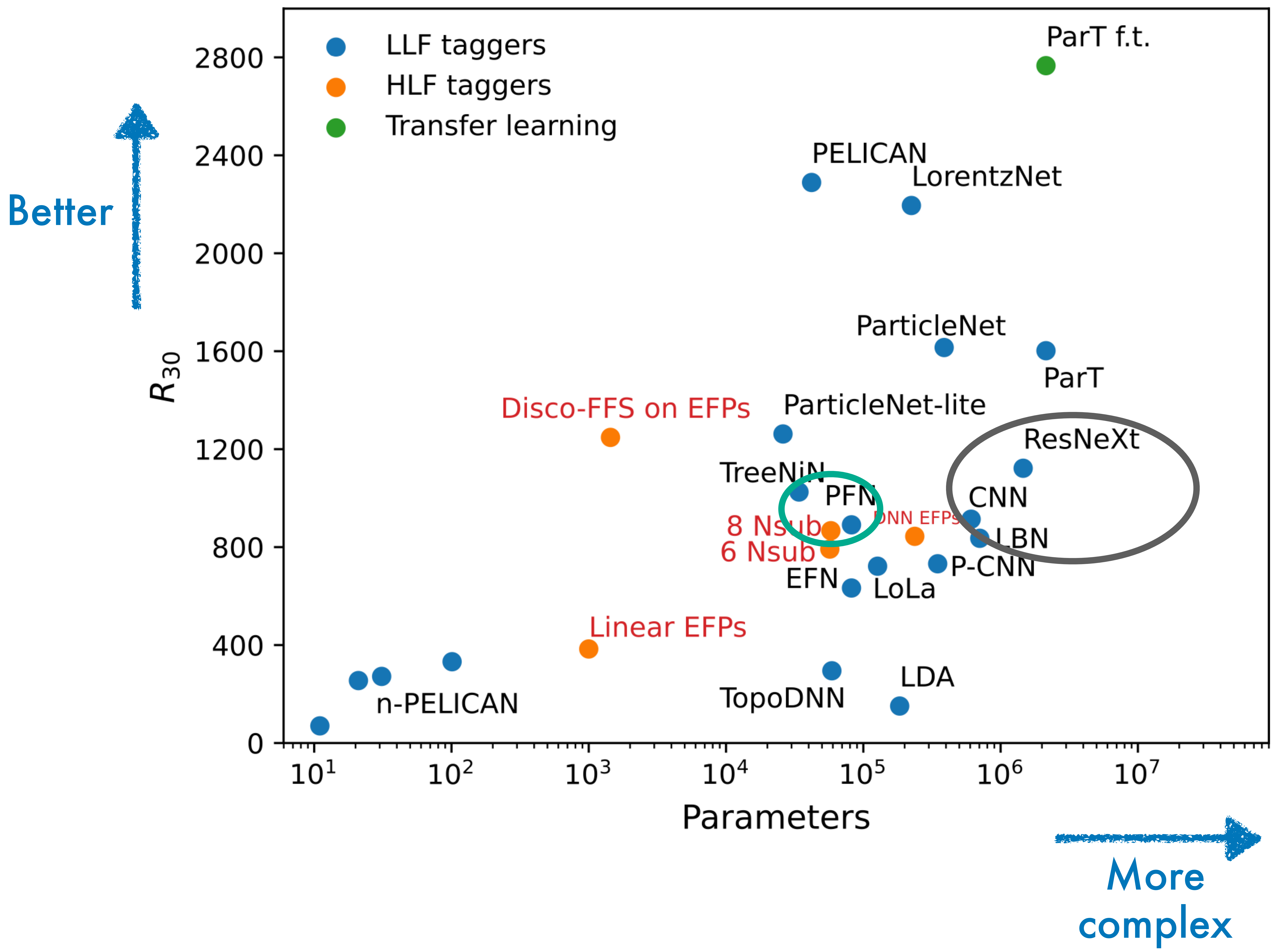


Evaluation metrics and results

- **Jets as images**
  [1701.08784, 1803.00107]

- **Point cloud**
  [PFN 1810.05165]

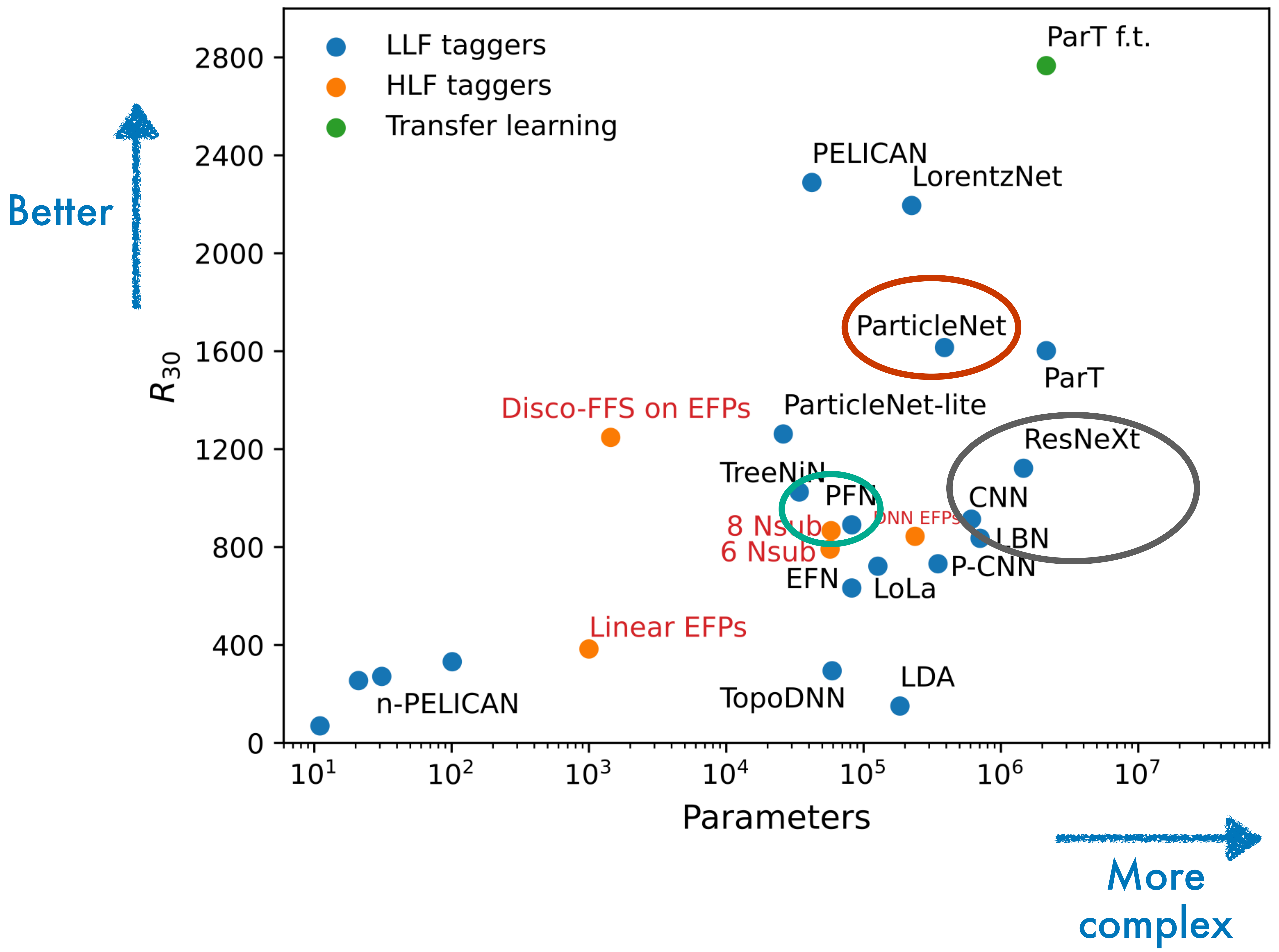
[2212.00046] + G. Kasieczka



Evaluation metrics and results

- **Jets as images**
  [1701.08784, 1803.00107]
- **Point cloud**
  [PFN 1810.05165]
- **Point cloud with Graphs**
  [1902.08570, 2007.13681]

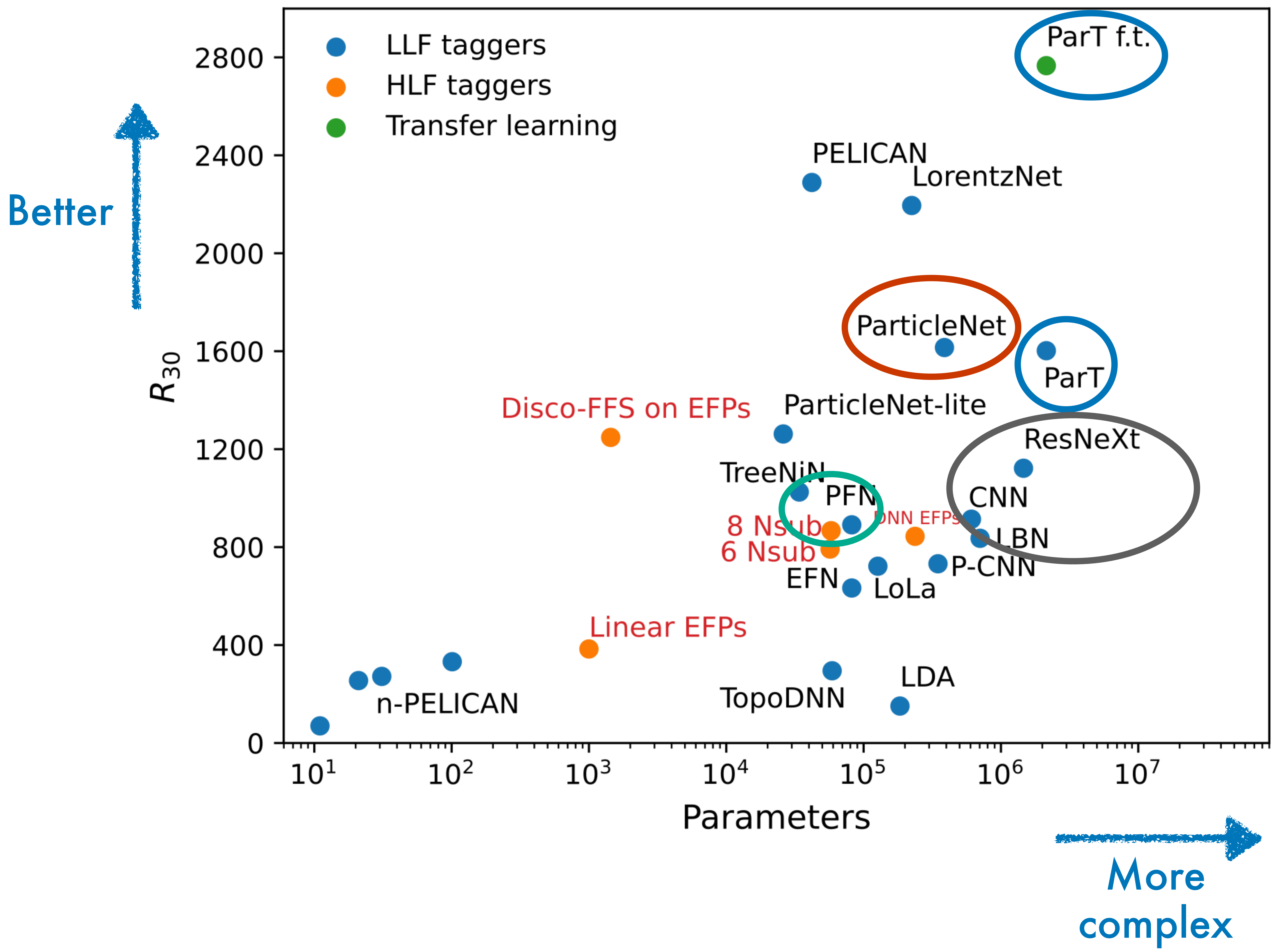
[2212.00046] + G. Kasieczka



Evaluation metrics and results

- **Jets as images**
  [1701.08784, 1803.00107]
- **Point cloud**
  [PFN 1810.05165]
- **Point cloud with Graphs**
  [1902.08570, 2007.13681]
- **Point cloud with attention**
  [2202.03772]

