SMASH
machine learning for science and humanities postdoctoral program

Jožef Stefan Institute

I FEEL SLOVENIA

Co-funded by the European Union

MACHINE LEARNING FOR MODEL-AGNOSTIC SEARCHES FOR NEW PHYSICS

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in collaboration with

Sabine Kraml, Kazuki Sakurai & David Shih

Particle Physics and Cosmology Seminar 05-11-2026

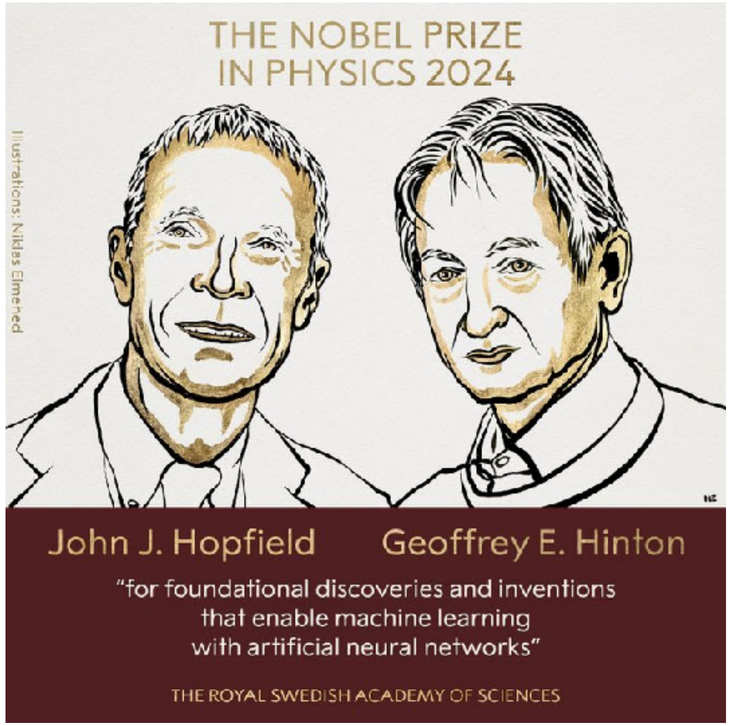
This project has received the funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 101081355. The operation (SMASH project) is co-funded by the Republic of Slovenia and the European Union from the European Regional Development Fund.

Presentation plan

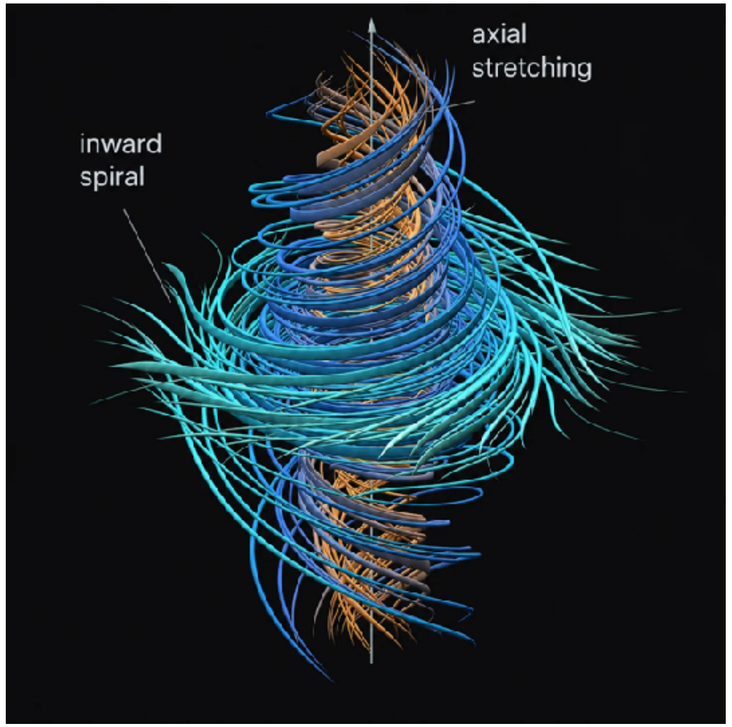



WHAT IS MACHINE LEARNING?
Mazury, Poland

Why should you care?



Nobel Prize in physics



Navier-Stokes
millenial problem
proof

OpenAI

772 math papers

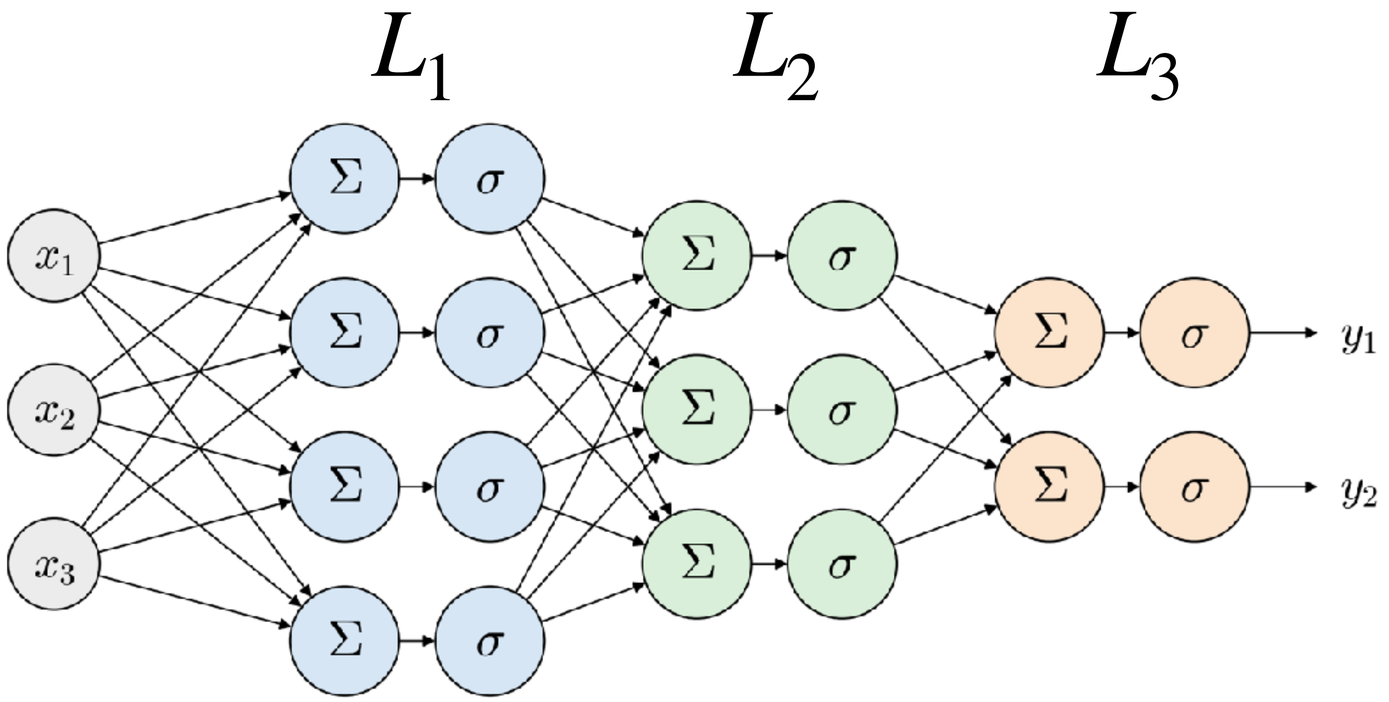
What is Machine Learning?

"Machine learning is the study and use of algorithms that improve their performance on a task by learning from data or experience, rather than by following explicitly programmed instructions."

"Machine learning is a glorified curve fitting."

Artificial neural network = parametrised function

input data $\vec{x}$



output $\vec{y}$

$$\mathrm{NN}(\vec{x}; W, b) = L_{W_3,\vec{b}_3} \circ L_{W_2,\vec{b}_2} \circ L_{W_1,\vec{b}_1}(\vec{x}) \qquad \mathrm{L}(\vec{x})_{W_i,\vec{b}_i} = \sigma\left(W_i \vec{x} + \vec{b}_i \right)$$

Training — iterative optimisation of parameters W, b by minimising the loss function $\mathscr{L}\left(\vec{x}, \vec{y}\right)$:

$$W_i^{t+1} = W_i^t - \nabla_{W_i} \mathscr{L} \qquad b_i^{t+1} = b_i^t - \nabla_{b_i} \mathscr{L}$$

Common neural network tasks

$$\mathbb{X} \in \mathbb{R}^n$$

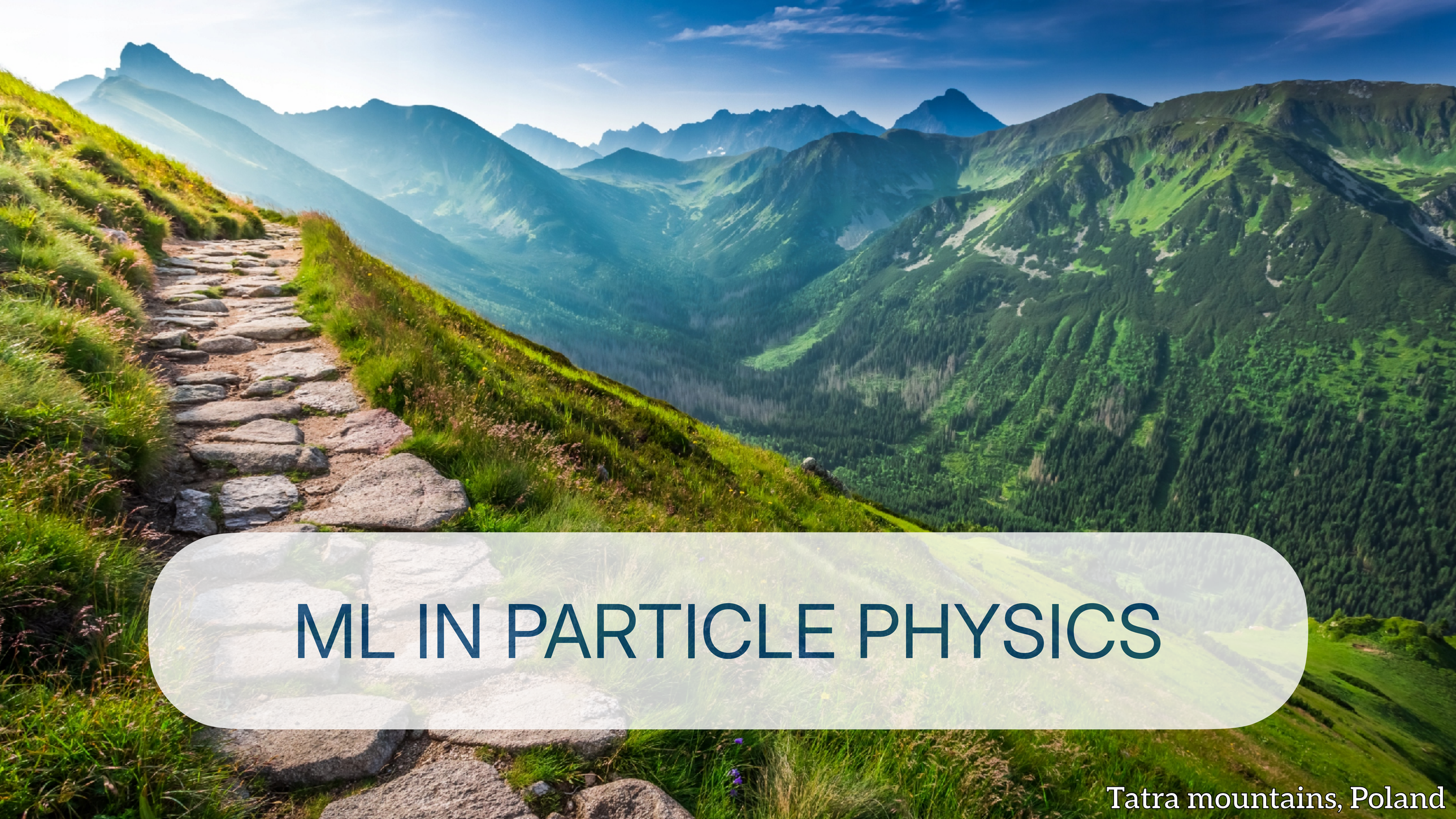
classification $\quad \mathbb{X} \xrightarrow{\text{NN}} \mathbb{Z}$

regression $\quad \mathbb{X} \xrightarrow{\text{NN}} \mathbb{R}^m$

embedding $\quad \mathbb{X} \xrightarrow{\text{NN}} \mathbb{R}^d, \quad d \ll n$

decision-making $\quad \mathbb{X} \xrightarrow{\text{NN}} \text{action}$

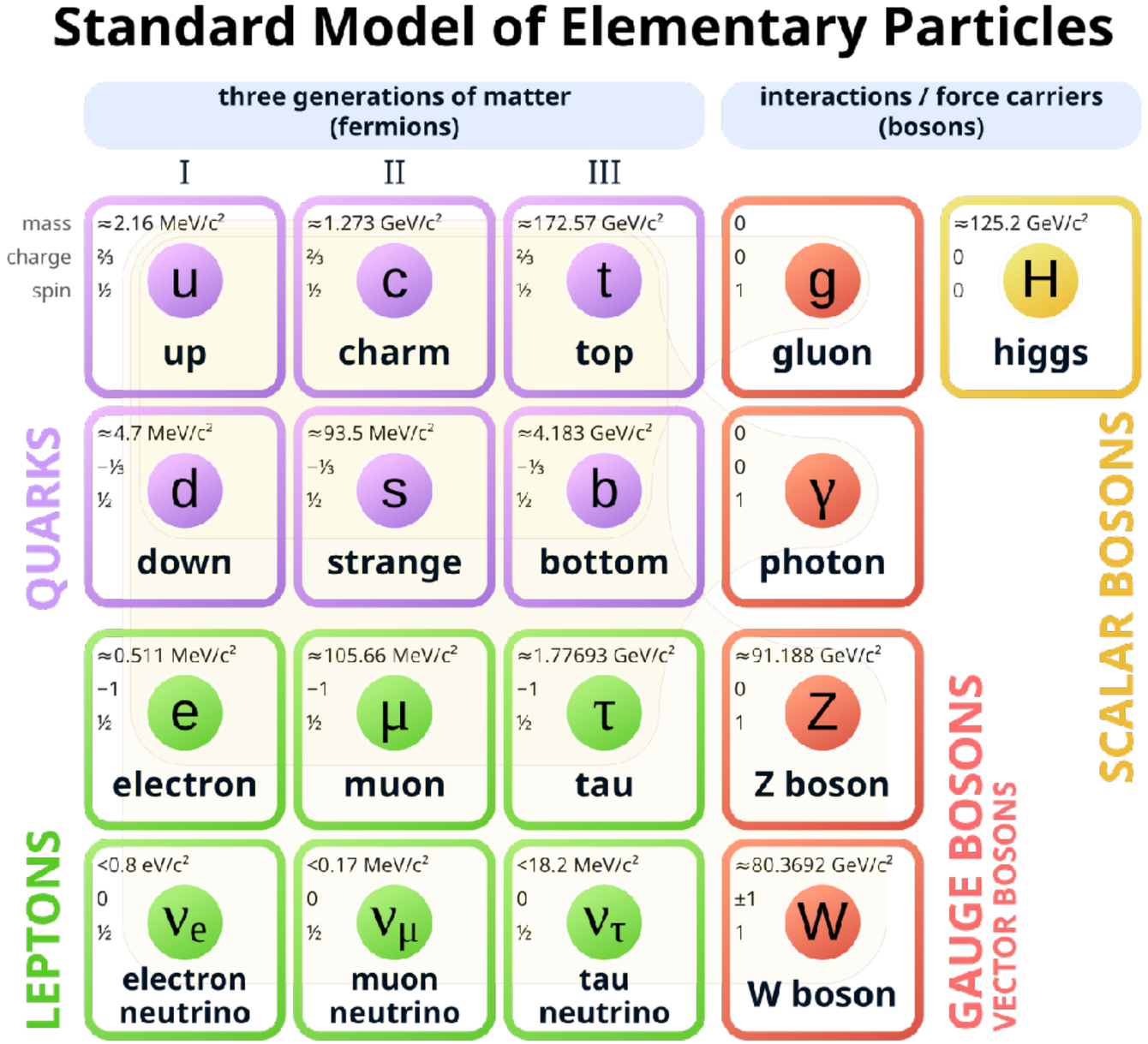
generation $\quad z \sim p(z) \xrightarrow{\text{NN}} \mathbb{X}$



ML IN PARTICLE PHYSICS

Tatra mountains, Poland

Status of the Particle Physics



IMG source: https://en.wikipedia.org/wiki/Standard_Model

Status of the Particle Physics

⚠ Dark Matter

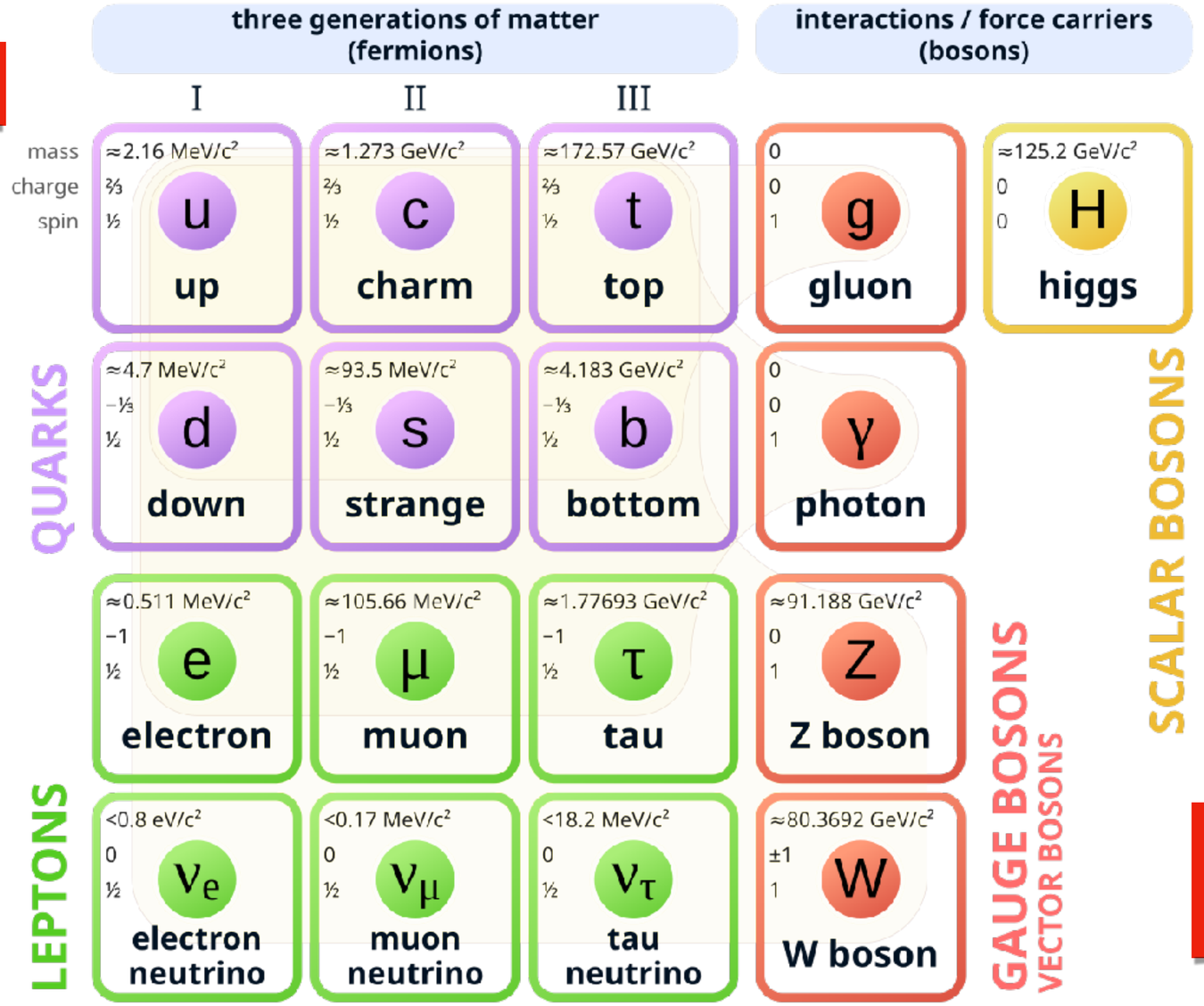
⚠ matter-antimatter asymmetry

⚠ neutrino masses

⚠ hierarchy problem

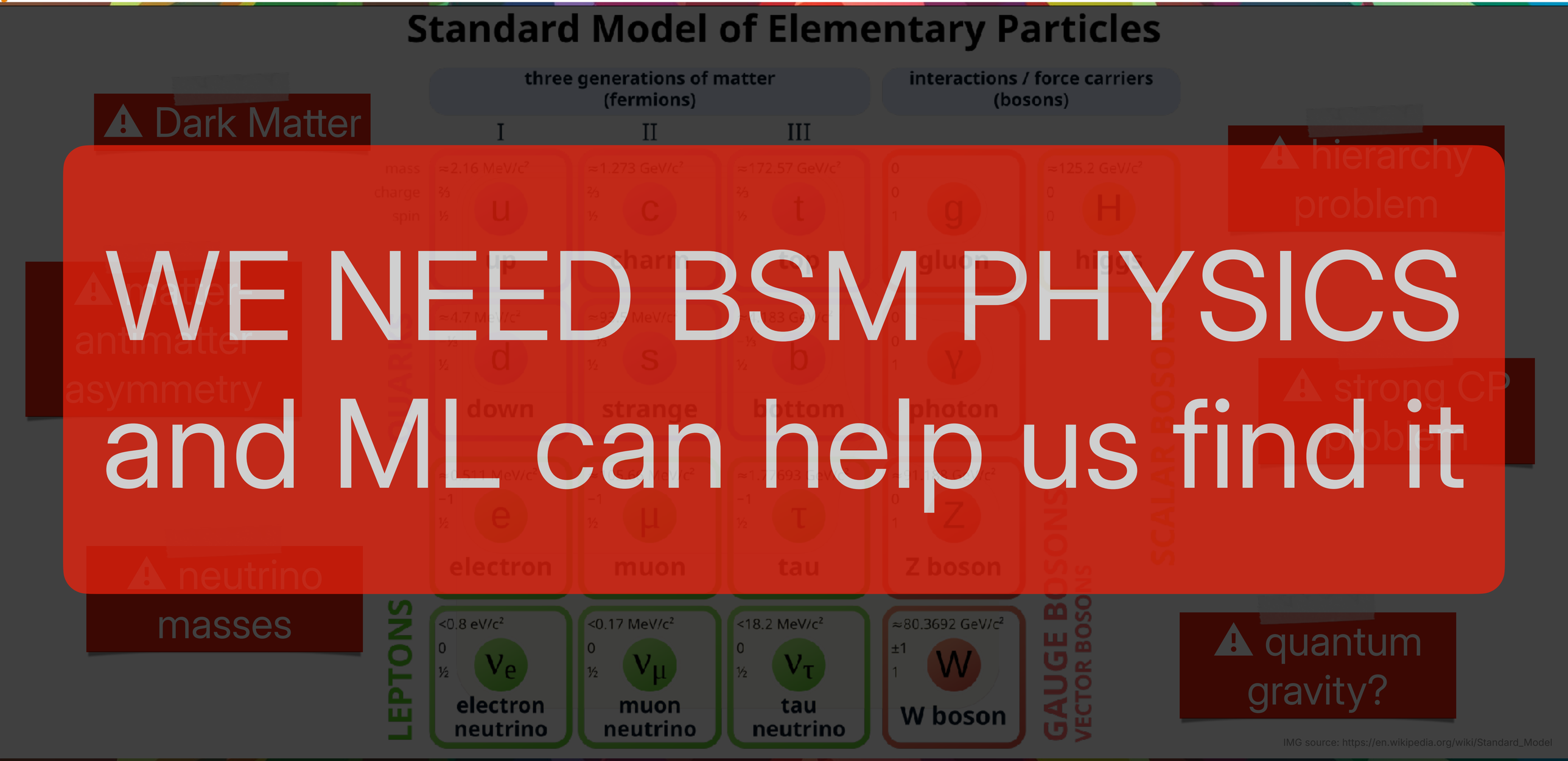
⚠ strong CP problem

⚠ quantum gravity?



