Unfolding Particle Detector Effects in HEP with Generative AI

Yaohang Li and the A(I)DAPT Collaboration

Department of Computer Science
Old Dominion University
Norfolk, Virginia 23529
yaohang@cs.odu.edu

Agenda

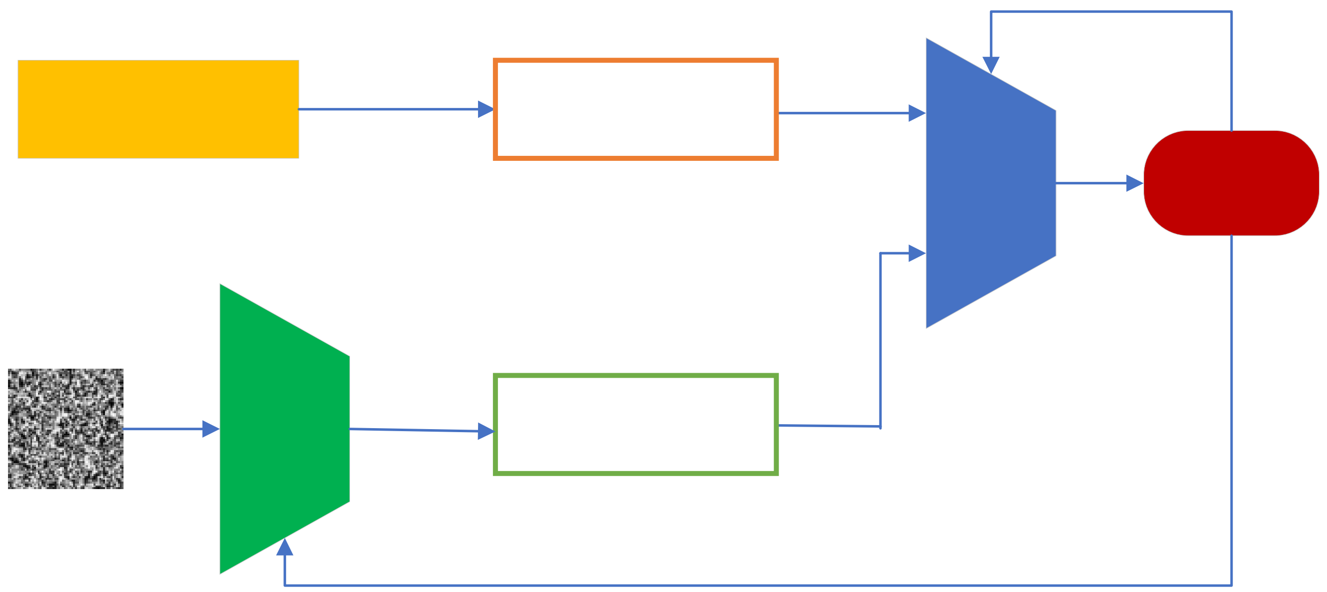
- **Initial Attempt in Exclusive Electron-Proton Scattering**
  - FAT-GAN
  - Conditional GAN
- **Unfolding Smearing Effects**
  - Electron-Proton Scattering
  - CLAS Exclusive 2π photoproduction
- **Unfolding Acceptance Effects**
  - Single-pion photoproduction reaction
- **Multiple Topologies**
- **Conclusion and Future Work**

2019-2020 Jefferson Lab LDRD Project: Universal Monte Carlo Event Generator (Wally, Sato)

- **Simulate Physics Events with Machine Learning**
  - Data-Driven: directly learning from event samples
- **Machine Learning-based Event Generators (MLEGs)**
  - Data preservation (JLab in a jump drive)
    - Compactified data storage utility
    - Derivation of physics properties
  - Faithful Representation of Nature
    - Model independent
    - Agnostic of theoretical assumptions about the microscopic nature of particle reactions
    - Accurately mapping out the underlying probability distributions
  - Much faster than MCEGs
    - Simulation of the complete pipeline of particle experiment can take minutes to generate an event
    - MLEGs can generate millions of events

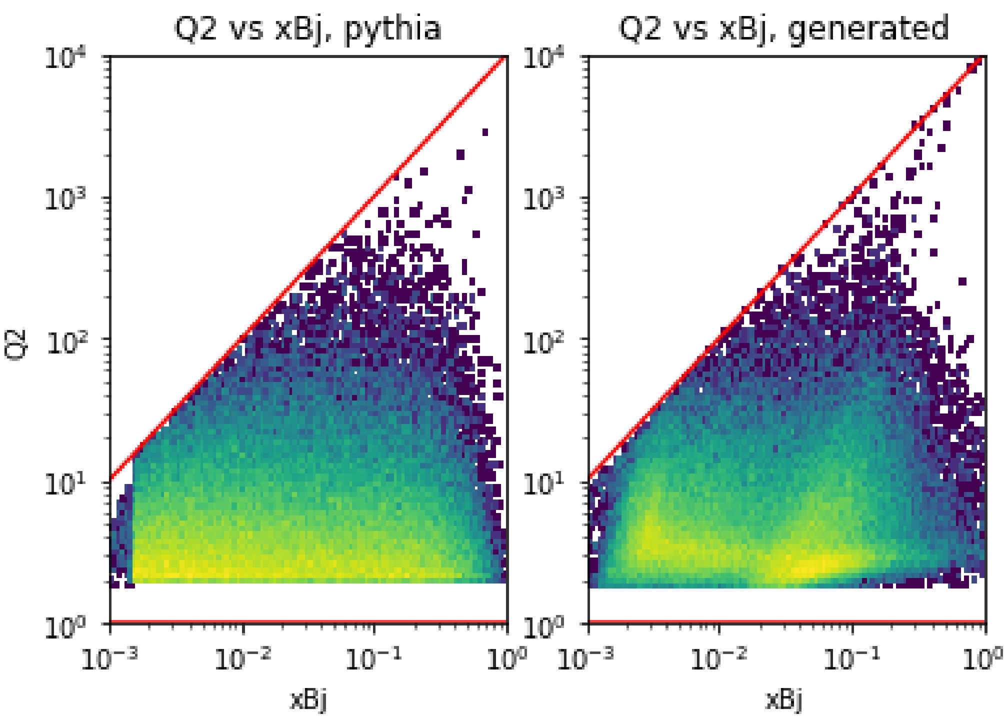
Initial Attempt: Electron-Proton Scattering

- **Direct Simulation Generative Adversarial Networks (GAN)**
- **Training Events**
  - Pythia Events with Center-of-mass energy of 100 GeV
- **Inclusive Simulation**
  - Only trained on the momenta of the final state electrons

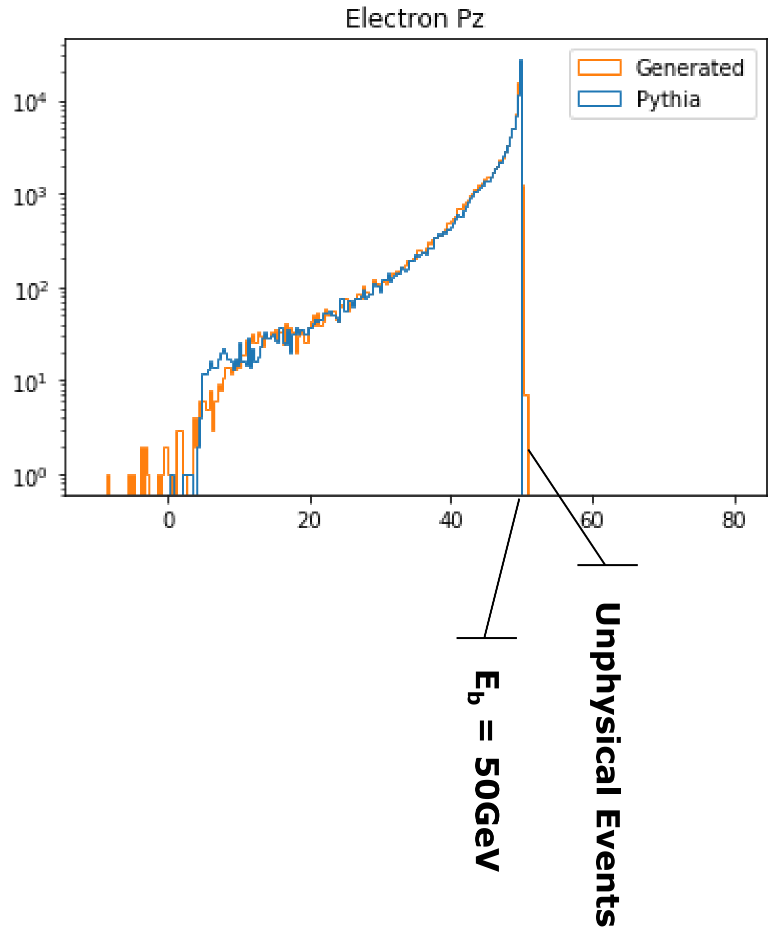


Alanazi et al., IJCAI 2021.

Results of Director Simulation GAN



$\chi^2 = 118.29$



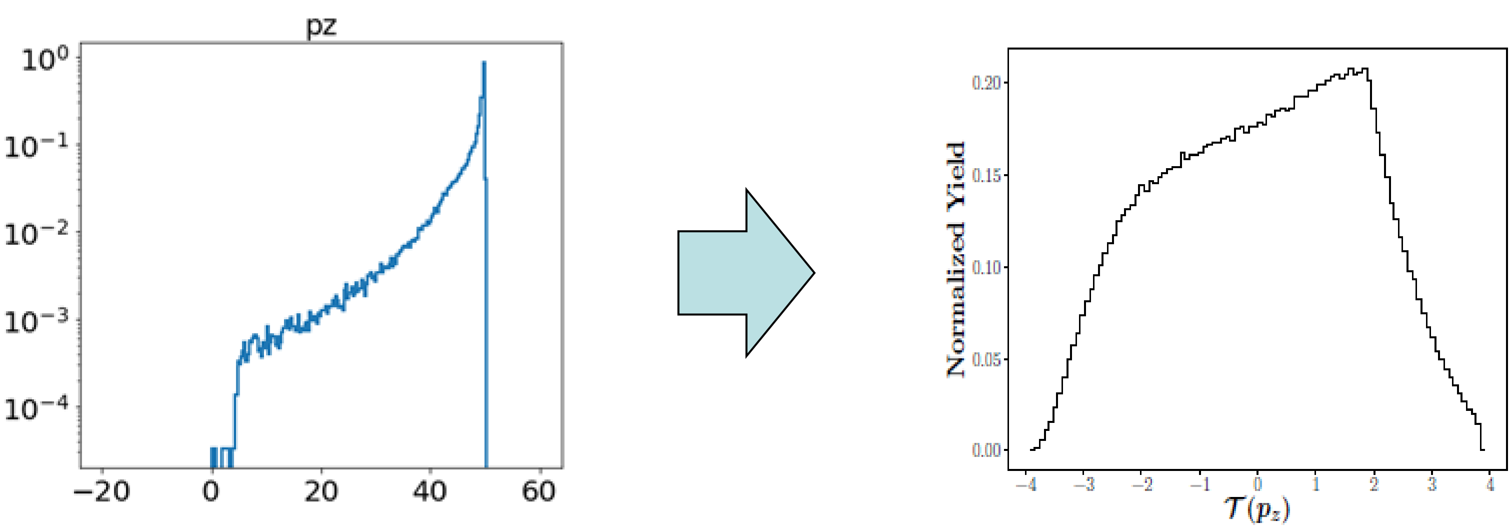
Challenges in GAN Training

- **Training a GAN is notoriously difficult**
  - Perfect Discriminator
  - Mode Collapse
  - Non-convergence
  - Imbalance Generator and Discriminator Training
  - Model parameter oscillation
  - Destabilization
  - Vanishing gradient
- **Additional Requirements for Physics Event Generation**
  - Precise Event Feature Distributions
    - Replicate the nature of particle reactions faithfully
  - Obeying the Fundamental Physics Laws
    - Energy Conservation
    - Momentum Conservation