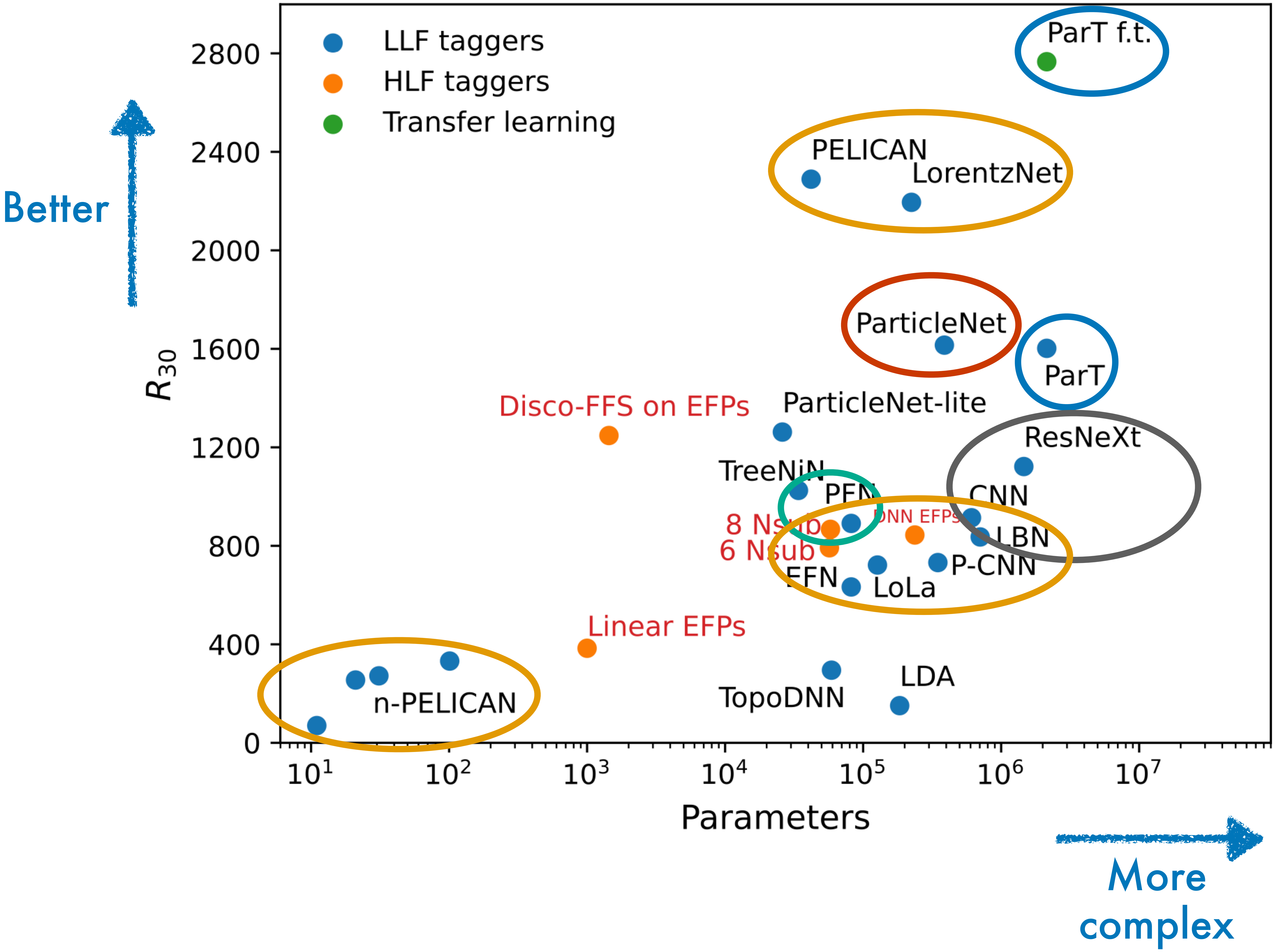
[2212.00046] + G. Kasieczka



Evaluation metrics and results

- **Jets as images**
  [1701.08784, 1803.00107]
- **Point cloud**
  [PFN 1810.05165]
- **Point cloud with Graphs**
  [1902.08570, 2007.13681]
- **Point cloud with attention**
  [2202.03772]
- **Lorentz symmetries**
  [1707.08966, 2201.08187, 2211.00454]

[2212.00046] + G. Kasieczka

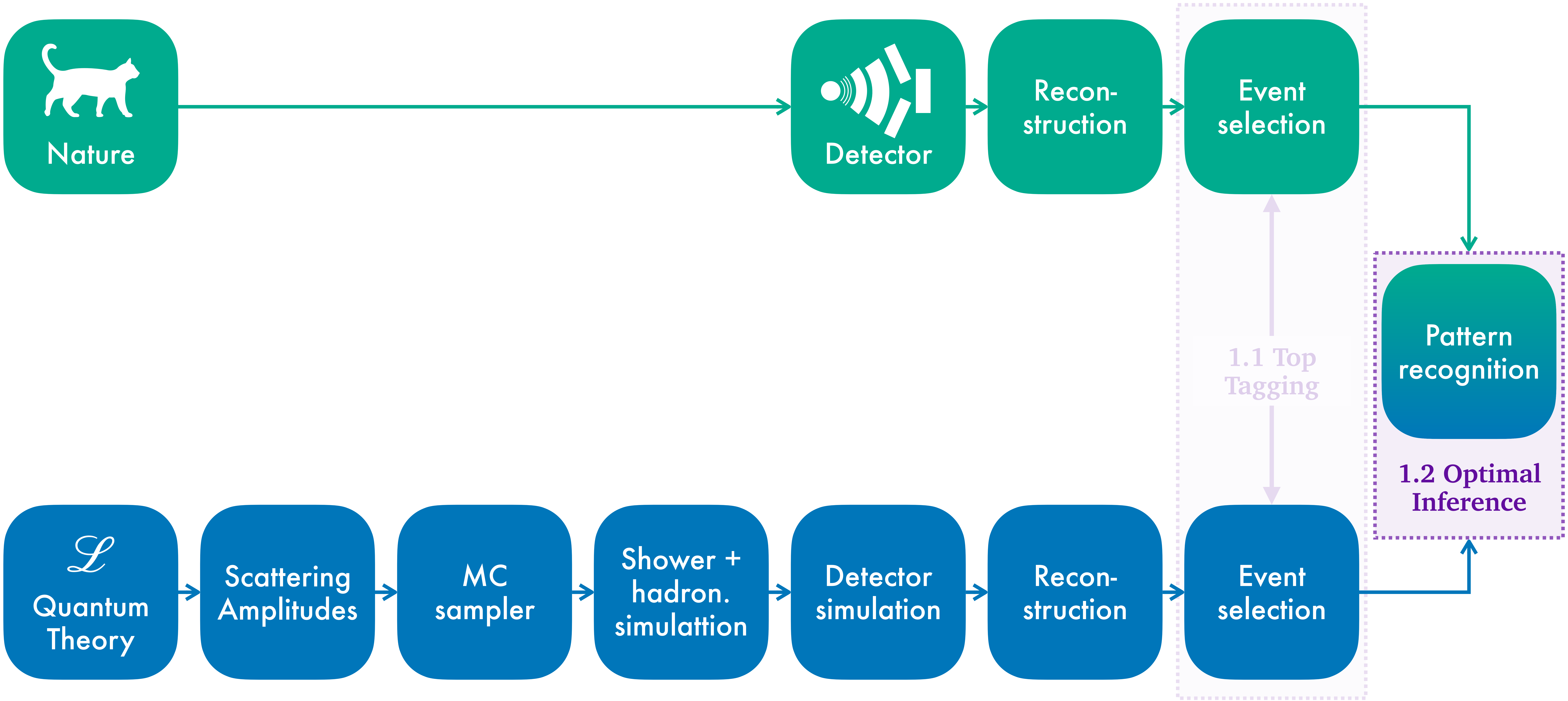


Example II

Regression with MadMiner

Brehmer, Cranmer, Louppe, Pavez [1805.00013, 1805.00020, 1805.12244]