IMG source: https://en.wikipedia.org/wiki/Standard_Model

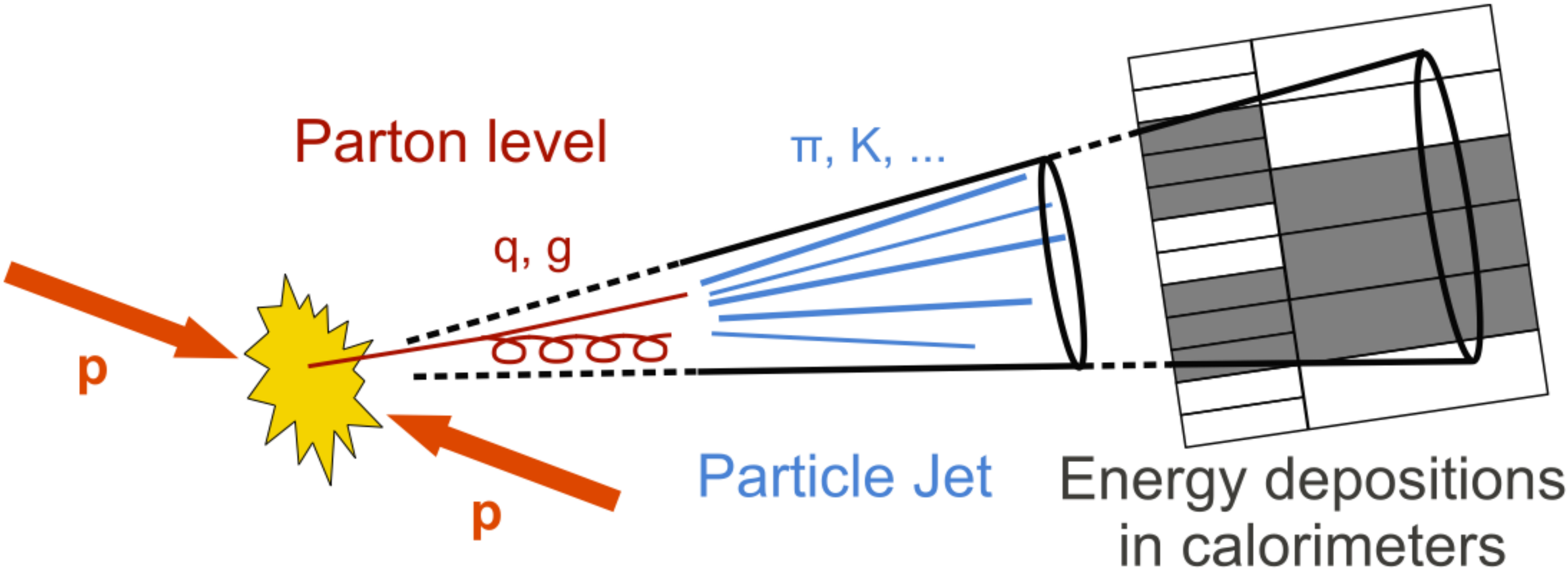
Status of the Particle Physics



WE NEED BSM PHYSICS and ML can help us find it

IMG source: https://en.wikipedia.org/wiki/Standard_Model

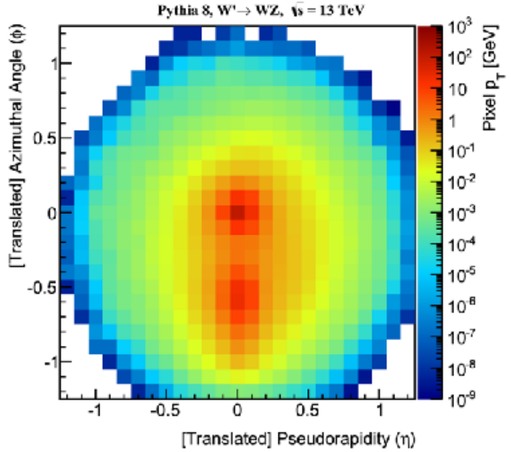
Jet tagging



Assign jet to type of elementary coloured particle → a classification problem

img source:https://www.ericmetodiev.com/post/jetformation/

Jet tagging



Convolutional Neural Networks
arXiv:1511.05190 [hep-ph]

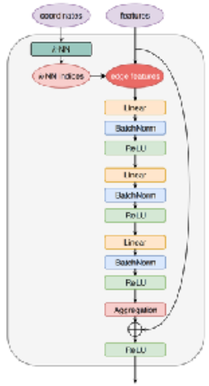
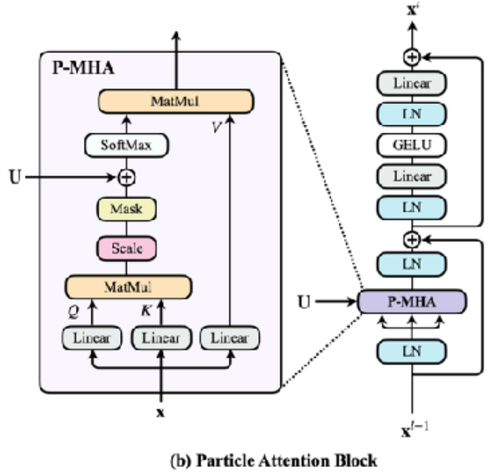


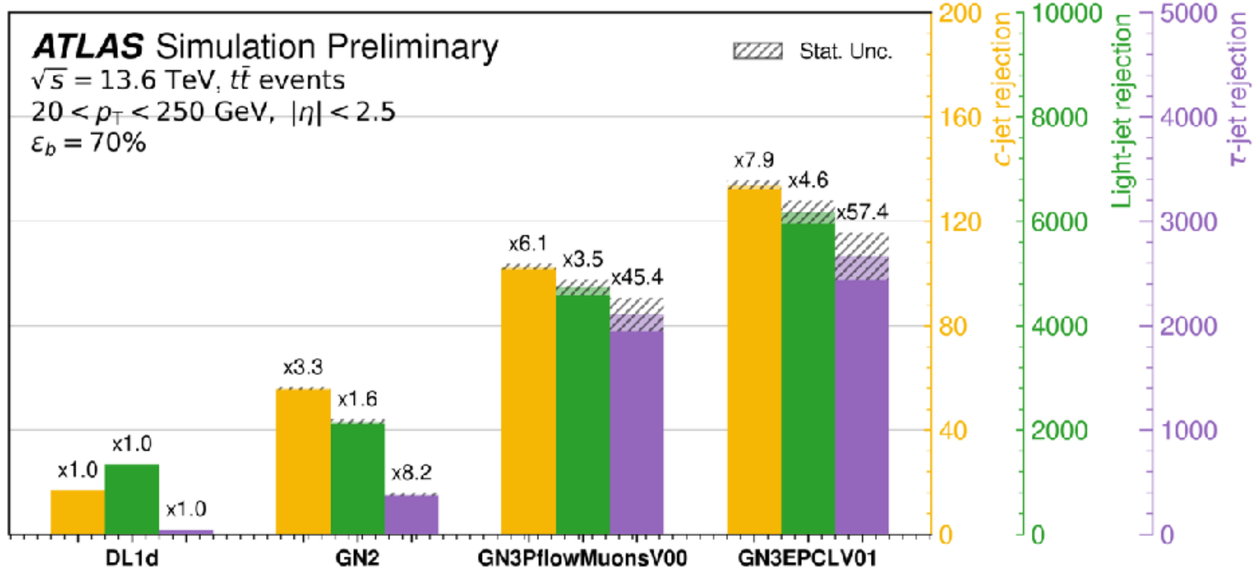
FIG. 1: The structure of the EdgeConv block.

ParticleNet
arXiv:1902.08570 [hep-ph]



(b) Particle Attention Block

Particle Transformer
arXiv:2202.03772 [hep-ph]



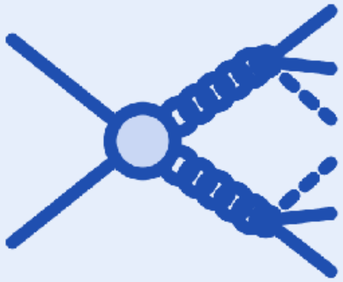
Heavy flavour tagging at ATLAS
FTAG-2026-07

Fast simulation

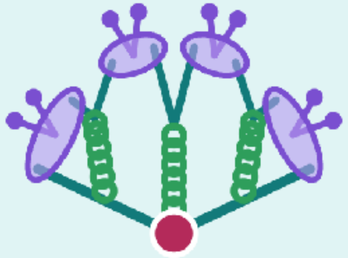
1 **Model**
Lagrangian

$\mathscr{L}$

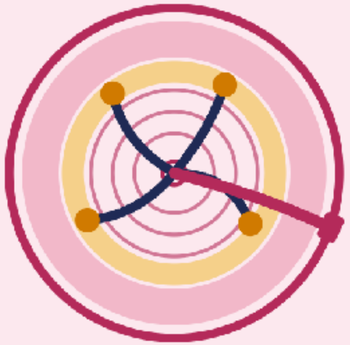
2 **Hard process**
MadGraph5



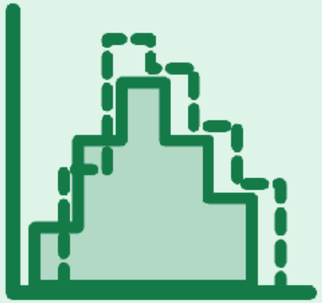
3 **Shower & hadronization**
Pythia/Herwig



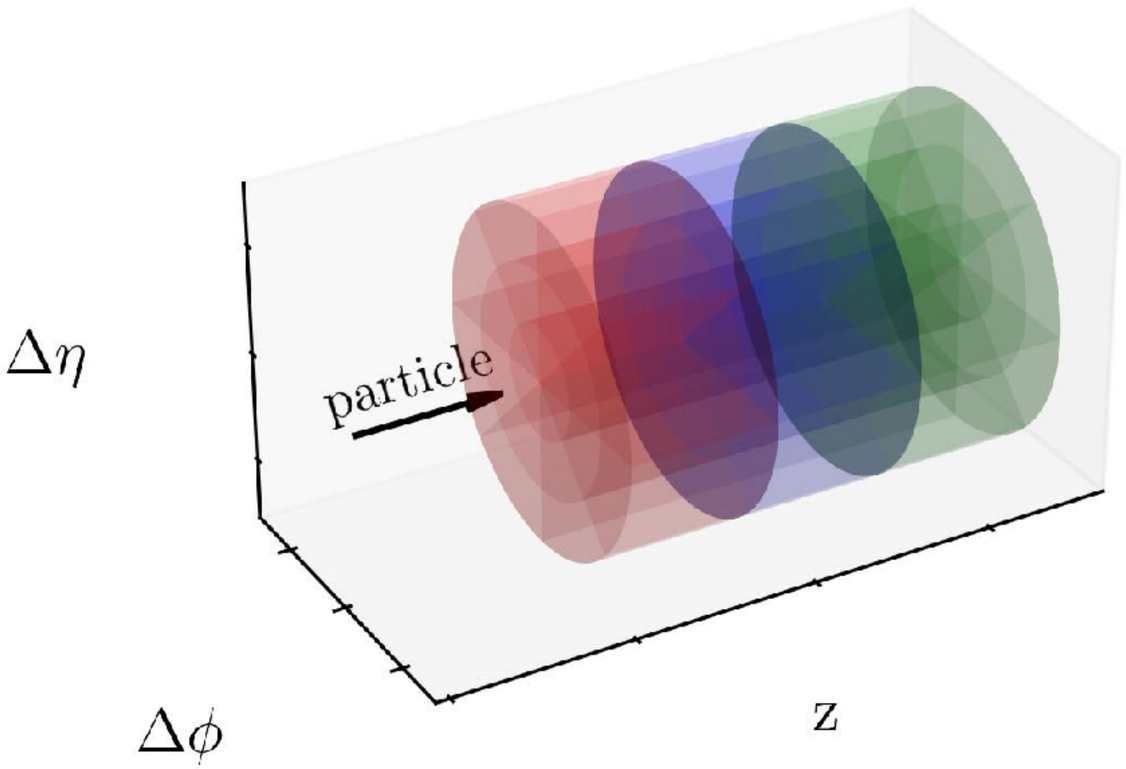
4 **Detector simulation**
Delphes/Geant4



5 **Analysis**
histograms, limits



Fast simulation



CaloChallenge
arXiv:2410.21611 [physics.ins-det]

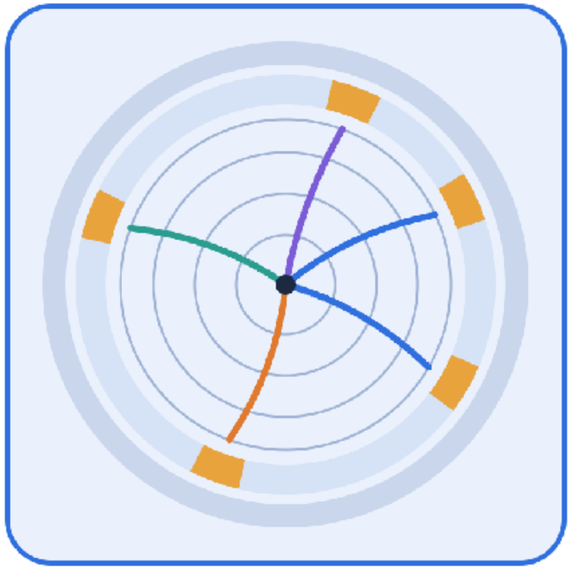
AtlFast3 (GAN, calo shower)
arXiv: 2109.02551 [hep-ex]

FlashSim (NF, detector)
EPJ WEB Conf 337, 2025

Lamarr (GAN + BDT, detector)
arXiv:2309.13213 [hep-ex]

Zero Degree Calorimeters
(Diff, detector subsystem)
arXiv:2507.18811 [cs.LG]

Foundation model



Large dataset

real or simulated

Pre-training

labels not needed



Foundation model

general physics knowledge

Fine-tuning

+ small labelled dataset

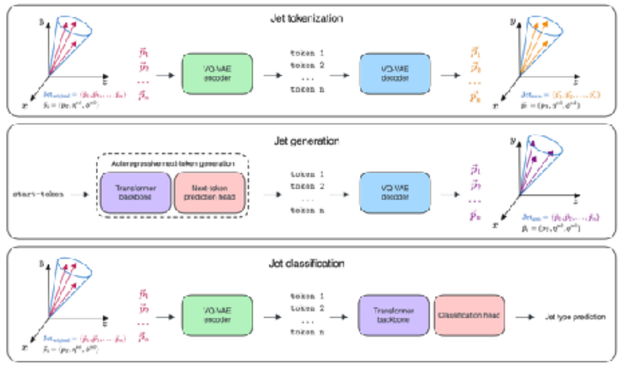
Downstream tasks

- Jet tagging
- Fast simulation
- Track-calo clustering
- Pileup mitigation
- Particle flow reconstruction
- Event analysis
- Unfolding
- Anomaly detection

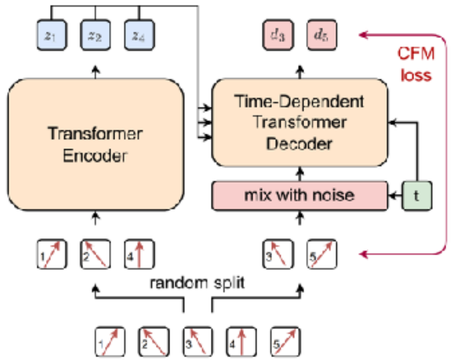
MISTRAL AI_

CERN

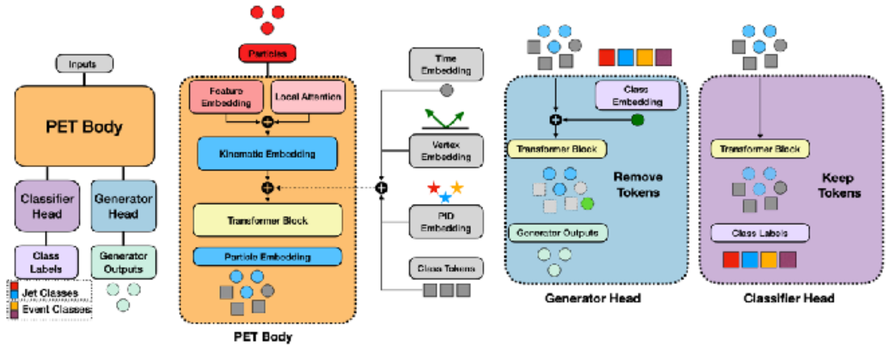
Foundation model



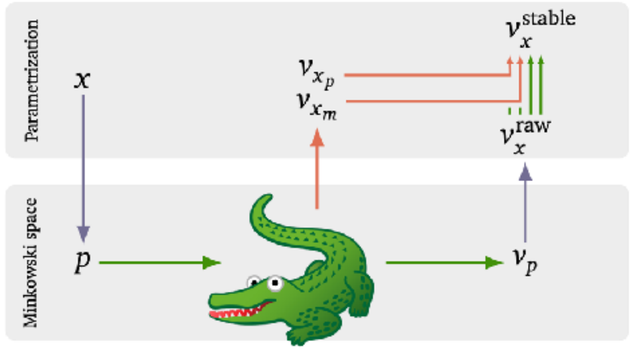
OmniJet-α
arXiv:2403.05618 [hep-ph]



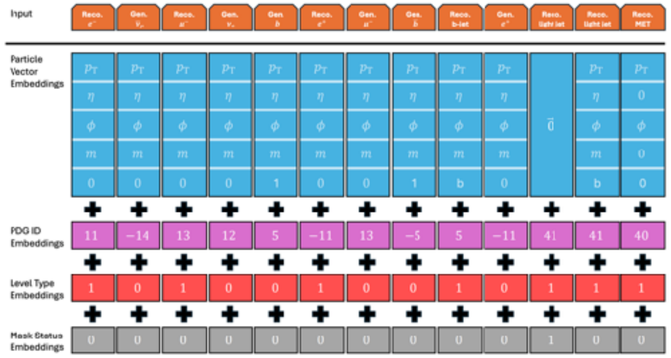
Set-to-set flow-matching model
arXiv:2409.12589 [hep-ph]



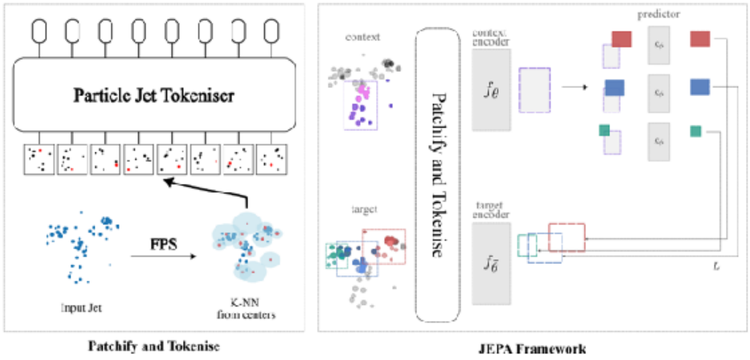
OmniLearned
arXiv:2510.24066 [hep-ph]



L-GATr
arXiv:2411.00446 [hep-ph]