Features Transformation

$$\mathcal{T}(p_z) = \log(E_\mathrm{b} - p_z)$$

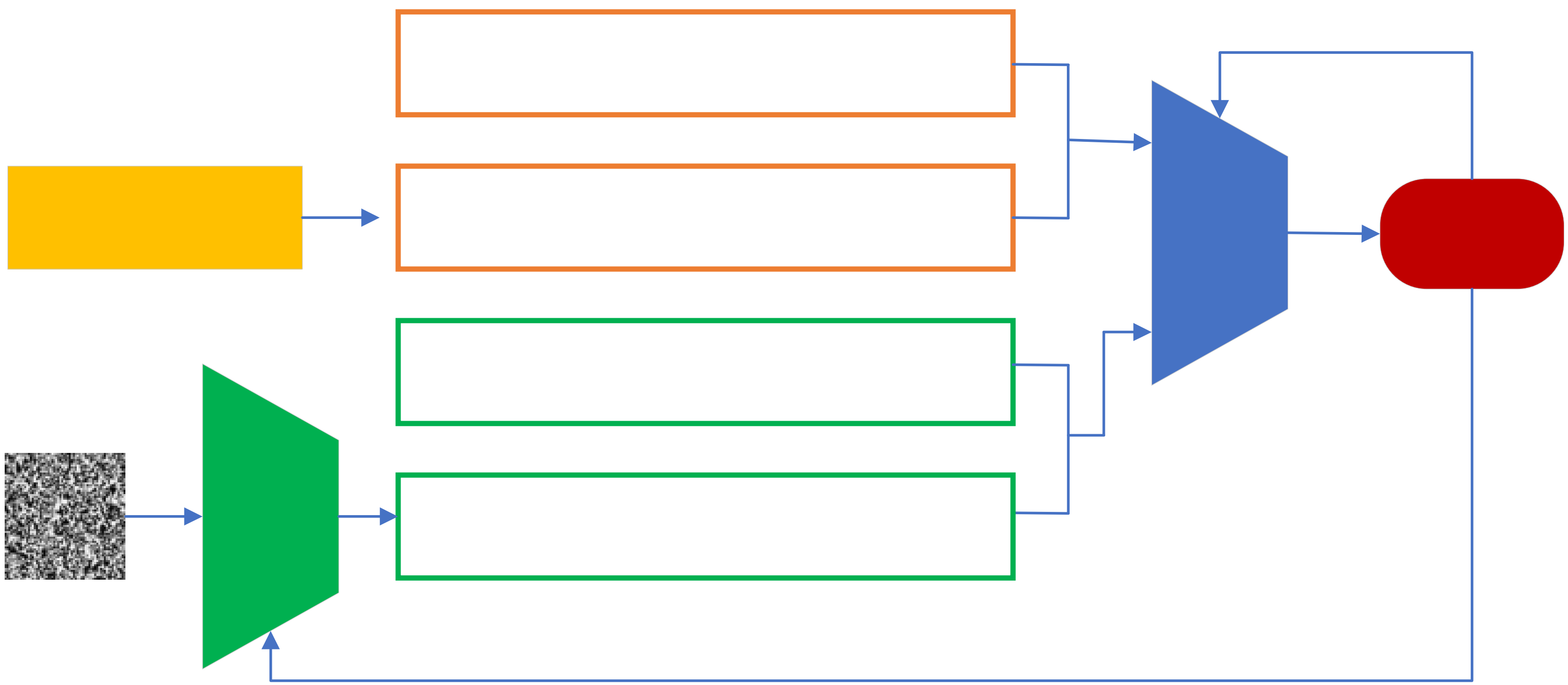
- **Conversion to eliminate sharp edges**
- **Guarantee no generation of non-physical electrons**



Alanazi et al., IJCAI 2021.

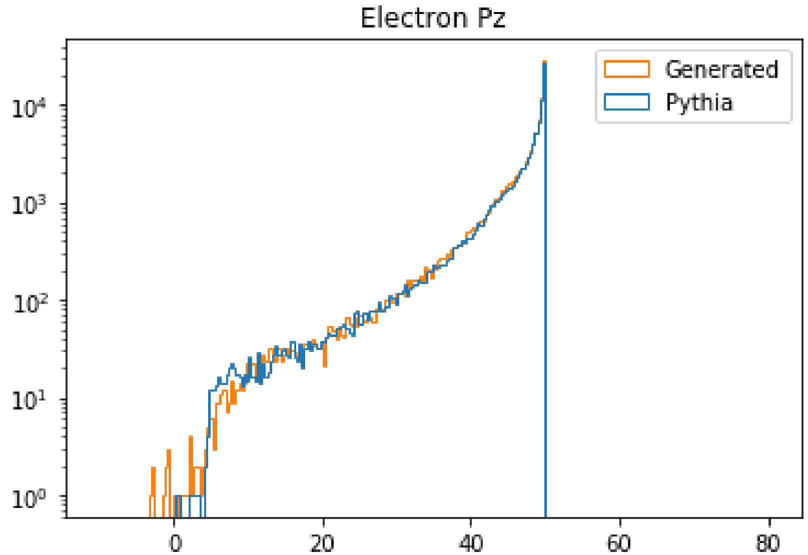
Features Augmentation and Transformation GAN (FAT-GAN)

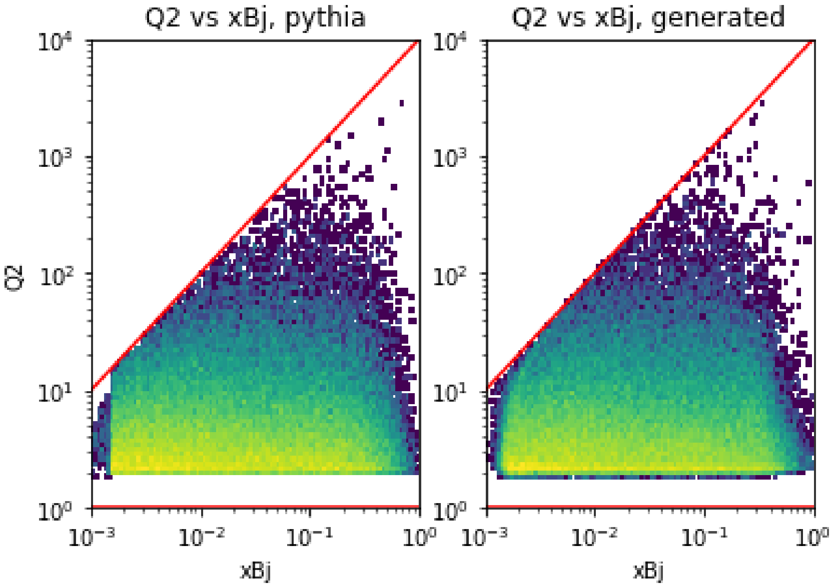
- Features Transformation
- Features Augmentation



Alanazi et al., IJCAI 2021.

Results of FAT-GAN



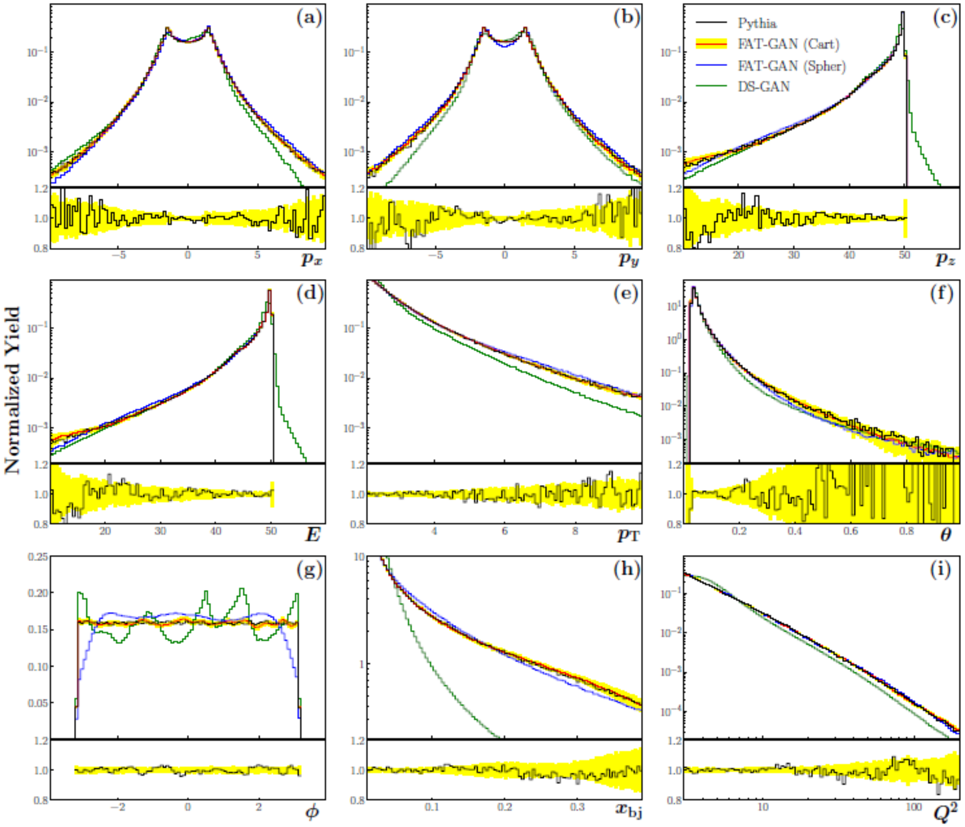


No more non-physical events with p_z > 50 GeV

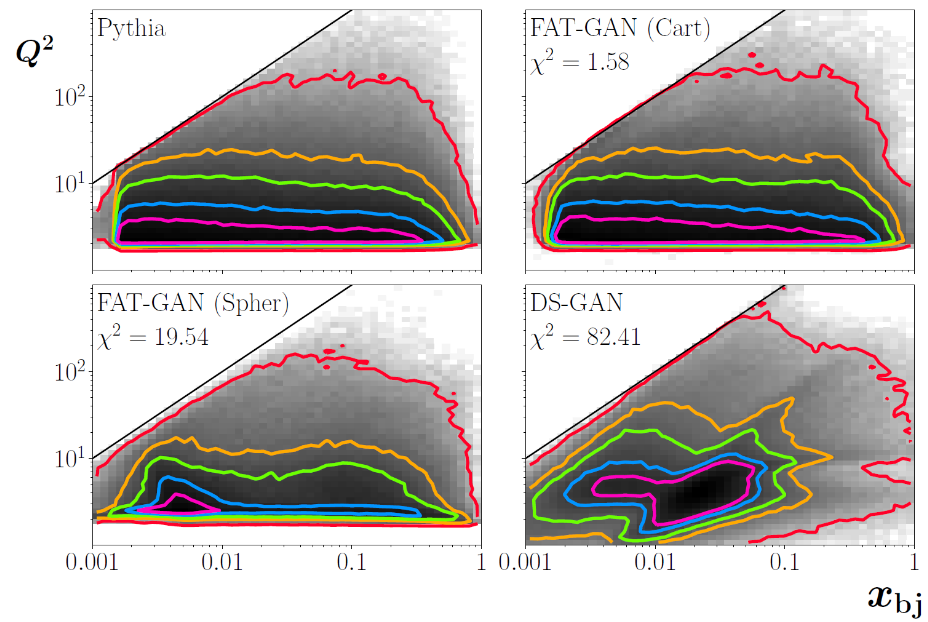
Good approximation of Q^2 and x_{Bj} correlation with $\chi^2 = 1.52$

Alanazi et al., IJCAI 2021.

