

MLEG

Status and plans

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MC4EIC
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Outline

Event generators in modern particle physics

Machine learning event generators:
Goals and methods
GAN

Electron-proton scattering:
FAT conditional GAN
Unfolding
Training on data

Horizon

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Event generators in modern particle physics

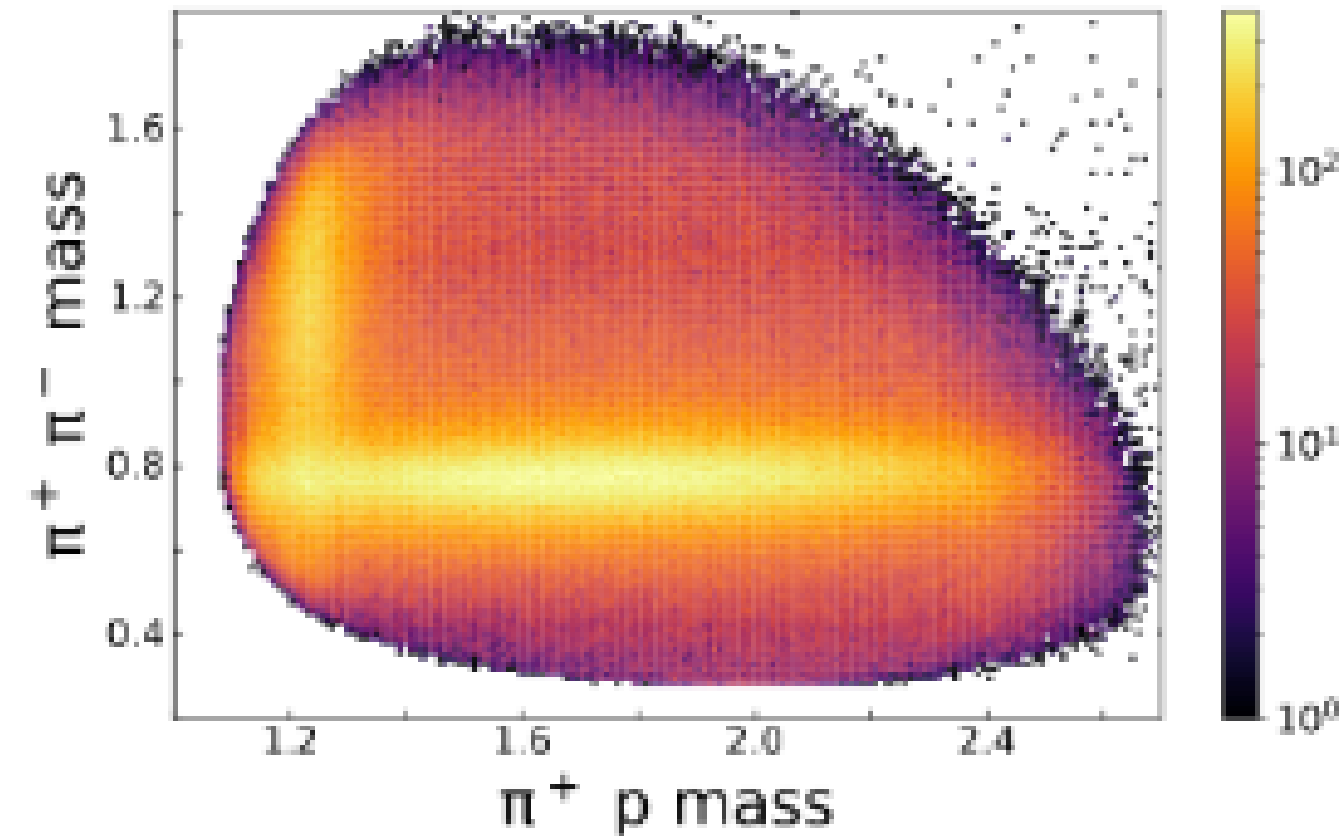
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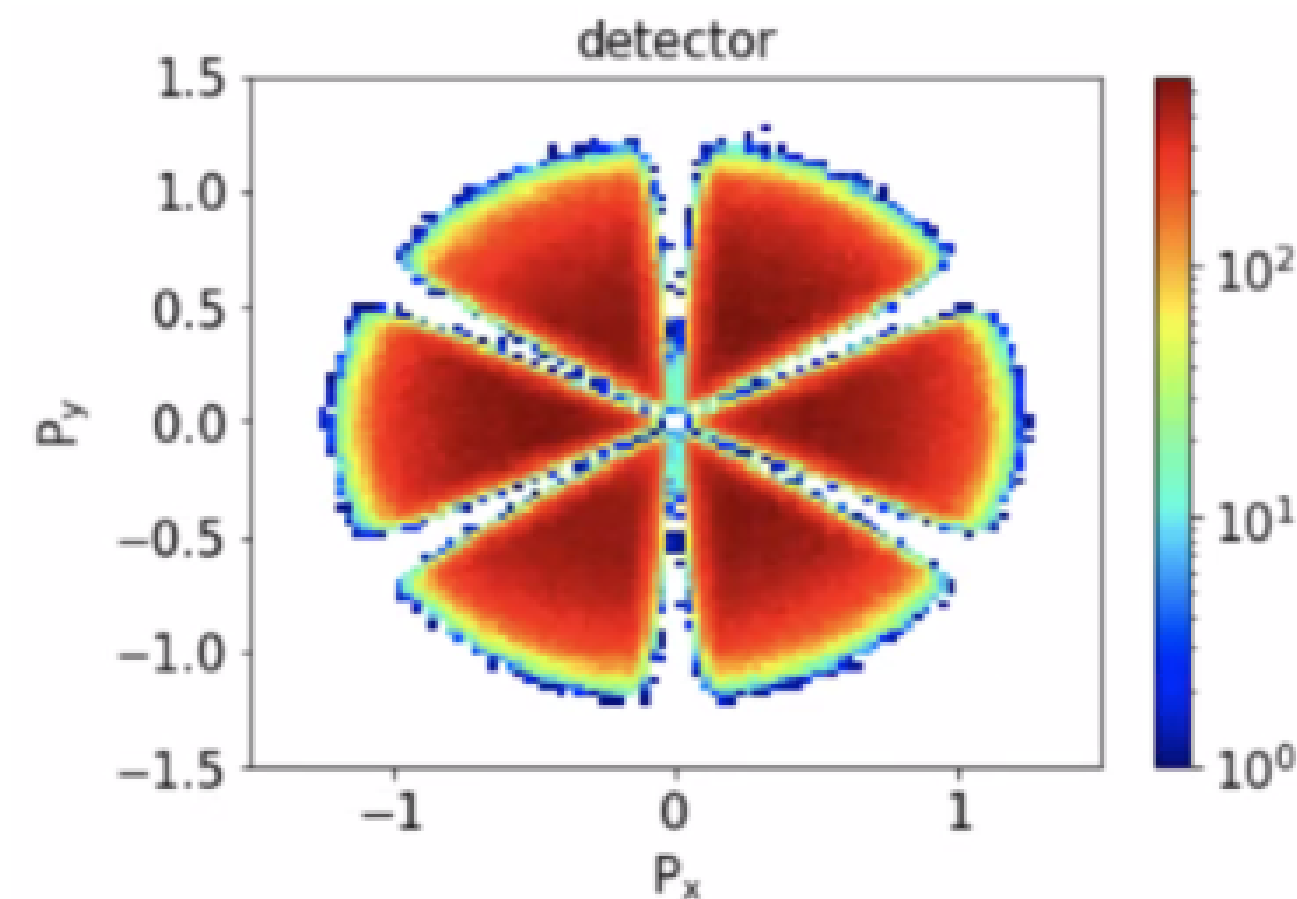
Challenges of modern particle experiments

Physics: high kinematic dimensionality, correlations lost in integration, multi-particle final states, resonance peaks.



Experimental apparatus: energy losses, decays, new particle production, multiple rescattering.

Detectors: limited acceptance, resolution, particle misidentification.



Simulations for experimental preparation and data analysis are indispensable.

Monte Carlo Event Generators (MCEG)

MCEG have been crucial to our physics knowledge to date.

They combine **high-precision experimental data** and the principles of **fundamental theory**, perturbative QCD.

The evolution towards the hadronic regime is well described with **factorization and hadronization phenomenology**.

Detector simulators are included to allow for direct experimental simulation.

Some caveats:

- event generation **can be slow** and once generated leads to **large data repositories**;
- phenomenology inputs introduce bias;
- limited physics scope: e.g. spin asymmetries in deep inelastic scattering have not yet been achieved;
- inverting the Markov chain can be done statistically, but with approximations in practice.

Bellagente et al., SciPost Phys. 8 (2020) 070

Machine Learning Event Generators (MLEG)

MLEG are a strong **complementary** tool for experimental simulation.

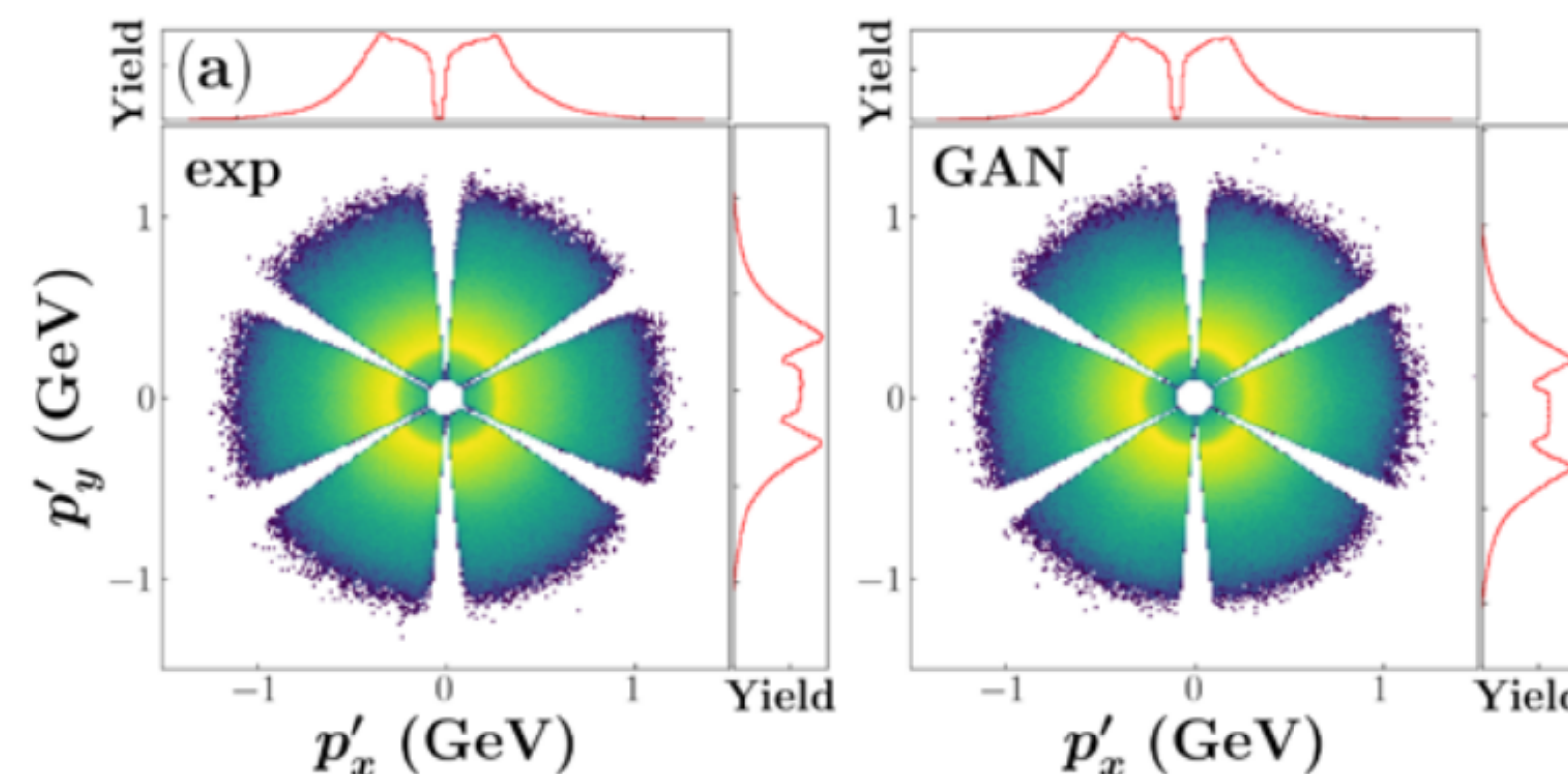
EIC Yellow Report: Abdul Khalek et al., Nucl. Phys. A 1026 (2022) 12247

When trained on MCEG data, they serve as compact and fast generators:
after training, the ML file of only a few MB can faithfully generate millions of events per second.