LHC analysis + ML



Recap — HEP analysis

Theory parameters

θ

Evolution

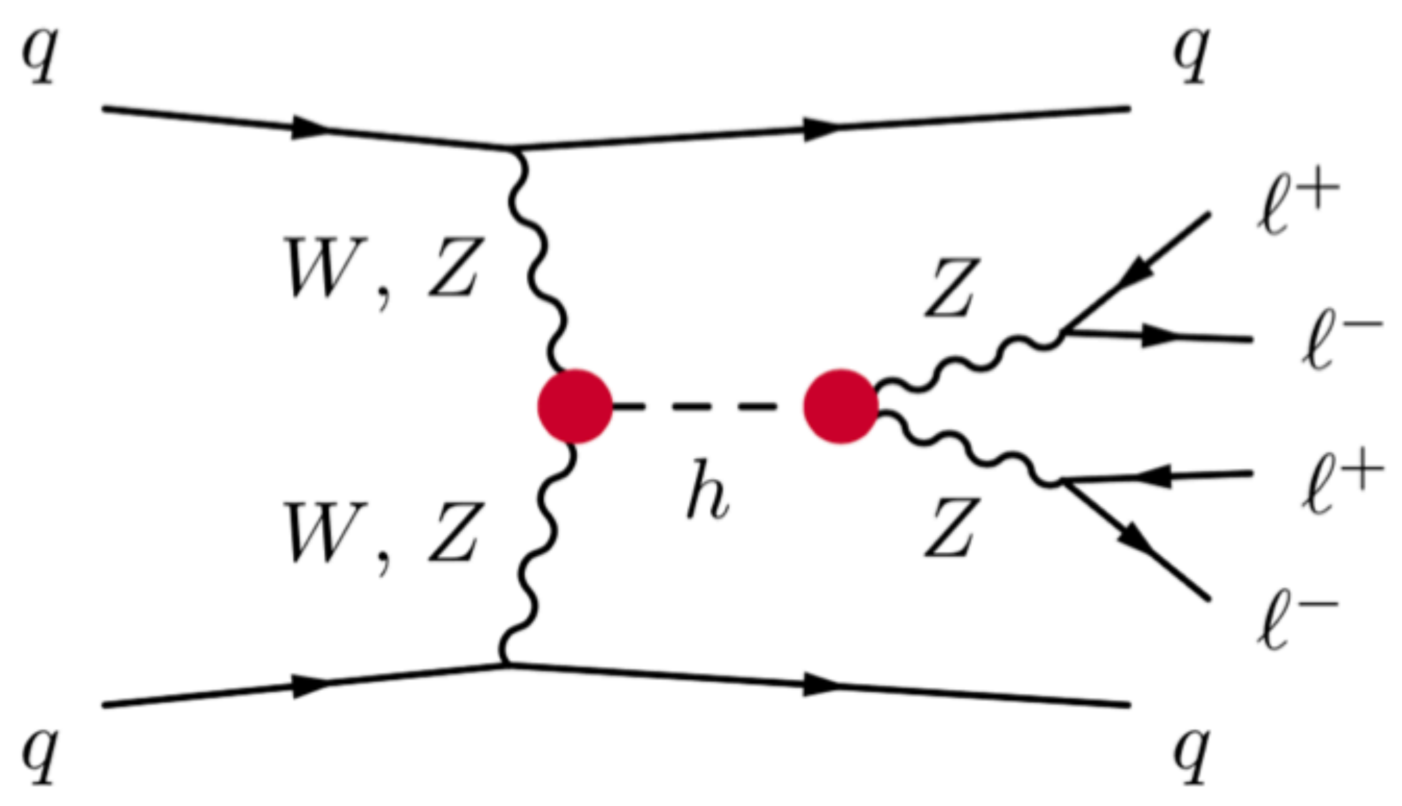
Recap — HEP analysis

Latent variables

Parton-level momenta

Theory parameters

$z_p \longleftarrow \theta$



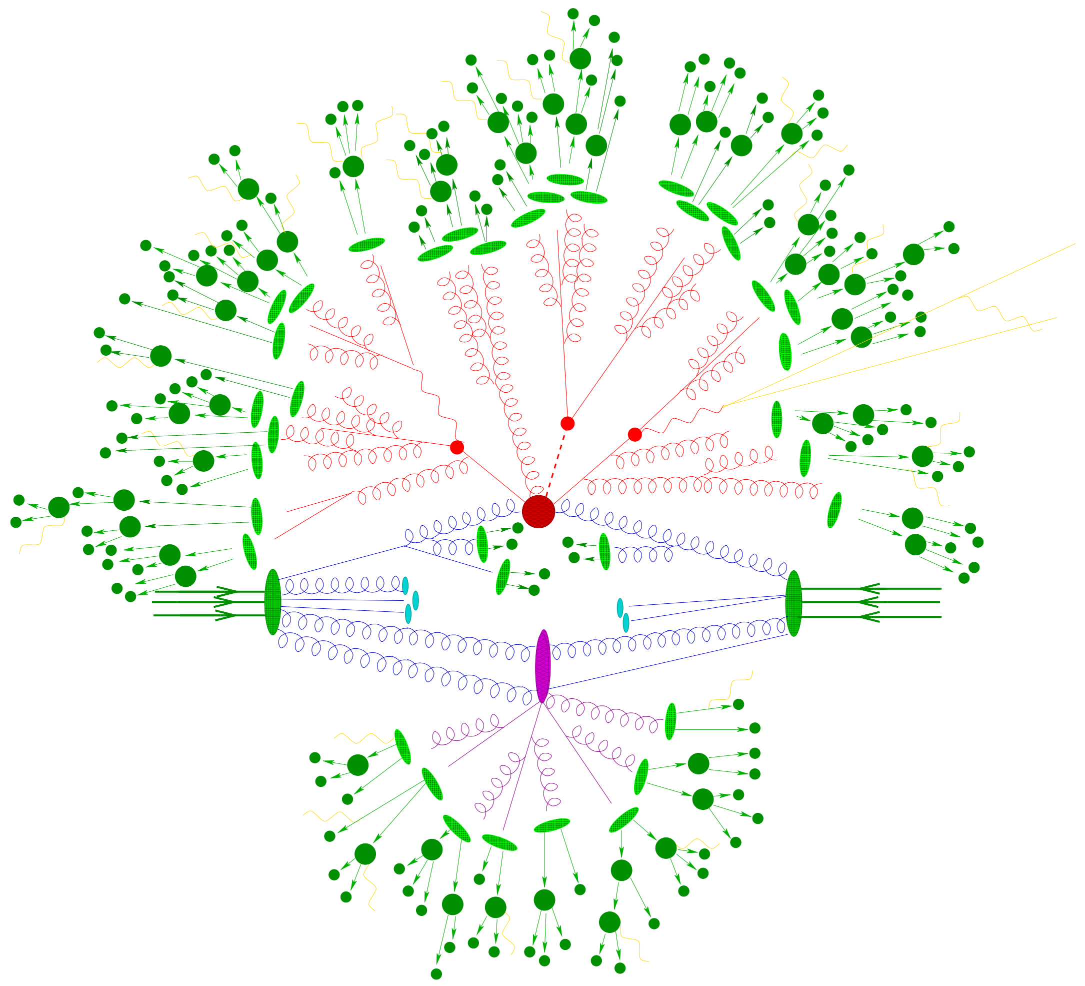
Evolution

Recap — HEP analysis

Latent variables

Shower splittings | Parton-level momenta | Theory parameters

$z_s \leftarrow z_p \leftarrow \theta$



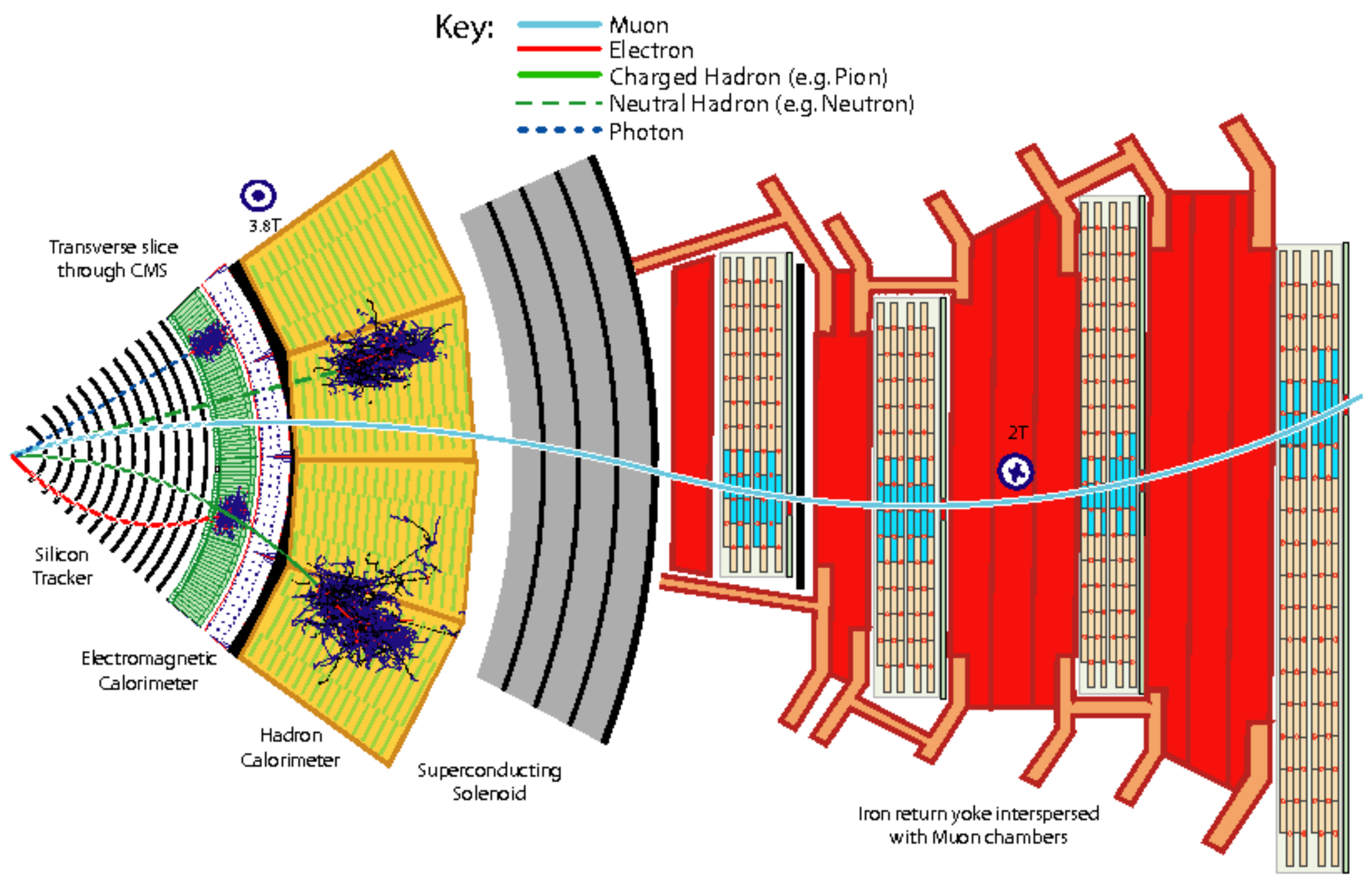
Evolution

Recap — HEP analysis

Latent variables

Detector Interactions	Shower splittings	Parton-level momenta	Theory parameters
z_d	z_s	z_p	θ

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



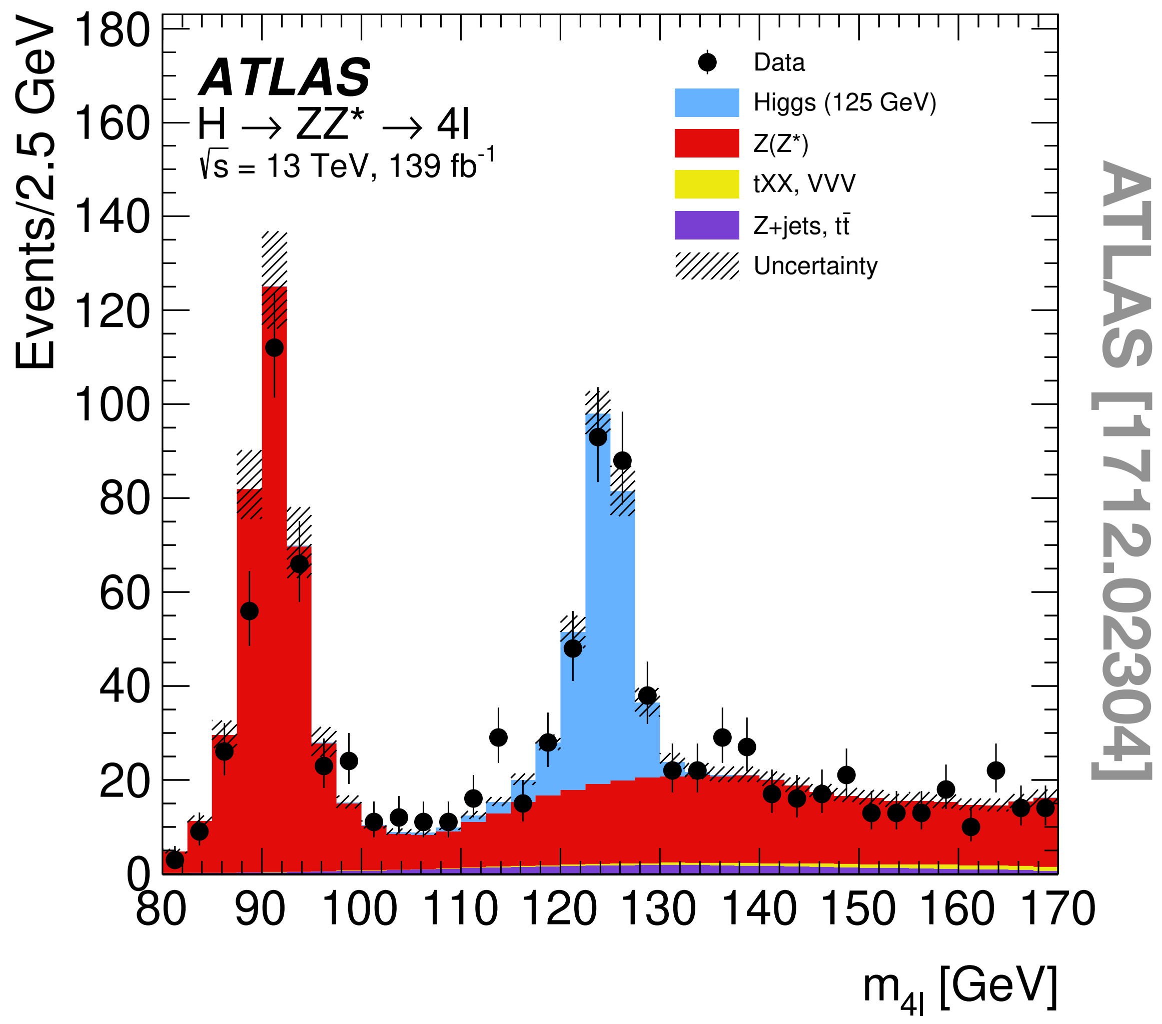
Evolution

Recap — HEP analysis

Latent variables

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

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



ATLAS [1712.02304]

Evolution

Recap — HEP analysis

Latent variables

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

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

Sample from $p(x \mid z_d)$ $\quad p(z_d \mid z_s)$ $\quad p(z_s \mid z_p)$ $\quad p(z_p \mid \theta)$

GEANT4
A SIMULATION TOOLKIT

DELPHES
fast simulation

MADGRAPH5
aMC@NLO

SHERPA

Prediction (Simulation)

Recap — HEP analysis

Latent variables

Observables	Detector Interactions	Shower splittings	Parton-level momenta	Theory parameters