Distributions of Generated Physical Properties



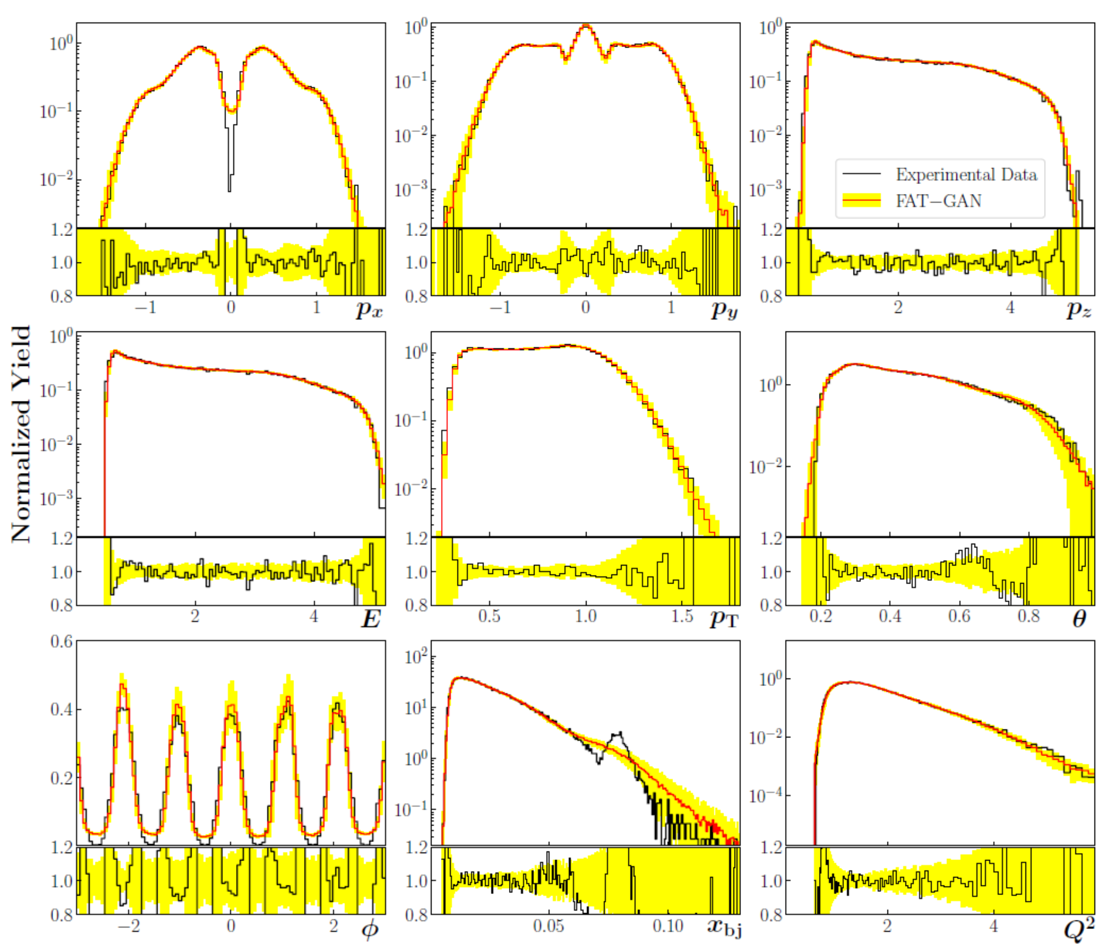
Distributions of Distributions of physical properties of the scattered electron, p_x, p_y, p_z, E, p_T , x_{bj} and Q^2



Joint distributions of Q^2 and x_{bj}

Alanazi et al., IJCAI 2021.

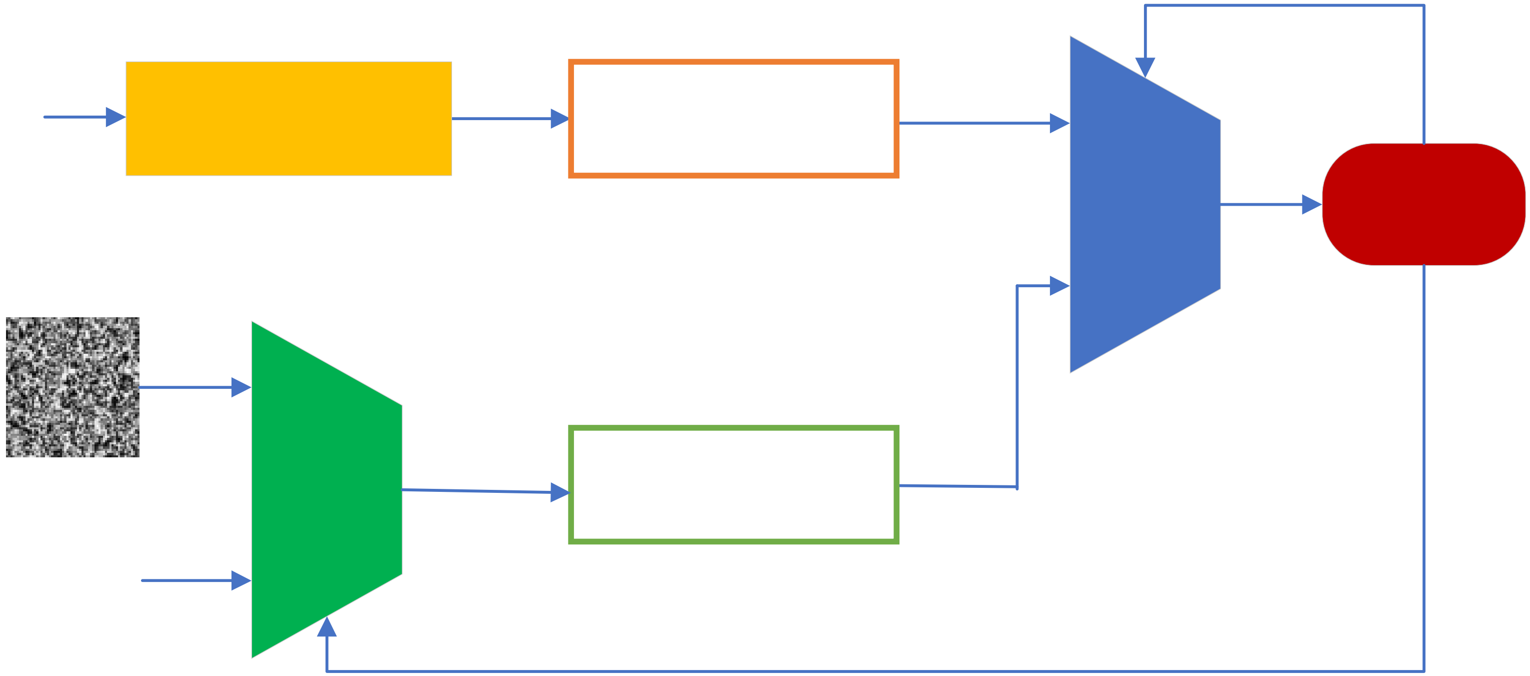
FAT-GAN on experimental electron-proton scattering data



Alanazi et al., IJCAI 2021.