Advantages for data distribution and storage.

Alanazi et al., IJCAI 2021, Survey Track, 4286; 2106.00643 [hep-ph]

When trained on experimental data, one can extract physics with **minimum bias**
and approaches to **unfold vertex-level physics from detector-level events** are underway.



**For the first time in the history of particle experiments,
we are in the unique position to incorporate ML tools from the beginning of experimental design.**

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The fitting procedure

Machine learning is ultimately a fitting procedure, which is very powerful in high-dimensional space.

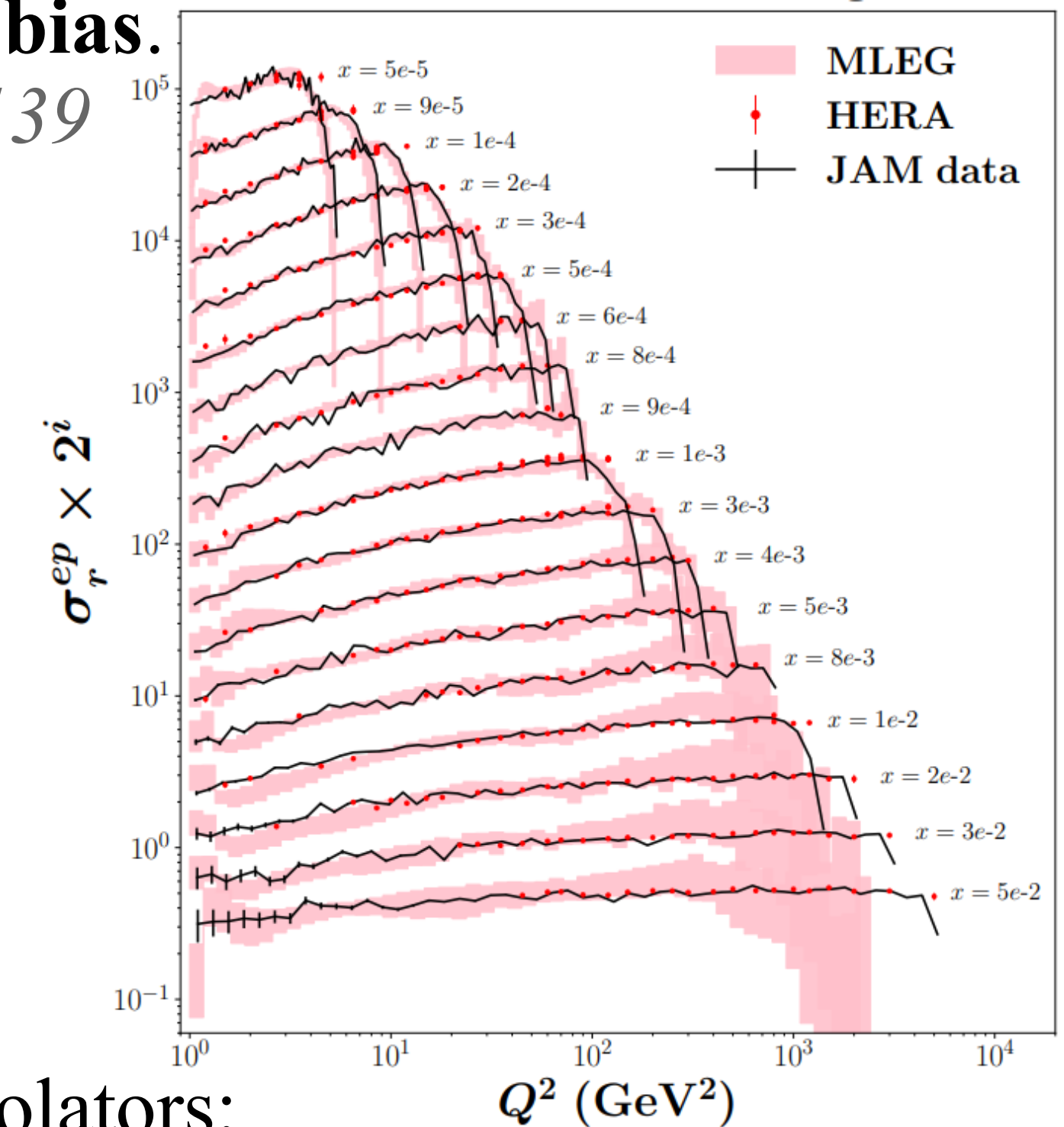
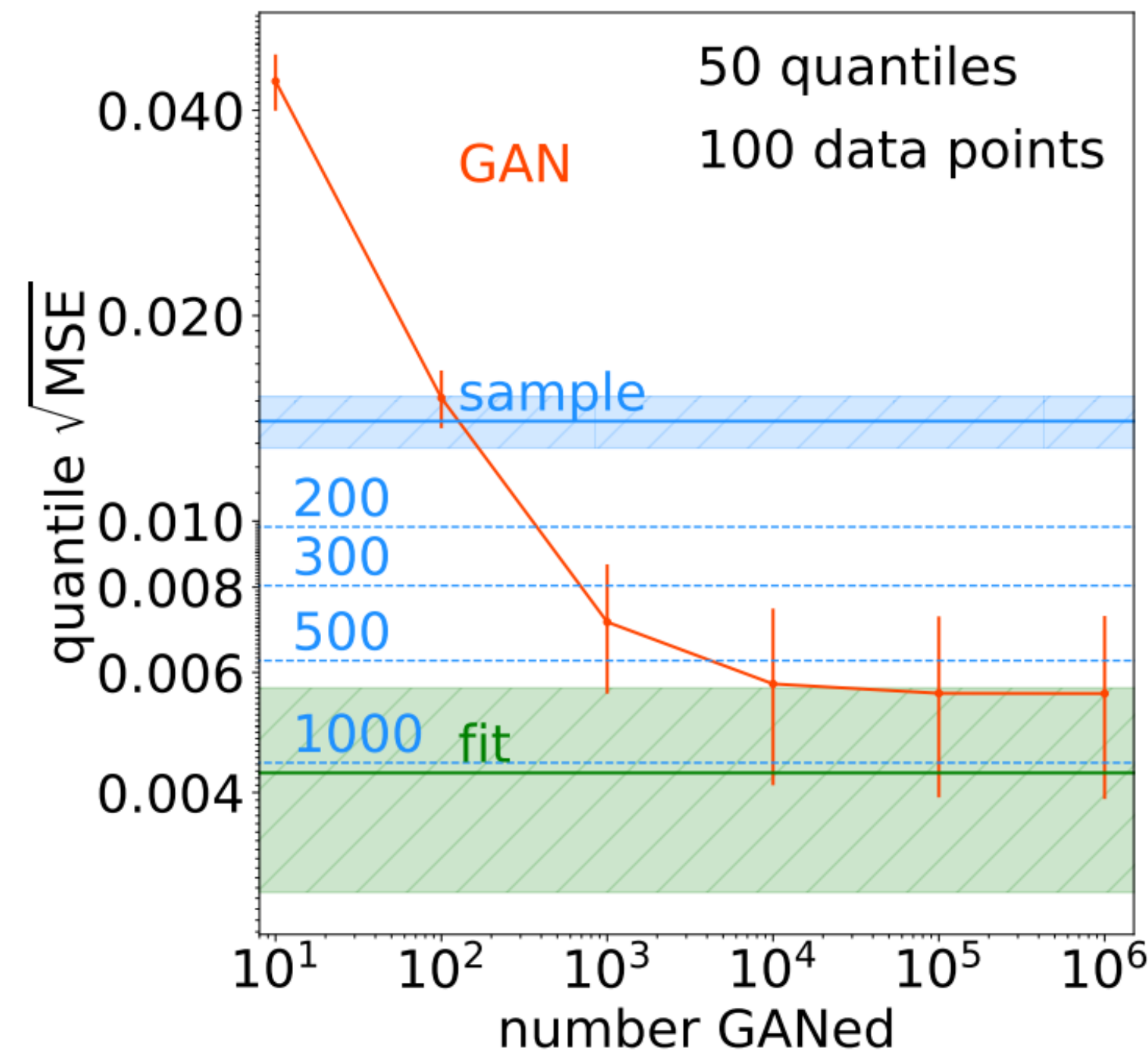
It can **NOT** outperform functional fits.

In most posed problems the theory function is unknown:

ML learns the underlying law without bias.

Butter et al., SciPost Phys. 10 (2021) 139

Data from **multiple experiments**
can be used in the training process.



Once trained, they serve as excellent interpolators:

data can be re-generated with high statistics without the need for binning/histogramming.

Y. Alanazi et al., Phys. Rev. D 106 (2022) 096002

Different methods on the market

Many MLEG approaches exist, also in the context of LHC physics.

Variational auto-encoders (VAE)

Otten et al., 1901.00875 [hep-ph]

Howard et al., 2101.08944 [hep-ph]

Normalizing flow

Gao et al., Phys. Rev. D 101 (2020) 076002

Decision trees

Darulis et al., 2207.11254

Generative adversarial networks (GAN)

Currently dominate the market of event generation, especially in our field.