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

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

$\longrightarrow$

Inference

Recap — HEP analysis

Latent variables

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

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

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

Known from theory

Inference

Recap — HEP analysis

Latent variables

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

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

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

Complicated integral

Known from theory

Inference

Recap — HEP analysis

Latent variables

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

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

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

Complicated integral

Likelihoods intractable

Known from theory

Inference

Recap — HEP analysis

Latent variables

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

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

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

Complicated integral

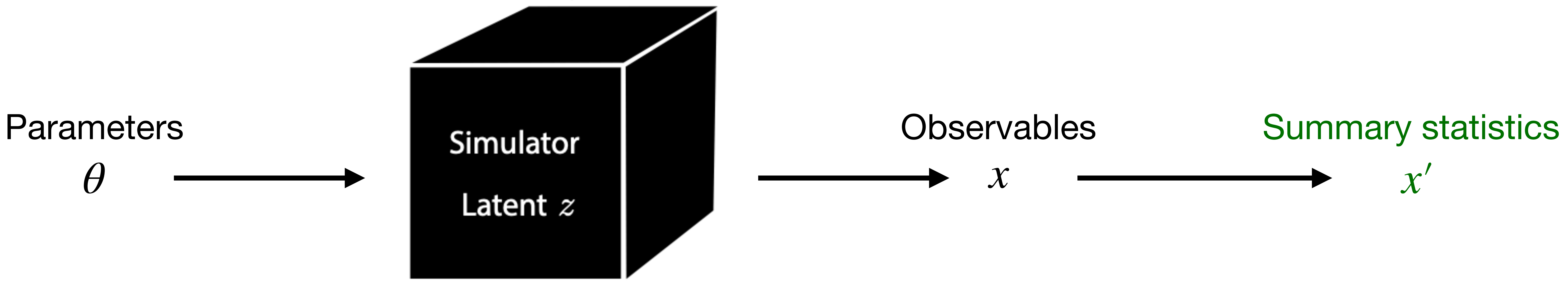
Likelihoods intractable

Known from theory

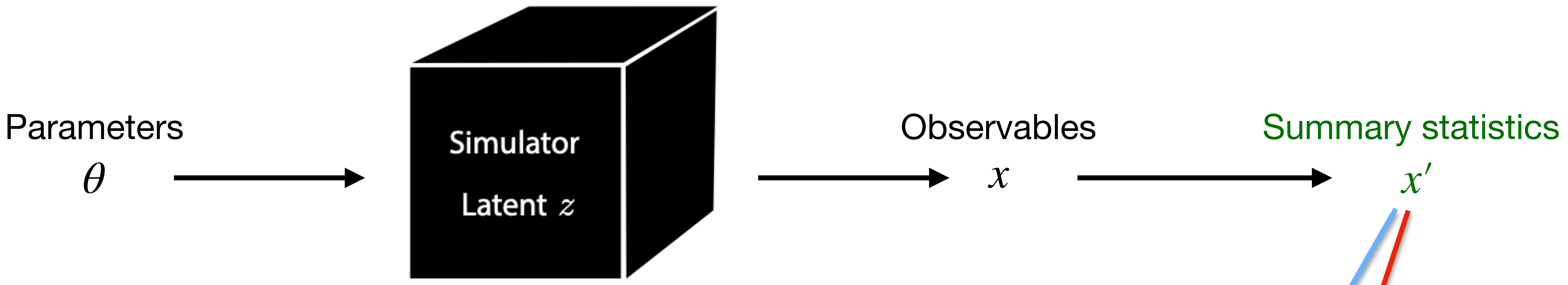
Why has that not stopped us so far?

Inference

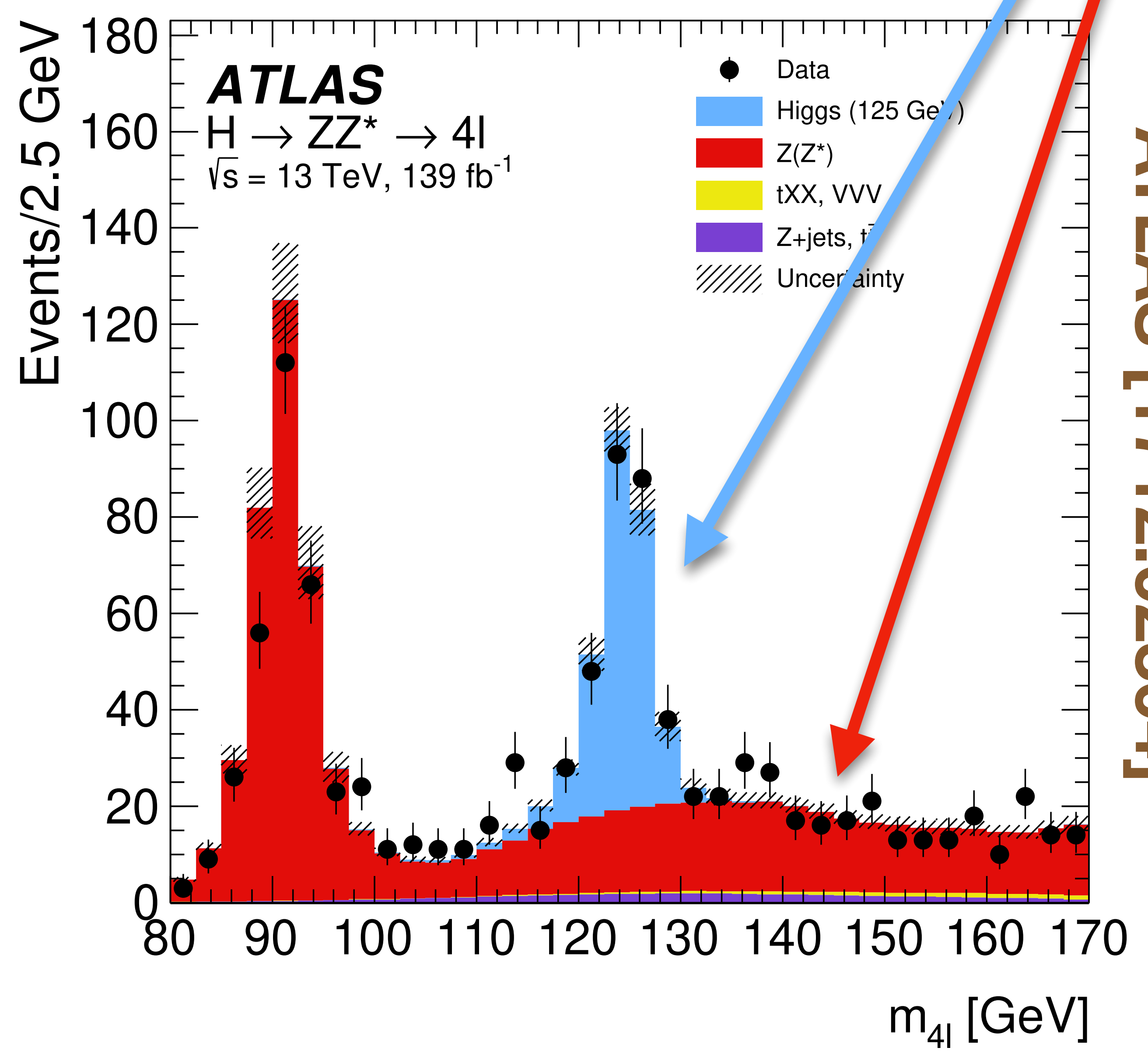
Solve it by histogramming summary statistics



Solve it by histogramming summary statistics



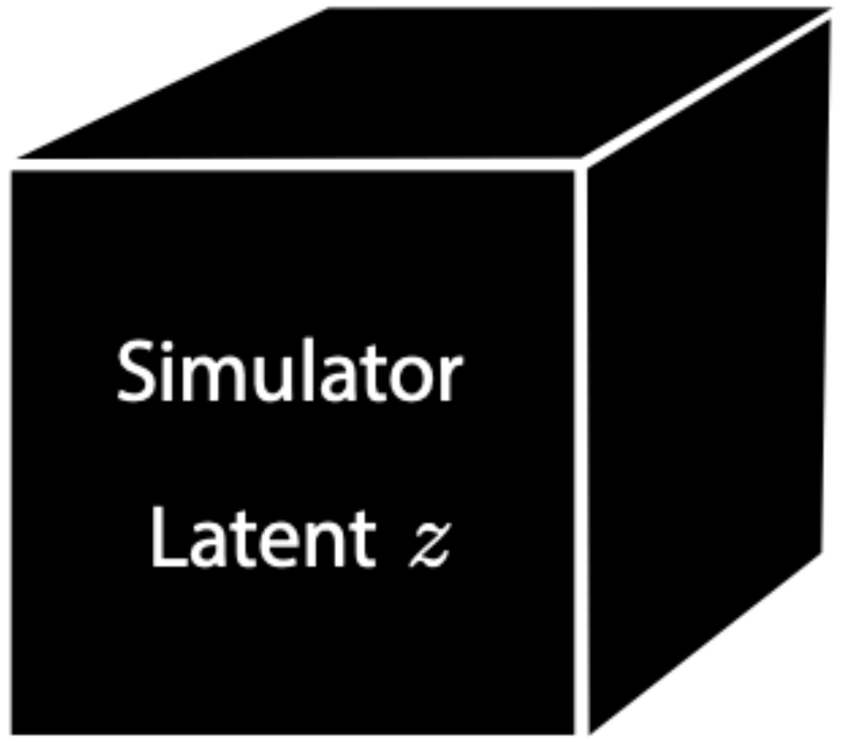
$$\hat{p}(x\,|\,\theta) = p(x'\,|\,\theta) =$$



ATLAS [1712.02304]

Run simulator for different θ, fill histograms

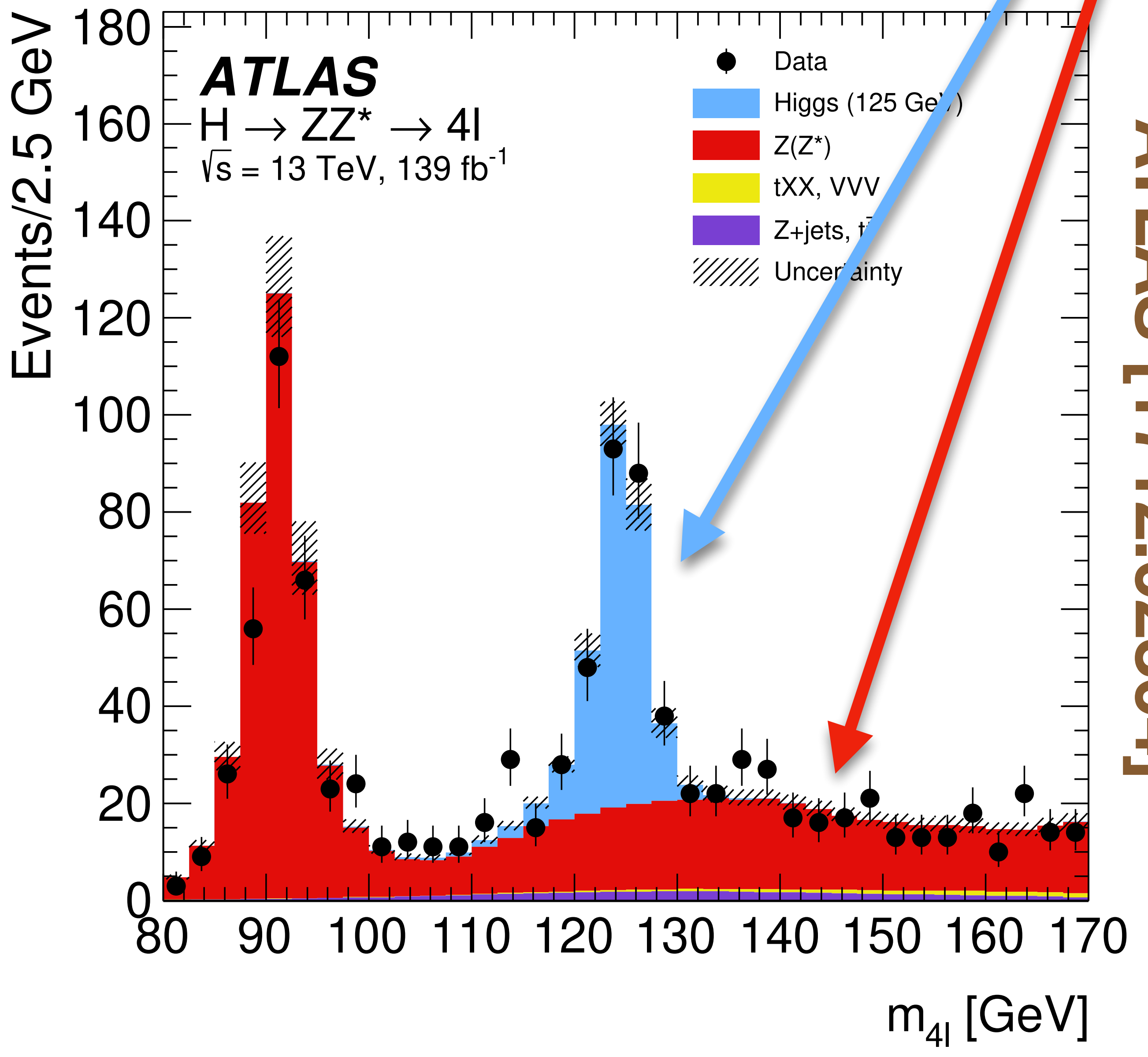
Solve it by histogramming summary statistics

Parameters θ → 

→ Observables x → Summary statistics x'

Run simulator for different θ, fill histograms

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



ATLAS [1712.02304]

- How to choose x' ? Standard variables often lose information **[1612.05261,1712.02350]**
- **Curse of dimensionality**: Histograms don't scale to high-dimensional x