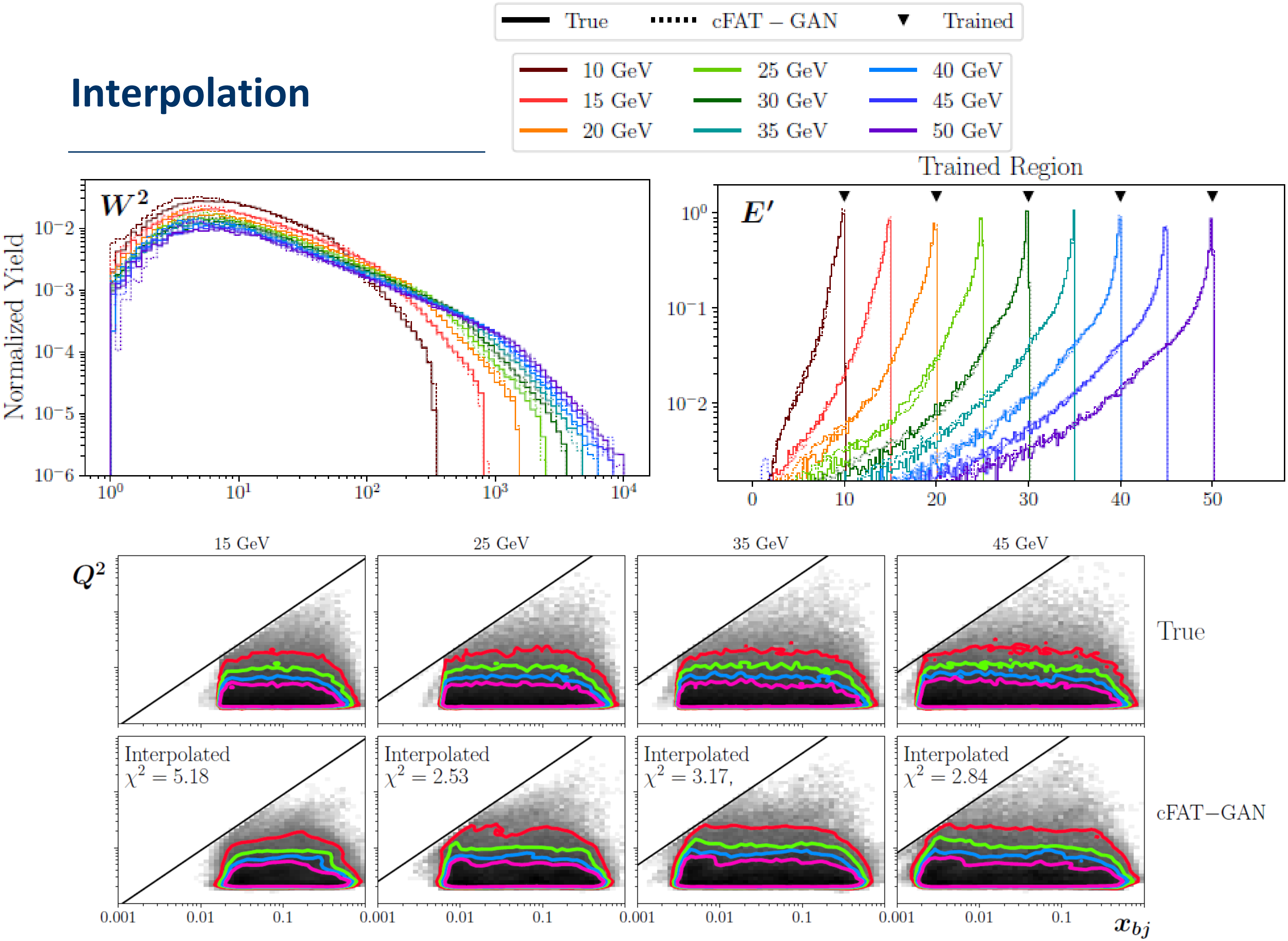
Conditional GAN

- **A GAN-based Event Generator w.r.t. Beam Energy Input**

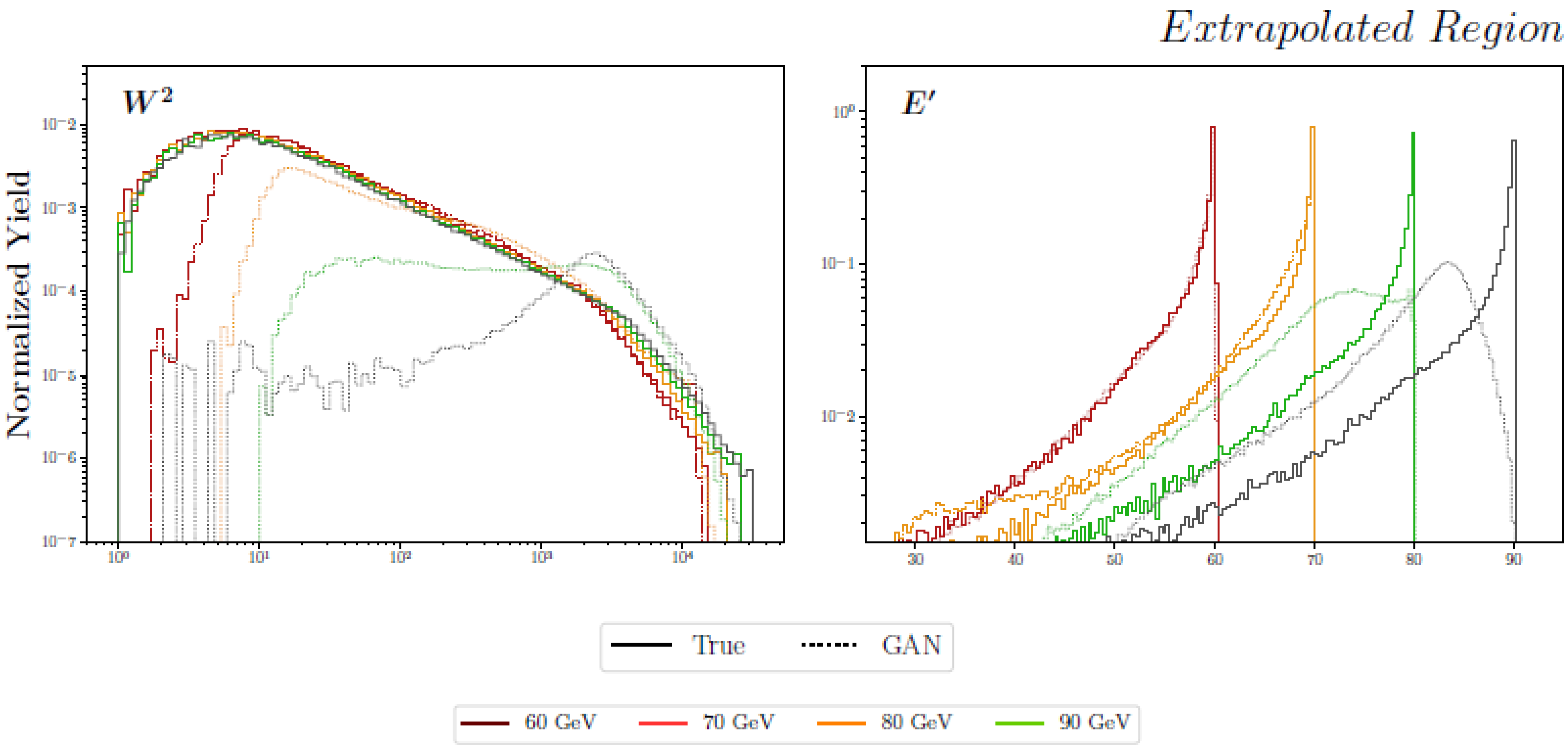


Velasco et al, ICMLA 2020

Interpolation

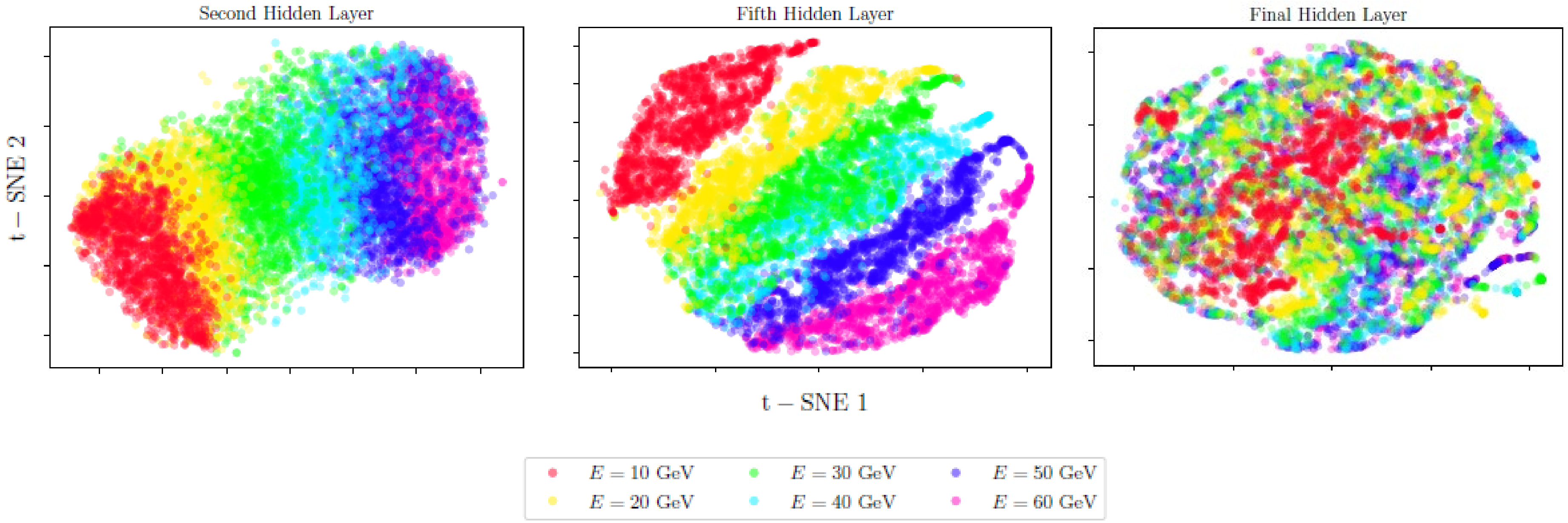


Extrapolation



Velasco et al, ICMLA 2020

Latent Space



Velasco et al, ICMLA 2020

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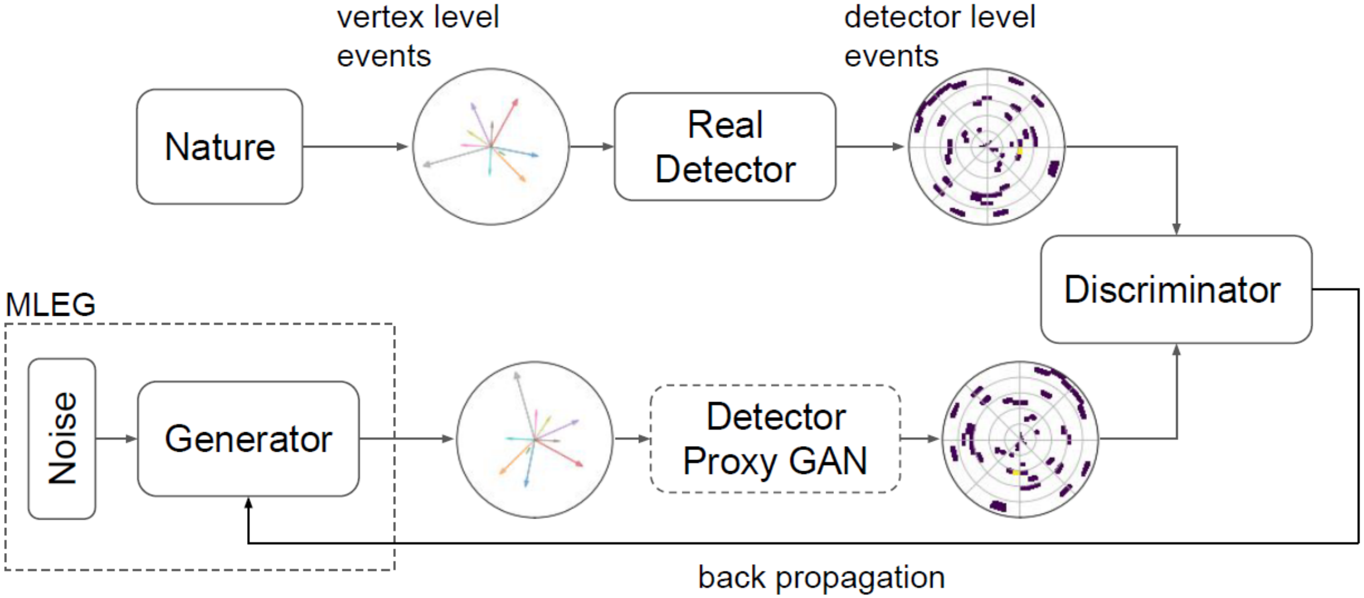
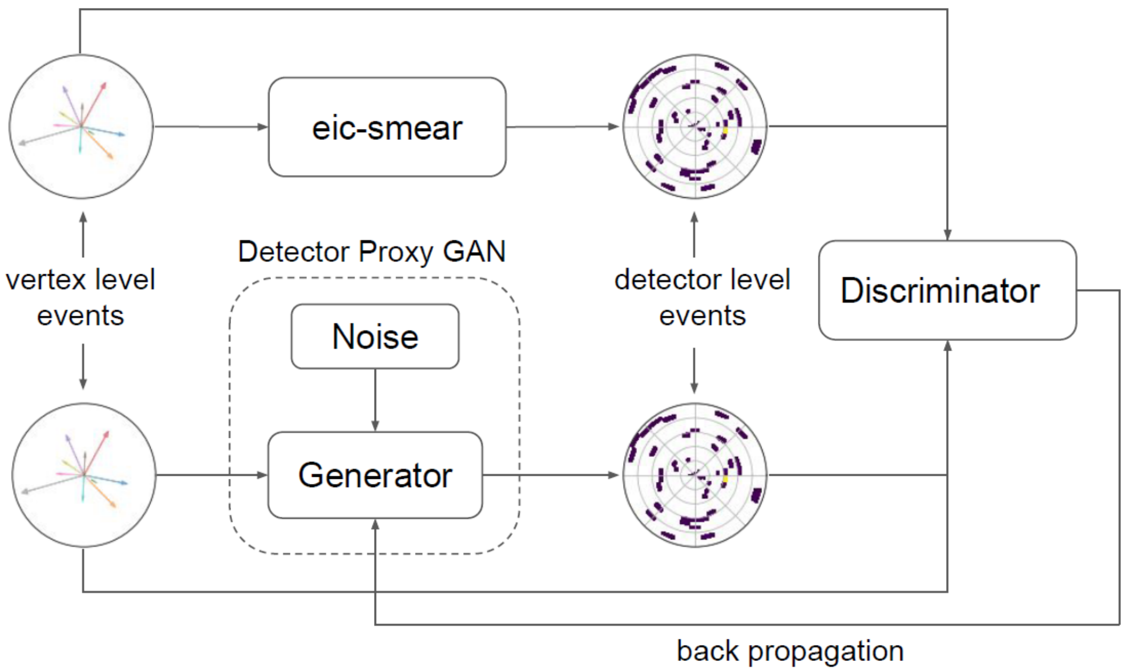
Unfolding Vertex-level Events from Detector-level Events

- **MLEG**
  - Transform noise into vertex-level simulated events
- **Detector Proxy (Surrogate) GAN**
  - Detected simulator
  - Mimic synthetic detector-level events
- **Discriminator**
  - Differentiate detector-level events



Detector Surrogate

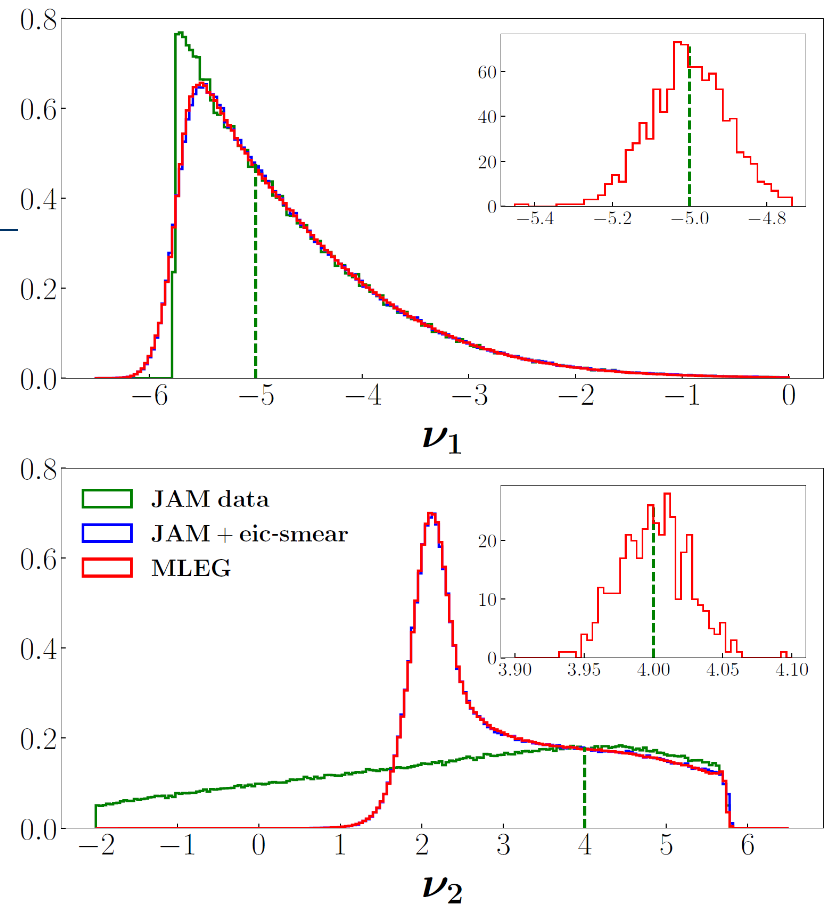
- **Detector Proxy GAN**
  - Conditional GAN
  - Training samples
    - From guessed vertex-level samples and corresponding detector-level samples using a detector simulator