Goodfellow et al., NIPS 2014

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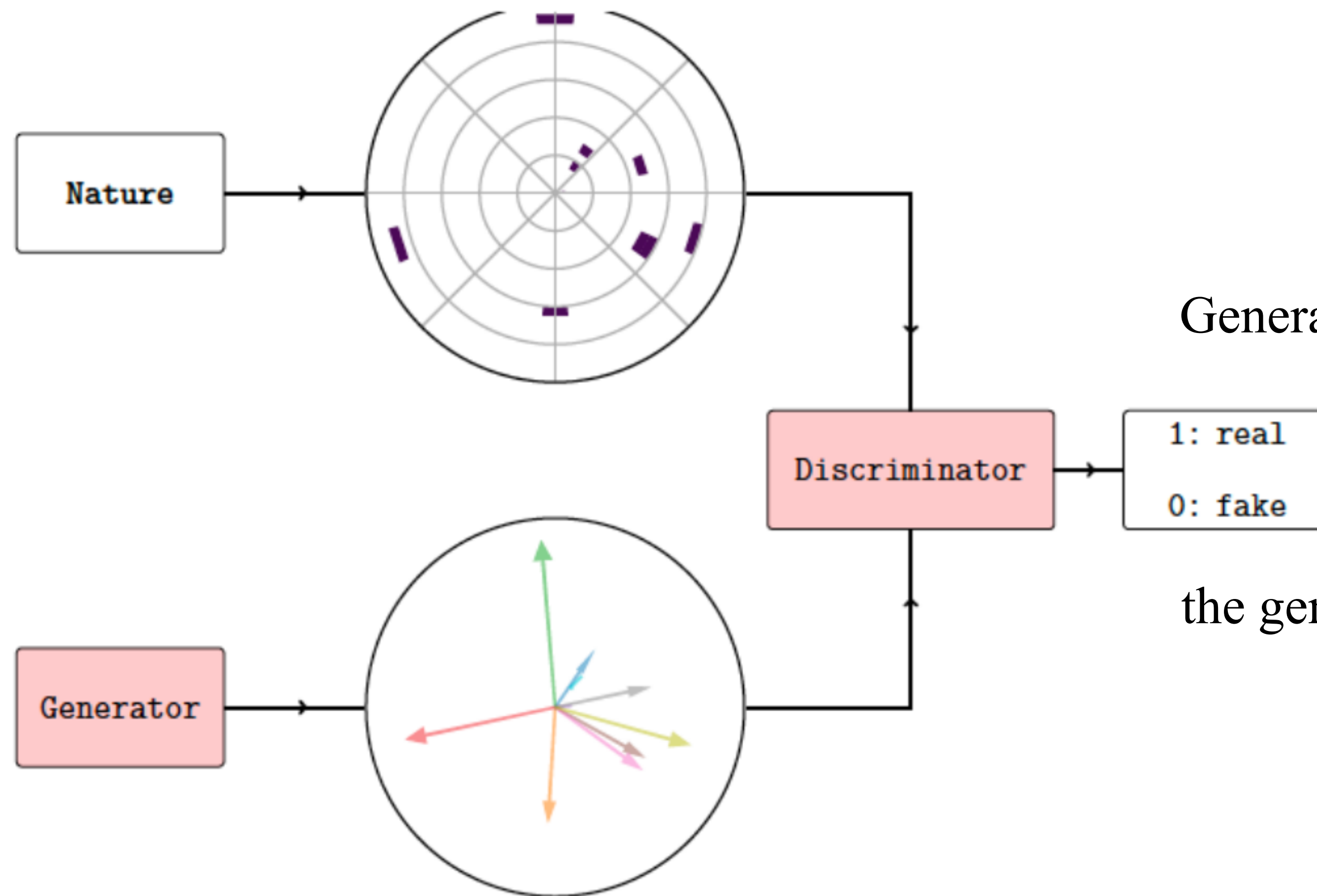
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Generative adversarial networks (GAN)

Discriminator trained to discern real (nature) from fake (generated) events.

Generator trained to create events so close to nature that they fool the discriminator.



Generator and discriminator are **trained** simultaneously, competing **adversarially**.

After training convergence, the generator can be used as a **compact data simulator**.

Panoply of good work

Calorimeter simulation, particle showers.

Paganini et al., 1705.02355, 1712.10321

Location-aware jet image training.

Oliveira et al., 1701.05927

Detector simulation.

Musella and Pandolfi, 1805.00850

Learning sharp local features of phase space, tails and peaks.

Butter et al., 1907.03764

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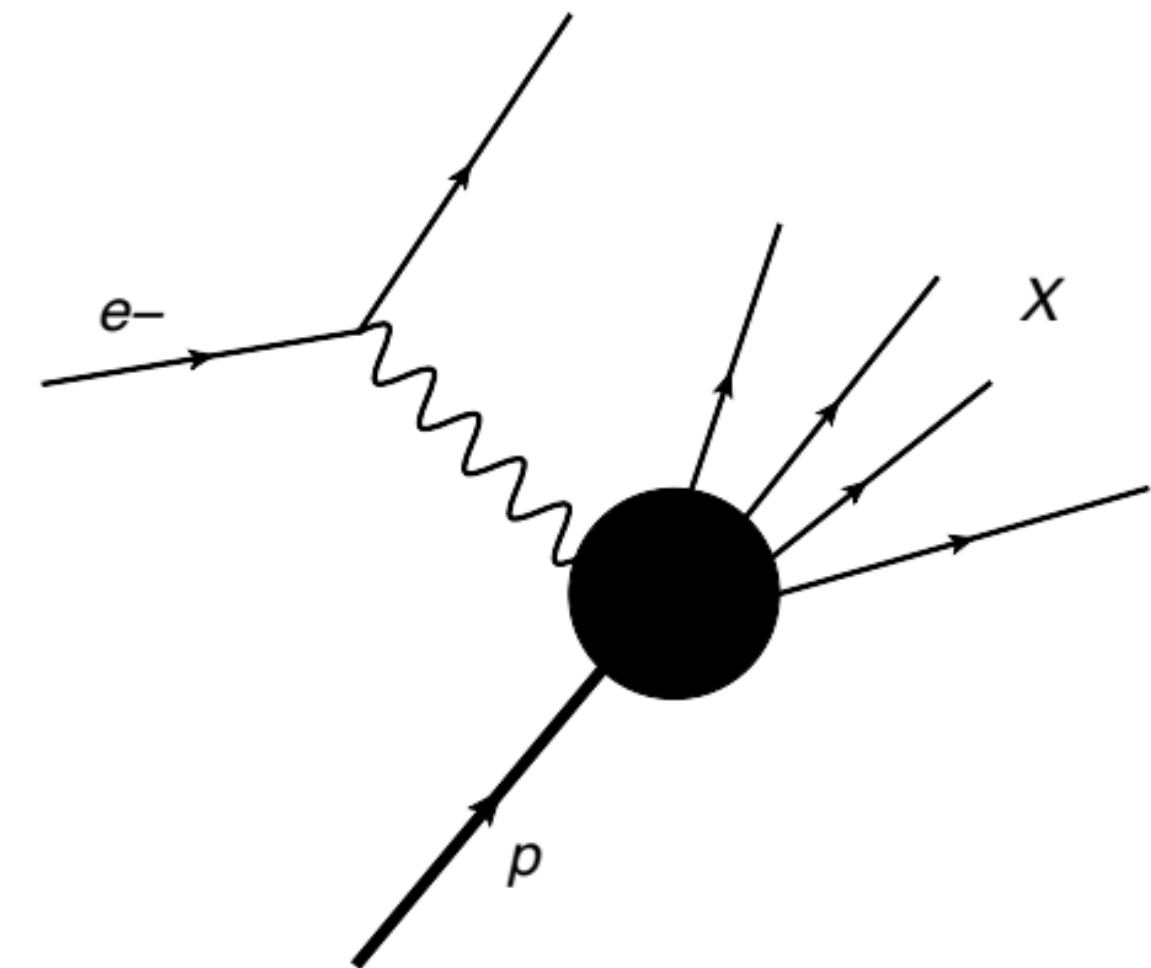
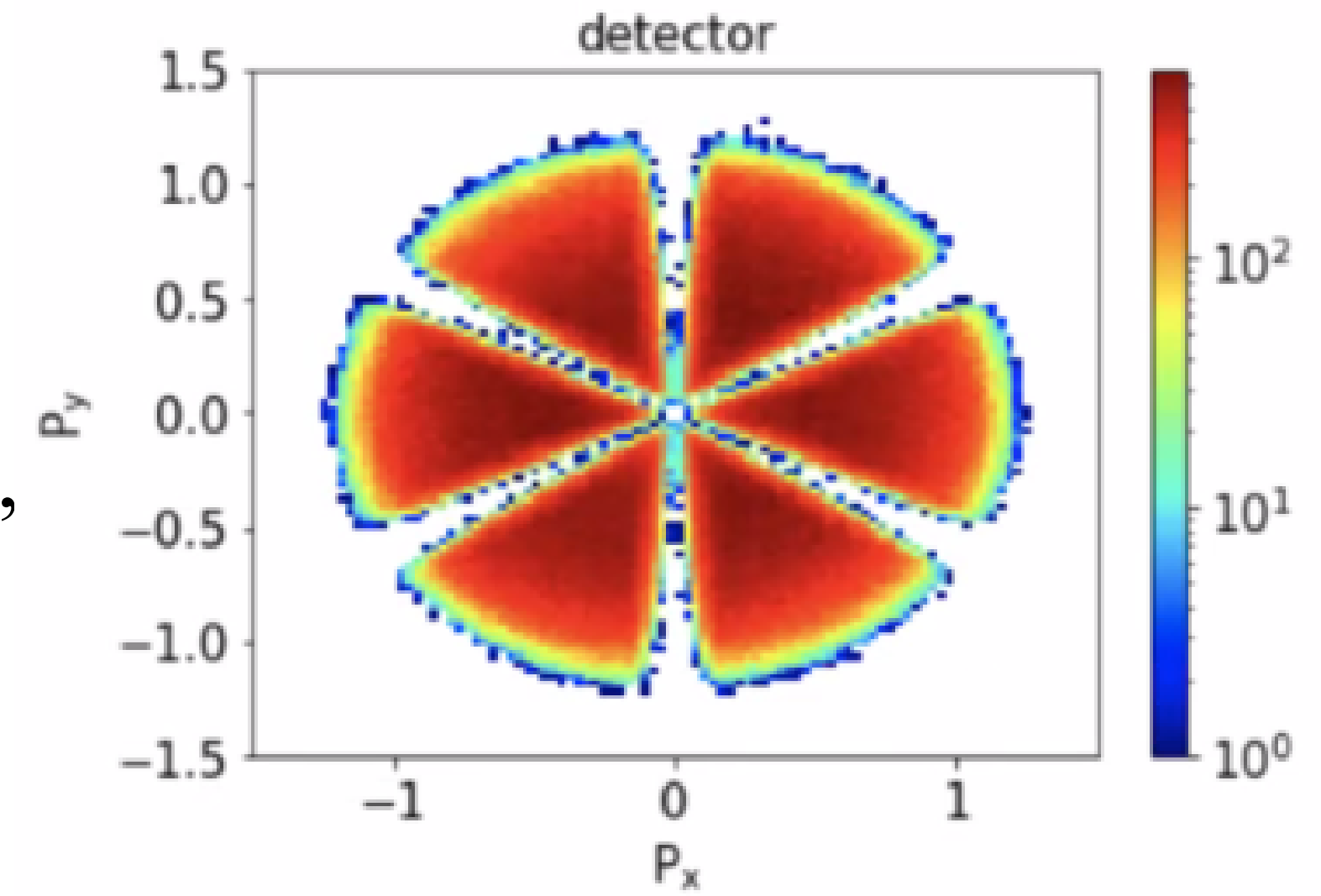
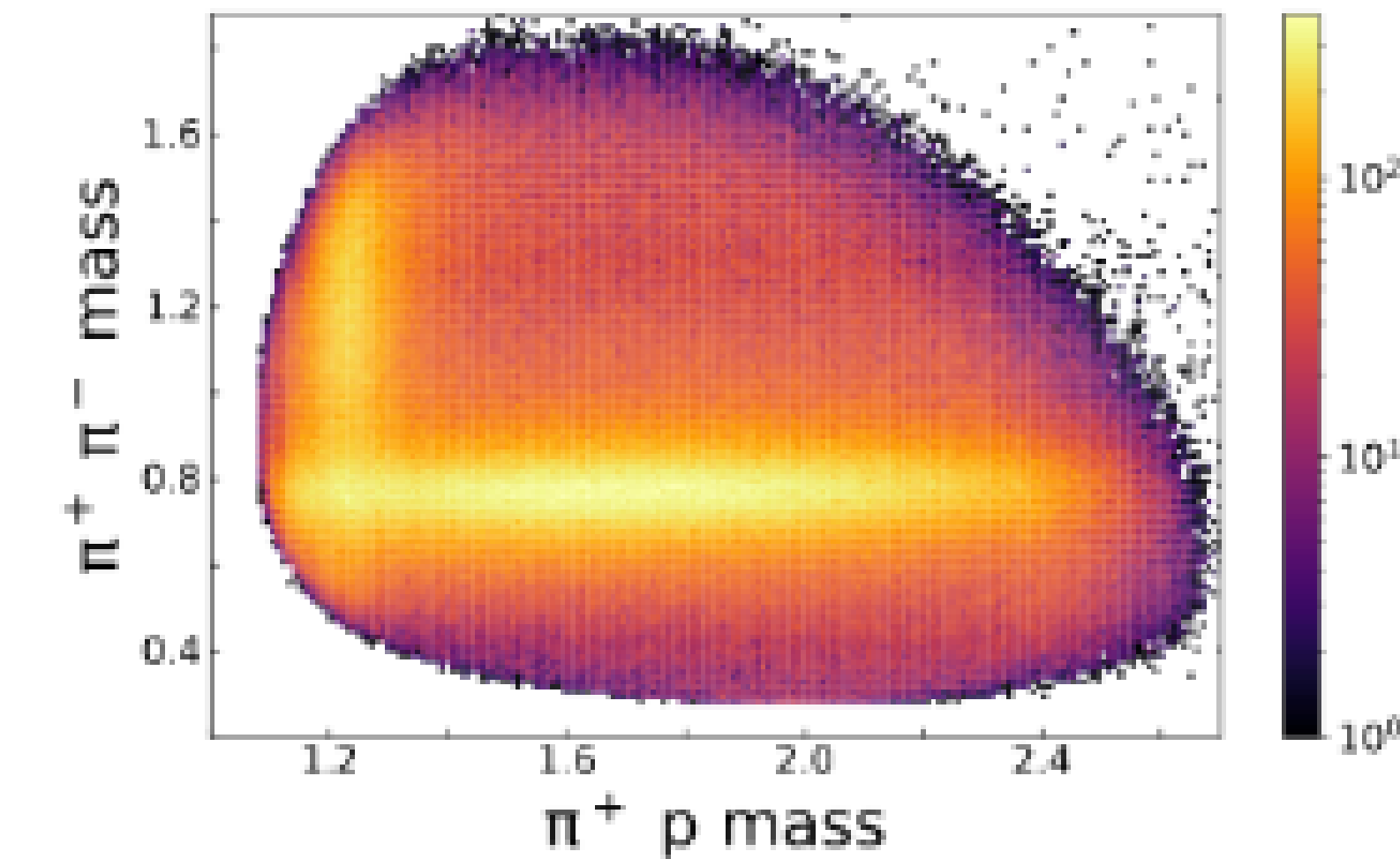
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Challenges and approaches