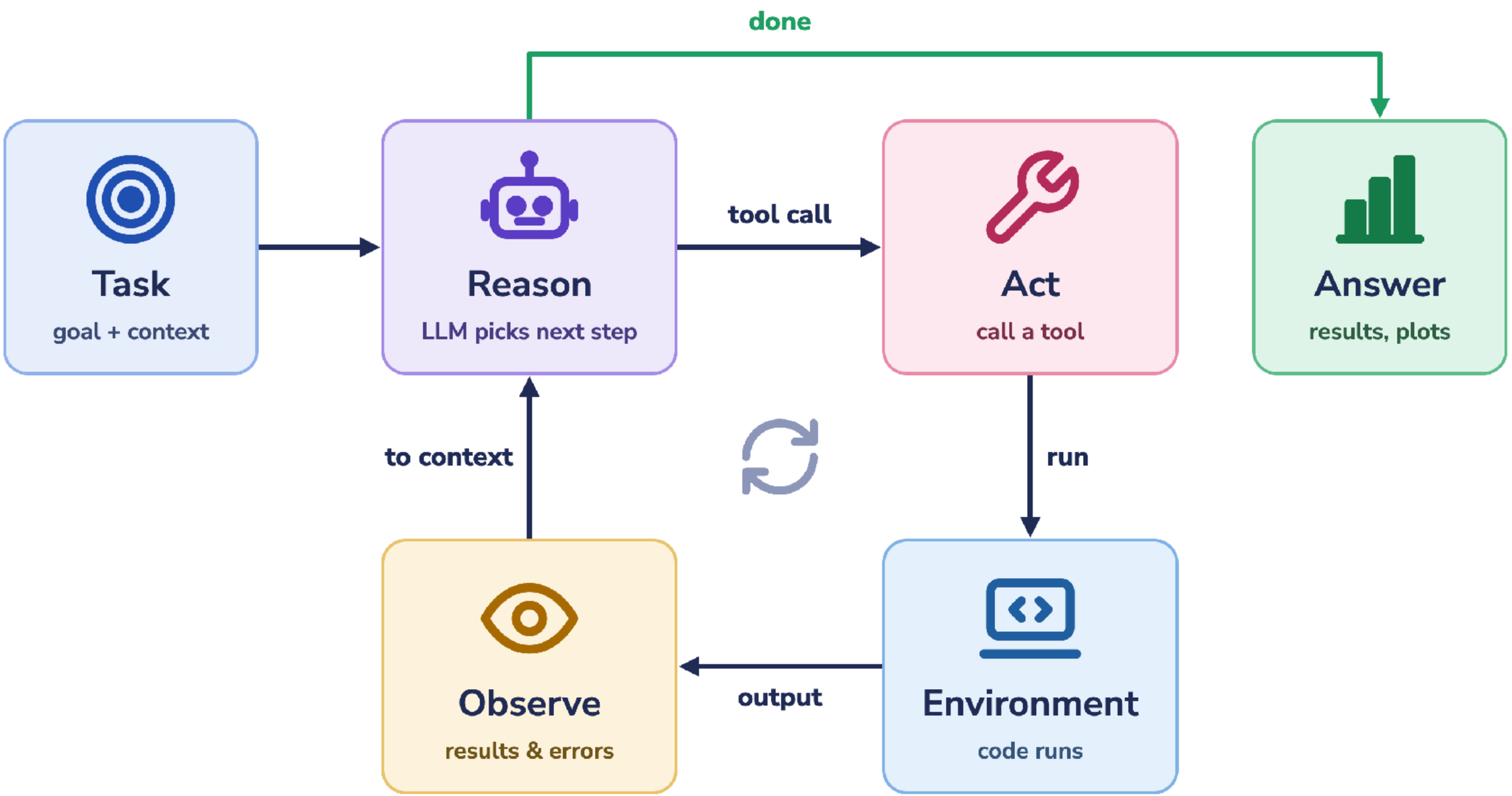


Bumblebee
arXiv:2412.07867 [hep-ph]



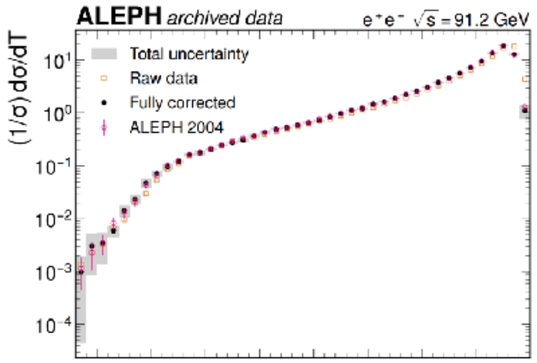
HEP-JEPA
arXiv:2502.03933 [hep-ph]

Agentic AI

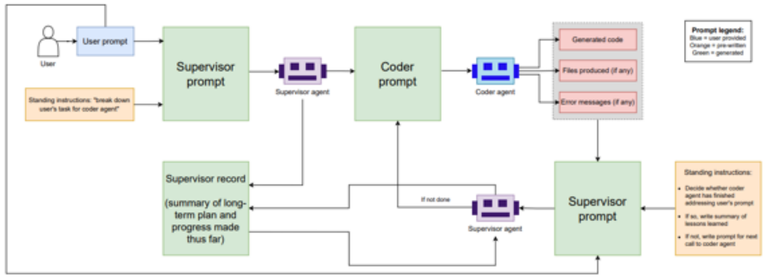

done
Task
goal + context
Reason
LLM picks next step
tool call
Act
call a tool
Answer
results, plots
to context
run
Observe
results & errors
output
Environment
code runs

Agentic AI

experiment

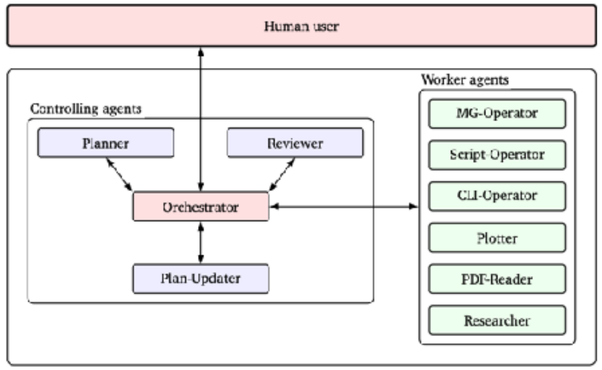


Thrust distribution measurement on LEP data
arXiv:2603.05735 [hep-ex]

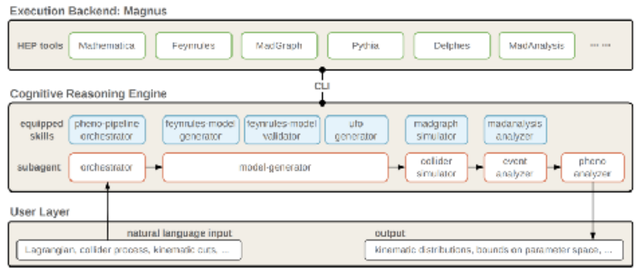


H→γγ cross-section measurement on ATLAS open data
arXiv:2512.07785 [physics.data-an]

phenomenology

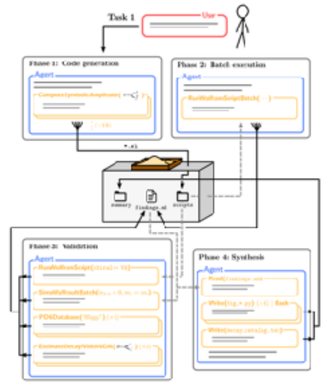


MadAgents
arXiv:2601.21015 [hep-ph]

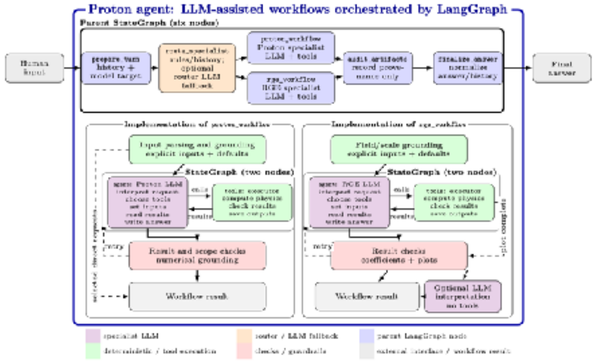


End-to-end phenomenology agent
arXiv:2603.14553 [hep-ph]

theory



Multi-step analytical calculations
arXiv: 2603.26990 [hep-ph]



Gauge Coupling Unif. & Proton Decay
arXiv:2610.33593 [hep-ph]

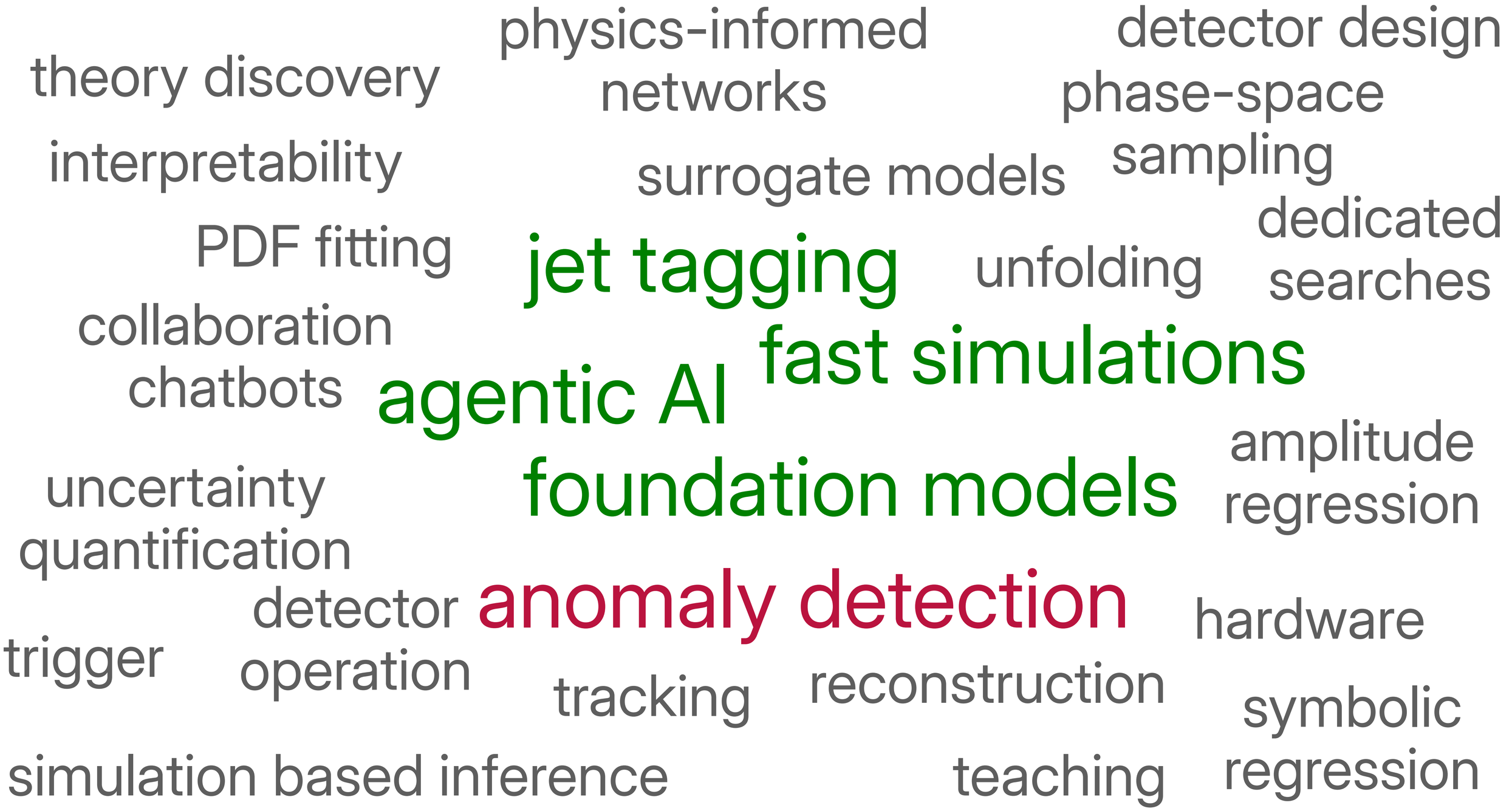
jet tagging

fast simulations

agentic AI

foundation models

anomaly detection


physics-informed networks
detector design
theory discovery
phase-space sampling
interpretability
surrogate models
dedicated searches
PDF fitting
jet tagging
unfolding
collaboration
fast simulations
chatbots
agentic AI
amplitude regression
uncertainty quantification
foundation models
anomaly detection
detector operation
hardware
trigger
tracking
reconstruction
symbolic regression
simulation based inference
teaching

Community

Conferences

ML4JETS

EuCAIFcon

CHEP

ACAT

BOOST

Inter-experimental ML workshop

AI+HEP in East Asia

Scientific Networks

EuCAIF

MLQC4FC CA

AIFORIA CA

CERN WGs

SMASH

Institutes

IAIFI

AISSAI

Challenges

LHC-Olympics

CaloChallenge

Higgs Uncertainty Challenge

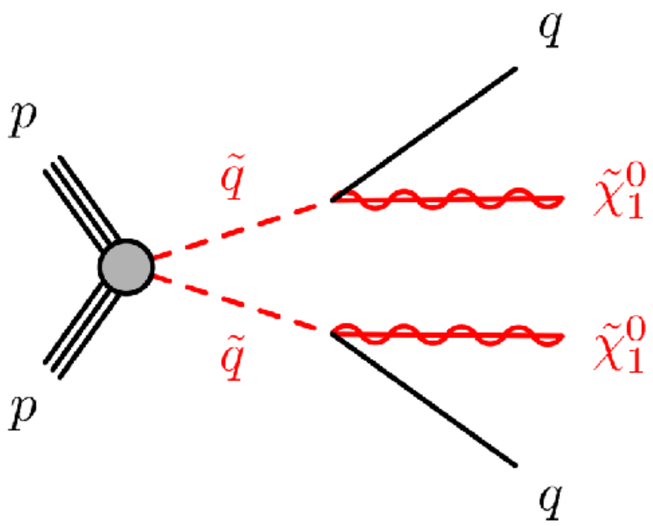


MODEL AGNOSTIC SEARCHES

Hel peninsula, Poland

Classical approach to BSM searches

BSM scenario



limited by our biases

event selection

Signal Region	≥ 2-jet
$E_{\mathrm{T}}^{\mathrm{miss}}$	> 130
Leading jet p_{T}	> 130
Second jet p_{T}	> 40
$\Delta\phi(\mathrm{jet}, \vec{P}_{\mathrm{T}}^{\mathrm{miss}})_{\mathrm{min}}$	> 0.4
$E_{\mathrm{T}}^{\mathrm{miss}}/m_{\mathrm{eff}}$	> 0.3
m_{eff}	> 1000

specific to BSM scenario

background estimation

BG/signal estimation (MC sim)

Z/γ+jets	32.3 ± 2.6 ± 6.9
W+jets	26.4 ± 4.0 ± 6.7
$t\bar{t}$+ single top	3.4 ± 1.6 ± 1.6
QCD multi-jet	0.22 ± 0.06 ± 0.24
SM total	62.4 ± 4.4 ± 9.3
$(m_{\tilde{q}}, m_{\tilde{\chi}_1^0}) = (1, 0.1)$ TeV	29.2 ± 5.1
Data	58

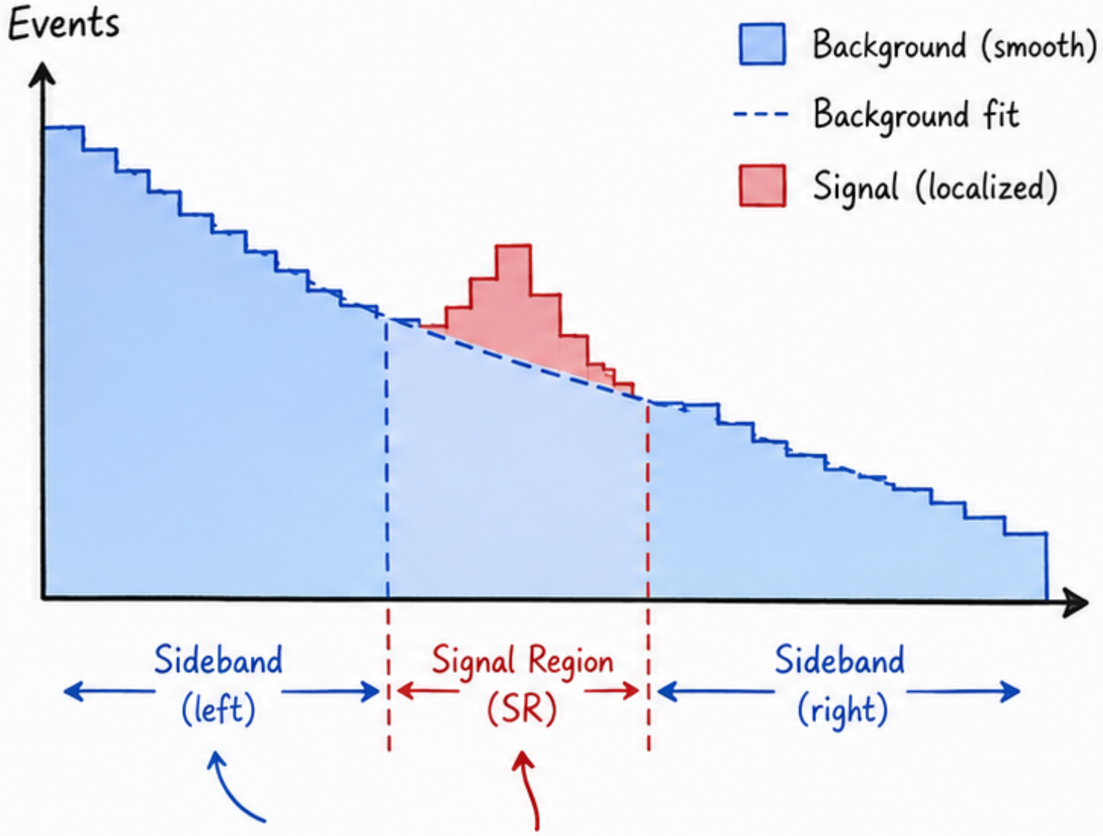
statistical consistency

simulation dependent

slide content borrowed from K. Sakurai

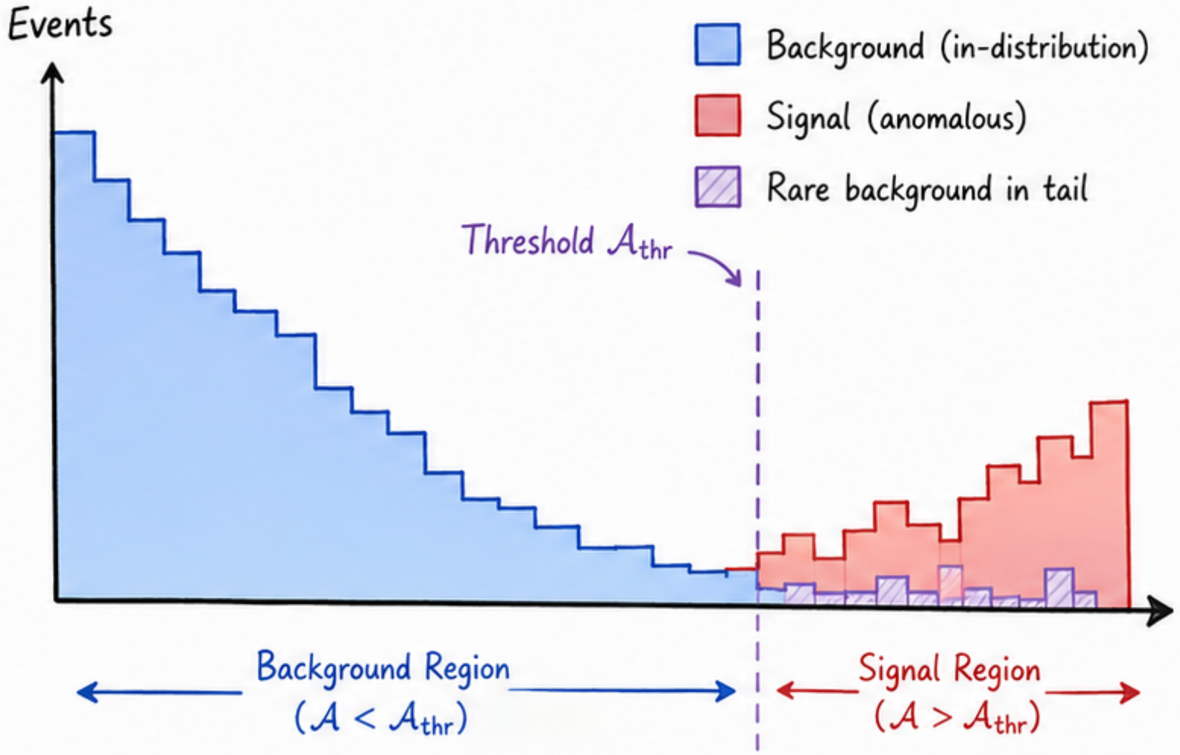
Anomaly searches in HEP

Overdensity (Bump Hunting)



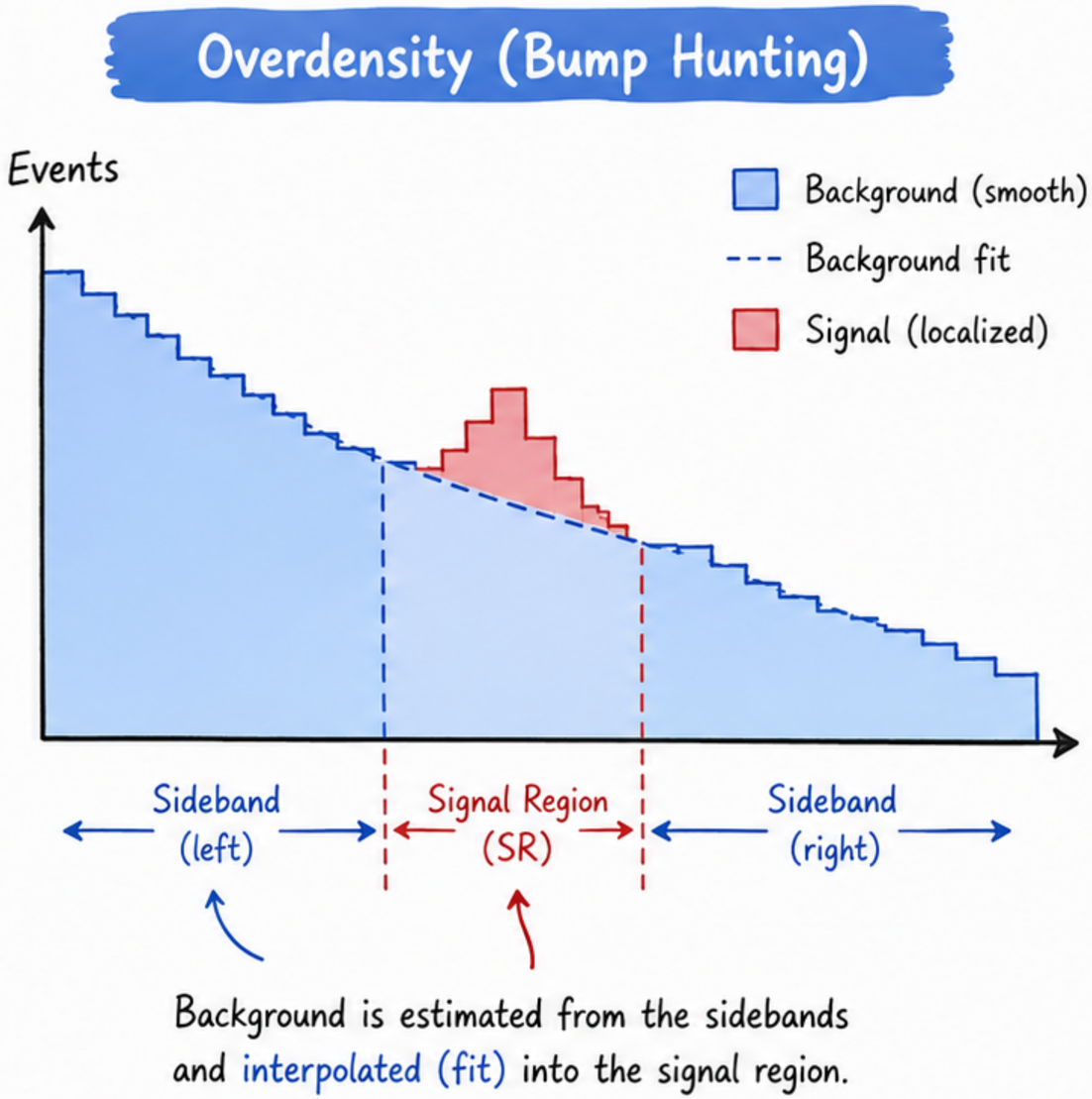
Background is estimated from the sidebands and interpolated (fit) into the signal region.