Alanazi et al., Phys. Rev. D 106, 096002, 2022

Detector Surrogate for Electron-Proton Scattering

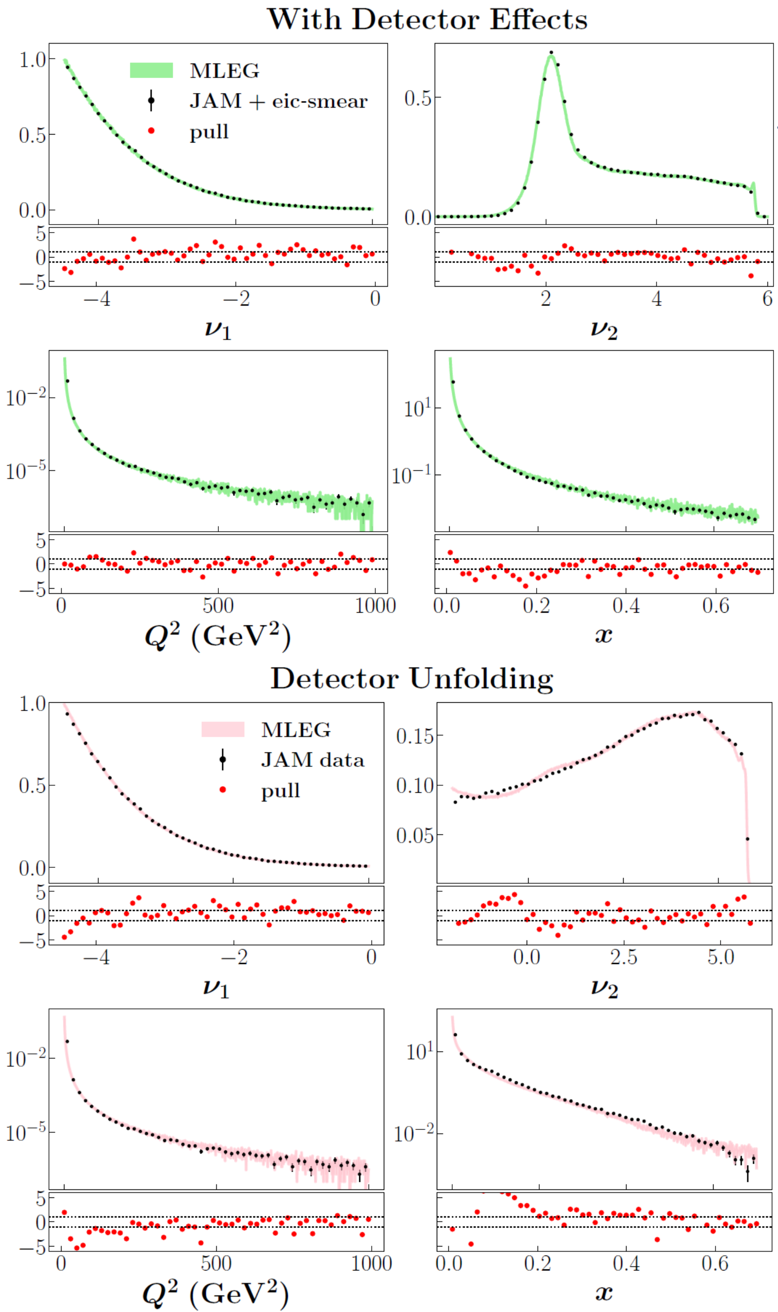
- **Detector Surrogate**
  - Conditional GAN Architecture
  - Translate vertex-level events to detector level events
  - Trained by detector parametrization provided by the eic-smear.
- **Vertex-level events**
  - JAM global QCD analysis
- **Detector-level events**
  - Simulated by EIC-smear
  - Vertex- and detector-level distributions for ν_1 and ν_2, where significant distortions are observed

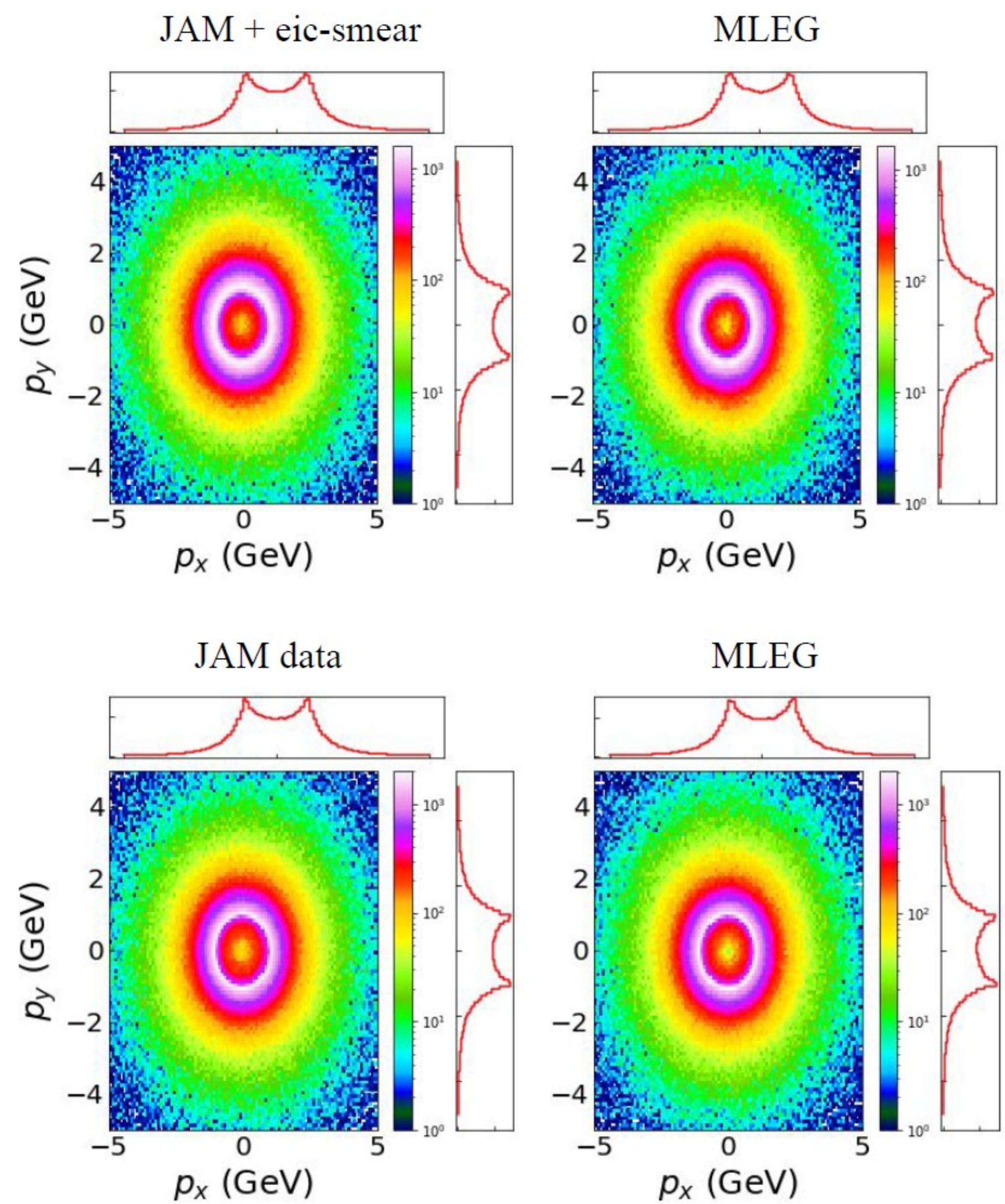


Comparison of training features at the vertex level (generated, green histograms) and detector level (smeared, blue histograms) with the MLEG generated synthetic data (red histograms). The insets illustrate the local smearing effect at the points indicated by the green vertical dashed lines.