Sharp structures (resonances, limits of phase space, holes in detector acceptance),
physics laws (momentum and energy conservation, correlations),
high dimensionality lead to

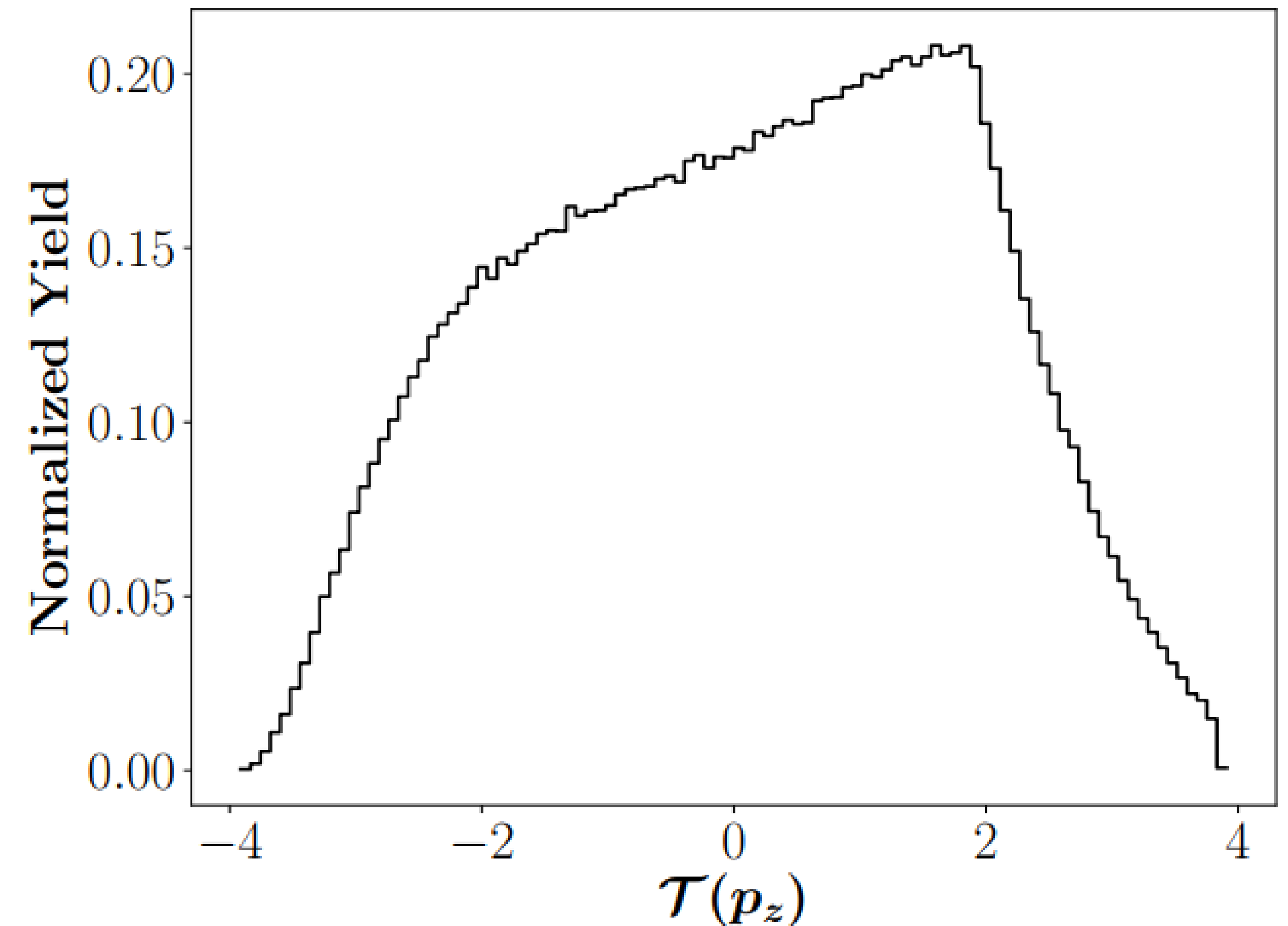
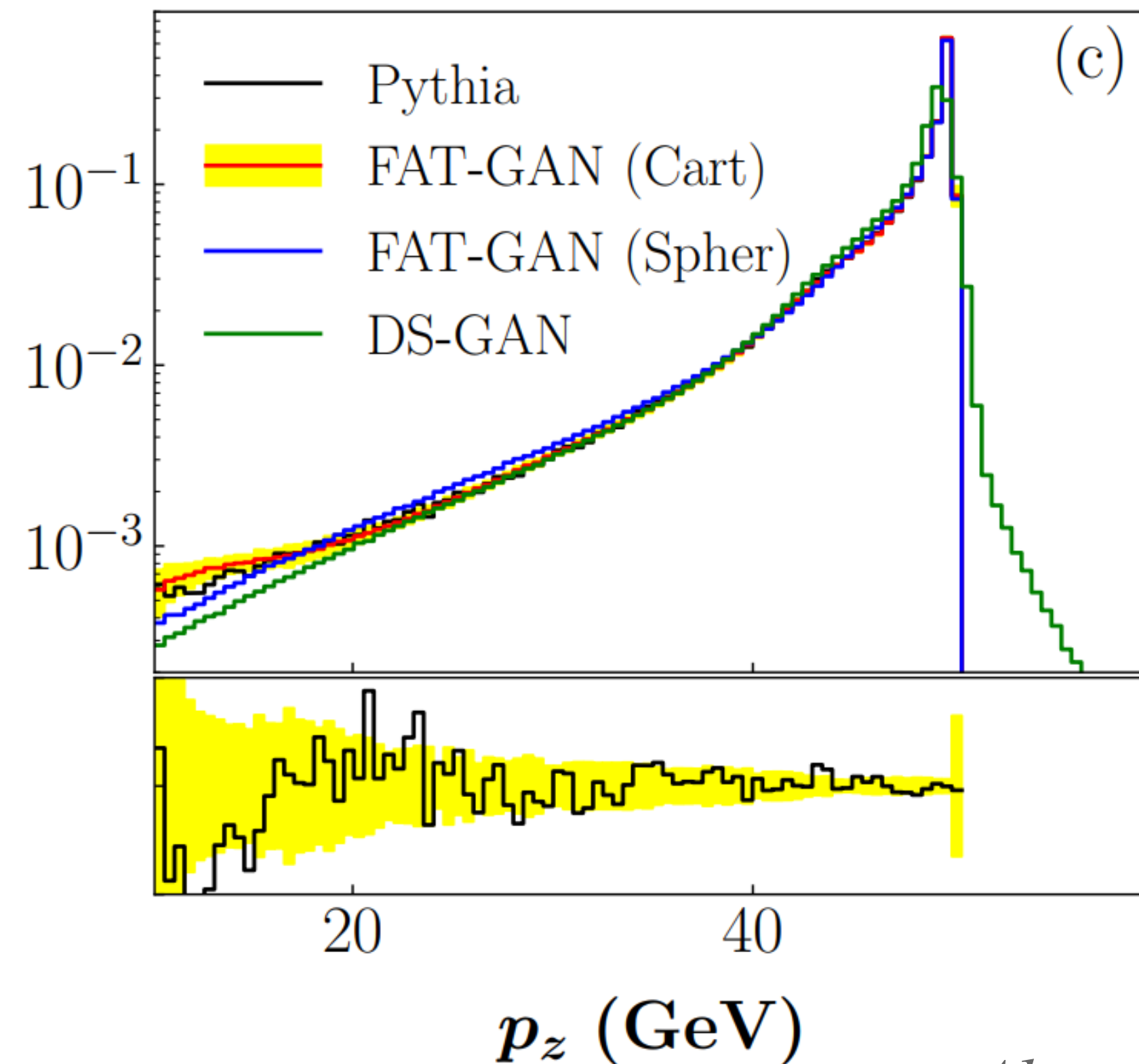
non-convergence and vanishing gradients,
parameter oscillation or **instability**,
mode collapse and **overfitting**.



- Improved approaches:
- **penalizing samples** too close to boundary;
 - **continuous** probabilistic output of what is fake and what is true;
 - feature **augmentation** and **transformation**;
 - **conditional** GAN.

Feature augmentation and transformation (FAT)

The corners of phase space are difficult to learn – the ML does not know that it has to obey physics laws.