Out-of-Distribution (OOD) Anomaly Search



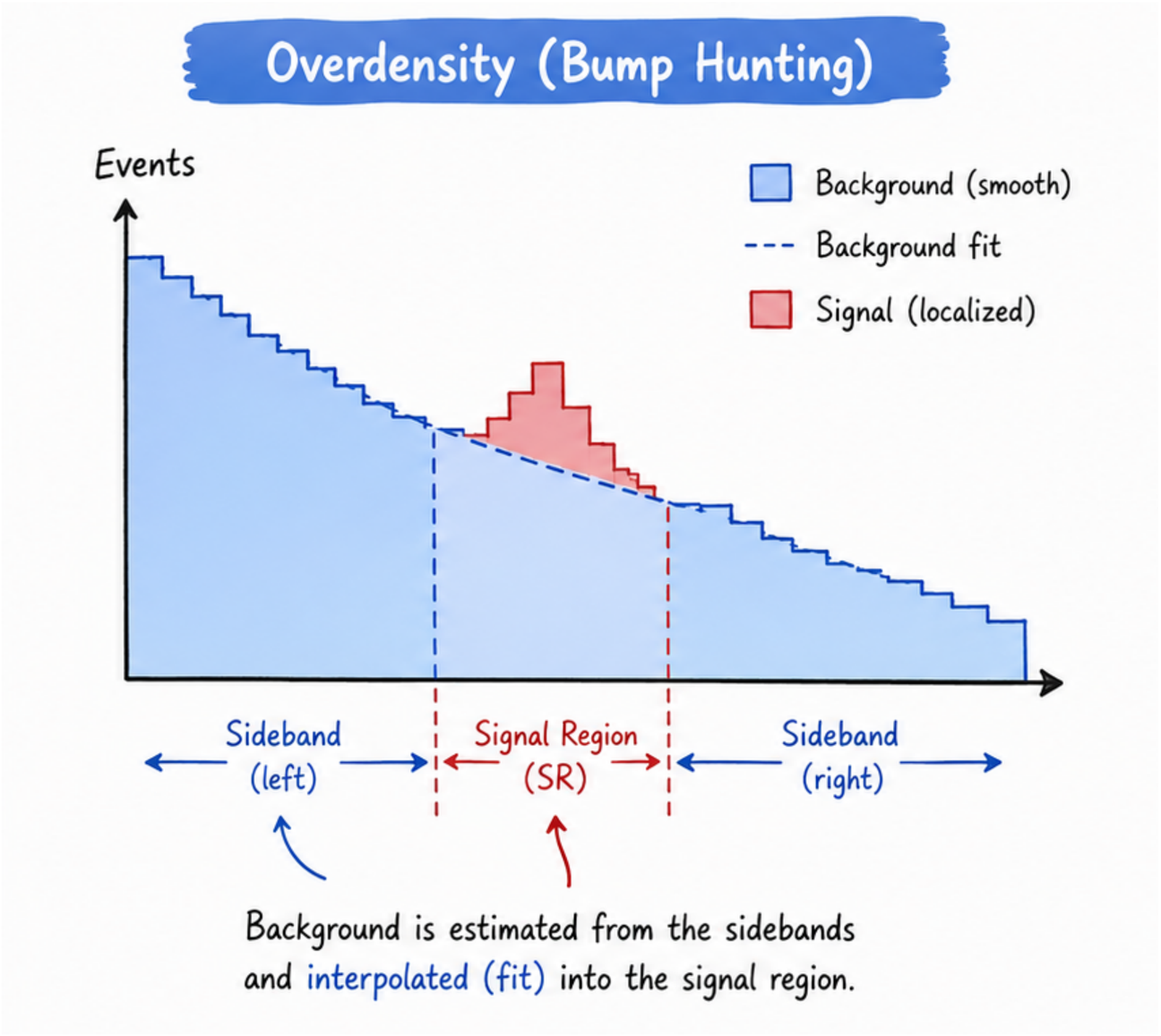
Events with anomaly score $\mathcal{A}$ greater than the threshold are considered anomalous.

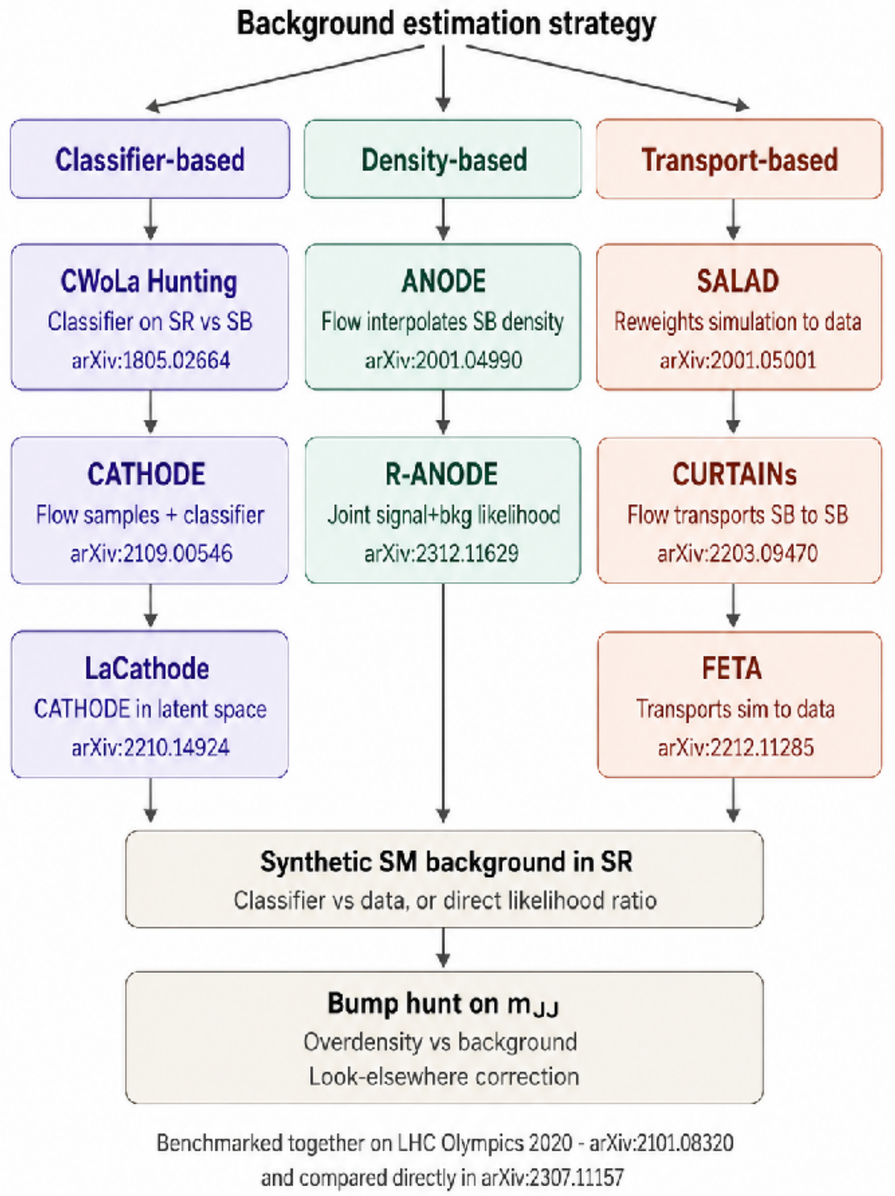
Anomaly searches in HEP



- Special resonant variable, e.g., m_{JJ}
- Signal localised
- Background smooth
- Define:
  - Signal region
  - Two adjacent sideband regions
- Look for an excess in the SR
- Classically: Bump Hunting
- ML: weakly-supervised methods using auxiliary variables

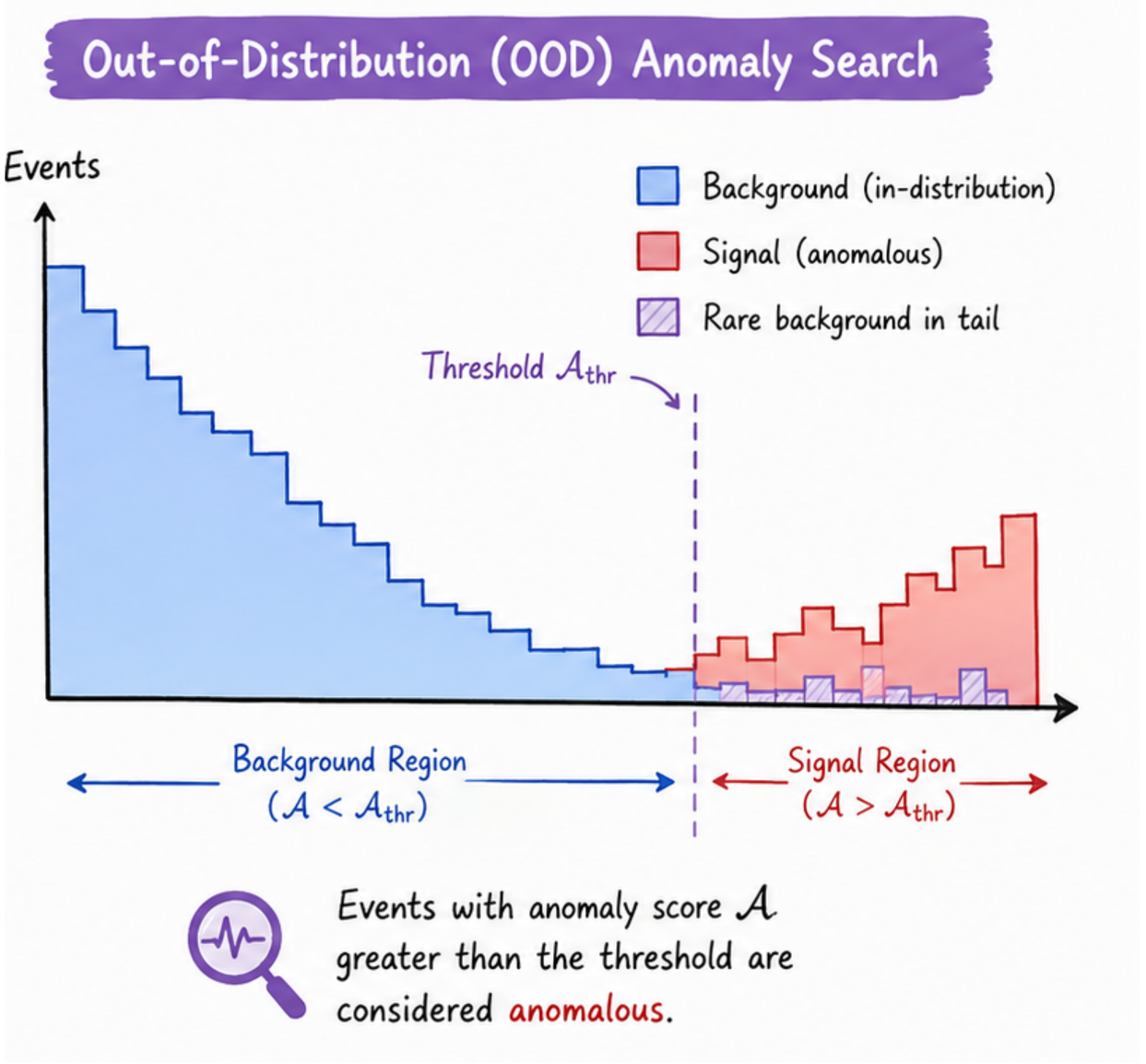
Anomaly searches in HEP





Anomaly searches in HEP

- Construct anomaly score A
  - Background events have small A
  - Signal events have large A
- Select a threshold: A_{thr}
- Define the signal region as $A > A_{thr}$

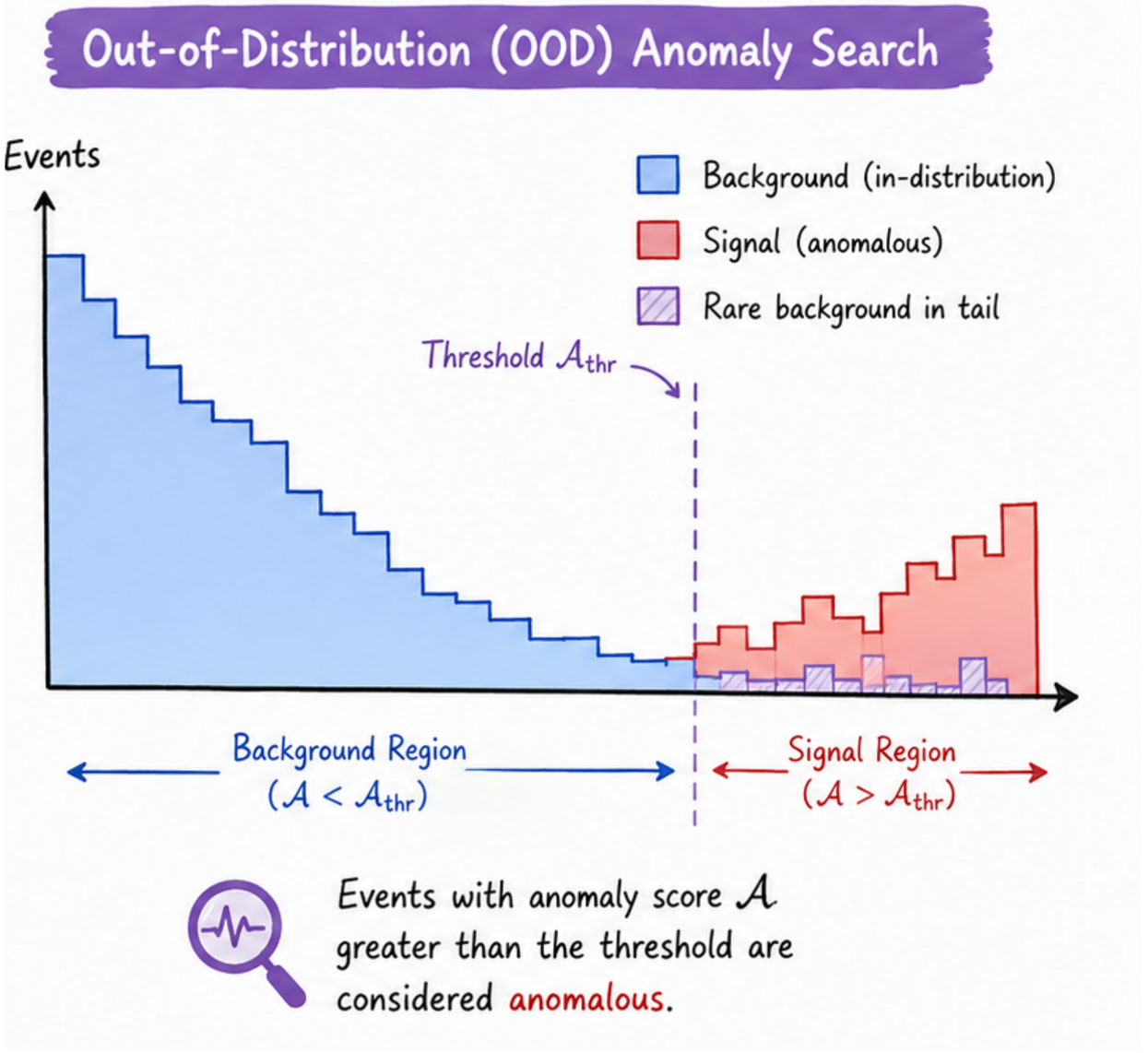


Anomaly searches in HEP

How?

- Construct anomaly score A
  - Background events have small A
  - Signal events have large A
- Select a threshold: A_{thr}
- Define the signal region as $A > A_{thr}$

What about background in the signal region?