Solve it by calculating the integral with ML

Latent variables

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

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

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

Known from theory

Solve it by calculating the integral with ML

Latent variables

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

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

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

Known from theory

Step 1

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

approximate **shower + detector effects**
into **transfer function**

Solve it by calculating the integral with ML

Latent variables

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

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

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

Known from theory

Solve it by calculating the integral with ML

Latent variables

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

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

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

(Less) complicated integral

Likelihood still intractable

Known from theory

Solve it by calculating the integral with ML

Latent variables

Observables

Detector Interactions

Shower splittings

Parton-level momenta

Theory parameters

θ

Matrix Element Method [K. Kondo 1988]

$$p(x \mid \theta) = \boxed{\int \mathrm{d}z_p} \; \boxed{p(x \mid z_p)} \; \boxed{p(z_p \mid \theta)}$$

(Less) complicated integral

Likelihood still intractable

Known from theory

Solve it by calculating the integral with ML

Latent variables

Observables

Detector Interactions

Shower splittings

Parton-level momenta

Theory parameters

θ

Matrix Element Method [K. Kondo 1988] + ML [2210.00019, 2310.07752]

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

(Less) complicated integral

Likelihood still intractable

Known from theory

Step 2

$$\boxed{\left\langle \frac{f(z_p)}{g_\omega(z_p)} \right\rangle}$$

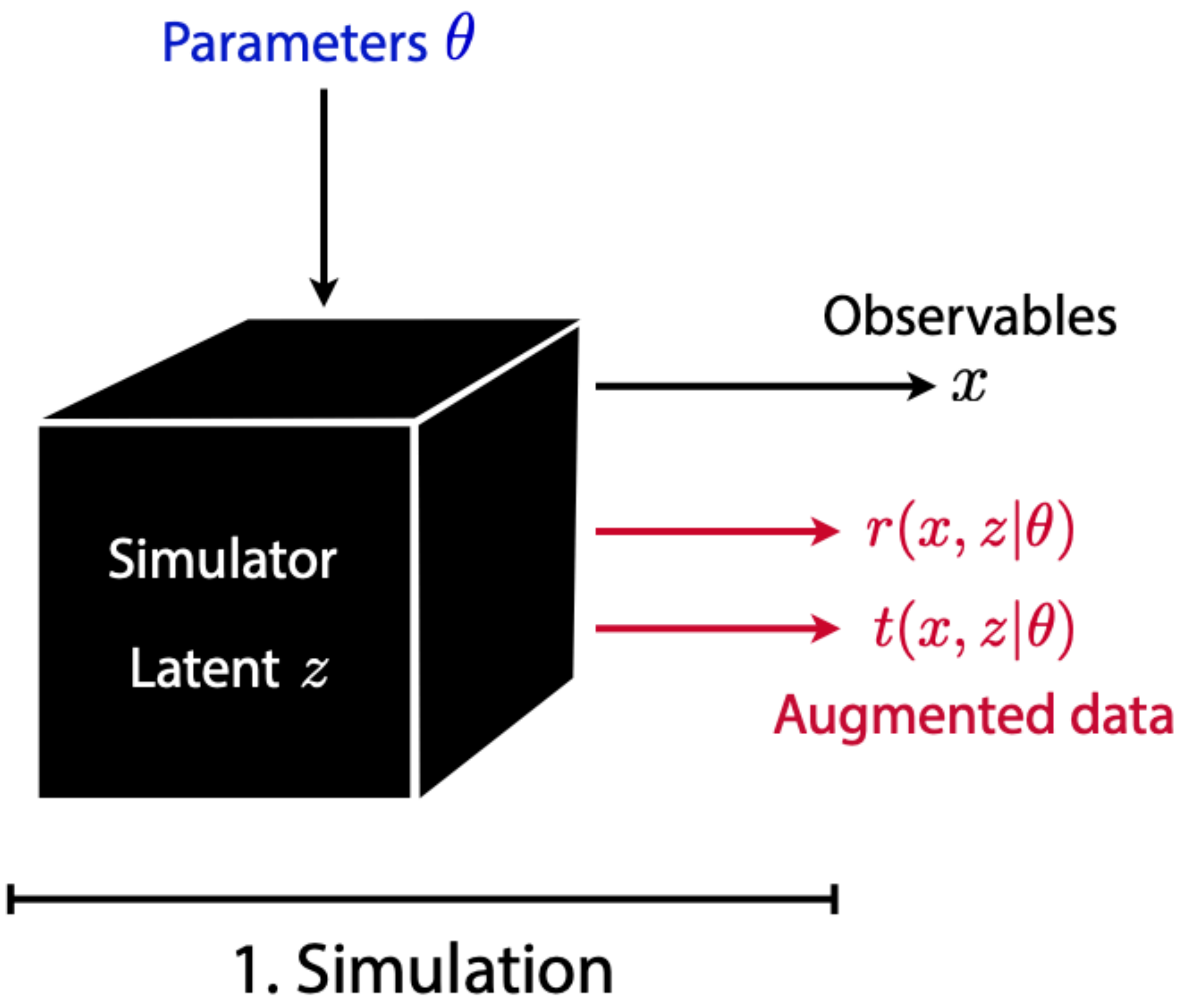
Use ML to speed-up integration

$$\boxed{\hat{p}_\omega(x\,|\,z_p)}$$

Use ML to parametrize transfer function

Solving it with likelihood-free inference

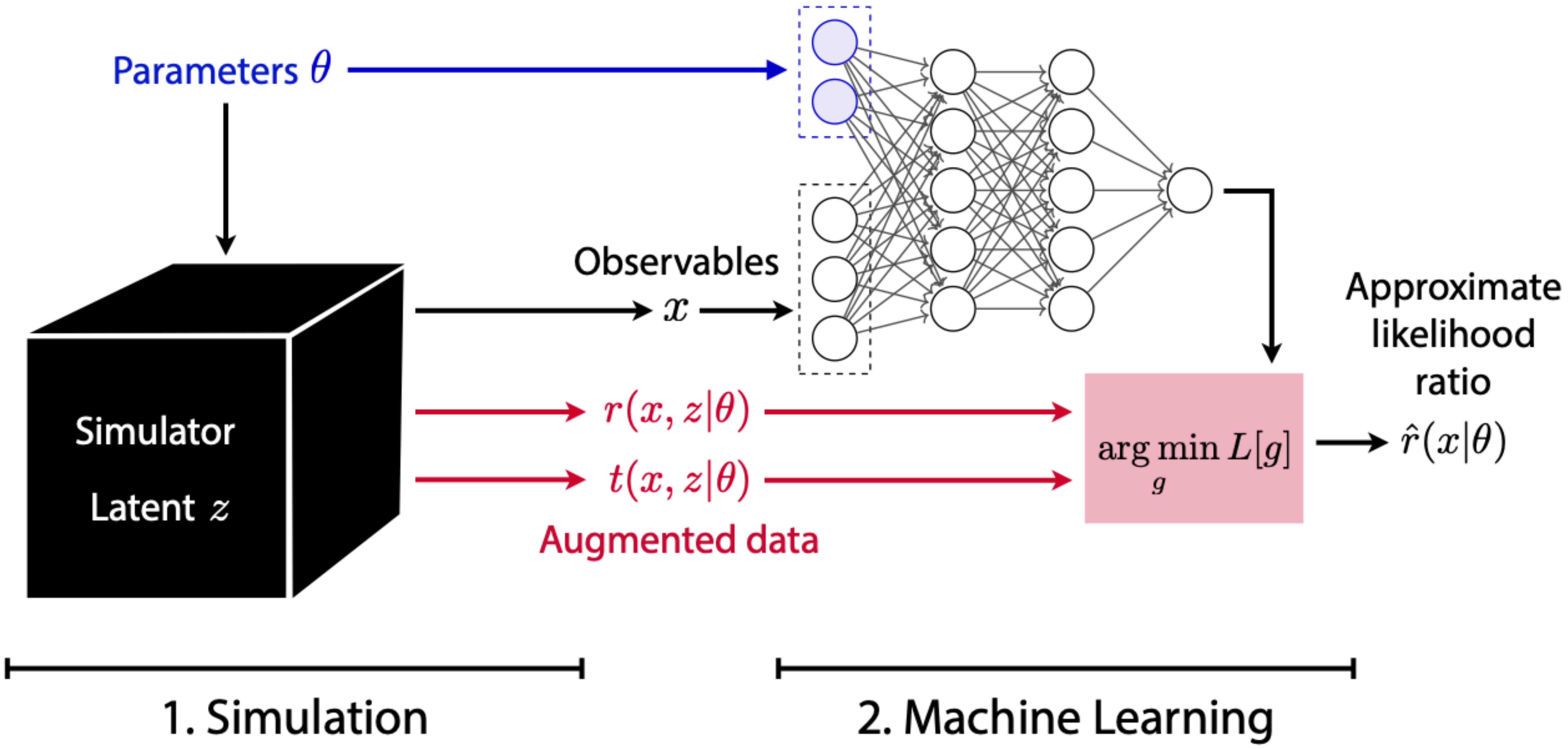
The MadMiner approach



“Mining gold”: Extract additional information from simulator

Brehmer, Cranmer, Louppe, Pavez [1805.00013, 1805.00020, 1805.12244]

The MadMiner approach

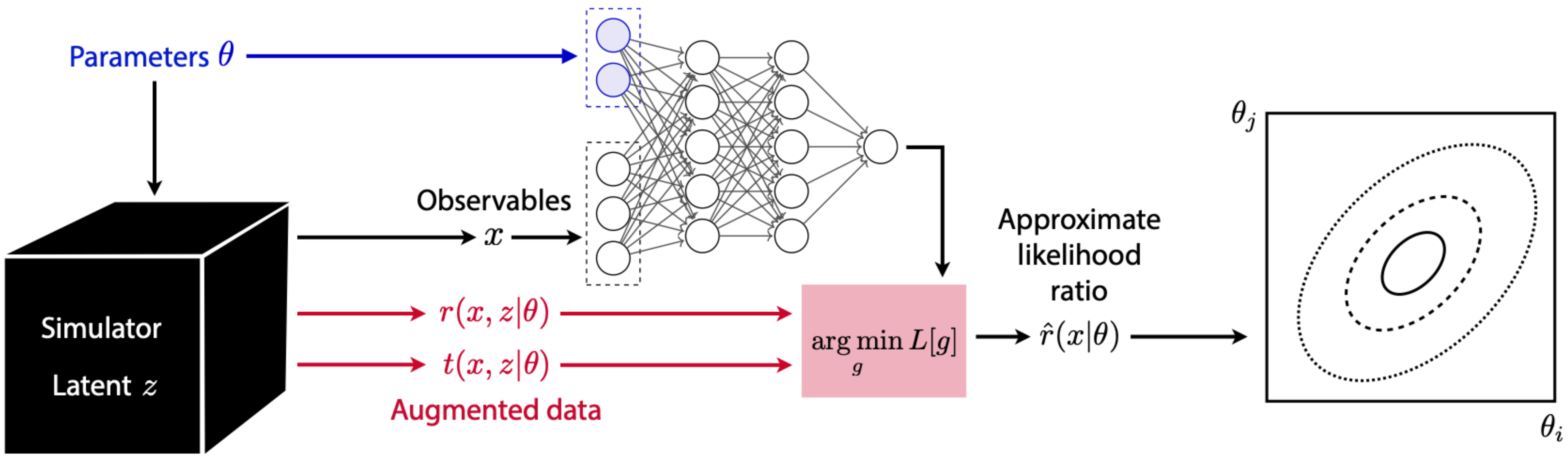


"Mining gold": Extract additional information from simulator

Use this information to train estimator for likelihood ratio

Brehmer, Cranmer, Louppe, Pavez [1805.00013, 1805.00020, 1805.12244]