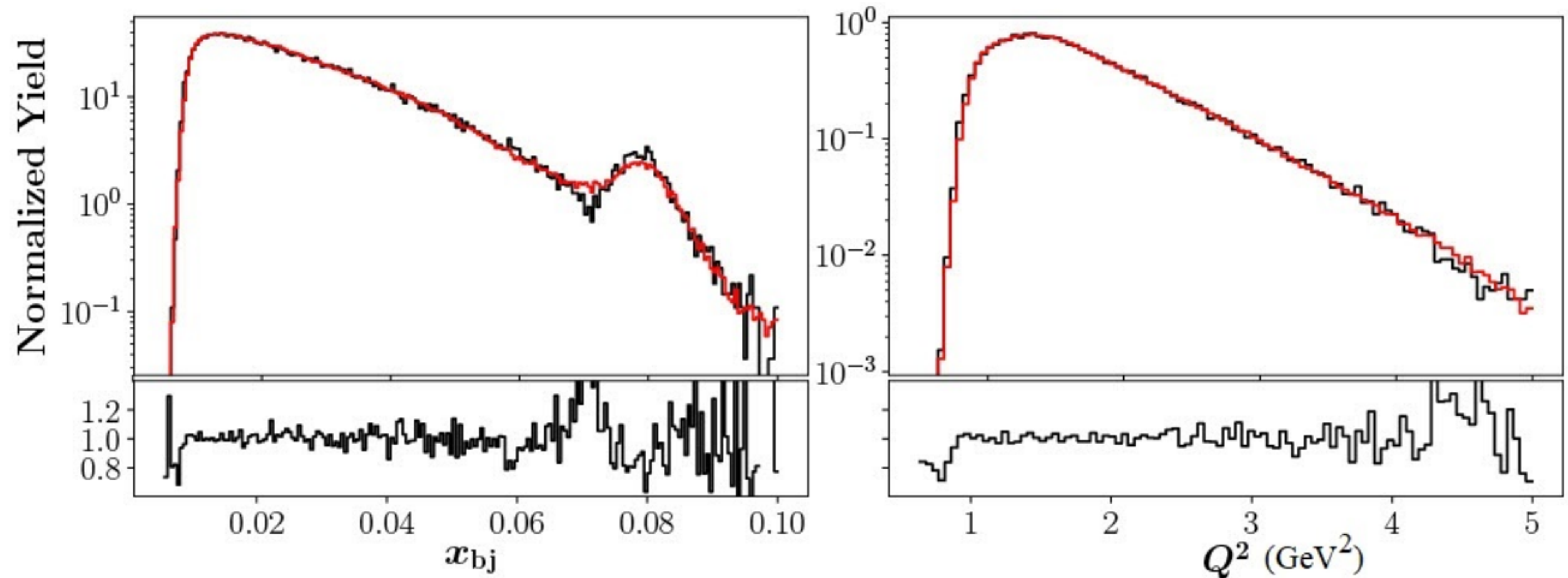
Alanazi et al., 2001.11103 [hep-ph]

Transformed features $\mathcal{T}(p_z) = \log \left(\frac{E_b - p_z}{1\text{GeV}} \right)$

Augmented features $p_x, p_y, \mathcal{T}(p_z), p_T, E, p_z/p_T$

Conservation of physics correlations

Even features untrained on are well generated: physics correlations are learned and kept in the generated data!
Physics validation shows that one can extract the same physics from MLEG as from original data.



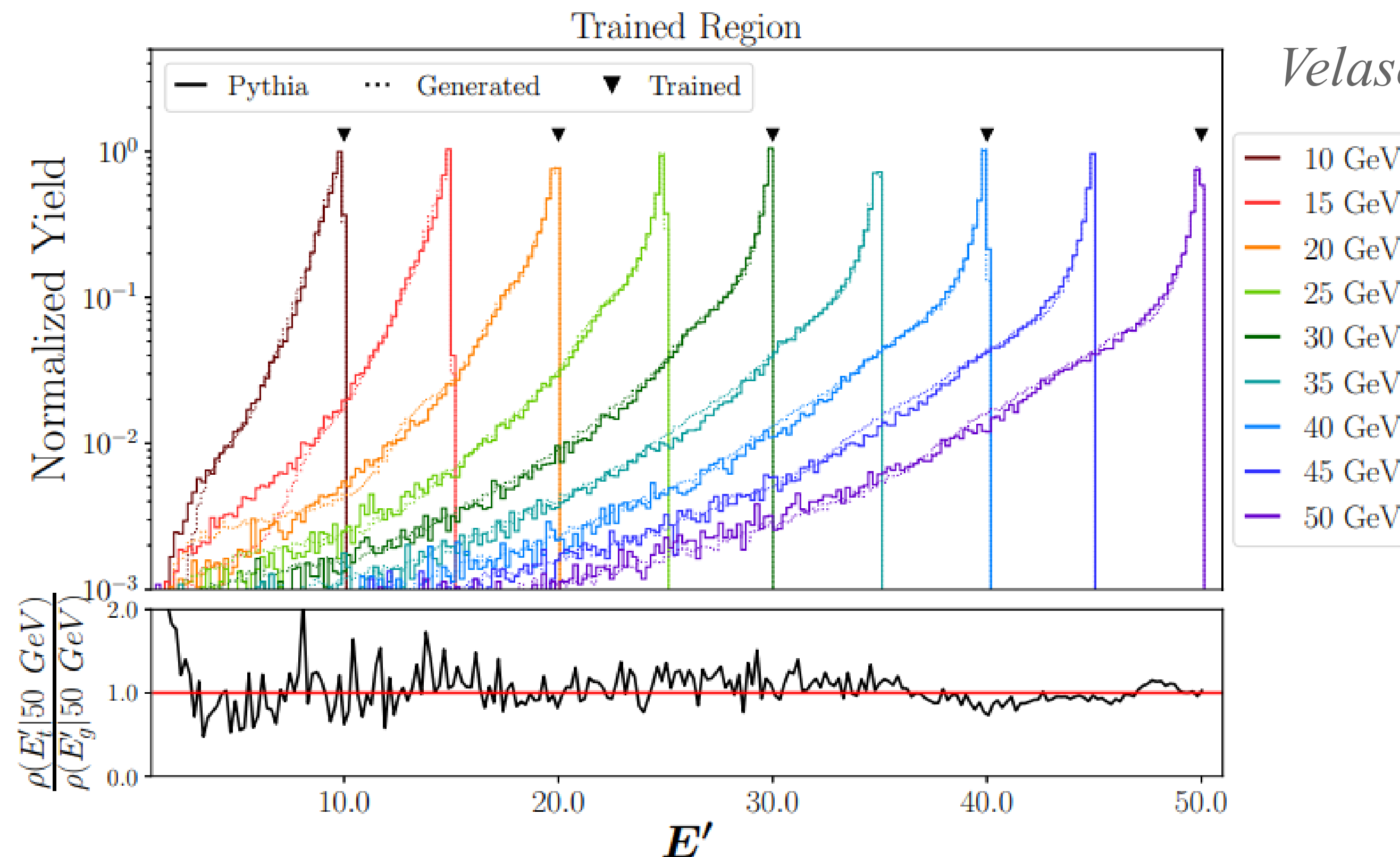
Alanazi et al., 2001.11103 [hep-ph]

Conditional FAT GAN

One wants to avoid training such that only one experiment (one energy setup) can be reproduced.

The cFAT-GAN receives:

- usual **input features**;
- **additional conditions** to each training sample, e.g. beam energy.



Velasco et al., ICMLA (2020) 372

The cFAT-GAN has excellent agreement with data **interpolation** region, even for those beam energies **NOT trained on**.

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From vertex to detector and back again

Experimental apparatus effects distort nature into detector-level events.

Unfolding from detector to vertex-level events is a physics reconstruction strategy.

Datta et al., 1806.00433 [physics.data-an]

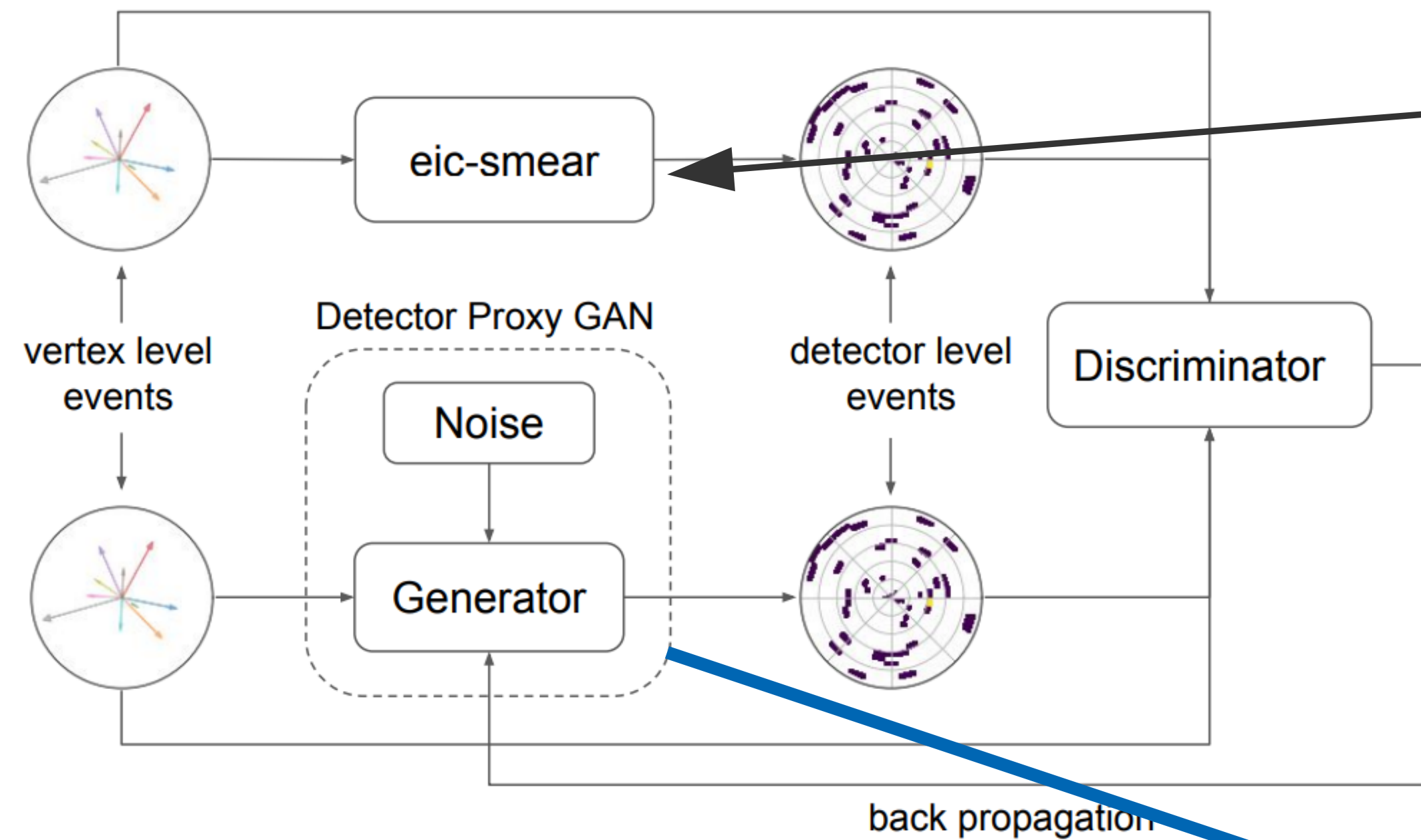
Andreassen et al., Phys. Rev. Lett. 124 (2020) 182001

Conditional GAN can invert from detector to vertex level by conditioning the training on detector input.