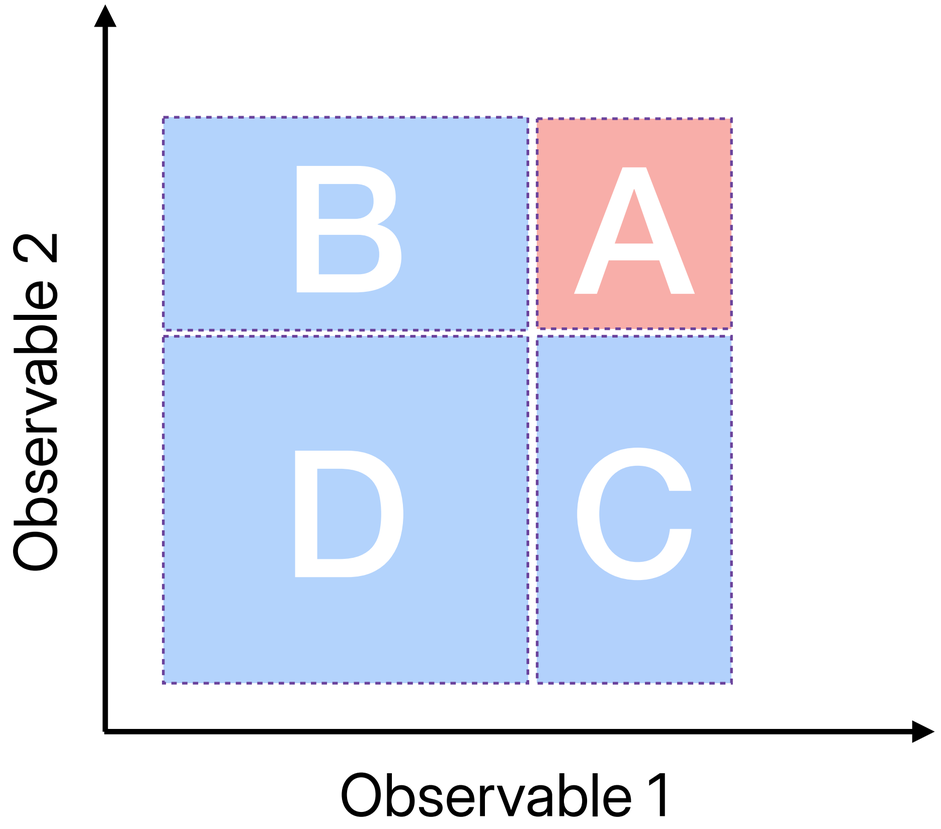


METHODOLOGY

Moszna Castle, Poland

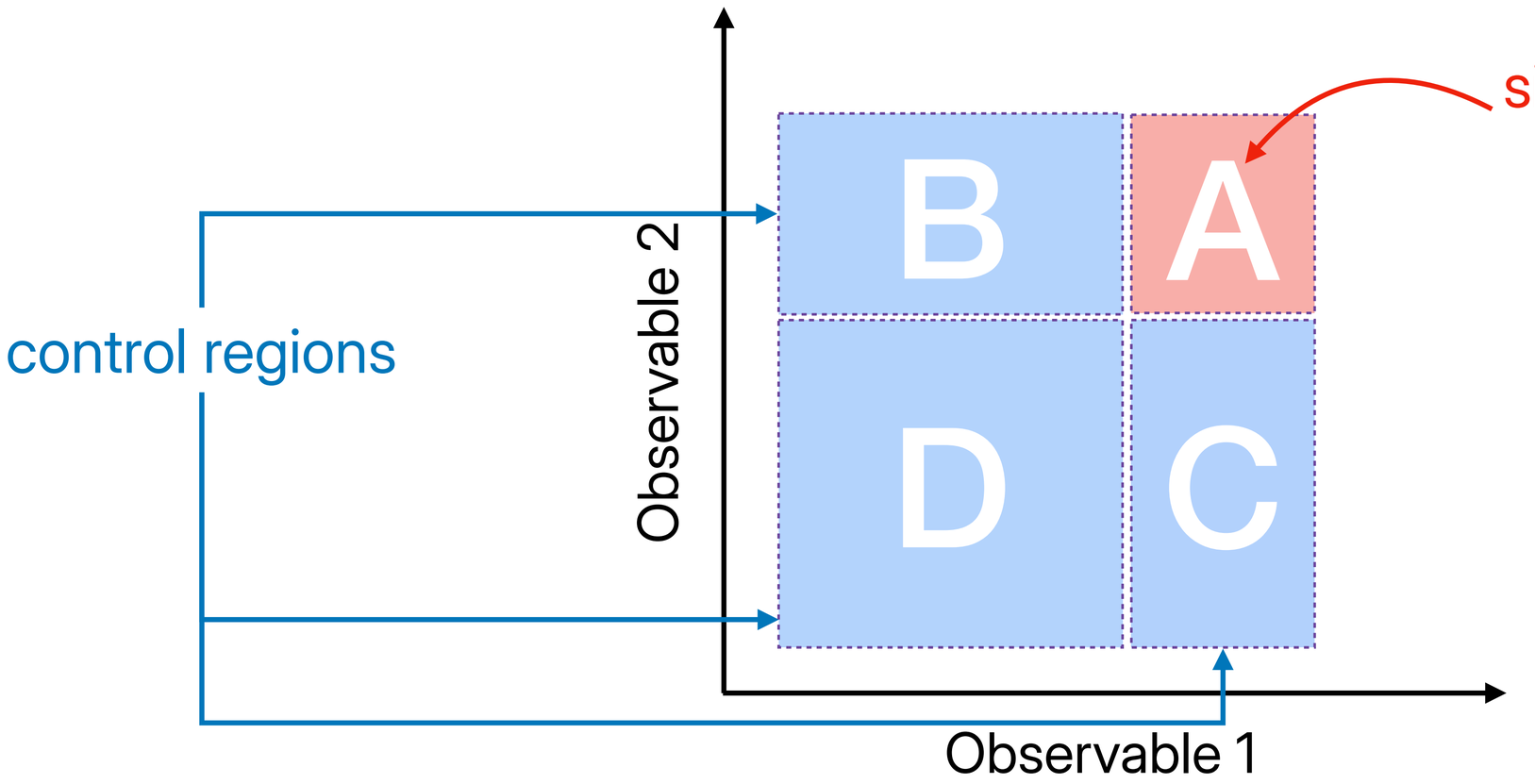
ABCD matrix method

Established method for data-driven background estimation



ABCD matrix method

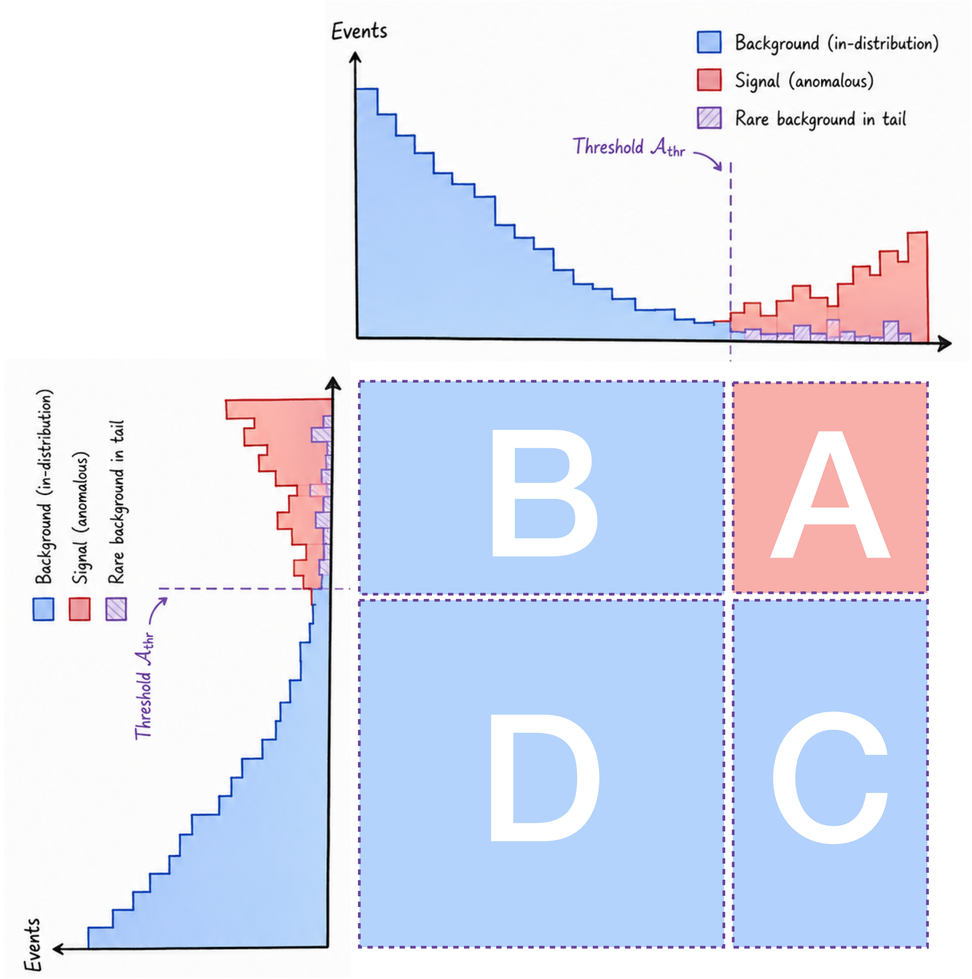
Established method for data-driven background estimation



$$N_A^{\text{bkg}} = N_B^{\text{bkg}} \frac{N_C^{\text{bkg}}}{N_D^{\text{bkg}}}$$

ABCD matrix method

Established method for data-driven background estimation



$$N_A^{\text{bkg}} = N_B^{\text{bkg}} \frac{N_C^{\text{bkg}}}{N_D^{\text{bkg}}}$$

Both anomaly scores have to be independent!

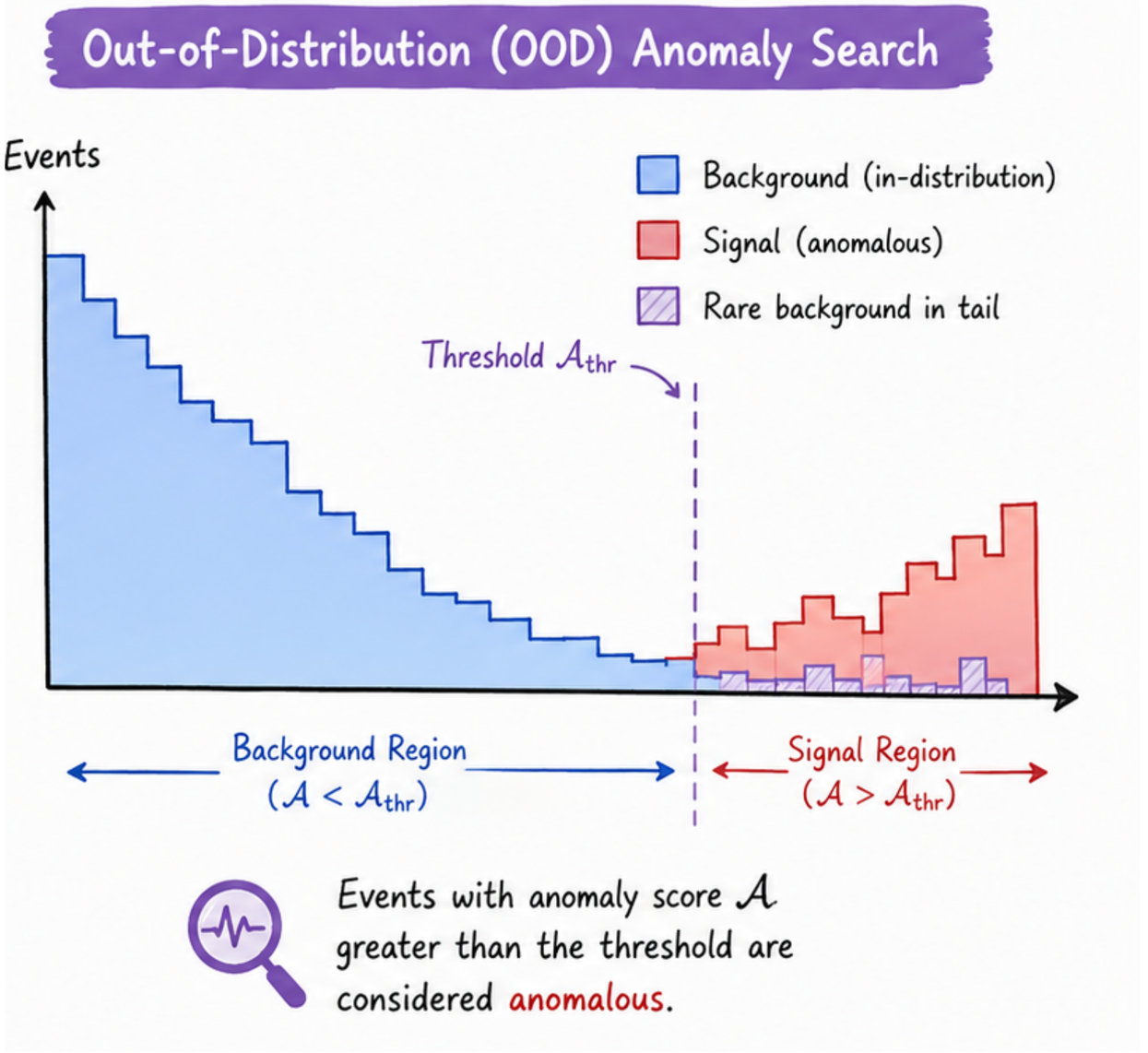
Relevant past works:
→ Kasieczka, Nachman, Schwartz, Shih [2007.14400]
→ Mikuni, Nachman, Shih [2111.06417]

Anomaly searches in HEP

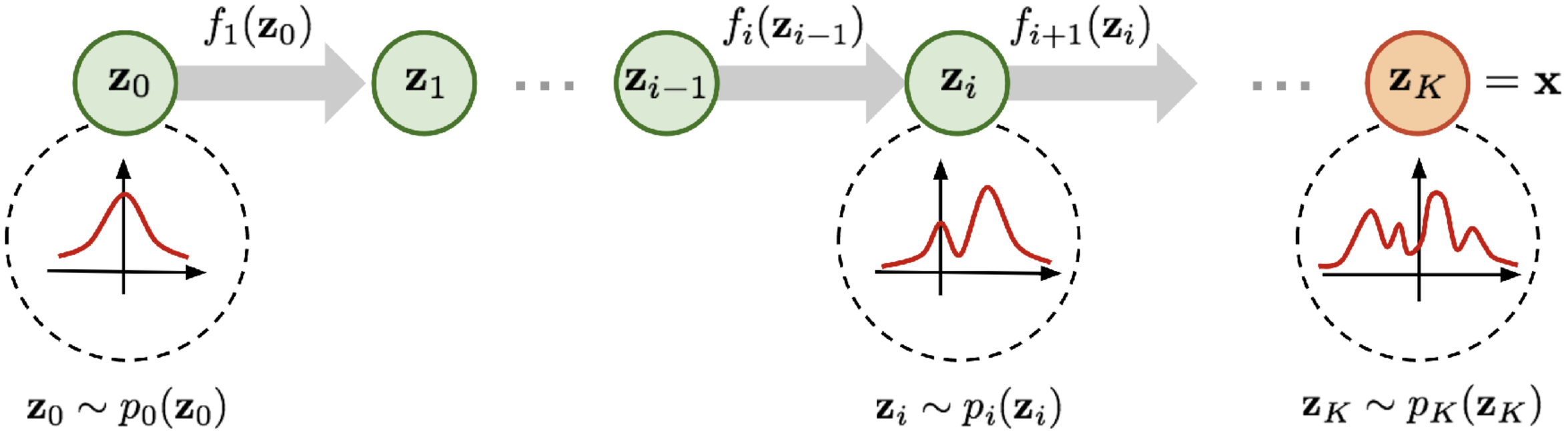
How?

- Construct anomaly score *A*
- Background events have small *A*
- Signal events have large *A*
- Select a threshold: A_{thr}
- Define the signal region as A> A_{thr}

What about background in the signal region?



Normalizing Flows

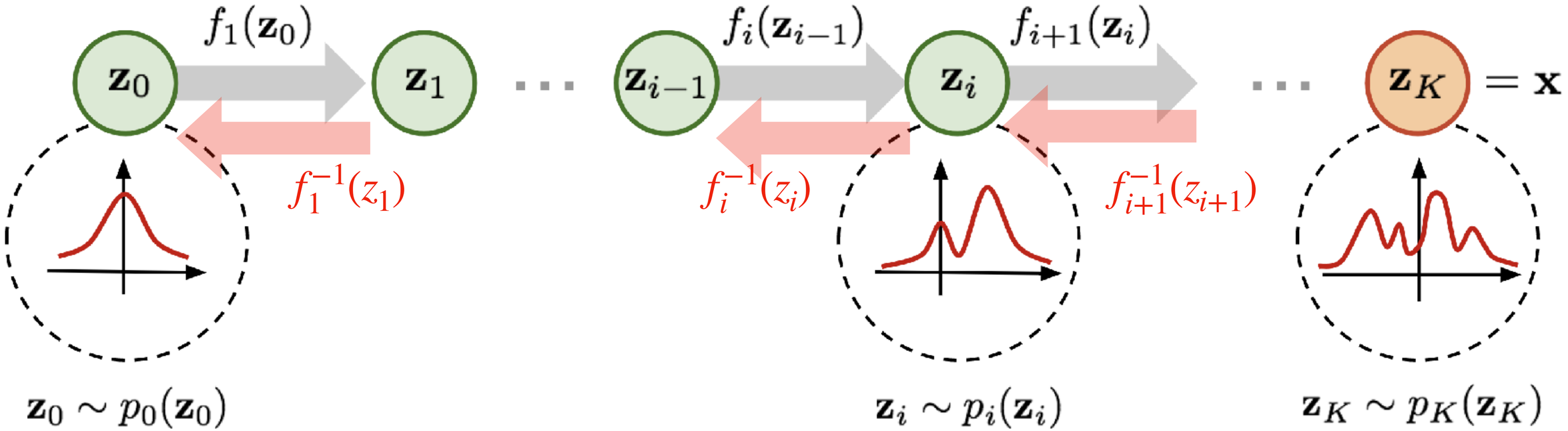


$$x = f_\theta(z_0) = f_K \circ \ldots \circ f_2 \circ f_1(z_0) \qquad \log p_K(x) = \log p_0(z_0) + \sum_{i=1}^{K} \log \left| det \left(\frac{\partial f_{\theta,i}}{\partial z_i} \right) \right|$$

$$\mathscr{L}_\theta = \mathscr{D}_{\mathrm{KL}} \left(p_{\mathrm{data}} || p_\theta \right) = \int p_{\mathrm{data}} \cdot \log \left(\frac{p_{\mathrm{data}}}{p_\theta} \right) dx$$

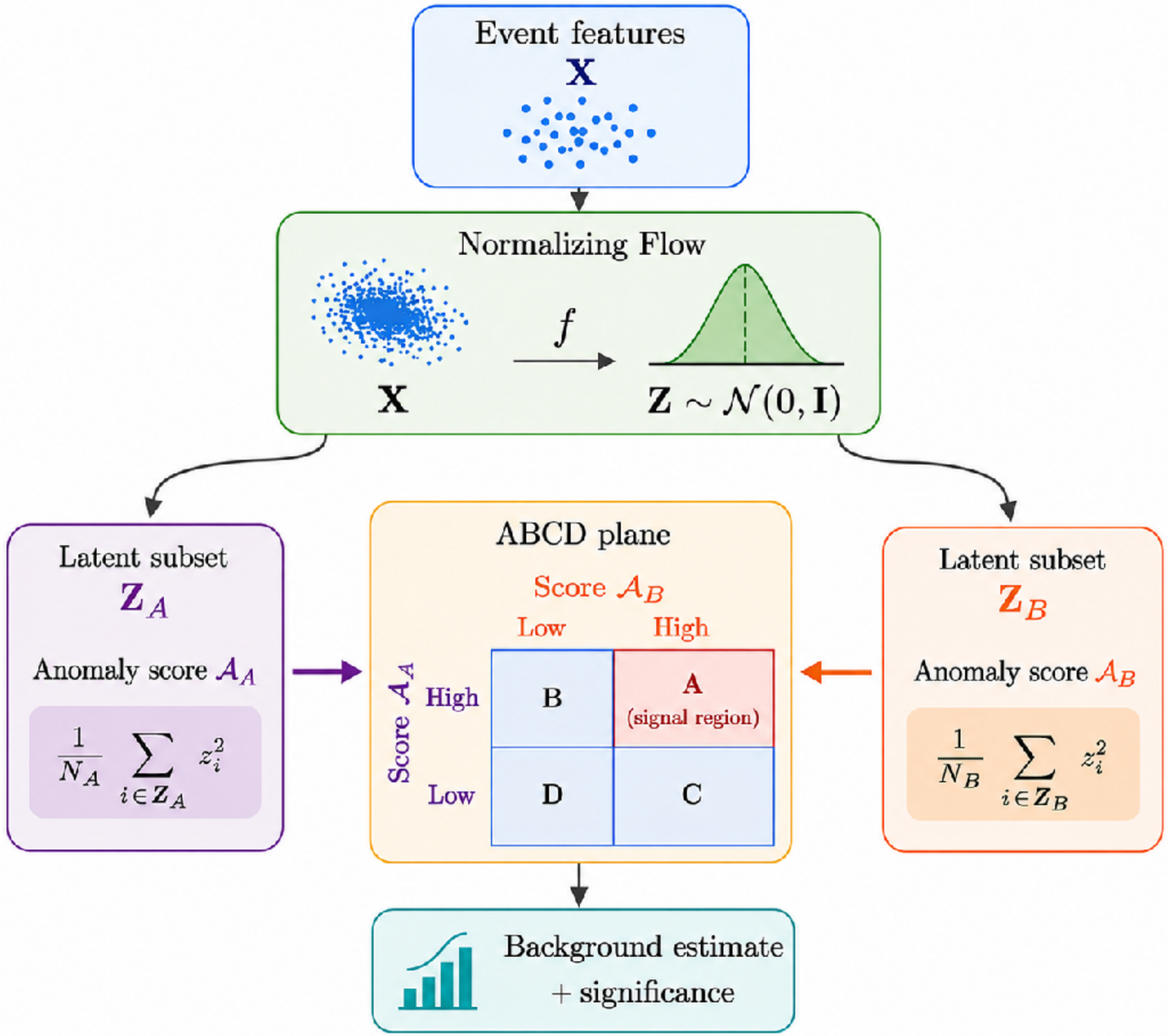
optimize network parameters θ
to minimize KL divergence (nll)

Normalizing Flows



Once we have trained the flow, we can reverse its direction to transform initial correlated variables into new approximately uncorrelated ones.