The MadMiner approach



1. Simulation

"Mining gold": Extract additional information from simulator

2. Machine Learning

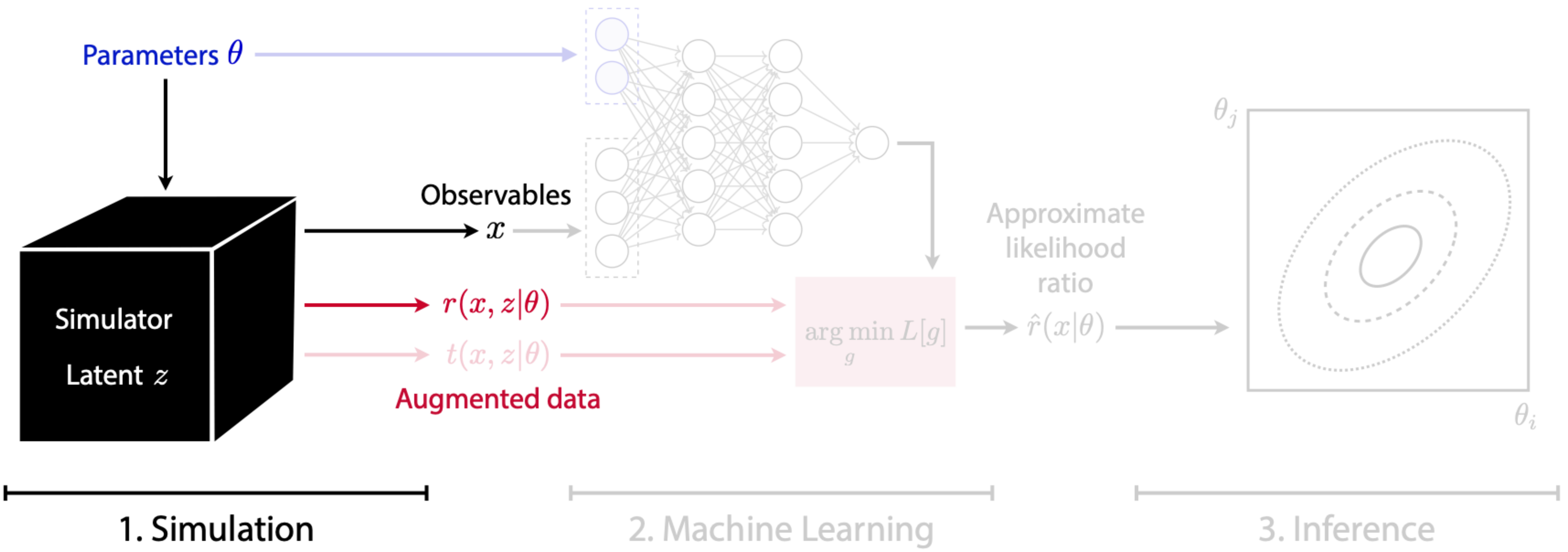
Use this information to train estimator for likelihood ratio

3. Inference

Set new constrains with standard hypothesis tests

Brehmer, Cranmer, Louppe, Pavez [1805.00013, 1805.00020, 1805.12244]

The MadMiner approach



Mining gold from the simulator

Latent variables

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

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

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

Intractable integrals

Mining gold from the simulator

Latent variables

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

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

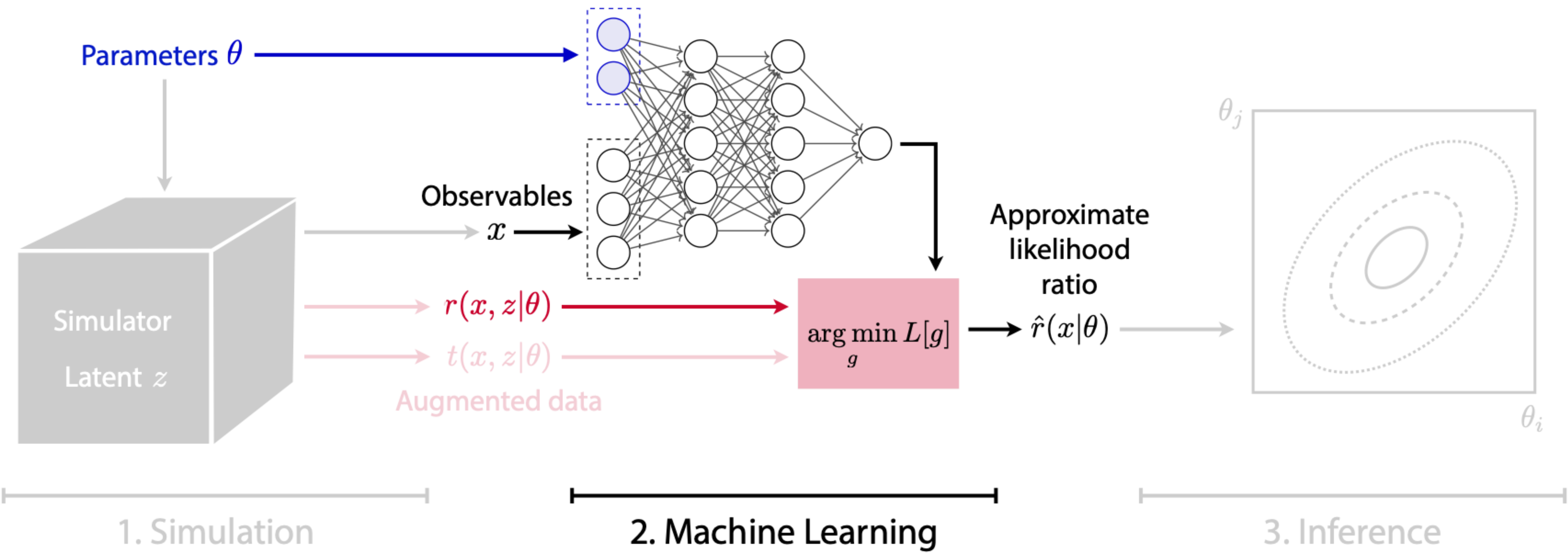
$$p(x|\theta) = \int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p \quad p(x|z_d) \quad p(z_d|z_s) \quad p(z_s|z_p) \quad \boxed{p(z_p|\theta)}$$

Parton-level likelihood can be evaluated!

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

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

The MadMiner approach



The value of gold

We can calculate the **joint likelihood ratio**

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

$$\downarrow$$

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**

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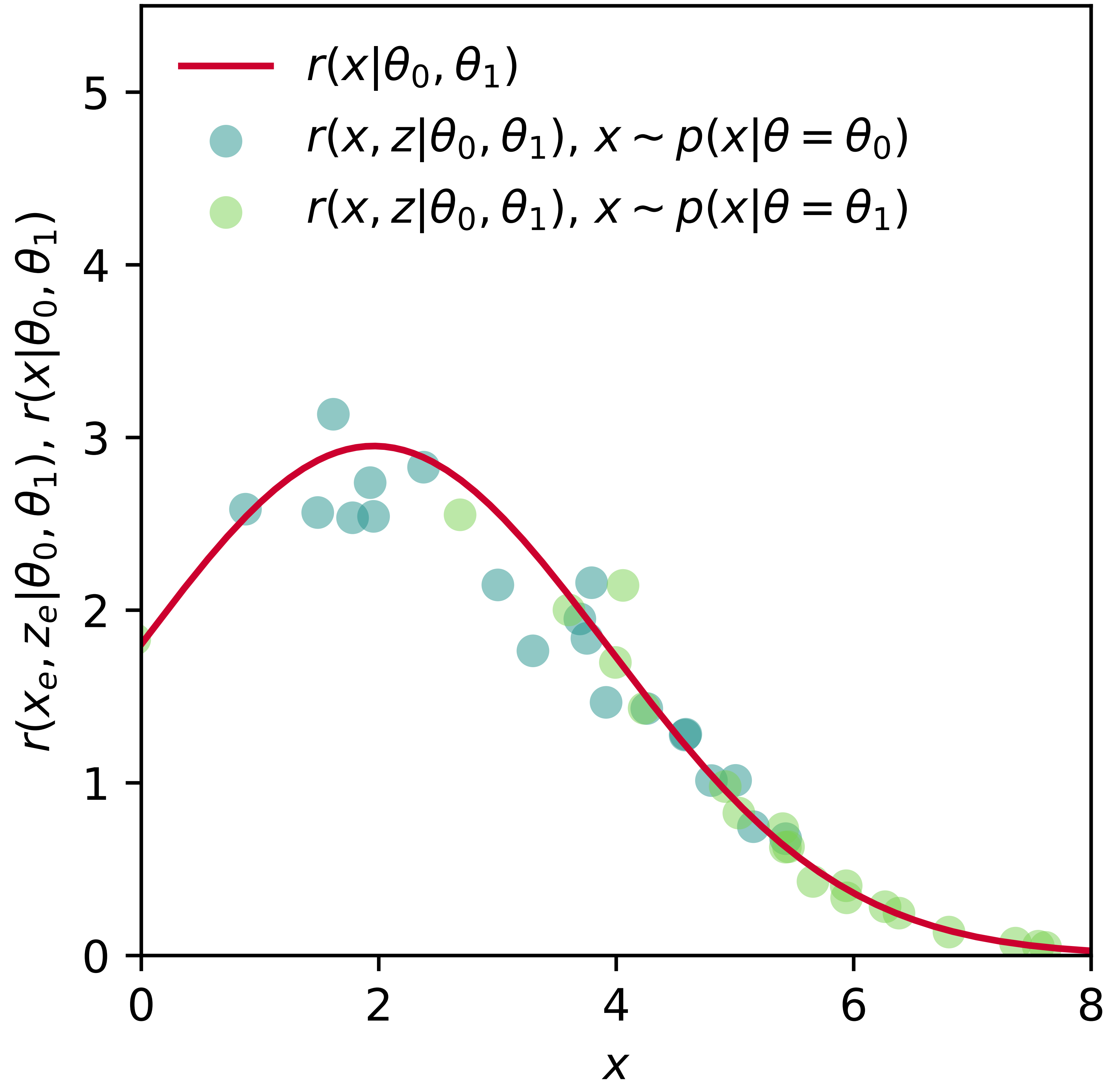
We want the **likelihood ratio function**

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

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

[1805.00020]



The value of gold

We can calculate the **joint likelihood ratio**

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

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

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

One can show it is minimized by

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

We want the **likelihood ratio function**

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

Machine learning = applied calculus

We can get a precise estimator by numerically minimizing a functional:

$$\hat{r}(x\,|\,\theta_0,\theta_1) = \underset{\hat{r}(x\,|\,\theta_0,\theta_1)}{\arg\min} \underbrace{\int \mathrm{d}x \int \mathrm{d}z\, p(x,z\,|\,\alpha_1)\ \left[\hat{r}(x\,|\,\theta_0,\theta_1) - r(x,z\,|\,\theta_0,\theta_1)\right]^2}_{L_r[\hat{r}(x\,|\,\theta_0,\theta_1)]}$$

Machine learning = applied calculus

We can get a precise estimator by numerically minimizing a functional:

$$\hat{r}(x\,|\,\theta_0,\theta_1) = \underset{\hat{r}(x\,|\,\theta_0,\theta_1)}{\arg\min} \underbrace{\int \mathrm{d}x \int \mathrm{d}z\, p(x,z\,|\,\alpha_1)\, \left[\hat{r}(x\,|\,\theta_0,\theta_1) - r(x,z\,|\,\theta_0,\theta_1)\right]^2}_{L_r[\hat{r}(x\,|\,\theta_0,\theta_1)]}$$

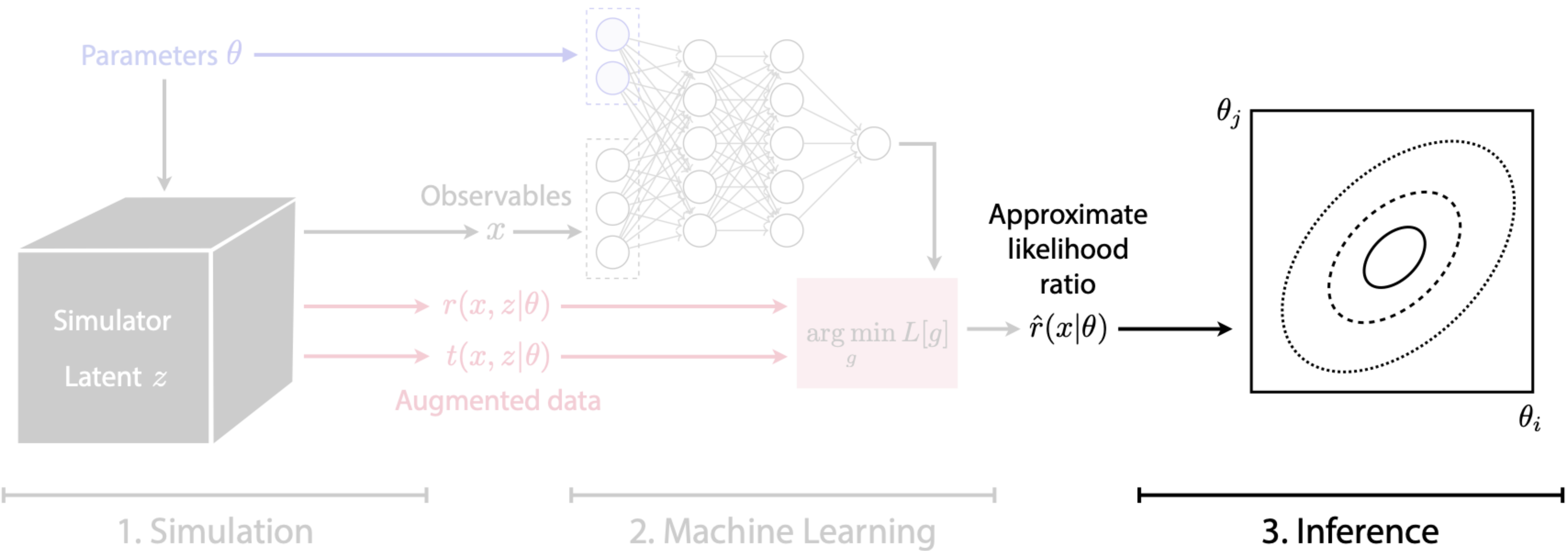
We do this via **Machine Learning:**

- Functional L_r → Loss function

$$\mathscr{L}_{\mathrm{MSE}} = \frac{1}{N}\sum_i \left[\hat{r}_\omega(x_i\,|\,\theta_0,\theta_1) - r(x_i,z_i\,|\,\theta_0,\theta_1)\right]^2$$