Bellagente et al., SciPost Phys. 8 (2020) 070

Y. Alanazi et al., Phys. Rev. D 106 (2022) 096002

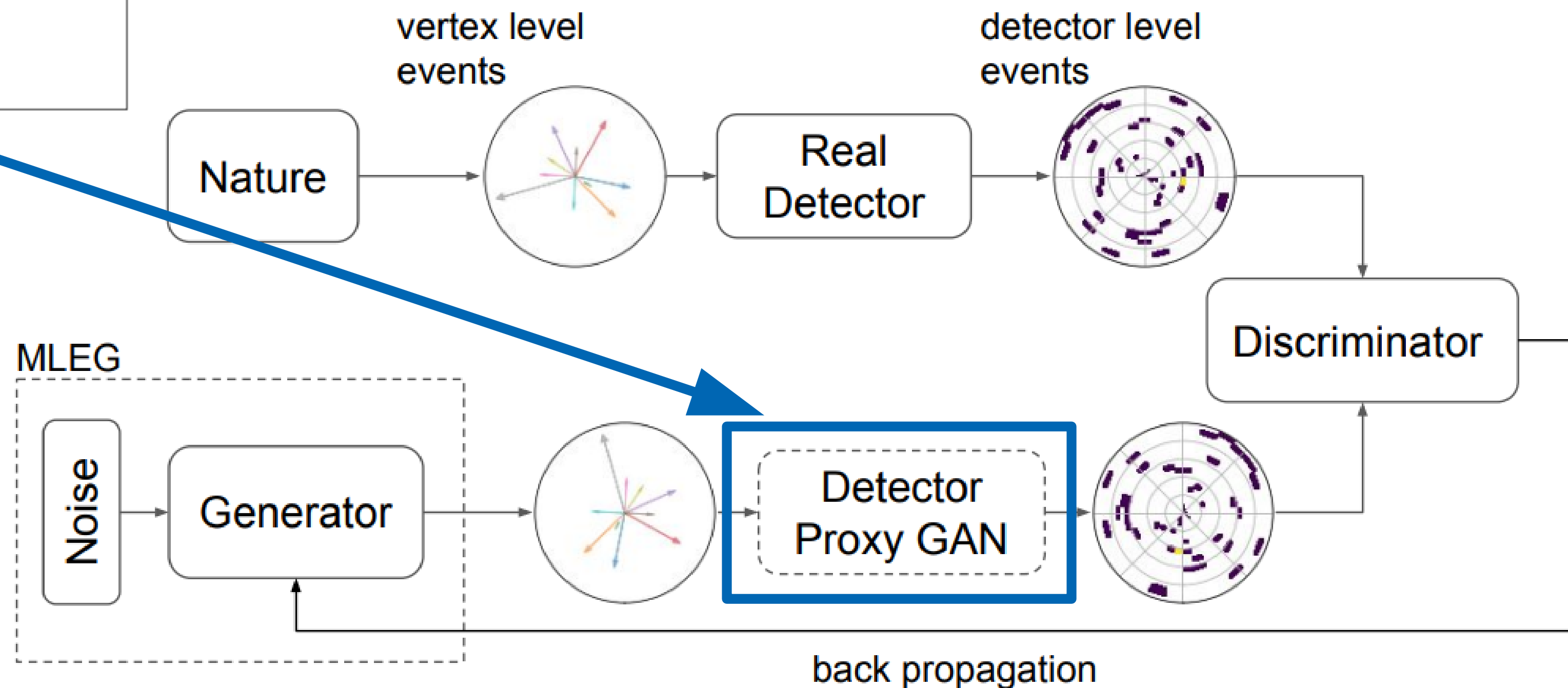
Unsupervised vertex learning



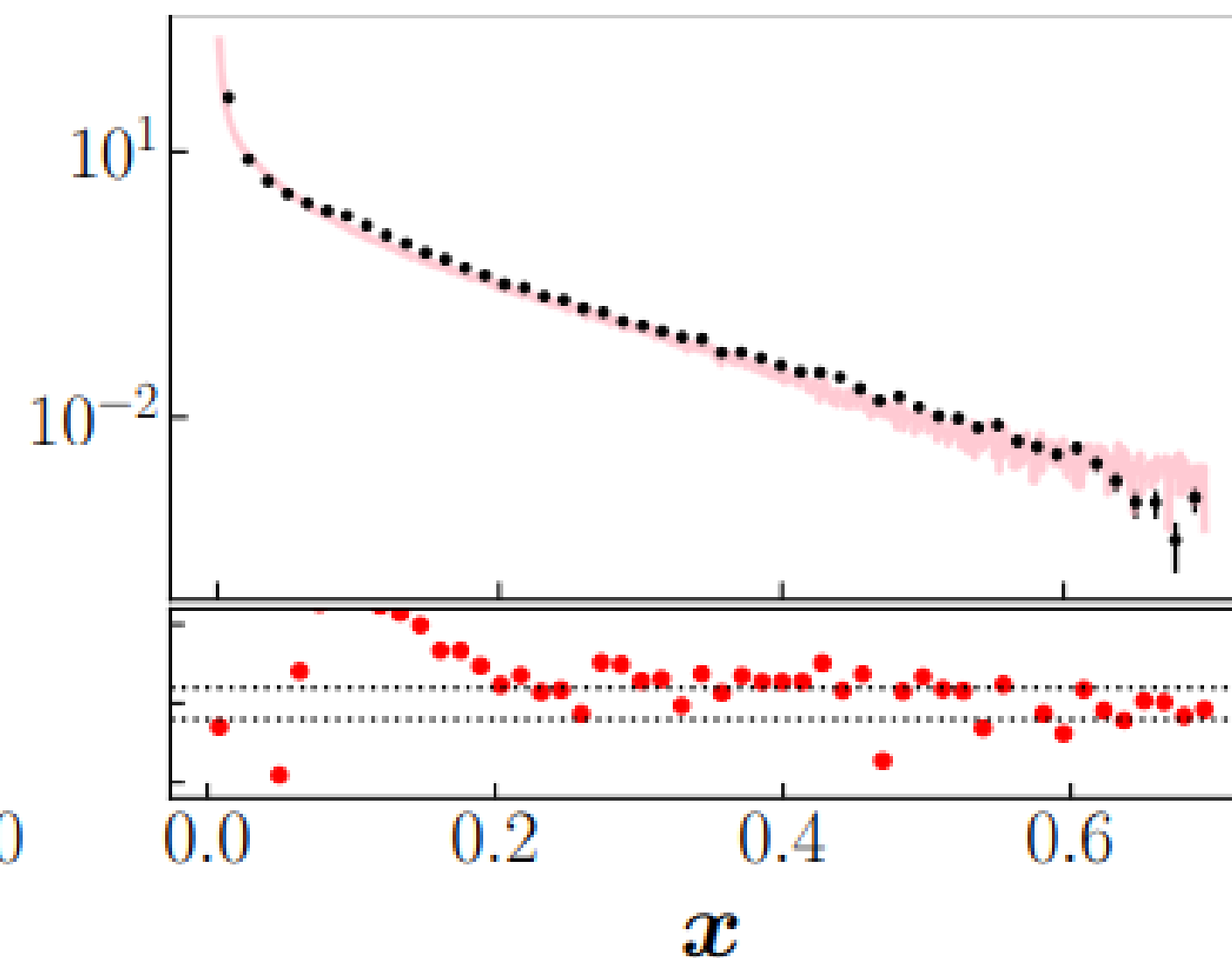
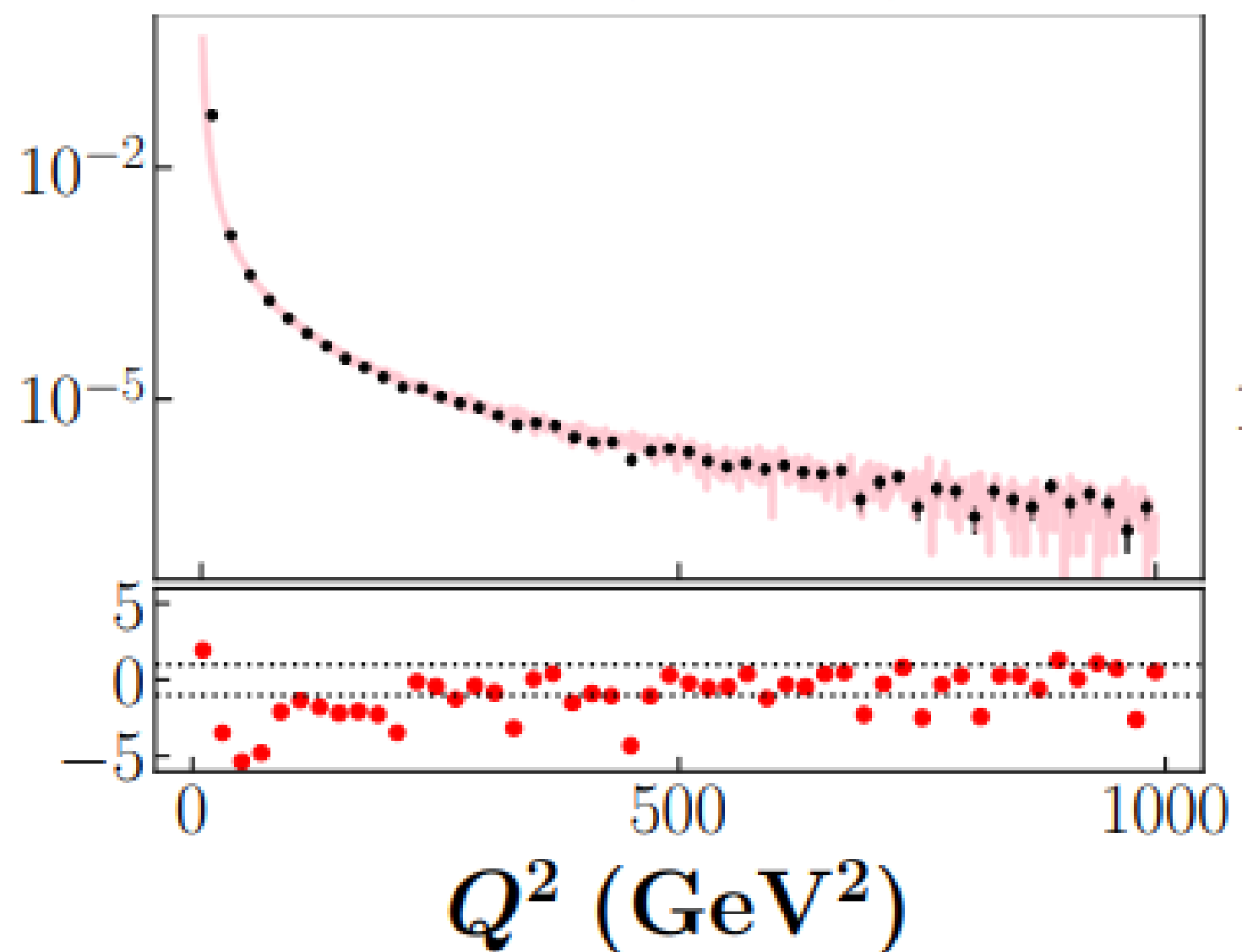
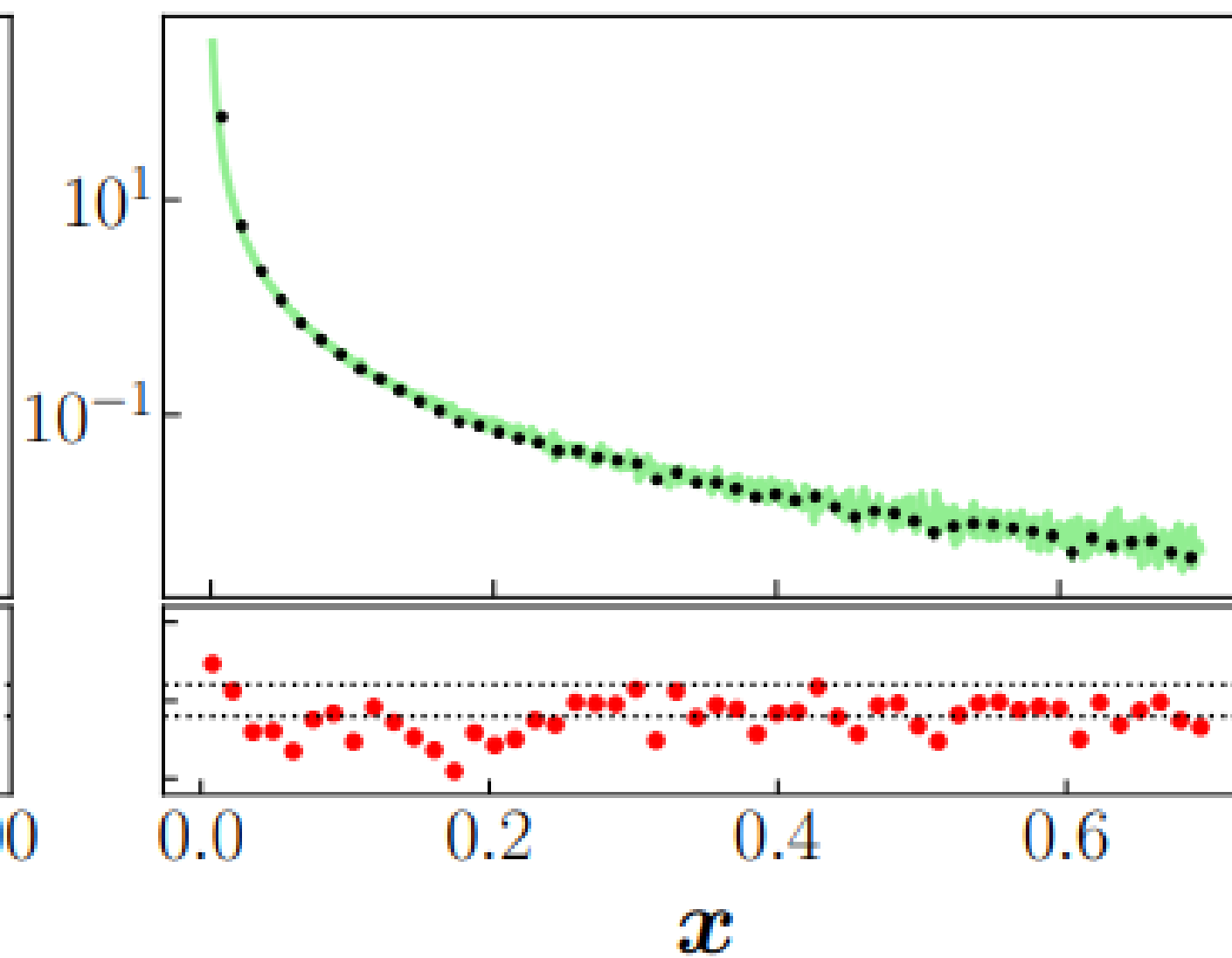
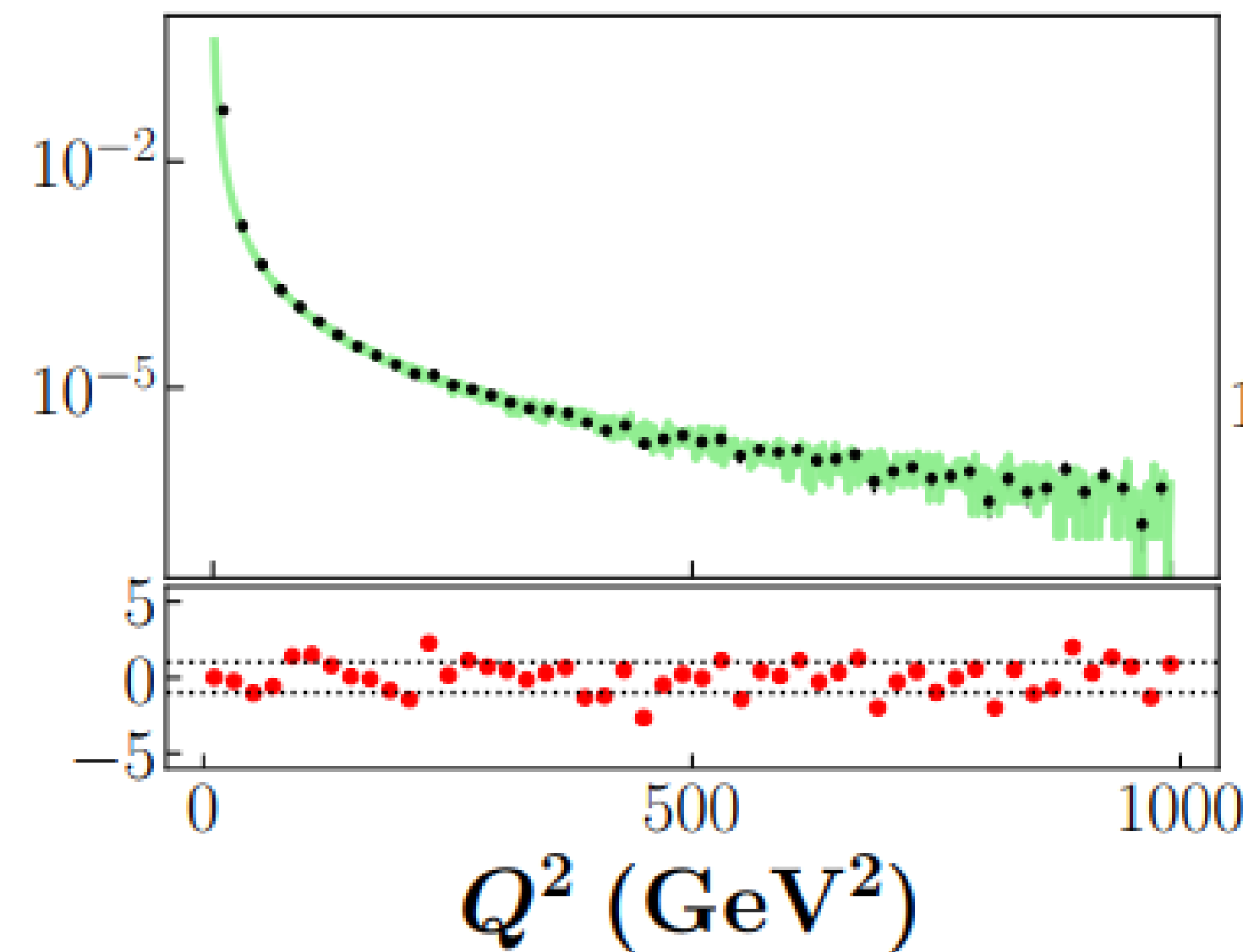
Smearing routine for the EIC
– mimics detector effects.