Overview of the method



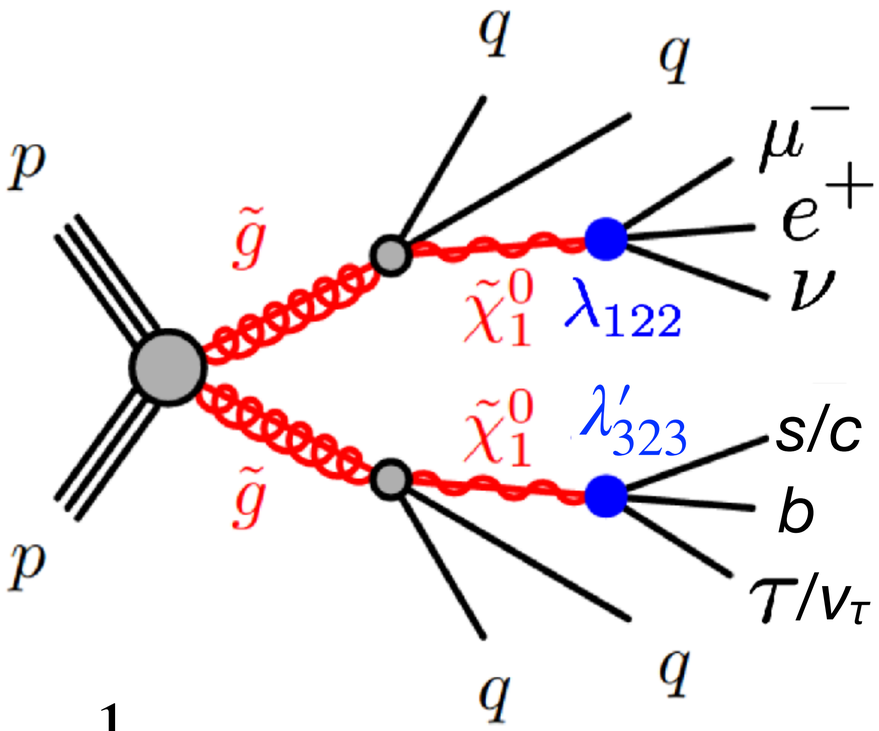


BENCHMARK

Książ Castle, Poland

Benchmark model

signal — RPV SUSY

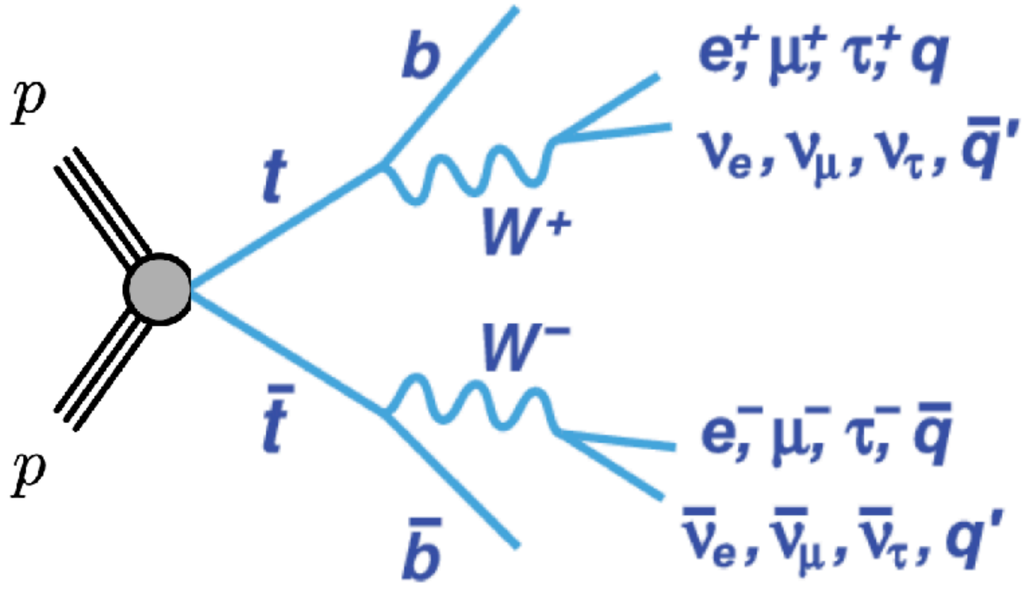


$$\mathscr{L} \ni \frac{1}{2}\lambda^{ijk} L_i L_j \bar{e}_k + \lambda'^{ijk} L_i Q_j \bar{d}_k$$

$$\lambda_{122} \simeq \lambda_{323} \neq 0$$

$$m_{\tilde{g}} = 1.8 \text{ TeV}$$
$$m_{\tilde{\chi}_1^0} = 1.7 \text{ TeV}$$

background — ttbar



Preselection & 16 original variables

Table 1: Data preselection cuts

#	Description
1	$N_{jets} \geq 3$
2	$N_{b-jets} \geq 1$
3	$N_{leptons} = 2$
4	opposite sign leptons
5	$p_T^{j1} > 60$ GeV
6	$p_T^{j2} > 30$ GeV
7	$p_T^{j3} > 30$ GeV
8	$\not{E}_T > 60$ GeV
9	$p_T^{l1} > 120$ GeV
10	$p_T^{l2} > 120$ GeV

#	Name
1	$\log p_T^{j1}$
2	$\log p_T^{j2}$
3	$\log p_T^{j3}$
4	$\log p_T^{l1}$
5	$\log p_T^{l2}$
6	$\log p_T^{miss}$
7	$\log H_T$
8	$\log M_{T2}$
9	$\lvert\eta^{j1}\rvert$
10	$\lvert\eta^{j2}\rvert$
11	$\lvert\eta^{j3}\rvert$
12	$\lvert\eta^{miss}\rvert$
13	$\Delta\phi(j_1, j_2)$
14	$\Delta\phi(l_1, l_2)$
15	$T_\perp$
16	S_T

L=3/ab

S = 432 S/B = 0.5%

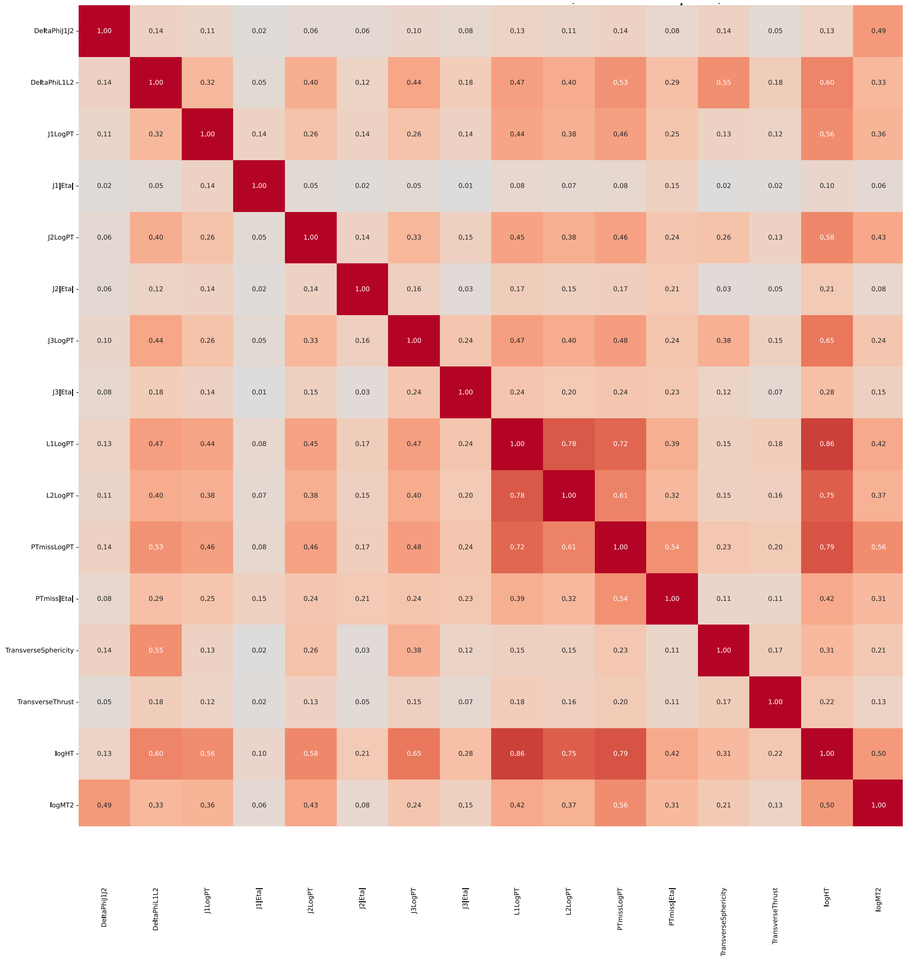
B = 80100 S/√B = 1.5



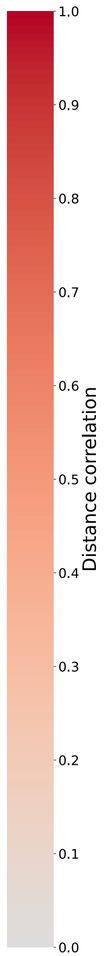
RESULTS
(semi-supervised)

Lublin Castle, Poland

Decorrelation in practice



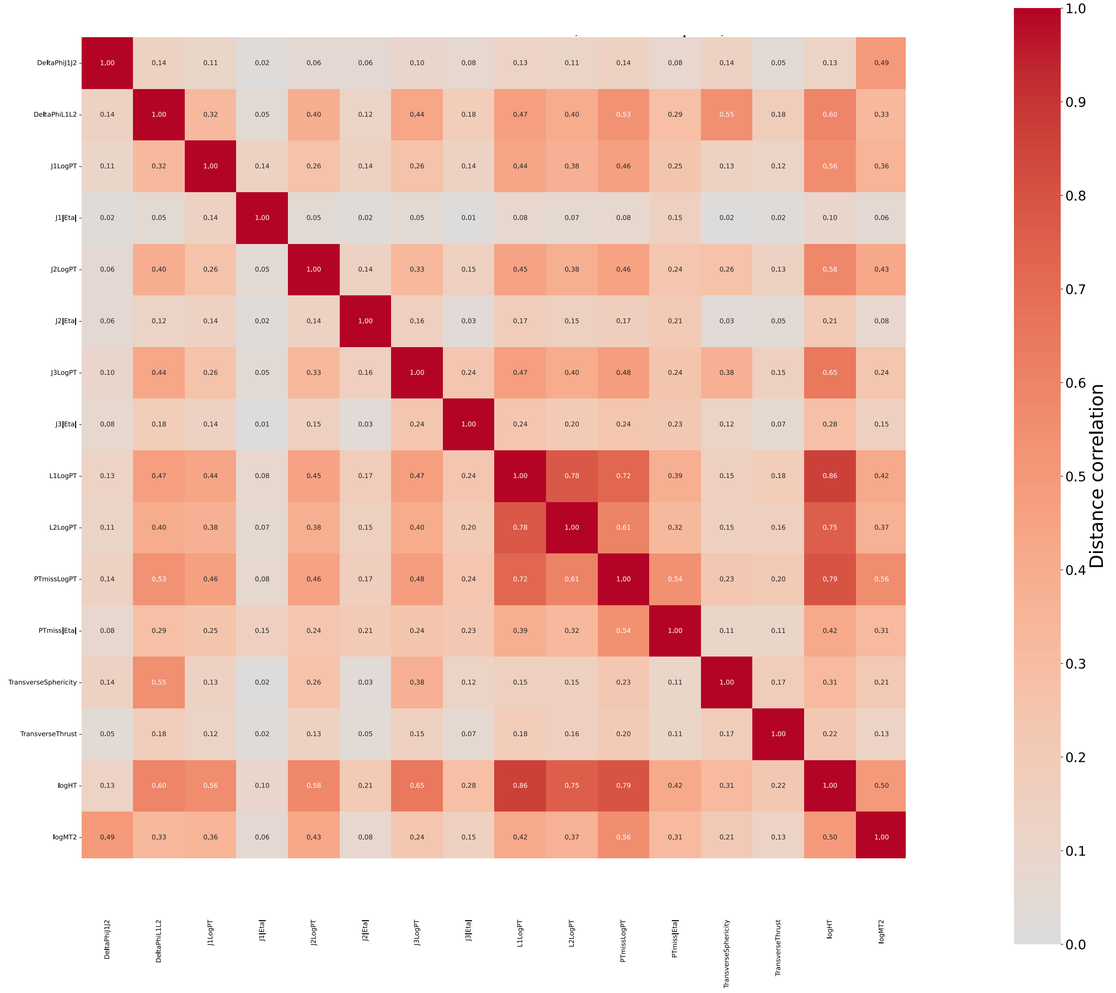
16 highly correlated variables



Fully correlated

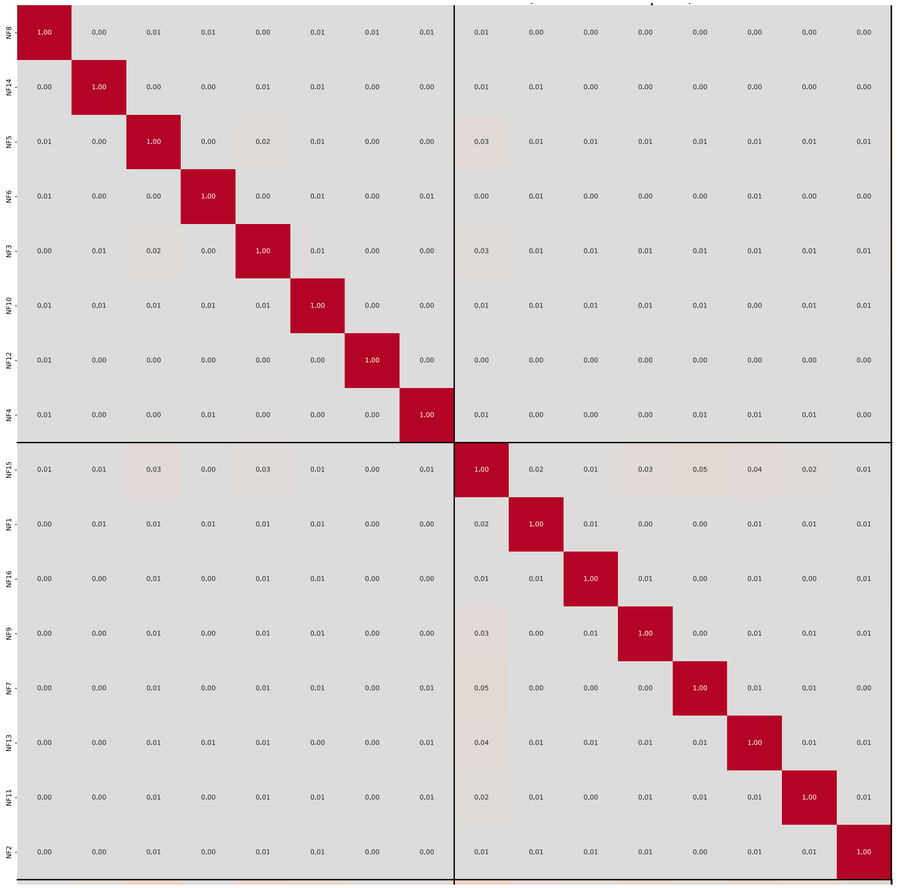
Uncorrelated

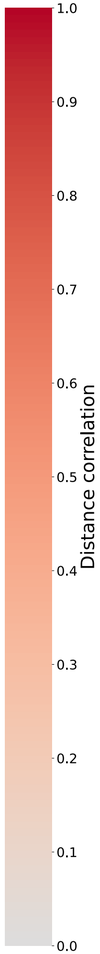
Decorrelation in practice



16 highly correlated variables

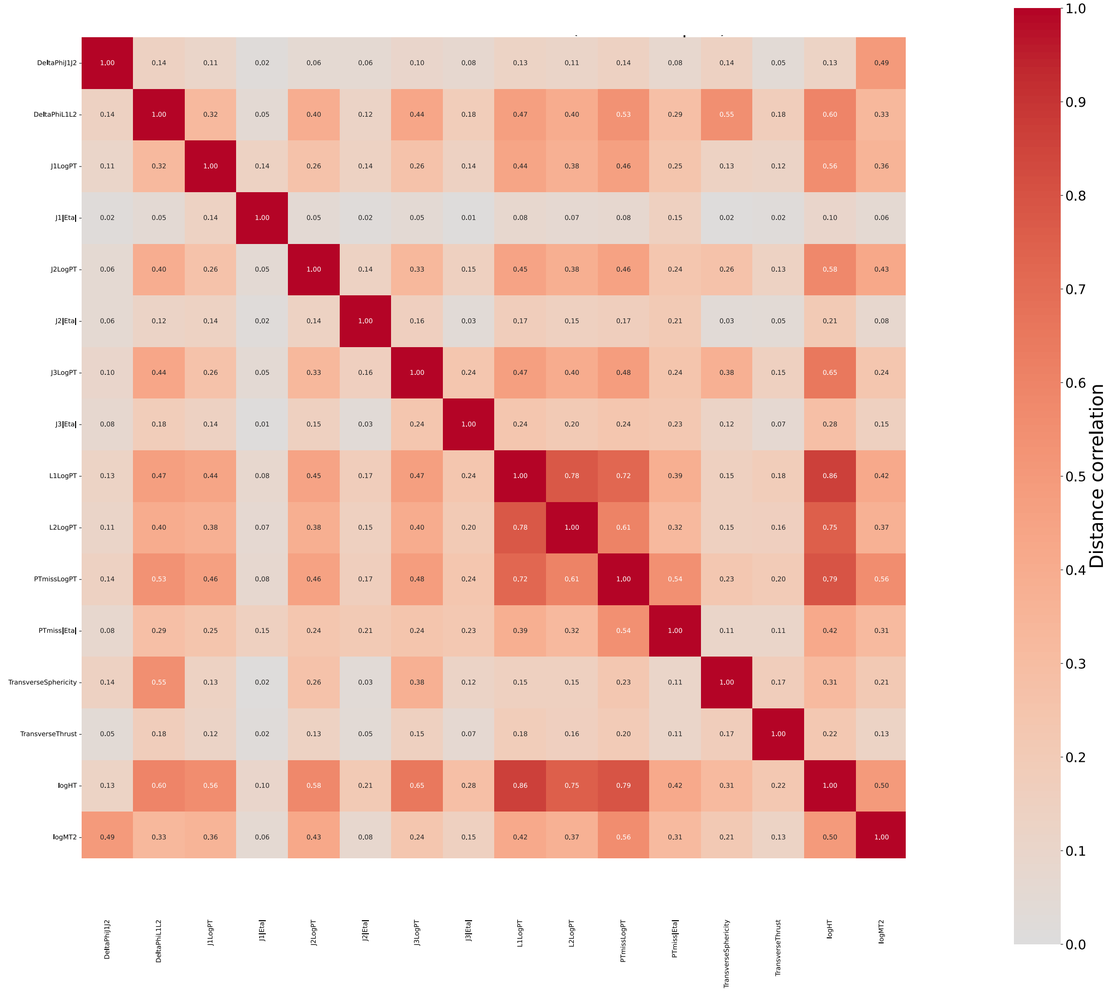
decorrelation



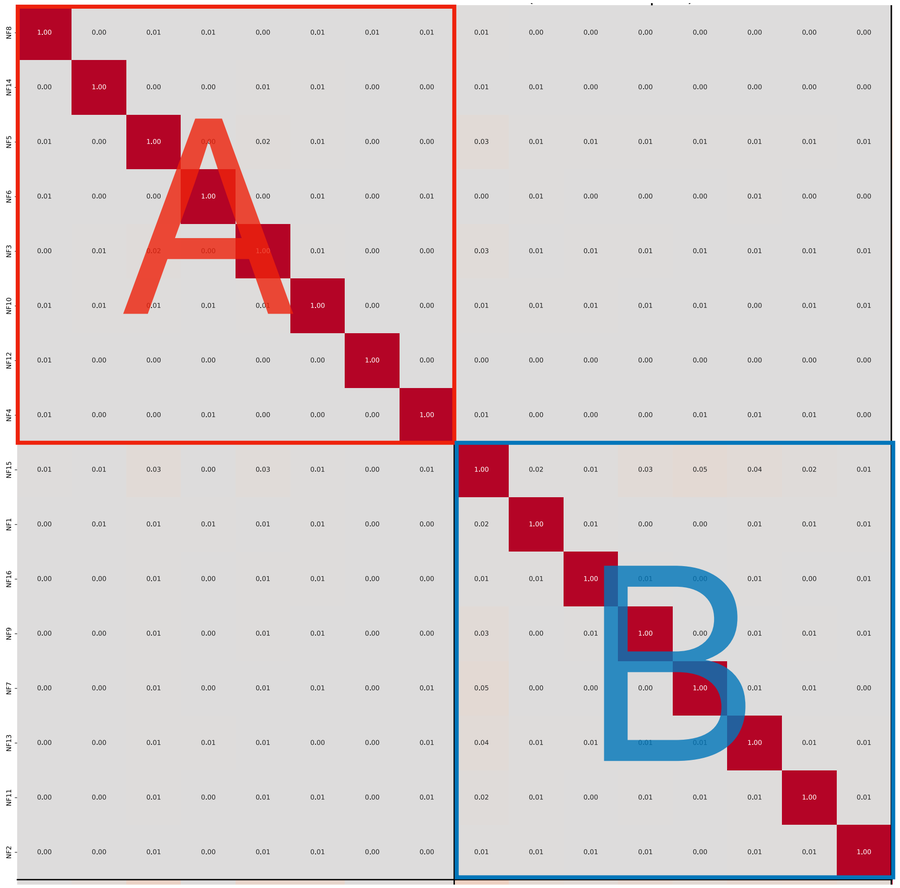


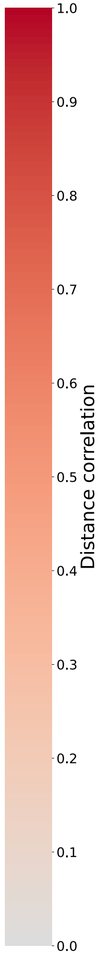
16 highly largely uncorrelated variables split into two subsets