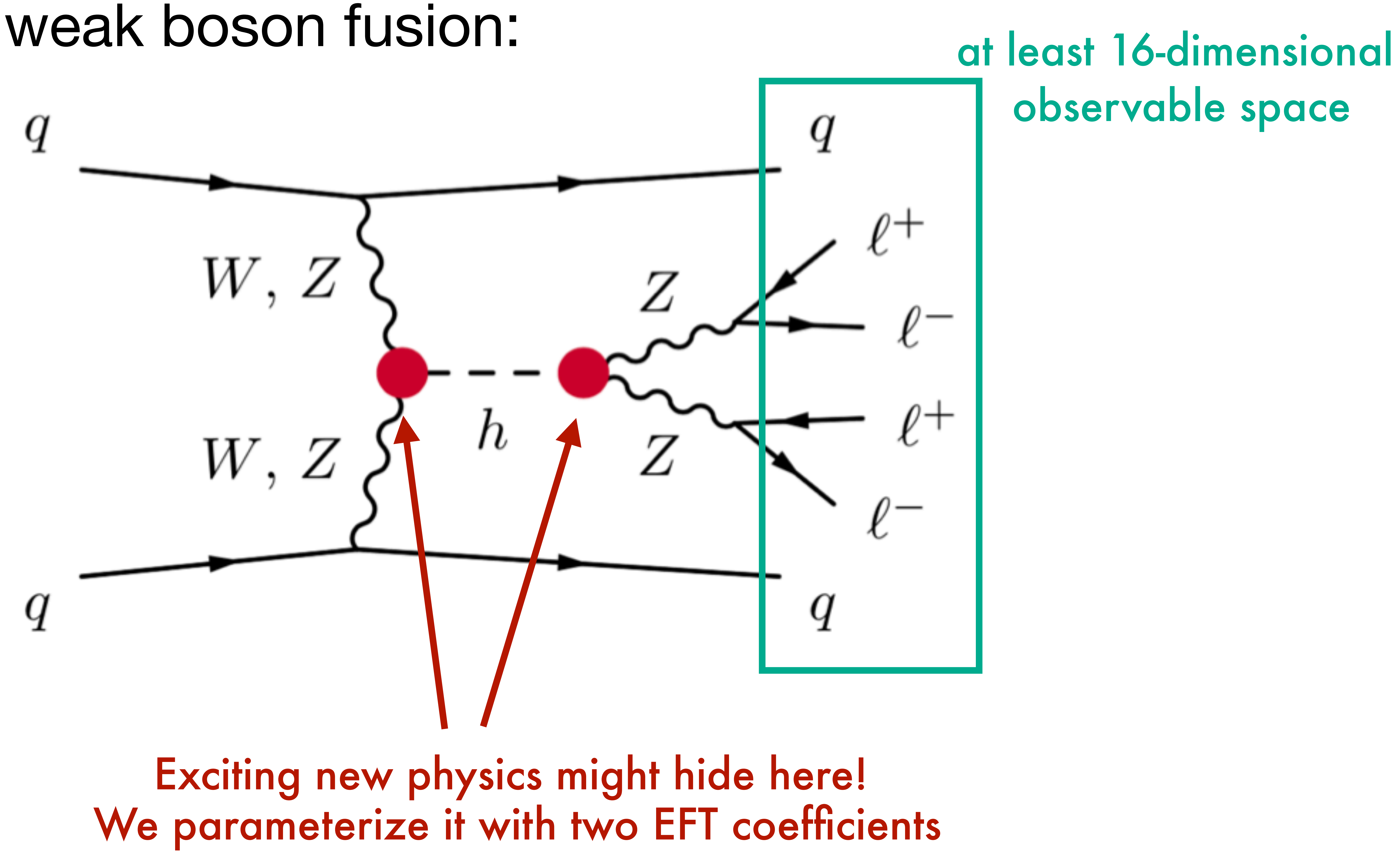
- Variational familiy $\hat{r}_\omega(x\,|\,\theta_0,\theta_1)$ → Flexible parametric function (e.g. neural network)
- Exact minimization → Numerical optimization algorithm (eg. Stochastic gradient descent)

The MadMiner approach



Constraining EFT parameters with ML

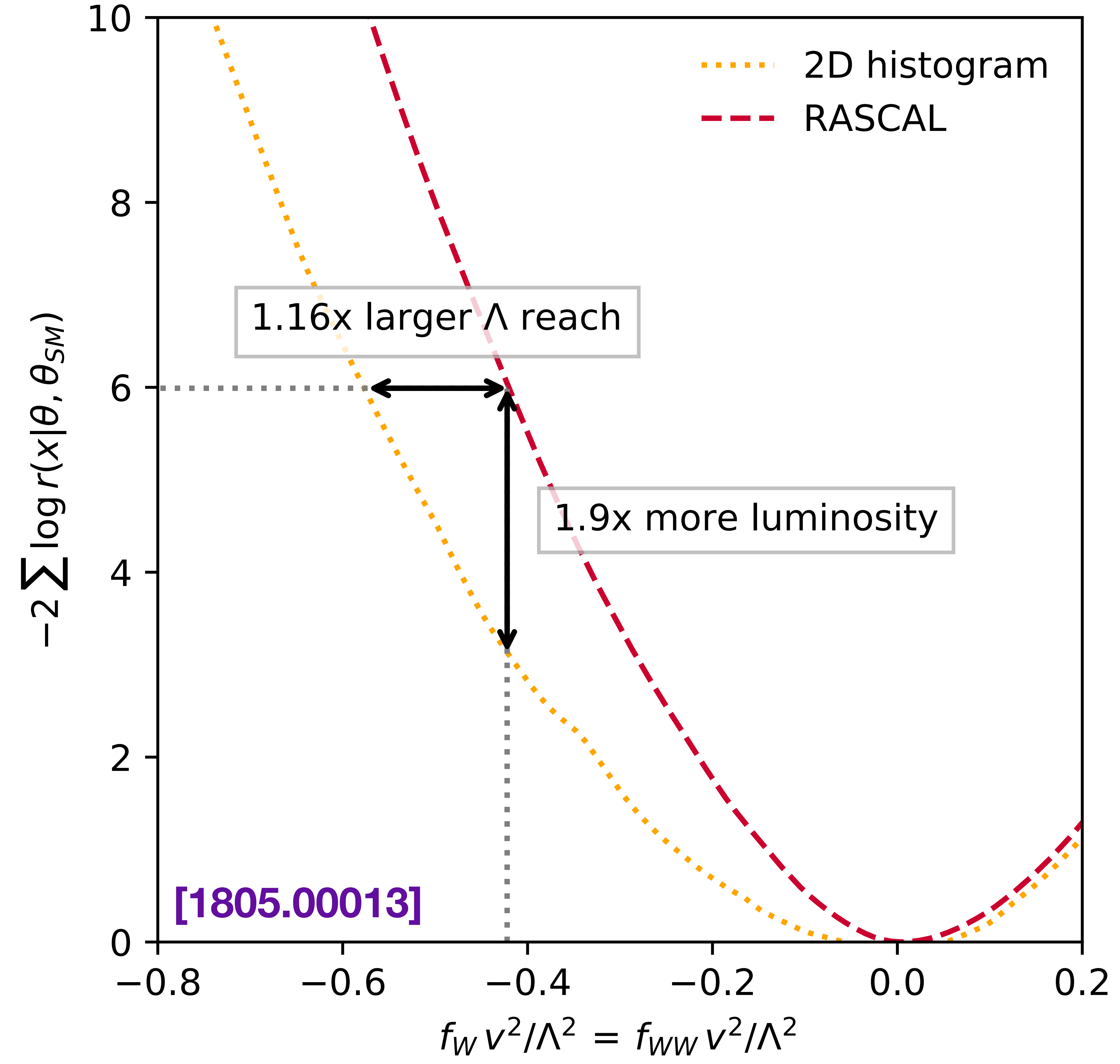
Higgs production in weak boson fusion:



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

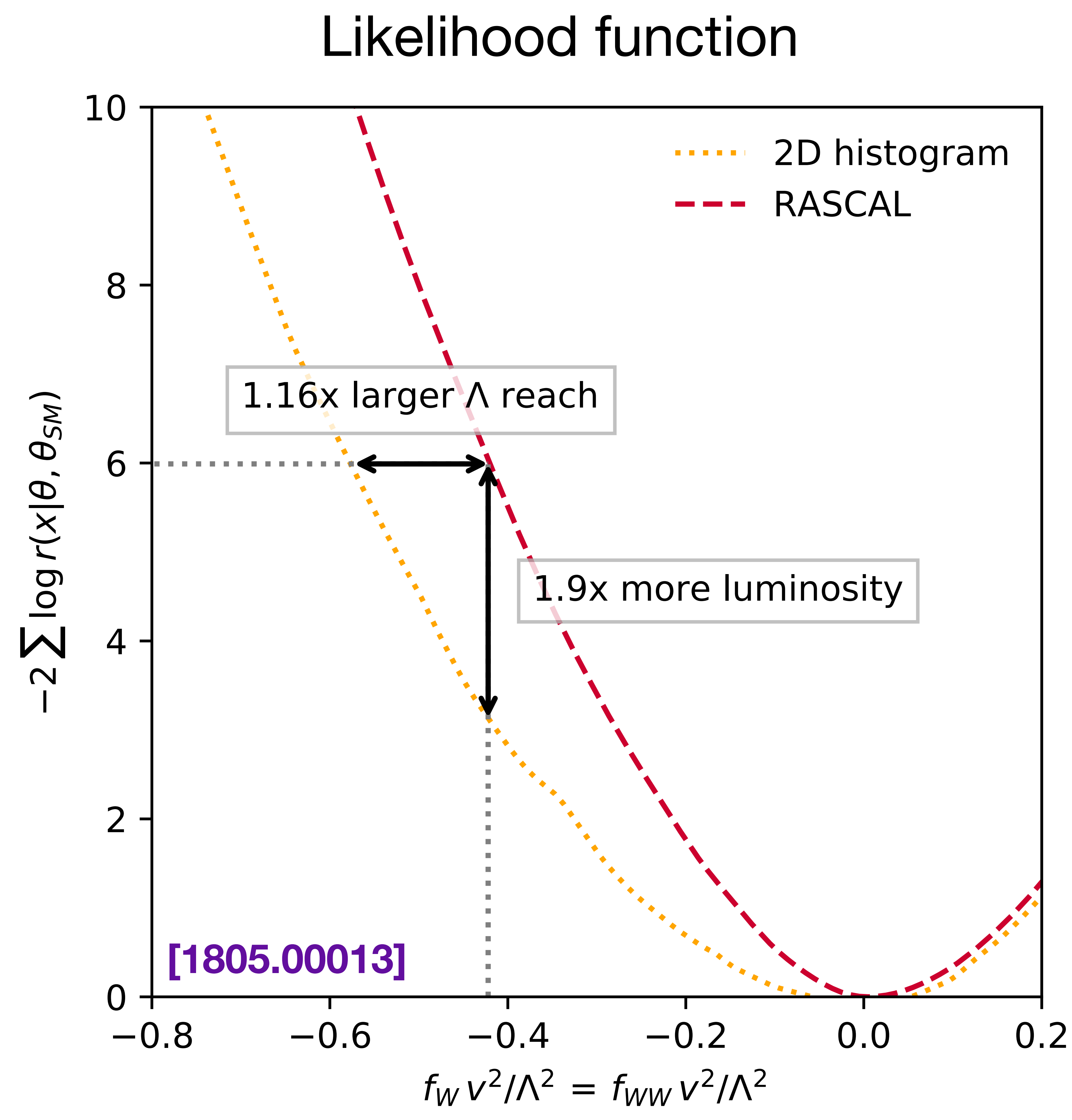
Better sensitivity to new physics

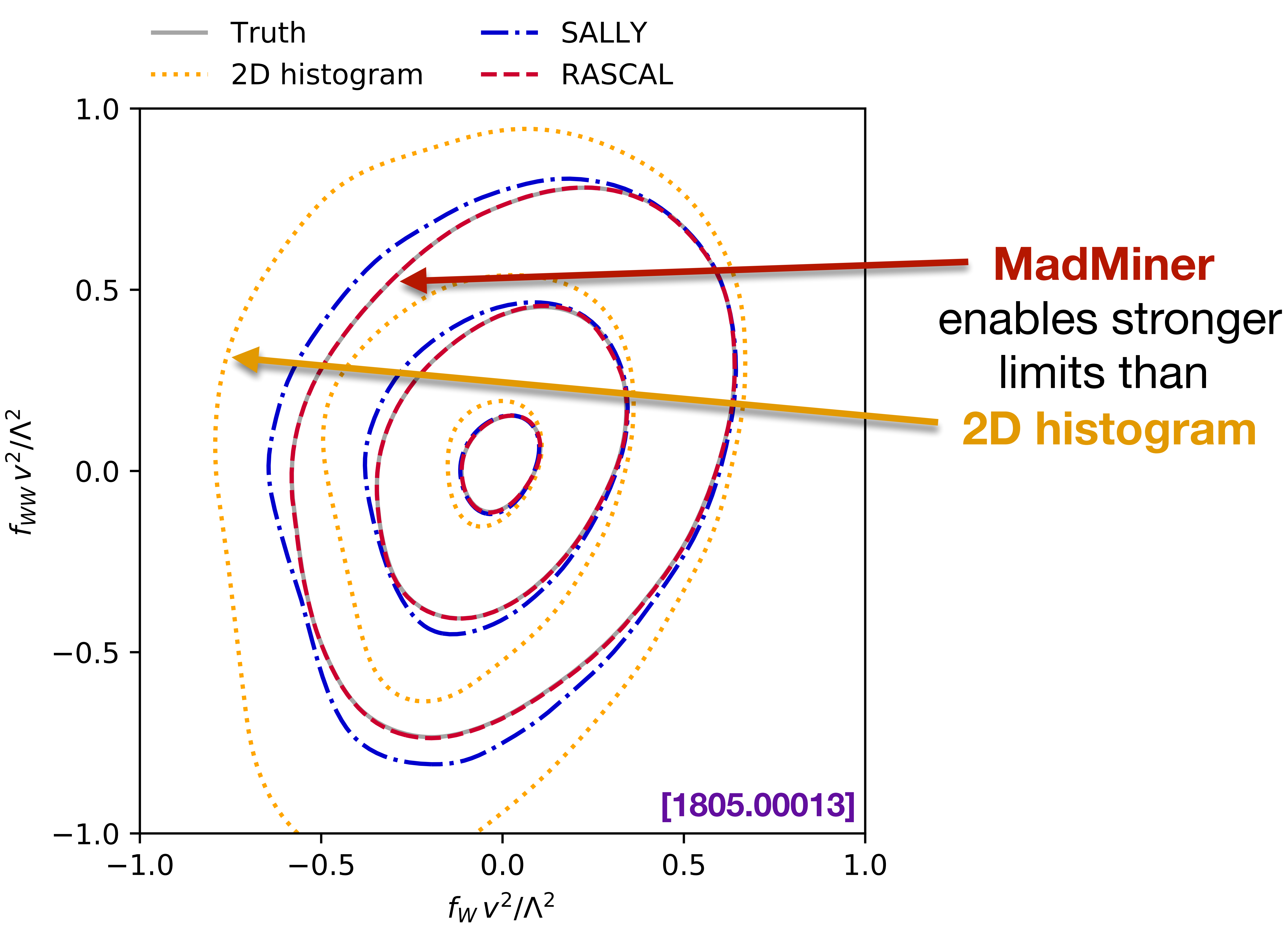
Likelihood function



Results are based on 36 observed events, assuming SM

Better sensitivity to new physics





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Better sensitivity to new physics

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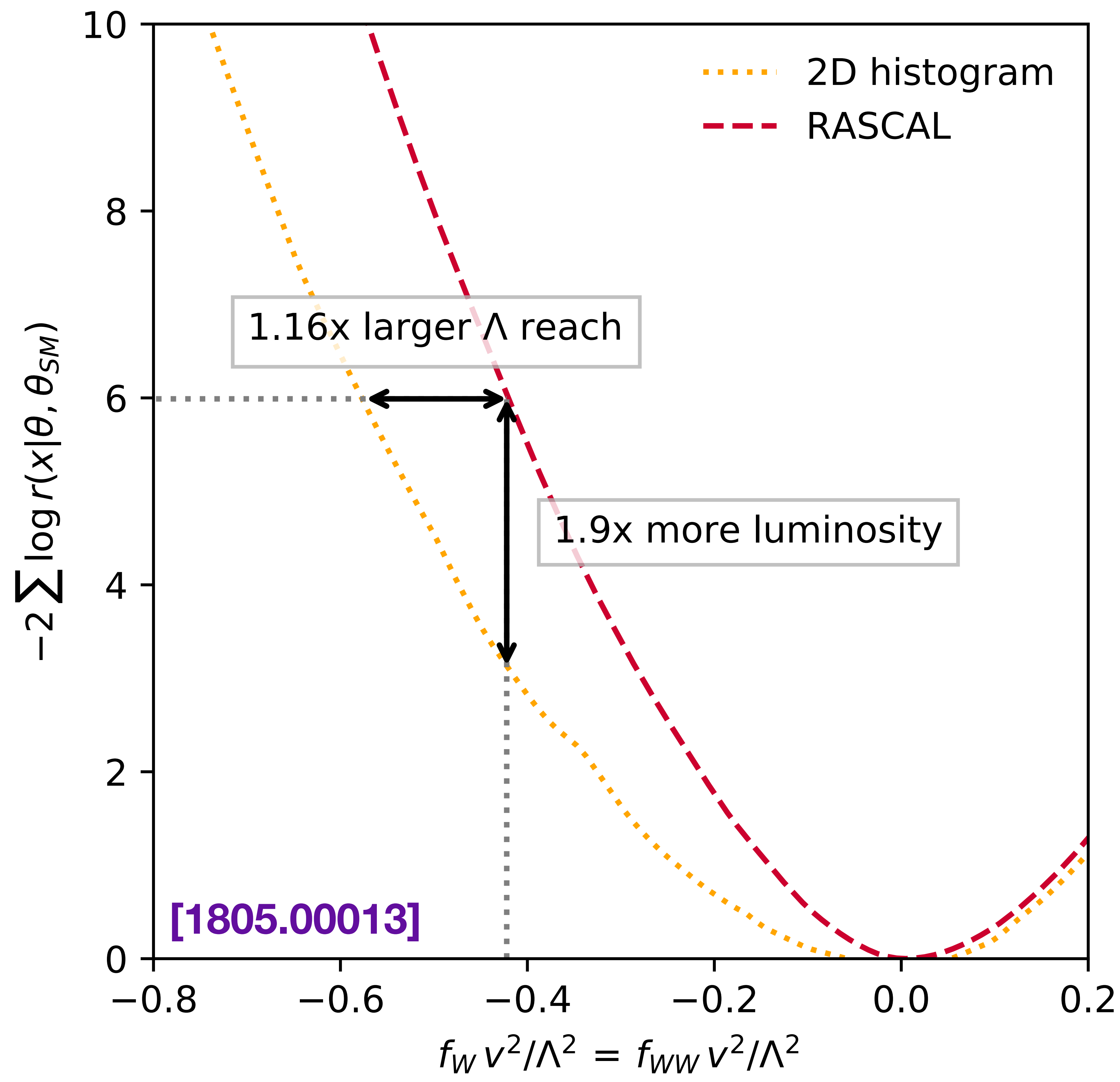
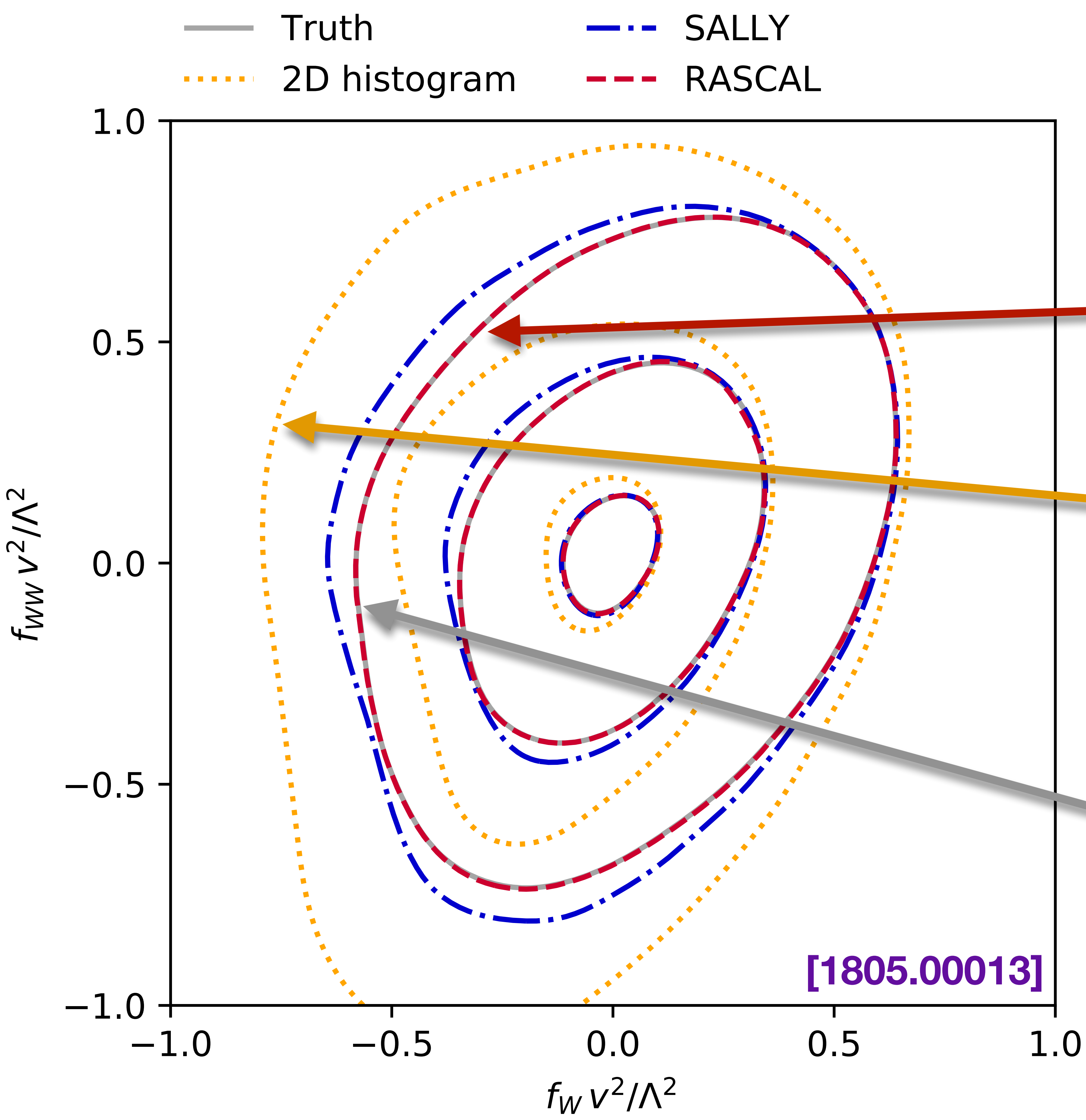


Expected exclusion limits at 68%, 95%, 99.7% CL



MadMiner enables stronger limits than **2D histogram**

Limits from **MadMiner** indistinguishable from **true likelihood** (usually we don't have that)

Results are based on 36 observed events, assuming SM

Appendix

Bonus material

Variational calculus

$$L[\hat{g}(x)] = \int \mathrm{d}x \int \mathrm{d}z\, p(x, z \,|\, \theta) \left[g(x, z) - \hat{g}(x)\right]$$

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

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

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

Choose

$$g(x, z) = \frac{p(x, z, \,|\, \theta_0)}{p(x, z, \,|\, \theta_1)}$$