Y. Alanazi et al., Phys. Rev. D 106 (2022) 096002

The detector proxy GAN is trained to transform vertex into detector events.
It is then built into the full architecture.



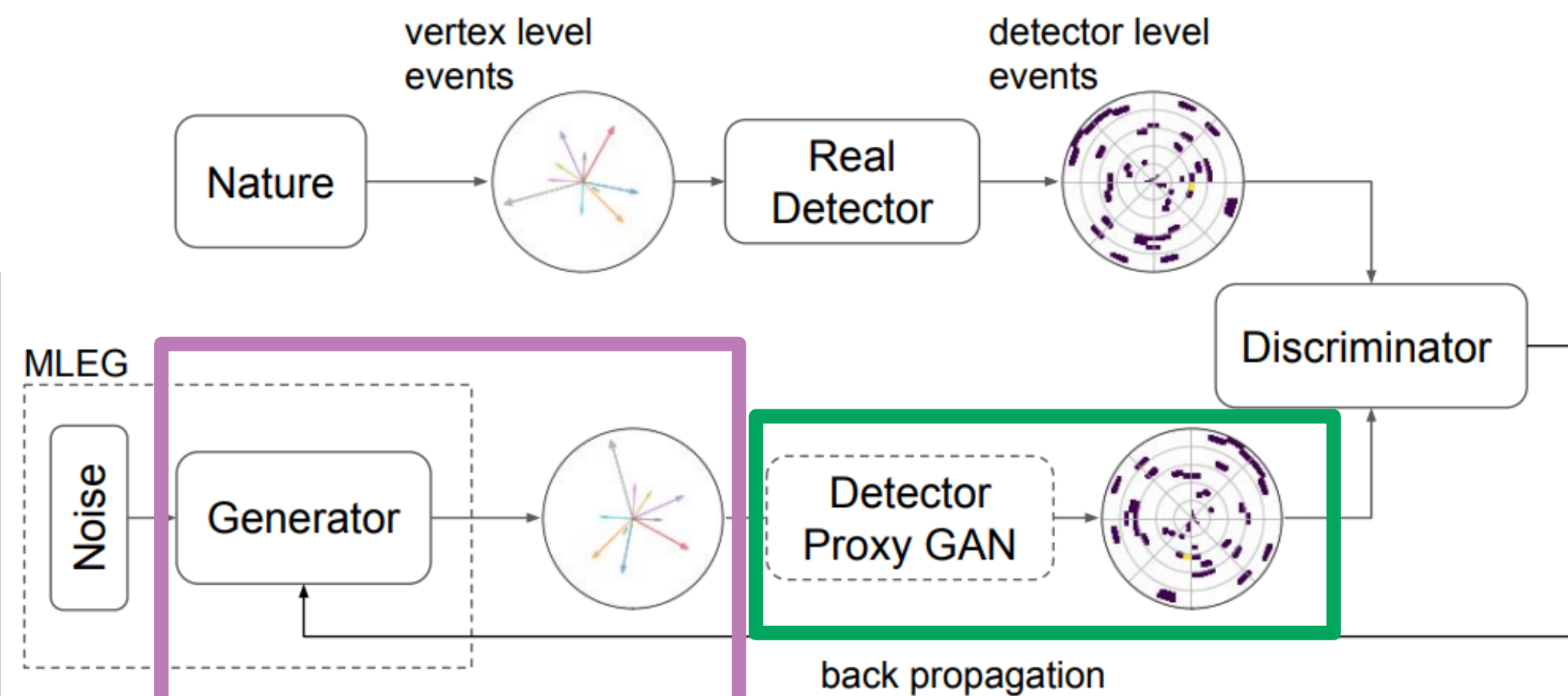
Closure tests and uncertainty quantification



Training supervised
on **detector-level** samples

Folding detector-level GAN output

$$P_{\text{pull}} = \frac{E_{\text{GAN}} - E_{\text{Data}}}{\sqrt{V_{\text{GAN}} - V_{\text{Data}}}}$$



Training **unsupervised**
on **vertex-level** samples

Unfolded vertex-level GAN output

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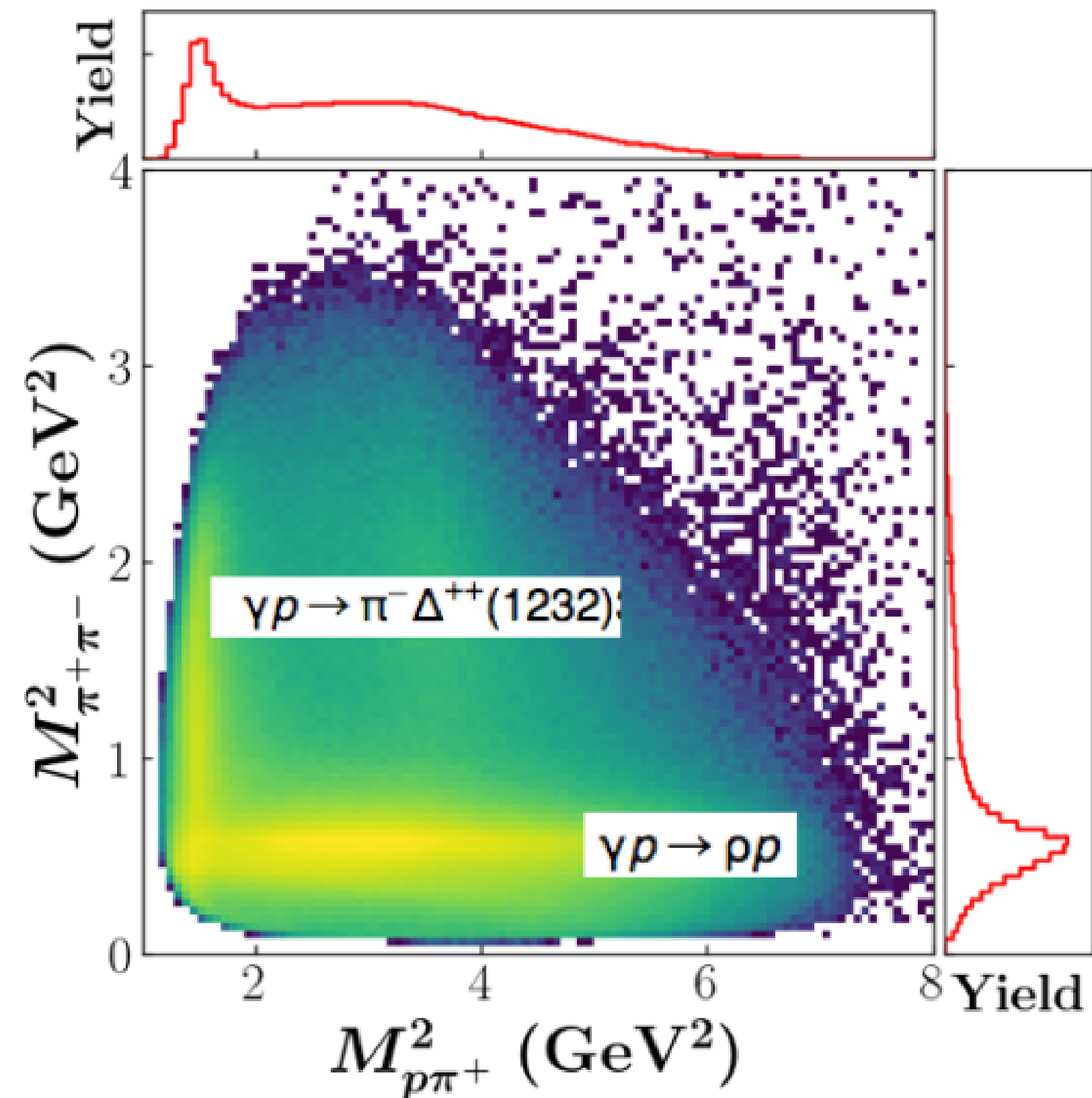
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Two-pion photoproduction data