Alanazi et al., Phys. Rev. D 106, 096002, 2022

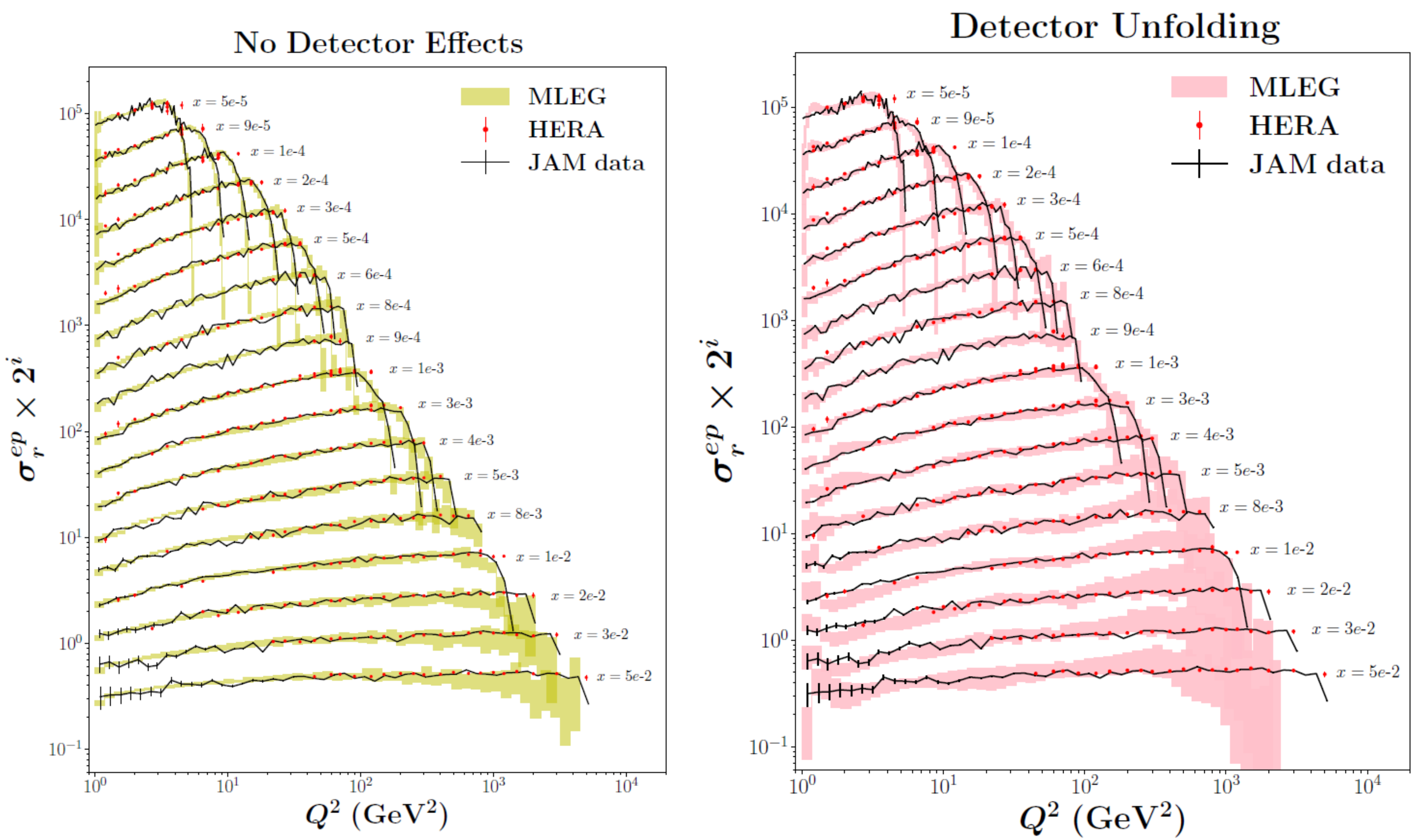
Unfolding Results





Alanazi et al., Phys. Rev. D 106, 096002, 2022

HERA



Alanazi et al., Phys. Rev. D 106, 096002, 2022

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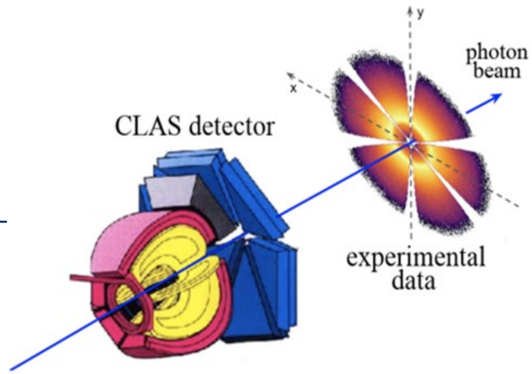
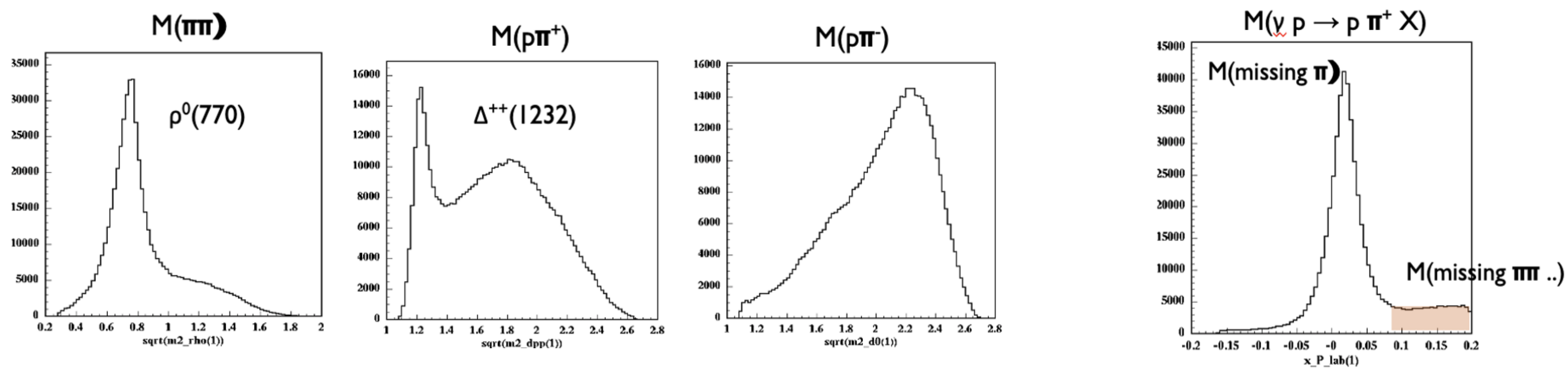
CLAS Exclusive 2π photoproduction



- **CLAS g11 kinematics**
  - Dataset used by CLAS Collaboration
    - M. Battaglieri et al. (CLAS Collaboration) Phys. Rev. Lett. 102, 102001
    - M. Battaglieri et al. (CLAS Collaboration) Phys. Rev. D 80, 072005
  - Focus on $\gamma p \rightarrow p\pi^+ \ (\pi^-)$
  - Fiducial cuts (p, θ, ϕ) are used
  - Final exclusive 2π state identified by missing mass technique
    - Variables are reconstructed by energy/momentum conservation



Unfolding Detector Effect for CLAS Exclusive 2π photoproduction

- **Two main components:**
  - **Detector Simulation GAN (DS-GAN): Simulate the smearing detector effects**

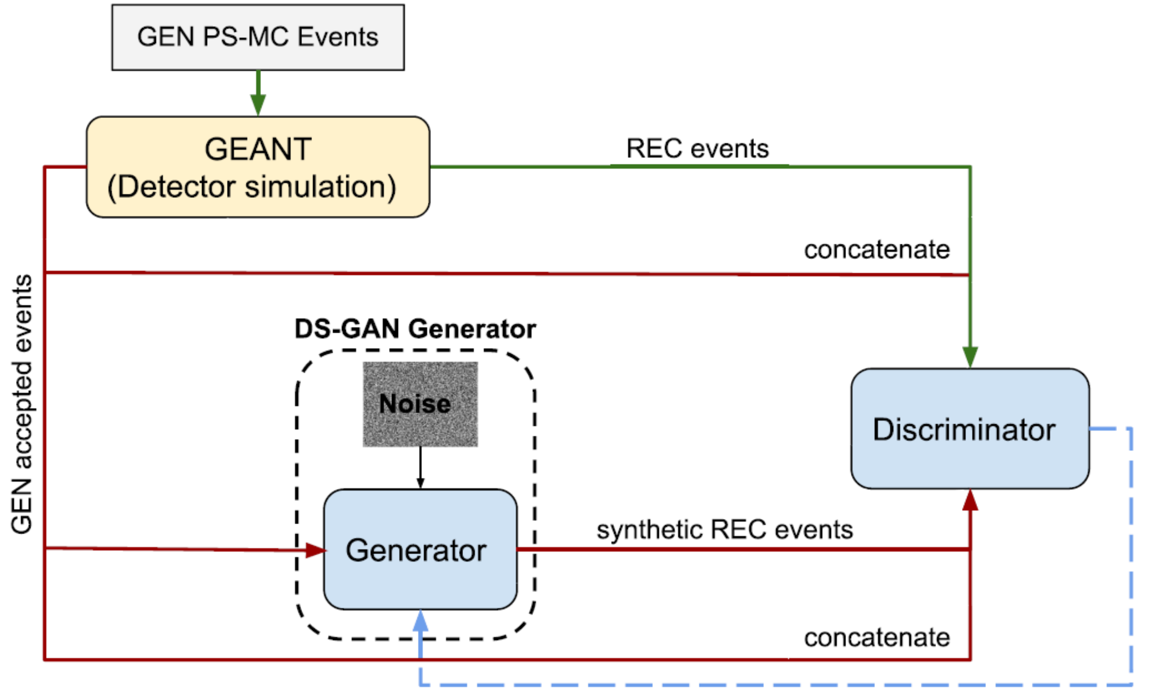
MC-Phase Space Events

  - **Unfolding GAN (UNF-GAN): Reconstruct the vertex-level events.**

MC-Realistic Events

Alghamdi et al., Phys. Rev. D 108, 094030, 2023

Detector Simulation GAN (DS-GAN)

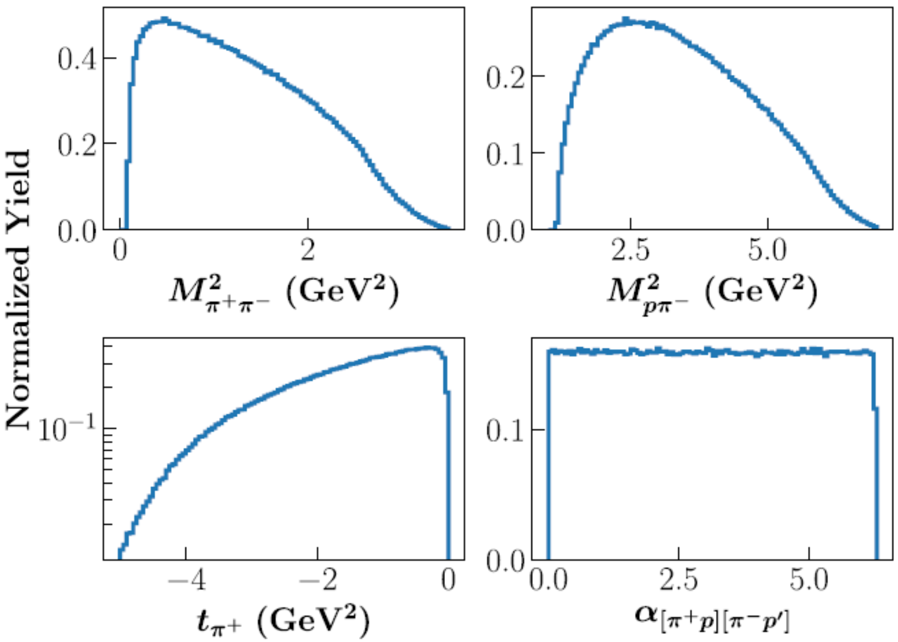


- Schematic view of DS-GAN
  - Generator converts input GEN vertex-level events features and noise into REC detector-level events.
  - The training is performed on PS-MC pseudodata passed through the GEANT simulation.
  - Synthetic REC and REC pseudodata are concatenated with GEN PS-MC events and fed to the discriminator.

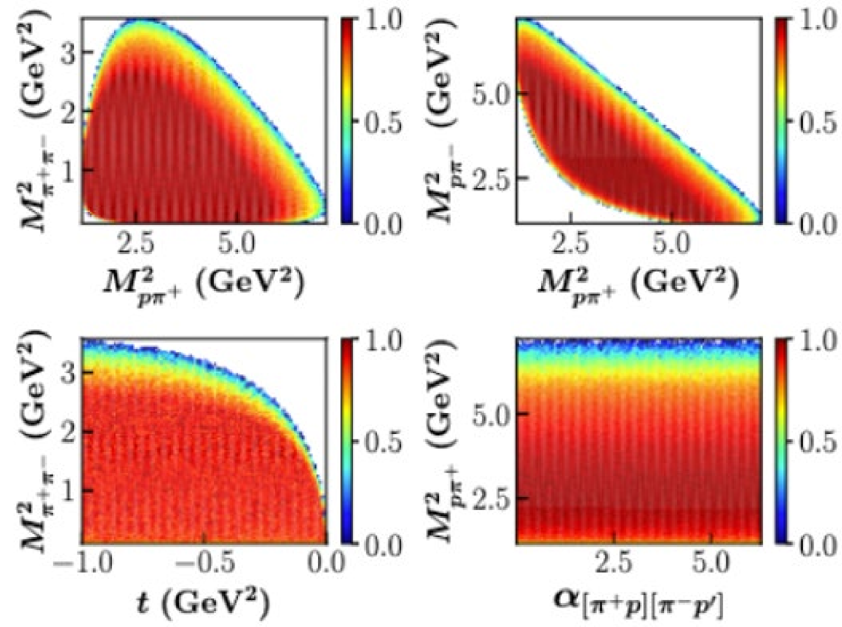
Alghamdi et al., Phys. Rev. D 108, 094030, 2023

Phase Space (PS-MC) Event Generator

Distribute final-state events according to the $\pi^+ \pi^- p$ phase space



1D-Projection



2D-Distribution

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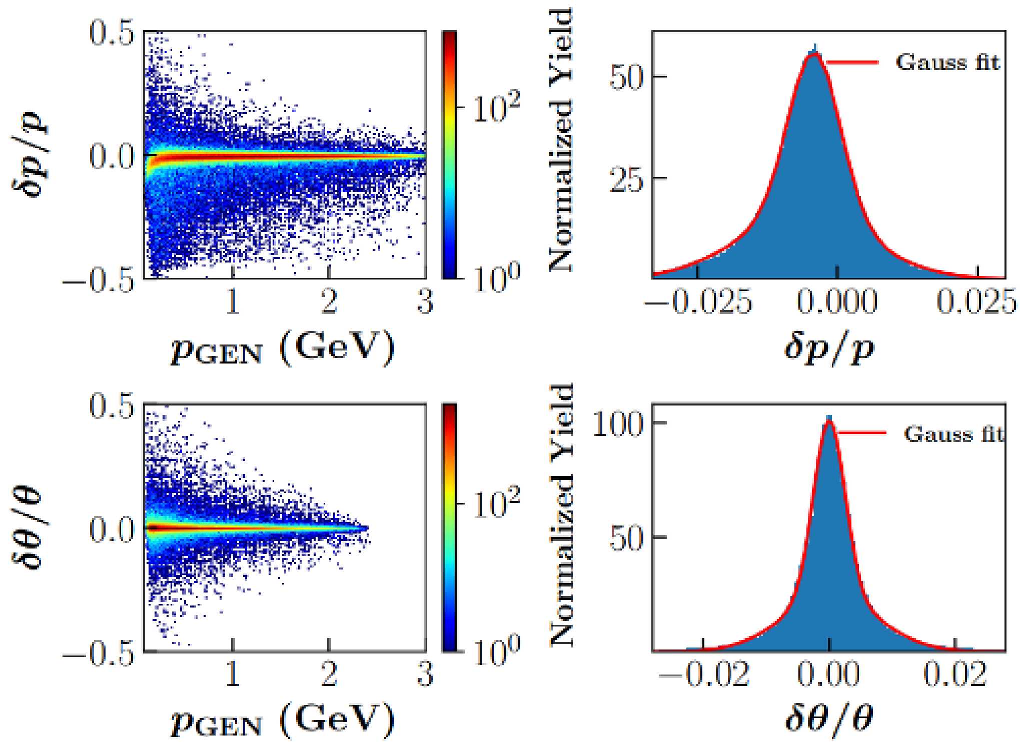
GSIM-GEANT for Detector Simulation