Decorrelation in practice



decorrelation

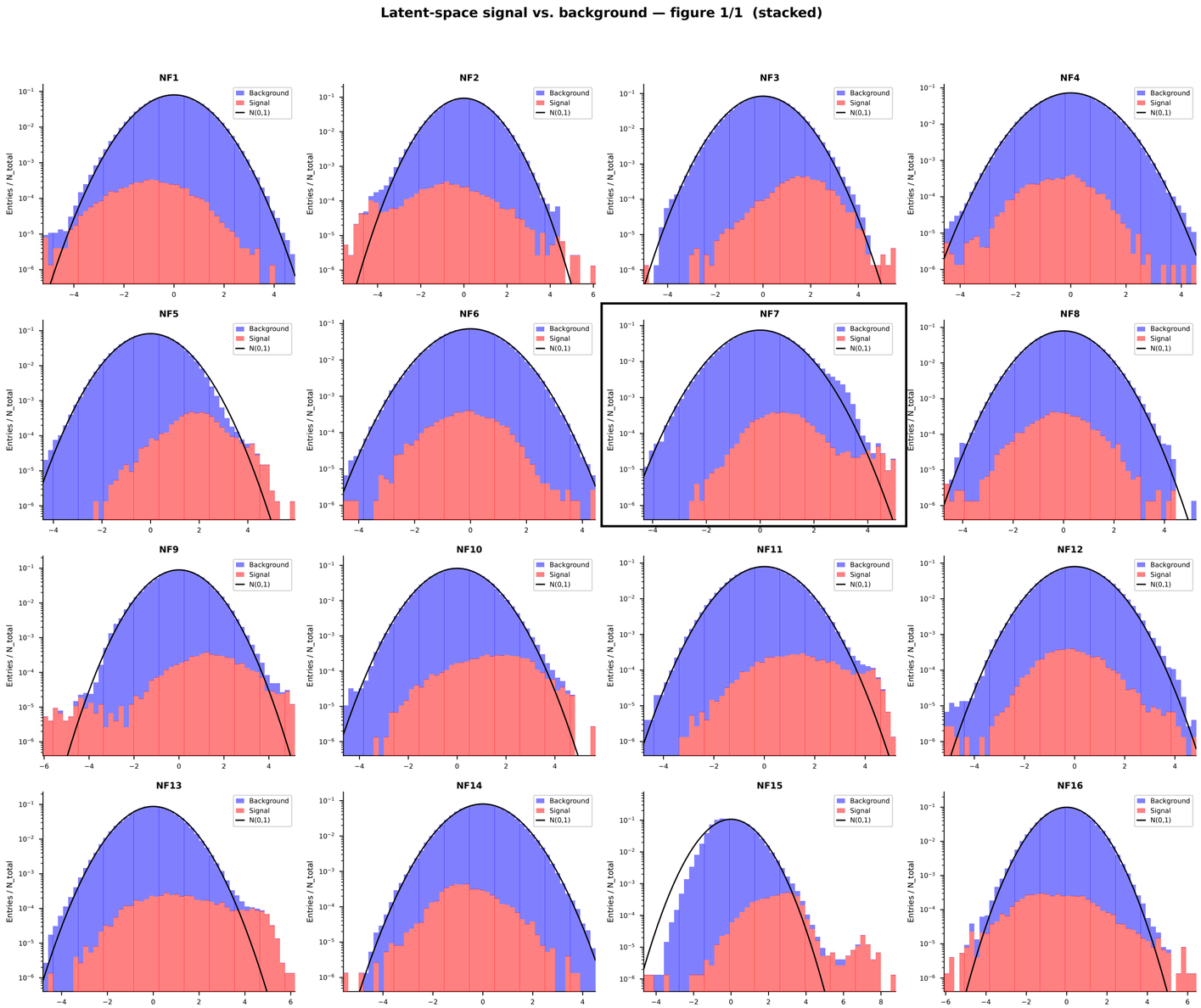


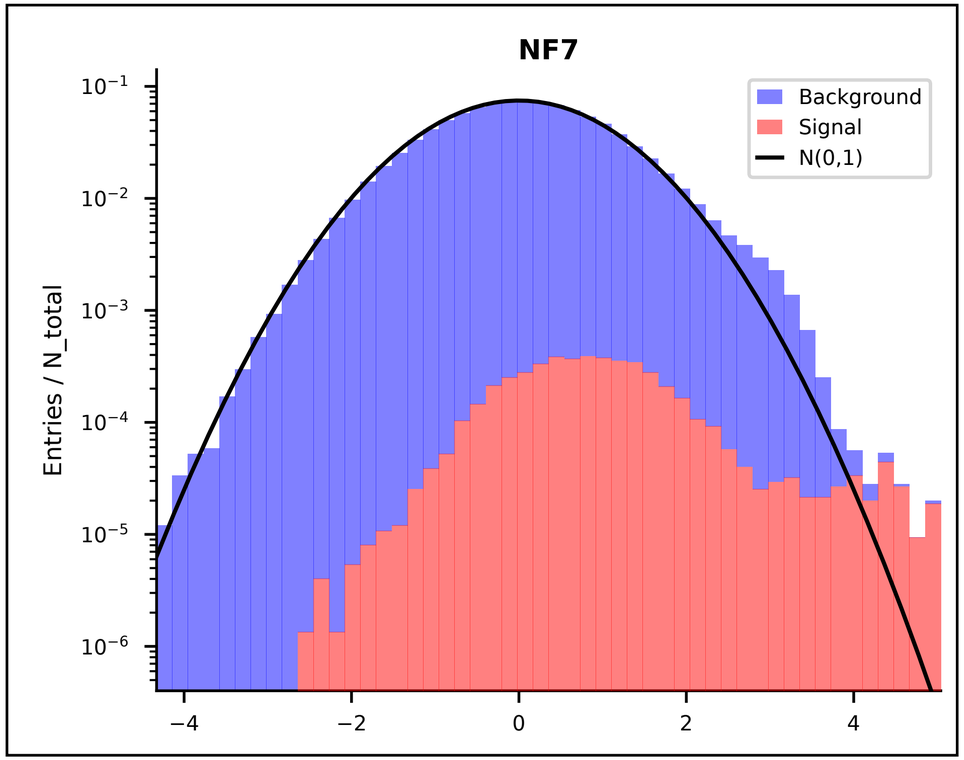


16 highly correlated variables

16 highly largely uncorrelated variables split into two subsets

Latent representation — semisupervised

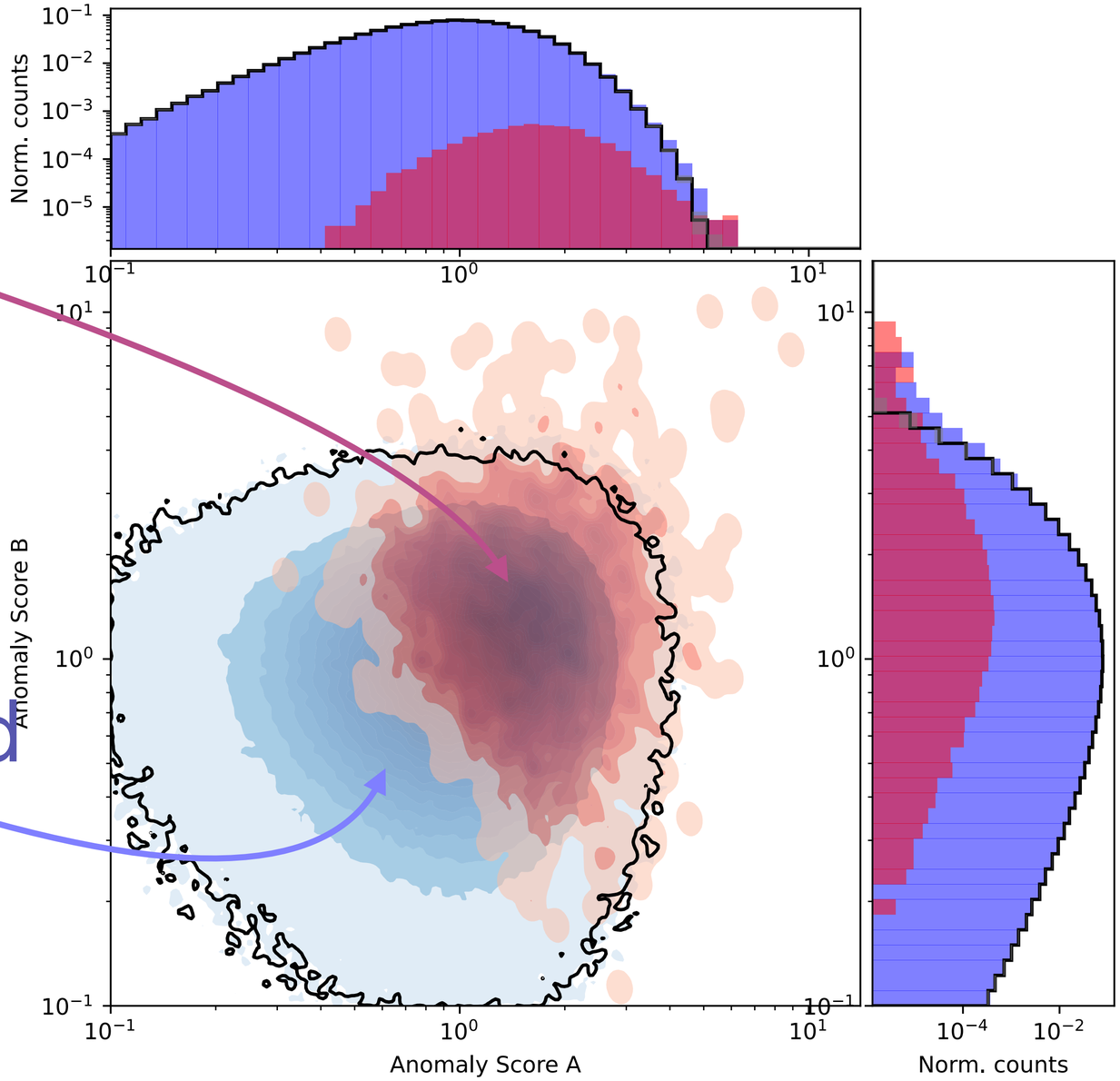




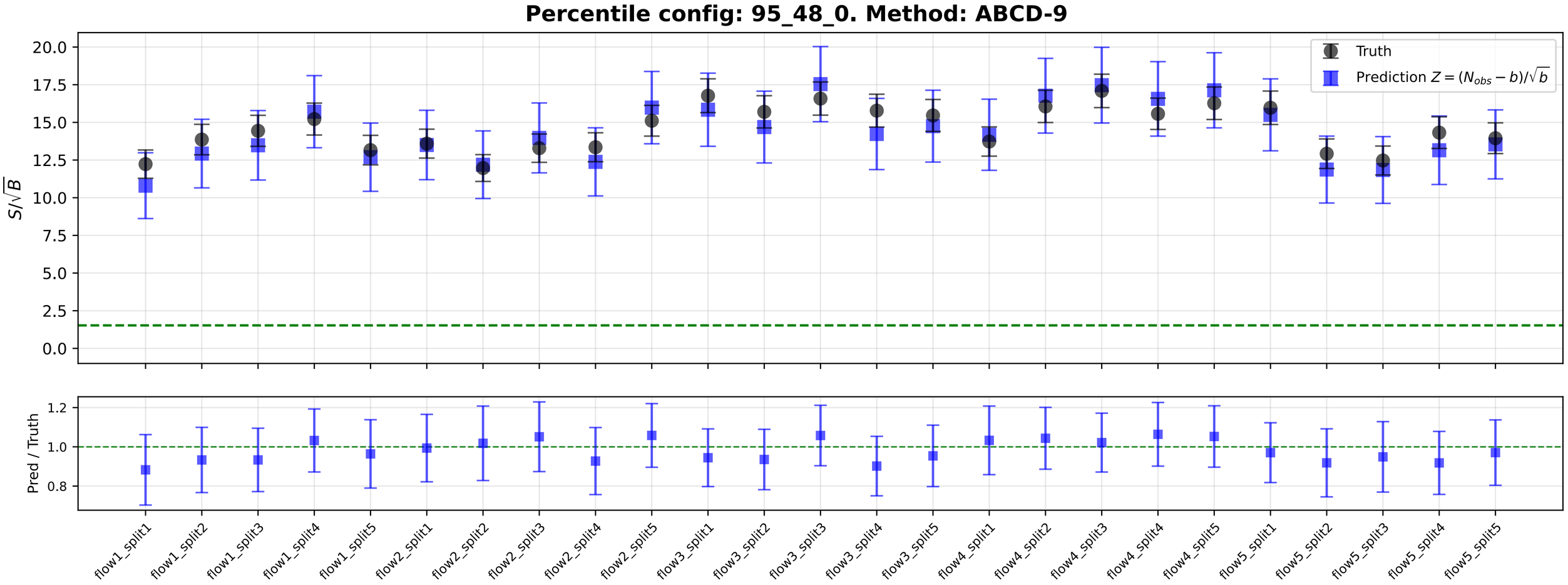
Anomaly score distribution

BSM signal

SM background



S/√B closure

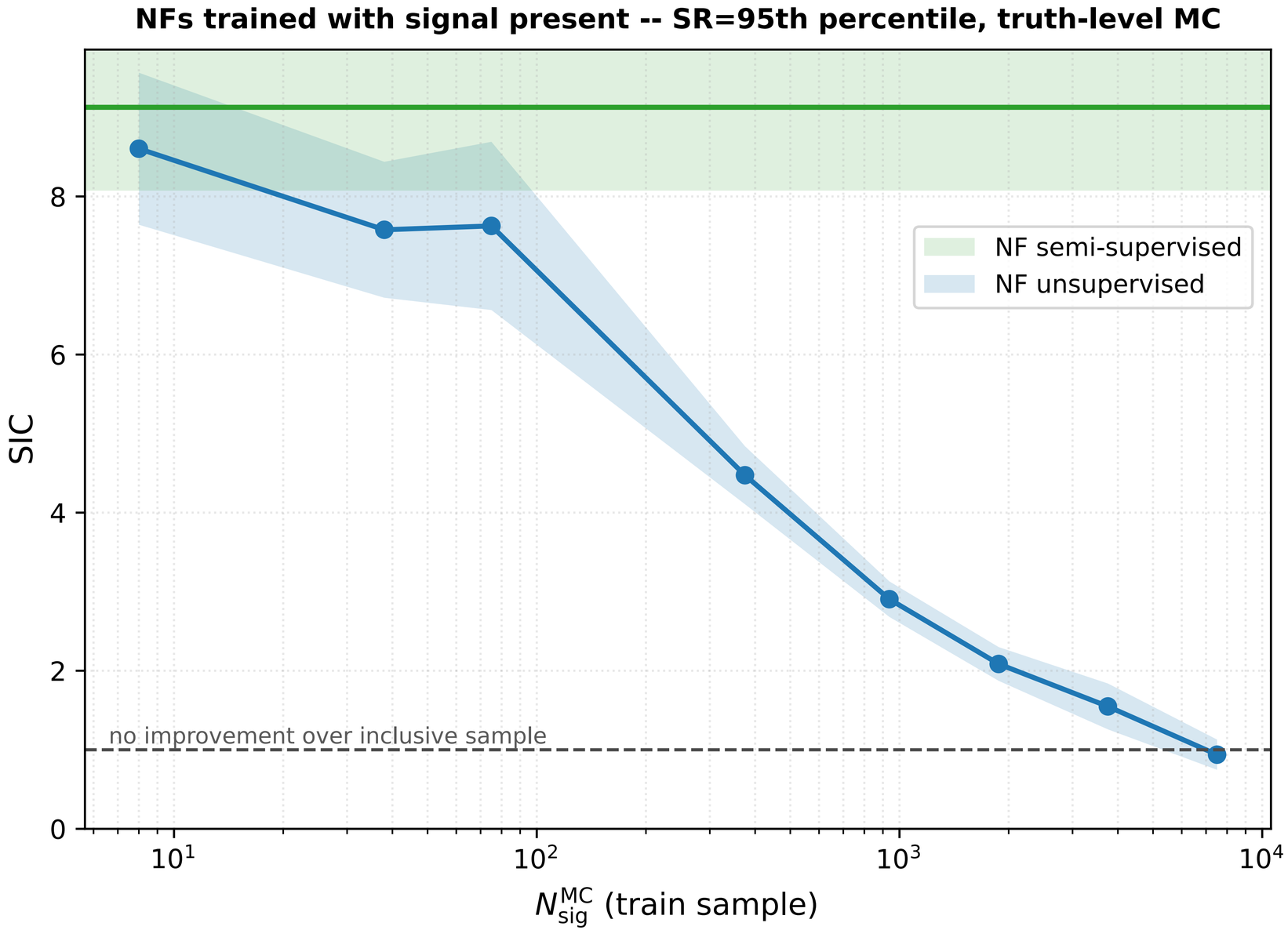

Percentile config: 95_48_0. Method: ABCD-9
Truth
Prediction $Z = (N_{obs} - b)/\sqrt{b}$
$S/\sqrt{B}$
Pred / Truth
flow1_split1
flow1_split2
flow1_split3
flow1_split4
flow1_split5
flow2_split1
flow2_split2
flow2_split3
flow2_split4
flow2_split5
flow3_split1
flow3_split2
flow3_split3
flow3_split4
flow3_split5
flow4_split1
flow4_split2
flow4_split3
flow4_split4
flow4_split5
flow5_split1
flow5_split2
flow5_split3
flow5_split4
flow5_split5



TOWARDS UNSUPERVISED

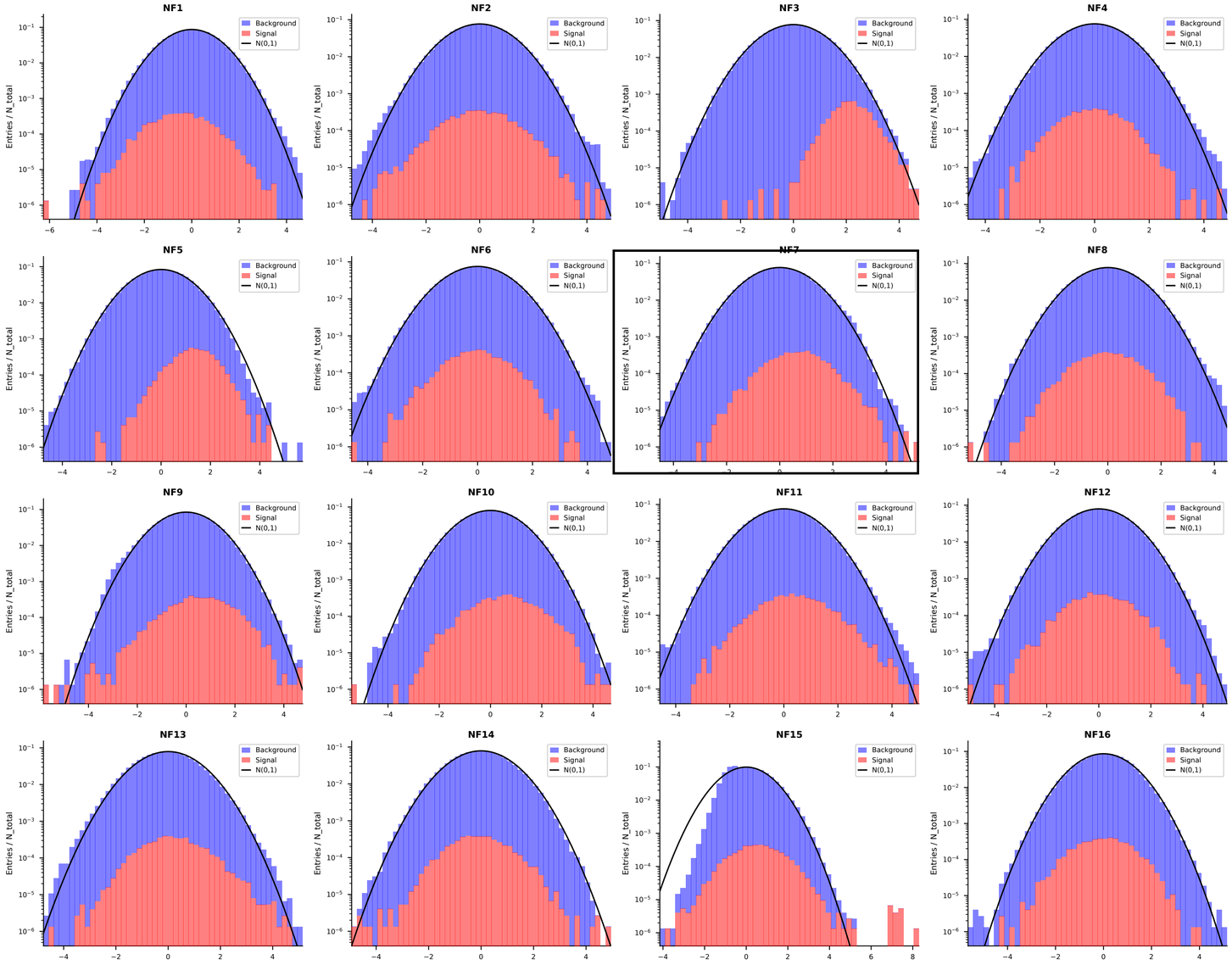
Marlbork Castle, Poland

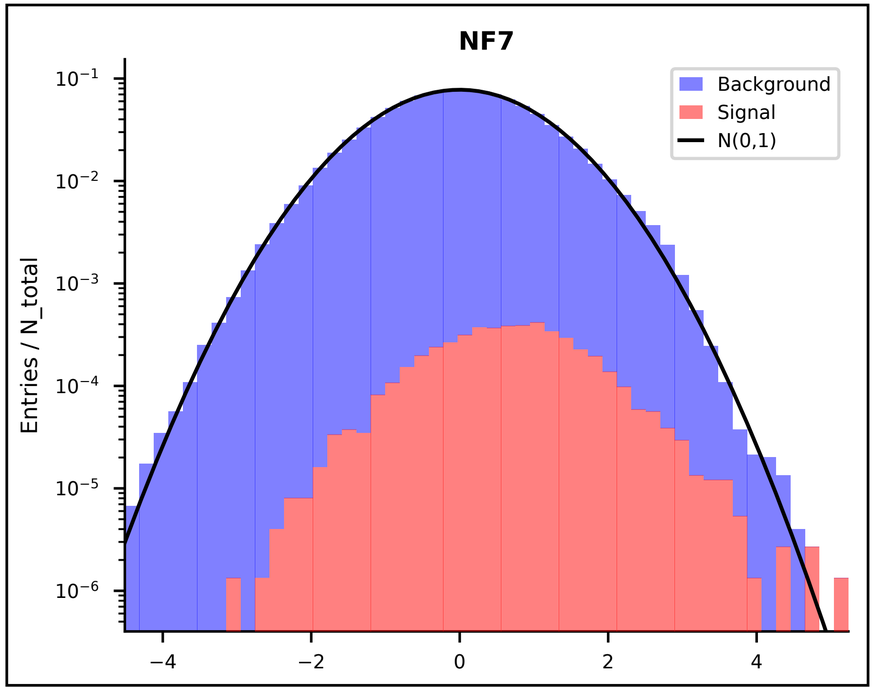
Significance improvement for unsupervised training



Latent representation — unsupervised

Latent-space signal vs. background — figure 1/1 (stacked)