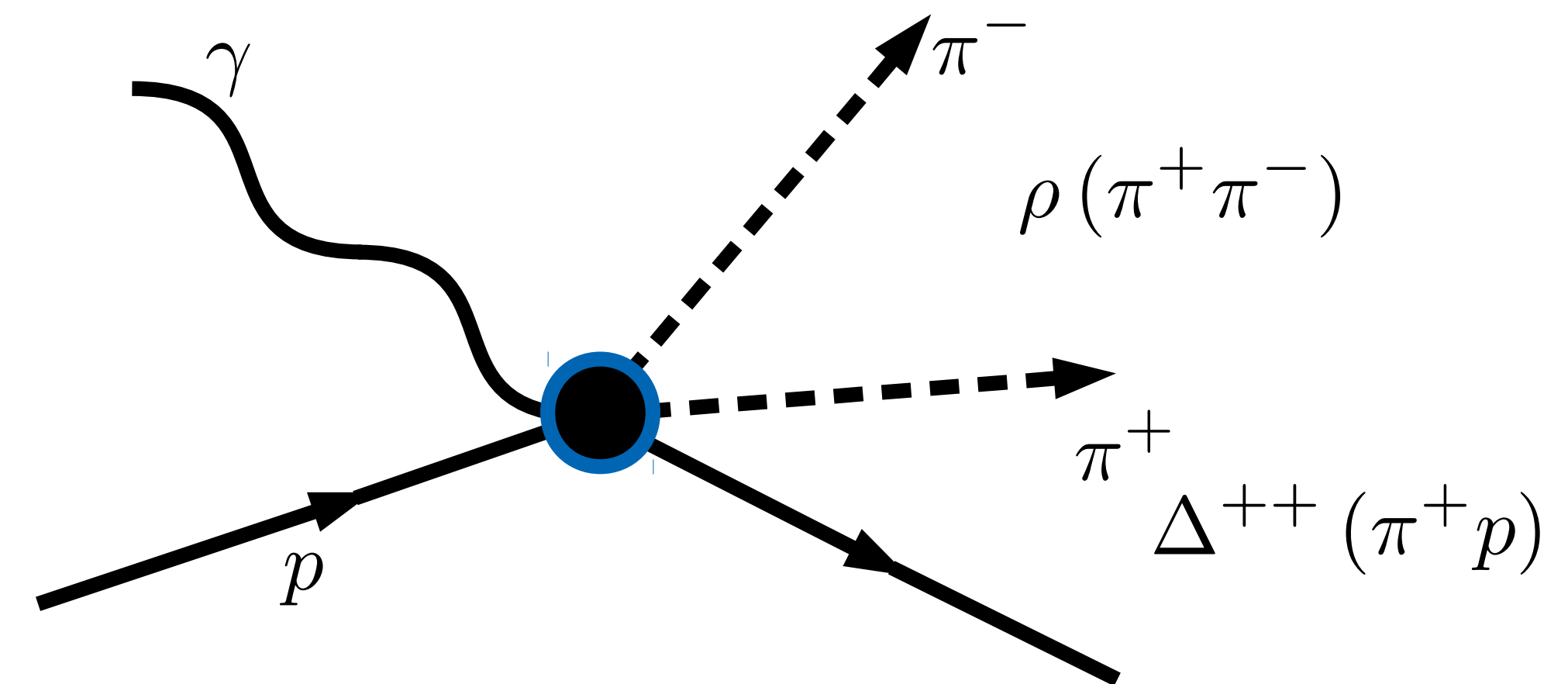
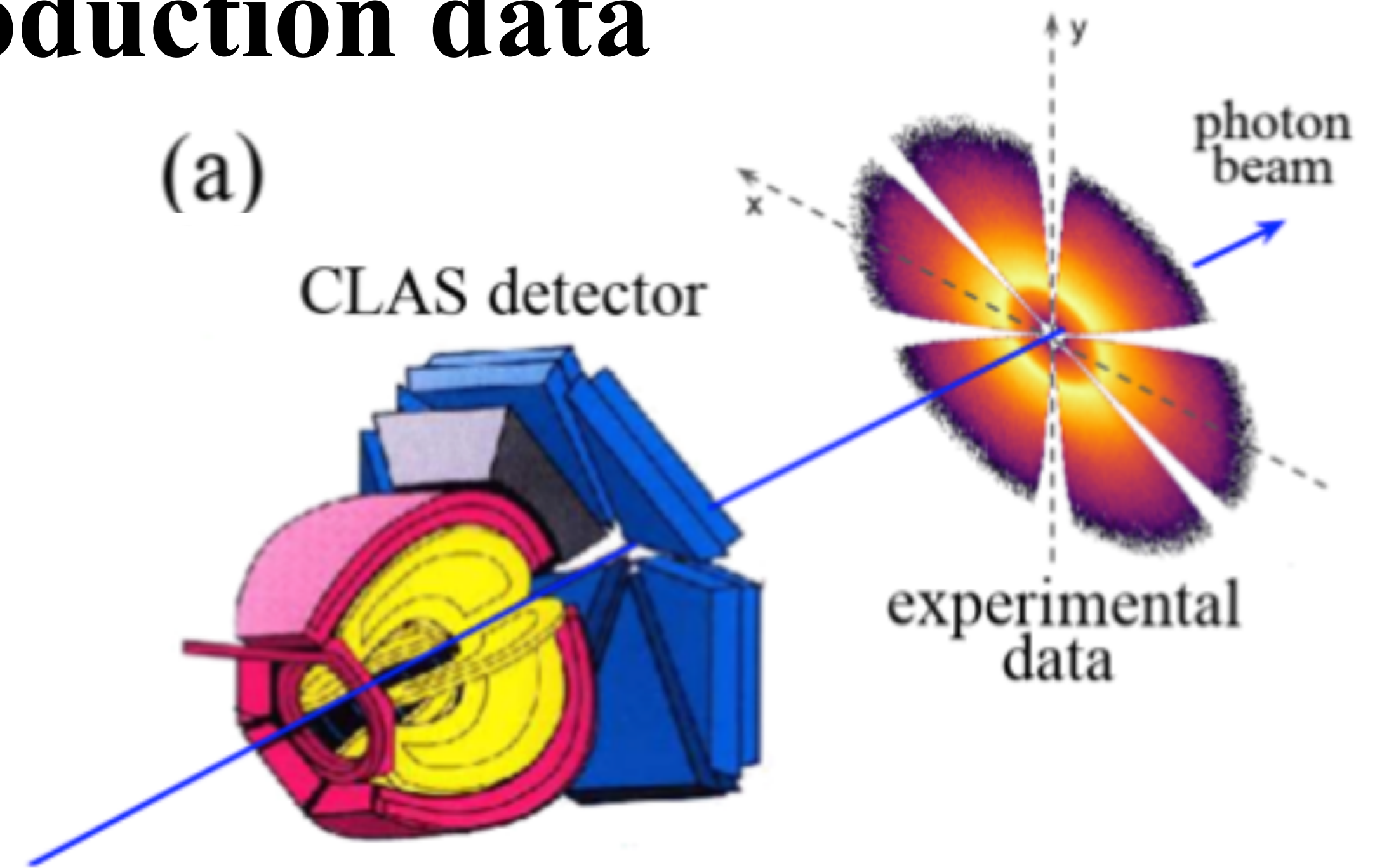
Narrow peaks, holes, steep edges, ...

Correlations between variables lost in integrated observables.

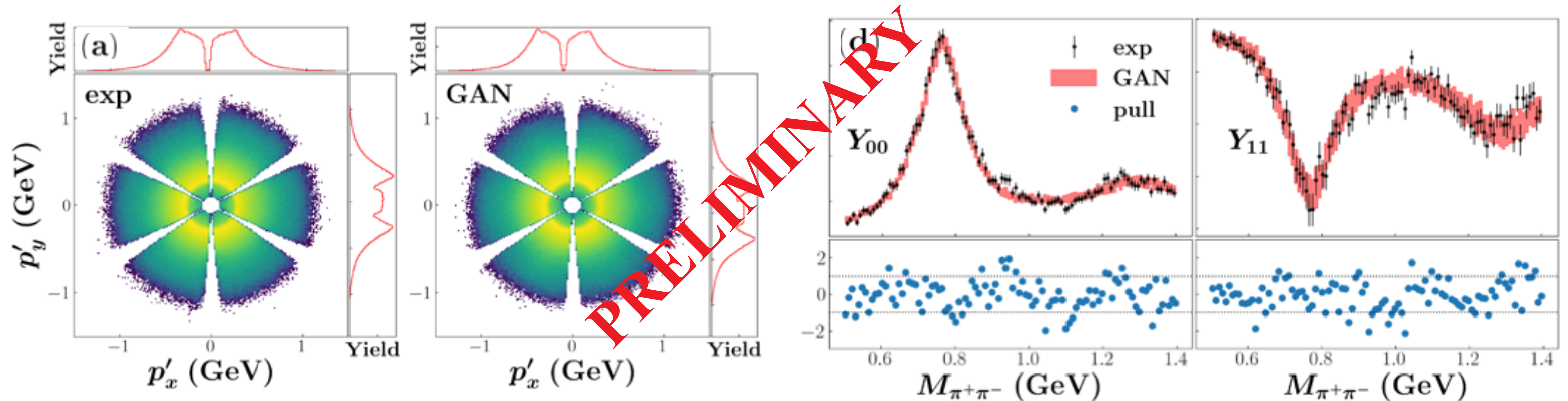
M. Battaglieri et al. (CLAS Collaboration)
Phys. Rev. D 80 (2009) 072005



(a)



Physics extraction



The GAN mimics the data despite the experimental distortions.

Observables extracted from GAN and data are compatible – **same physics can be extracted!**

The GAN serves as compact data generator ideal for data storage and distribution.

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Applications:

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Summary and future

Machine learning is a powerful complementary tool for event generation:

- data compression by training on Monte Carlo and real data, **capturing the original correlations**;
- possibility of unfolding **vertex-level physics** from detected data.

Currently available and ongoing works:

- generation of data with **sharp edges** from phase space, detector holes, resonances, ...;
- **interpolation** and combination of experiments with different setups;
- **closure tests** of vertex-level extraction, **uncertainty quantification** metrics and **physics validation**.

In future, these benchmarks will allow for:

- **EIC preparation and fast simulators**;
- interpolation and **minimum-bias** physics extraction.