Apply detector simulation package GSIM to simulate detector effects (acceptance and resolution) based on GEANT3

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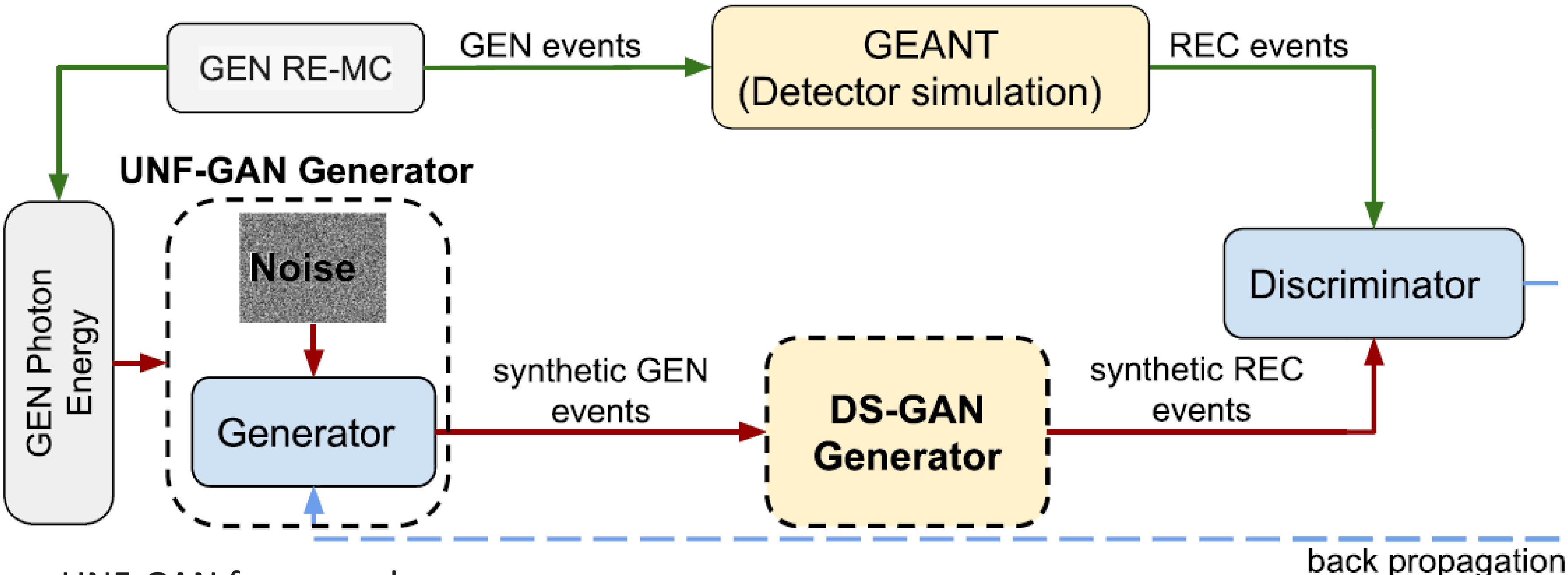
Unfolding GAN (UNF-GAN)



- UNF-GAN framework
  - Generator converts a GEN photon energy and random noise into synthetic GEN event features
  - DS-GAN introduces simulated detector effect and converts synthetic GEN events into synthetic REC event features.
  - Discriminator compares the features of the synthetic REC events and the REC events through GEANT.

Alghamdi et al., Phys. Rev. D 108, 094030, 2023

2π Photoproduction Closure Test

- **Generate events with a realistic MC (RE-MC) 2π Photoproduction model**
- **Apply detector effects with GSIM-GEANT**
- **Train a DS-GAN to learn detector effects using PS-MC + GSIM-GEANT**
- **Deploy the UNF-GAN that includes the DS-GAN, trained with RE-MC REC events**
- **Compare UNF-GAN GEN-SYNT events to RE-MC GEN events**

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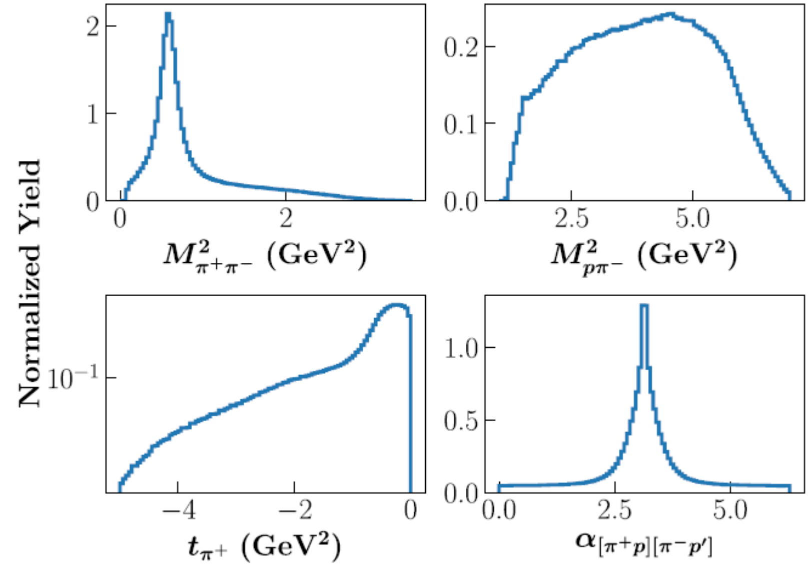
Realistic MC (RE-MC)

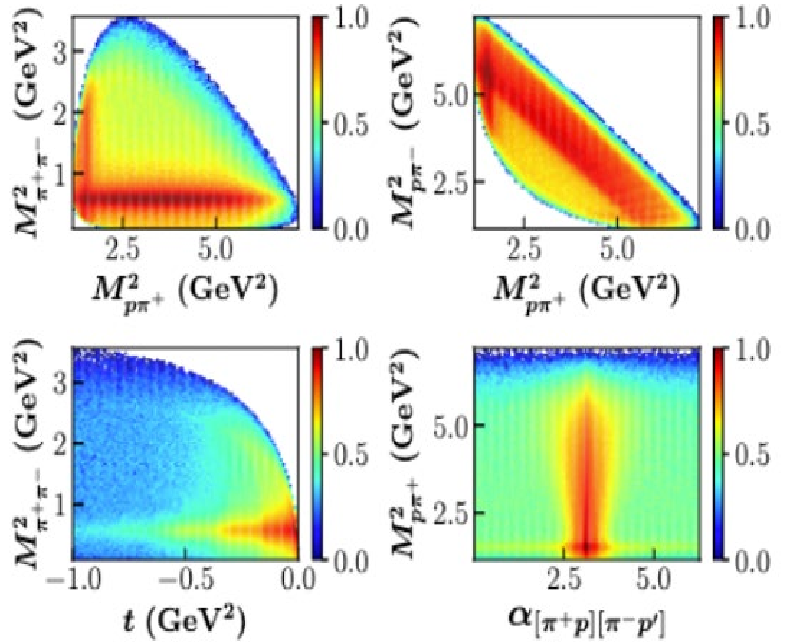
- Realistic MC (RE-MC)
  - Amplitude squared as an incoherent sum of the three dominant intermediate resonances observed,

    $\gamma p \rightarrow (p\rho^0; \Delta^{++}\pi^-; \Delta^0\pi^+) \rightarrow p\pi^-\pi^+$,

    added to a $\sim$10% constant that mimics the nonresonant two-pion photoproduction contribution.
  - Each process has been weighted with the corresponding contribution to the total cross section.
  - The angular distributions relative to resonance production are parametrized from measured differential cross sections.
  - The decays $p \rightarrow \pi\pi$ and $\Delta \rightarrow p\pi$ are described using the correct spin structure with the decay matrix elements.



1D-Projection



2D-Distribution

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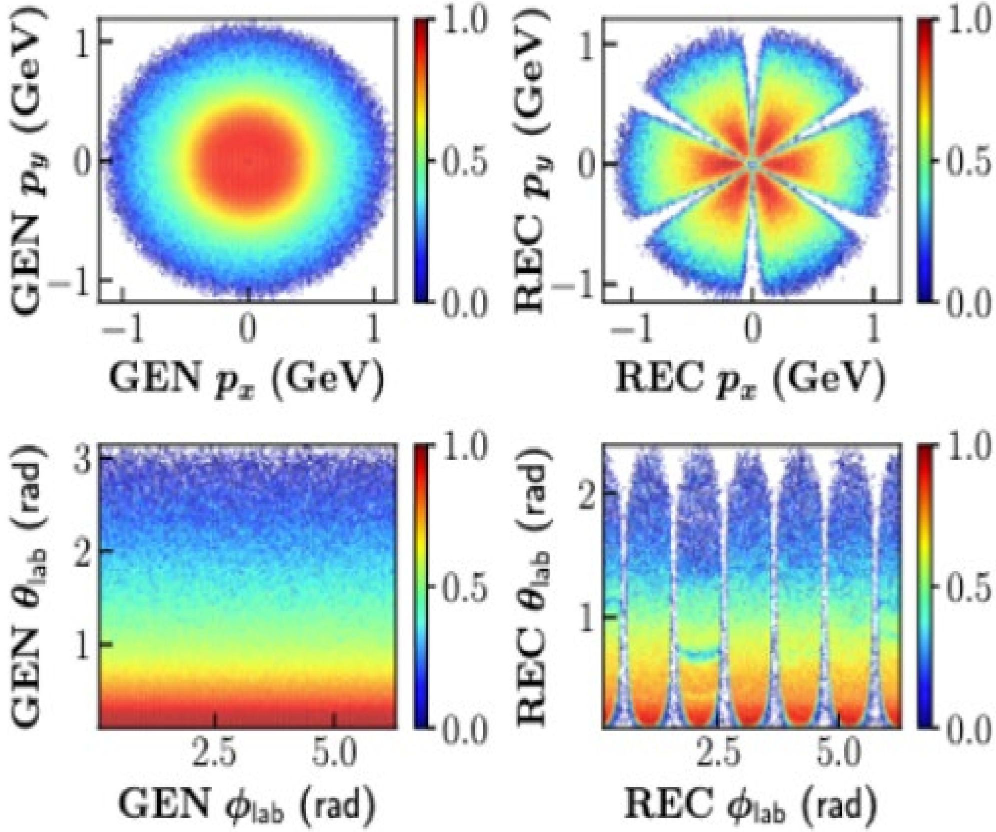
Detector Effects on RE-MC Events



The π^+ kinematic variables in the laboratory reference frame as GENerated with RE-MC (left) and REConstructed by CLAS (right)

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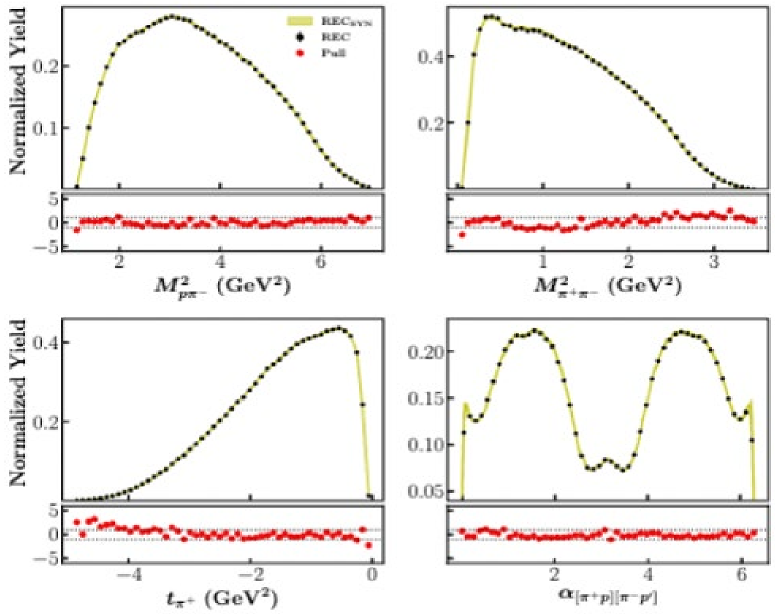
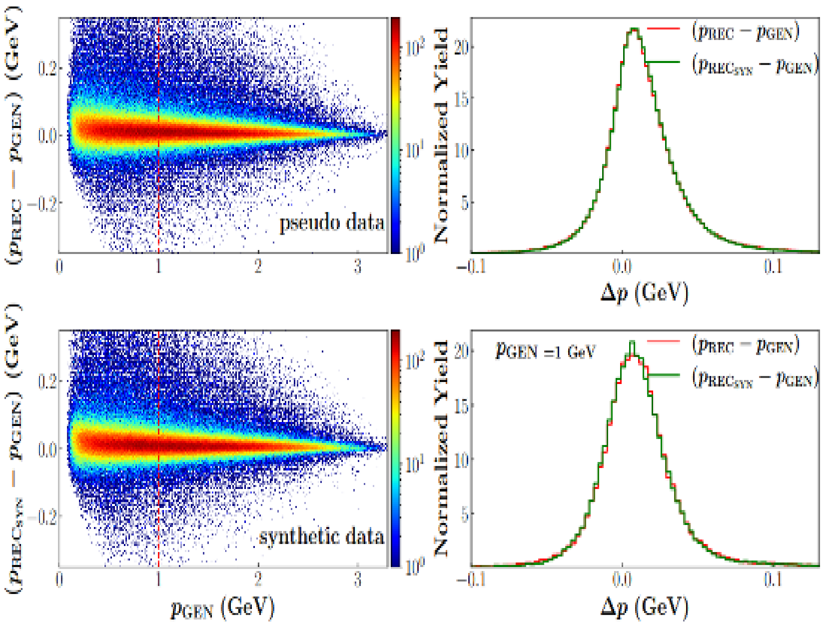
DS-GAN Results