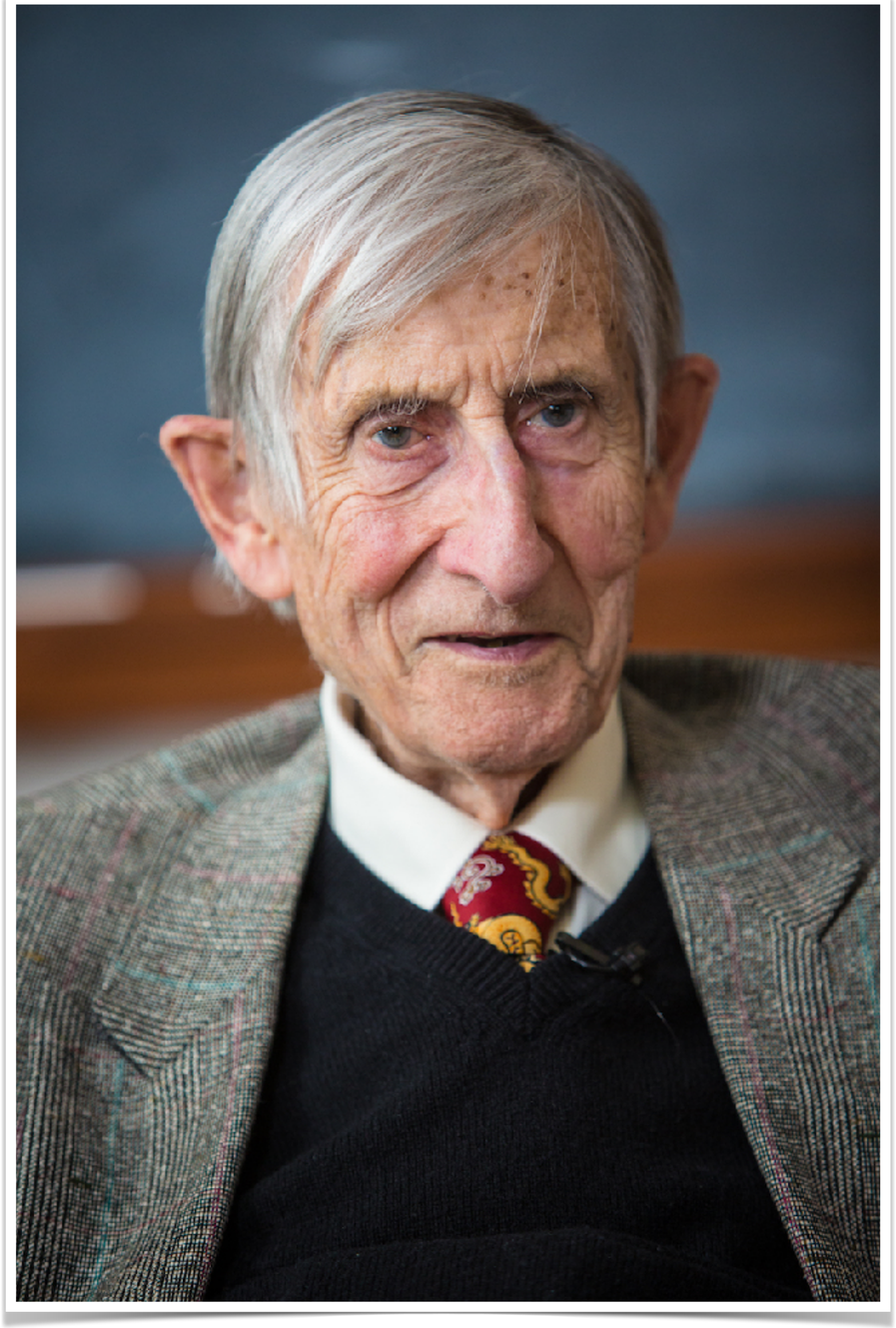


Summary

- Machine learning is enhancing various areas of particle physics
- Out-of-distribution anomaly detection methods allow for model-agnostic searches for BSM physics, but they are challenging:
  - How to construct a good anomaly score?
  - How to estimate the background in the SR?
- We propose combining NFs with the ABCD matrix method:
  - NF creates a new data representation with uncorrelated features
  - Anomaly scores are approximately uncorrelated
- The method **works very well** for semi-supervised training (NF trained on background-only data)
- For fully unsupervised training, the sensitivity drops when signal increases → opposite behaviour to weakly-supervised methods
- **The paper is going to be out soon!**

"Scientific revolutions are more often driven by new tools than by new concepts."

Freeman Dyson





Thank you for attention!

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BACKUP

Rafał Masełek

Particle Physics and Cosmology Seminar 05-11-2026

This project has received the funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 101081355. The operation (SMASH project) is co-funded by the Republic of Slovenia and the European Union from the European Regional Development Fund.

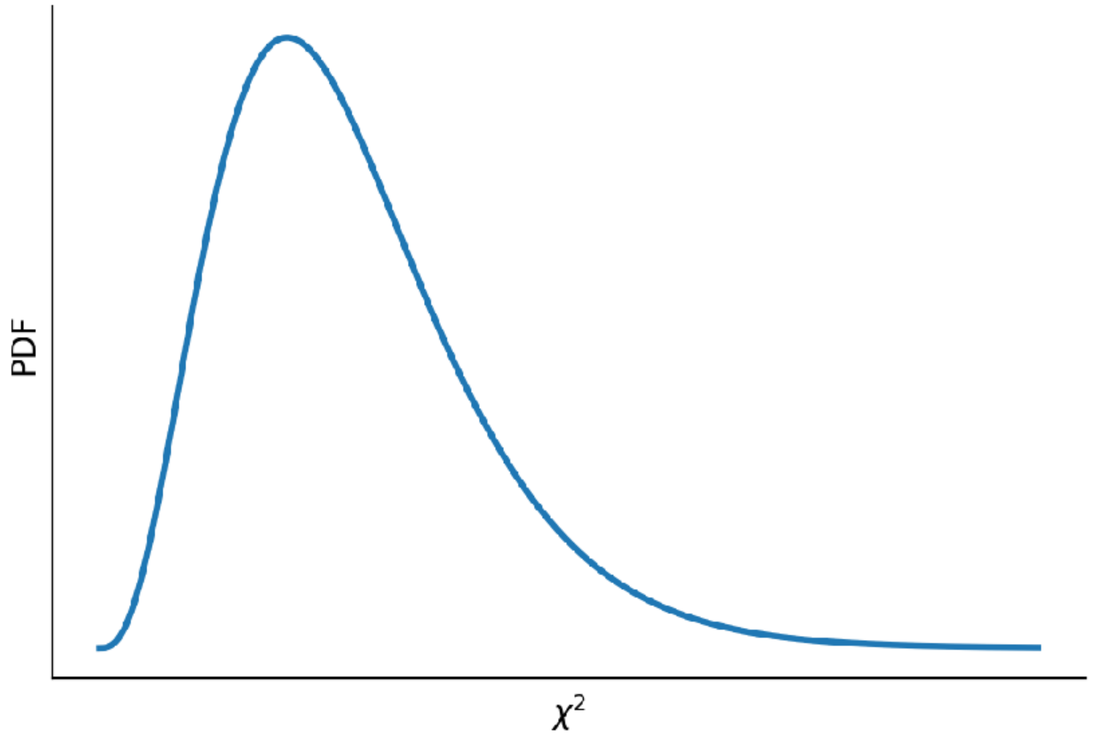
Anomaly score

anomaly scores

$$\mathscr{A}_A = \frac{1}{N_A} \sum_{z_i \in A} z_i^2$$ ← latent variables

$$\mathscr{A}_B = \frac{1}{N_B} \sum_{z_i \in B} z_i^2$$

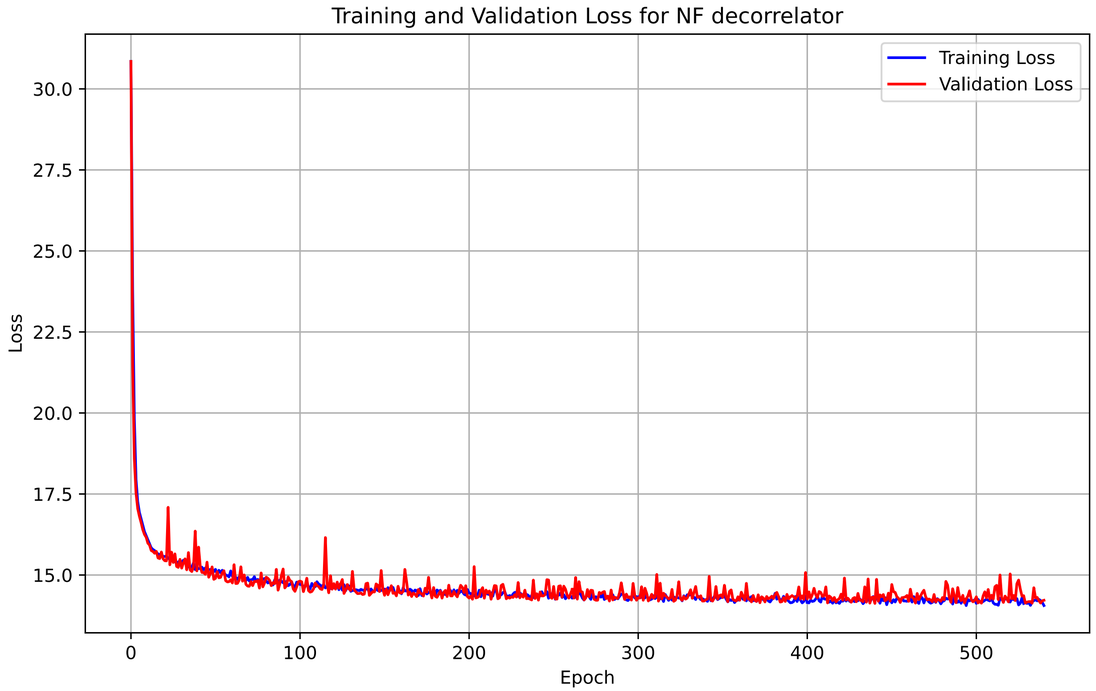
$$\mathscr{A} = \frac{1}{N} \sum_{i=1}^{N} z_i^2 = -\frac{2}{N} \log N(0,\mathrm{I}) - \log(2\pi)$$



$$\forall_{i,j} \left(z_i \sim N(0,1)\right) \wedge \left(z_i \perp\!\!\!\perp z_j\right) \implies \mathscr{A}_{A/B} \sim \chi^2(N_A/N_B) \wedge \left(\mathscr{A}_A \perp\!\!\!\perp \mathscr{A}_B\right)$$

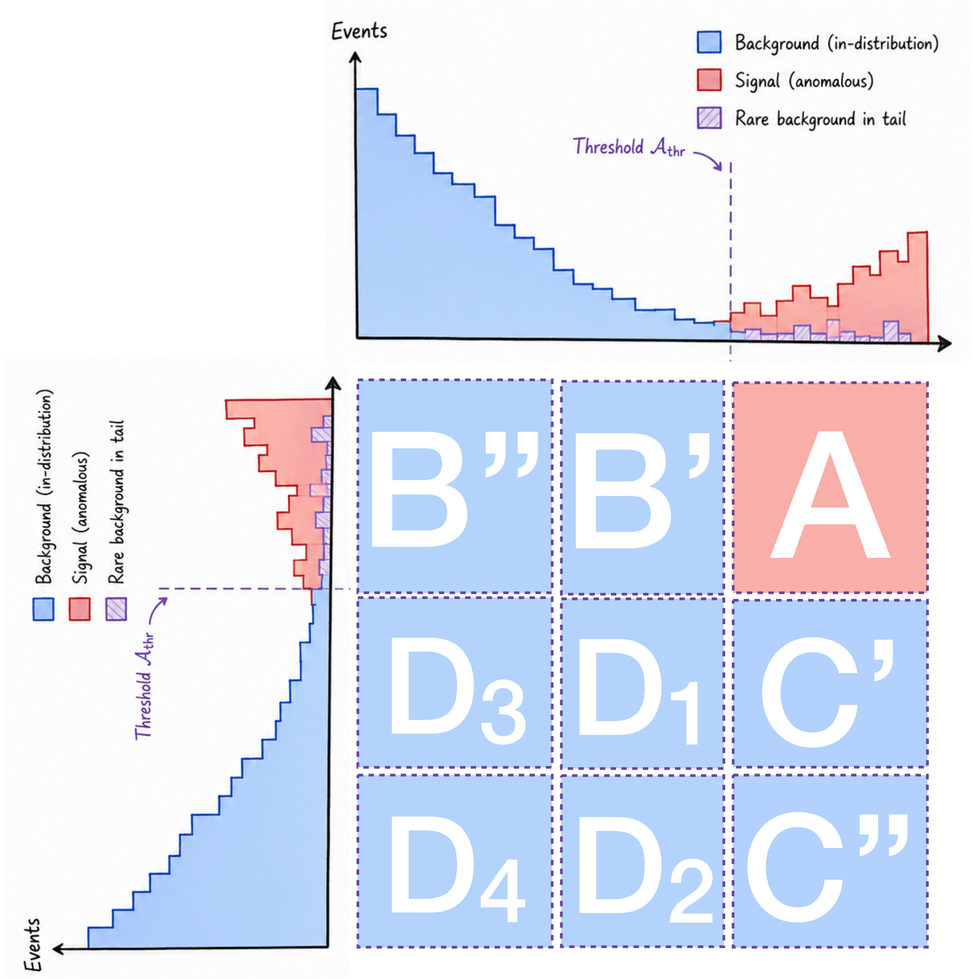
Training strategy

- The dataset consists of ~3M events.
- We randomly split the data 50-25-25 (train-val-test)
- We train a normalising flow on background-only data
- We randomly split the latent variables into two subsets and construct anomaly scores A and B
- We evaluate on background + BSM signal
- We repeat for 5×5 times



Extended ABCD matrix method

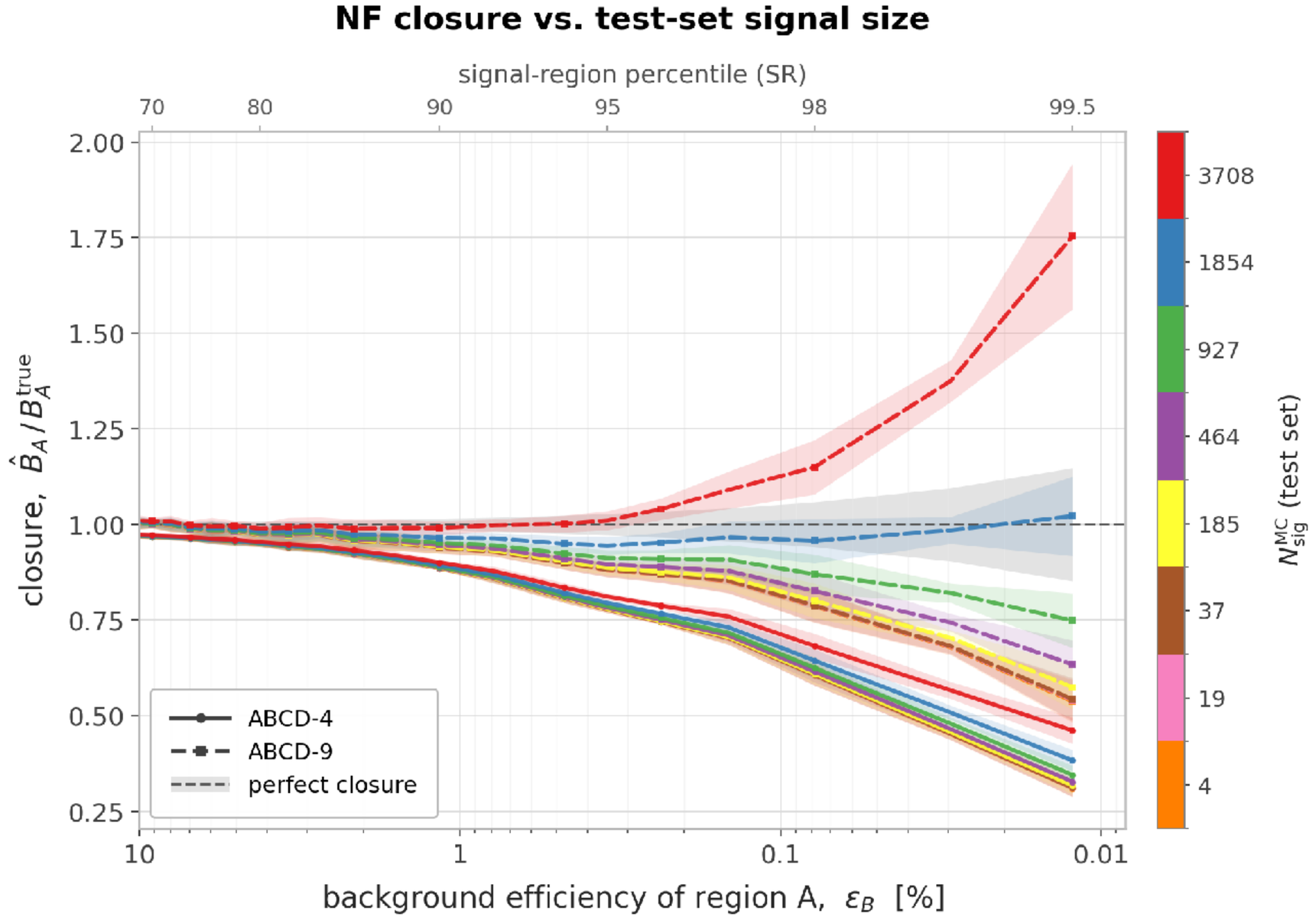
Established method for data-driven background estimation



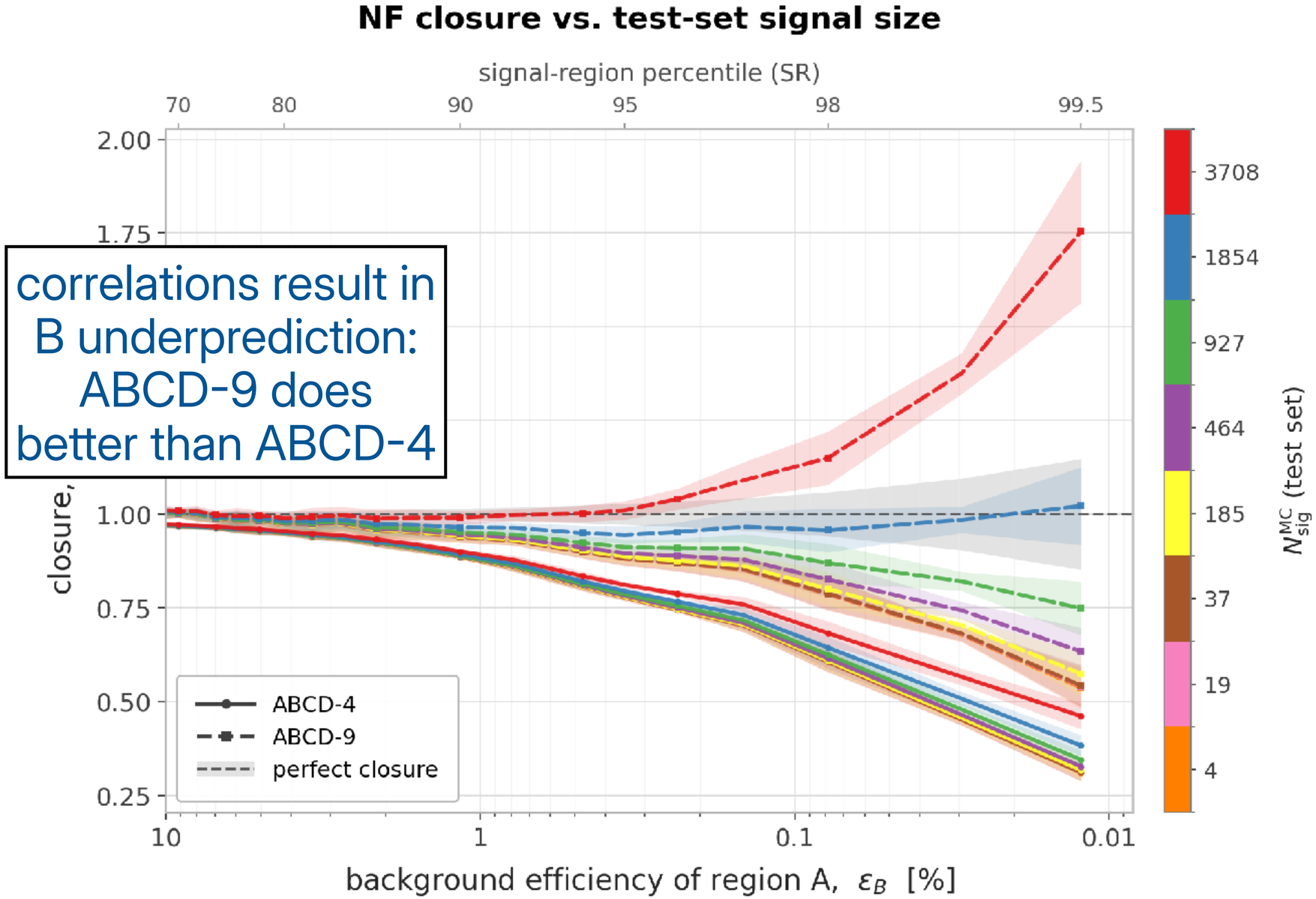
$$N_A^{\text{bkg}} = \frac{\left(N_{B'}^{\text{bkg}} N_{C'}^{\text{bkg}} N_{D_2}^{\text{bkg}} N_{D_3}^{\text{bkg}}\right)^2}{N_{B''}^{\text{bkg}} N_{C''}^{\text{bkg}} N_{D_4}^{\text{bkg}} \left(N_{D_1}^{\text{bkg}}\right)^4}$$

Both anomaly scores have to be independent!

Selecting the threshold



Selecting the threshold



correlations result in B underprediction: ABCD-9 does better than ABCD-4

Selecting the threshold