- **DS-GAN can learn the CLAS detector effect**





MC REC events vs DS-GAN synthetic events

CLAS Resolution

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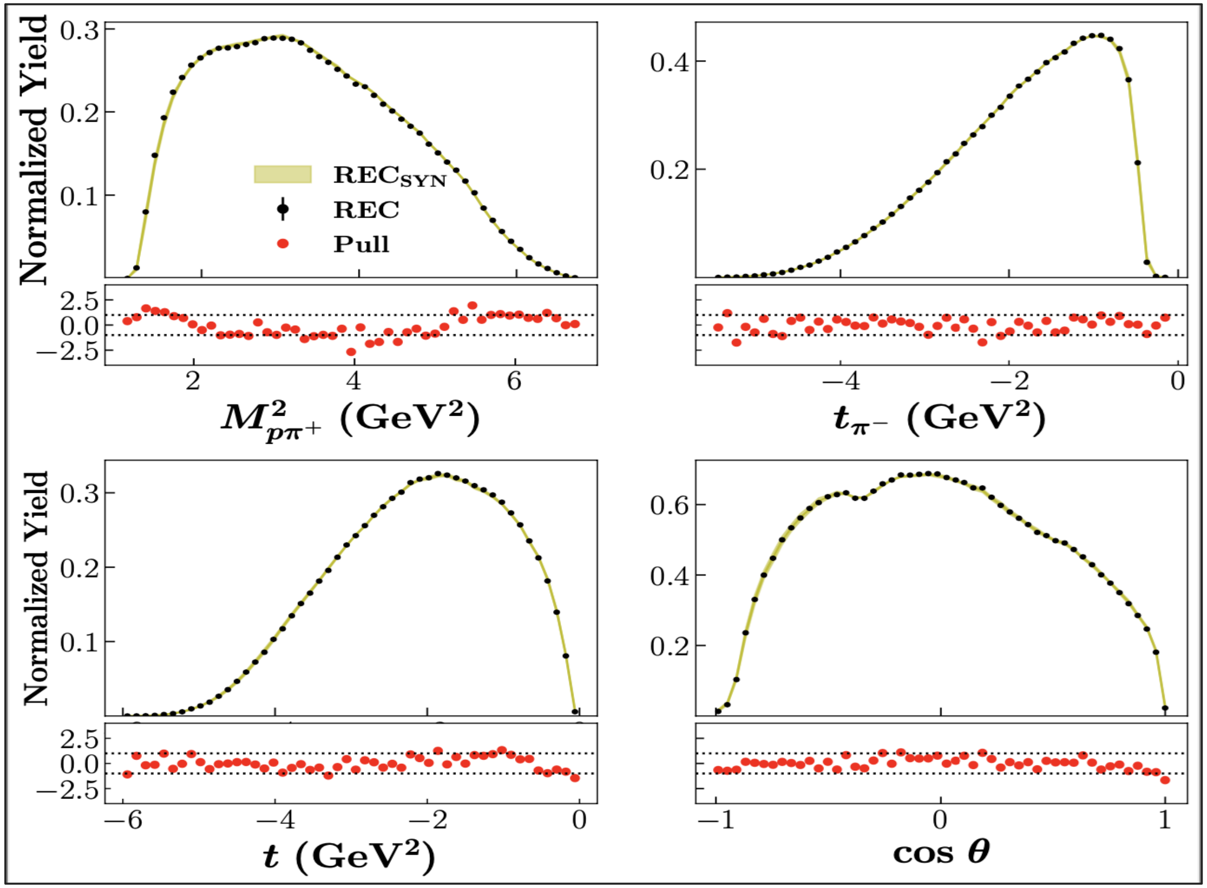
DS-GAN Results on Derived Variables

- **Derived Variables (not used in training)**



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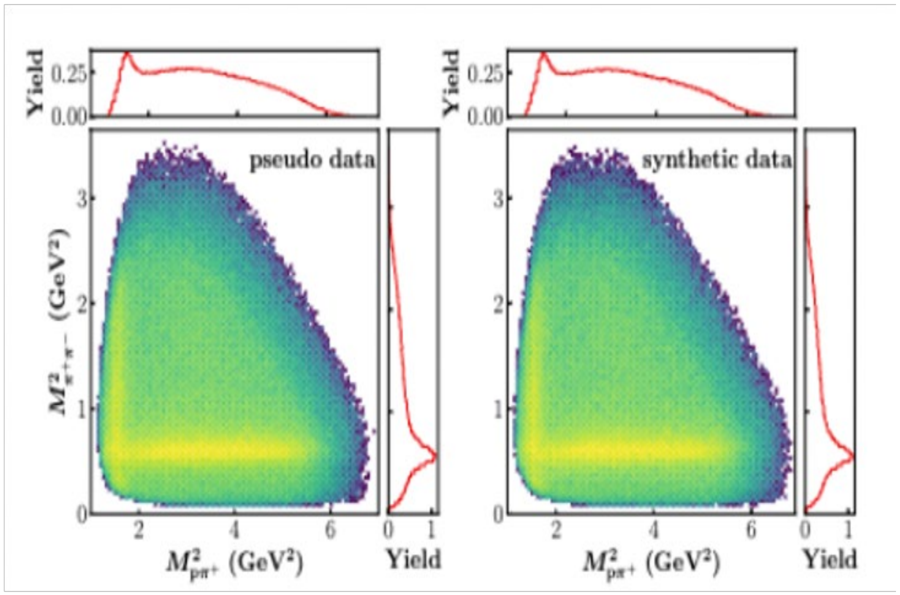
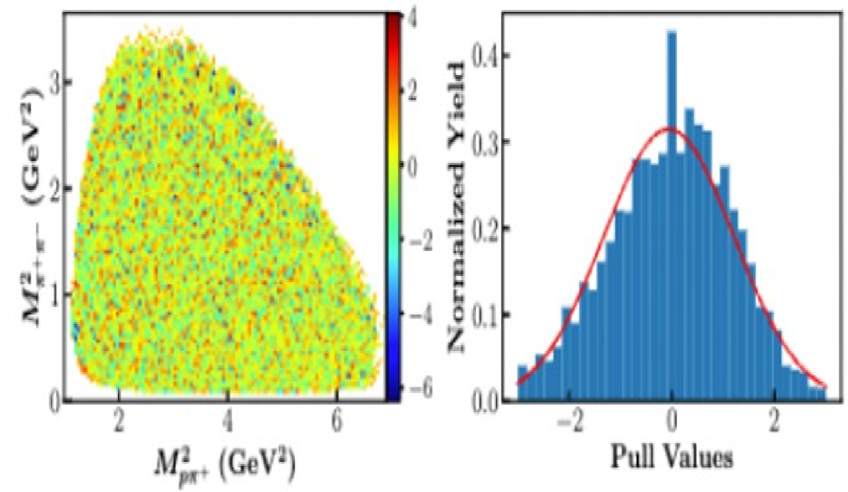
UNF-GAN Results (Unfolding Results)



RE-MC GEN events

UNF-GAN SYN events

$$\text{pull} = \frac{\mu_{\text{SYN}} - \mu_{\text{pseudodata}}}{\sqrt{\sigma^2_{\text{SYN}} + \sigma^2_{\text{pseudodata}}}}$$



2D Pull

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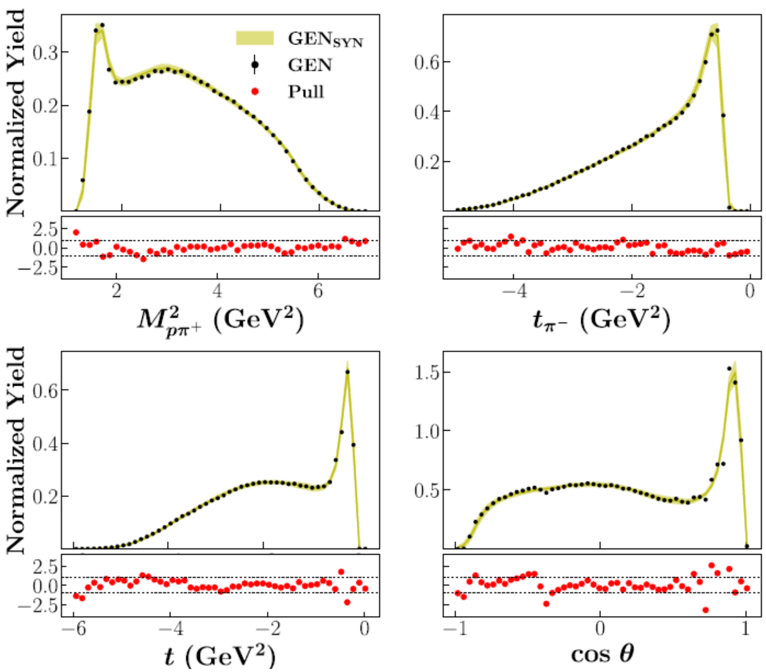
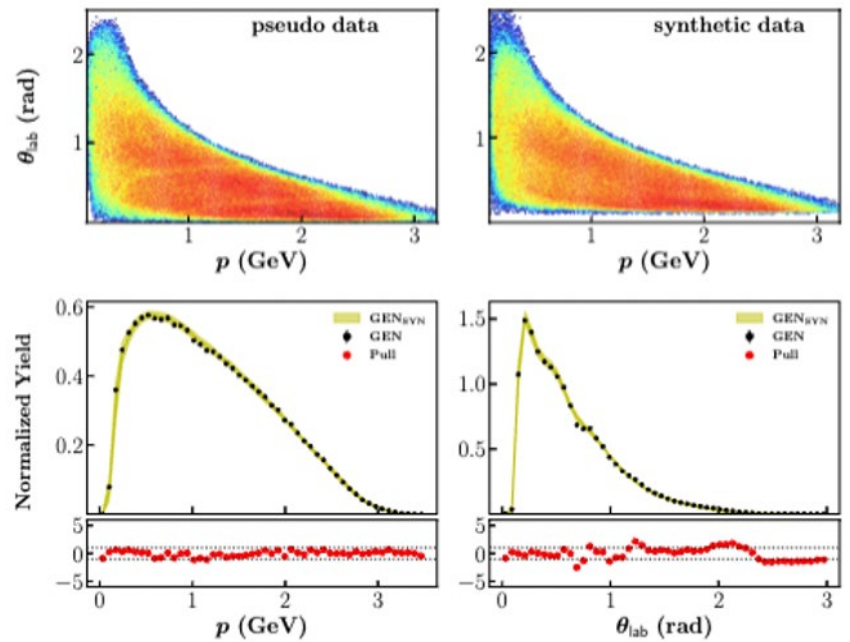
UNF-GAN Results on Derived Variables

- **Derived Variables (not used in training)**



CM Frame



Lab Frame

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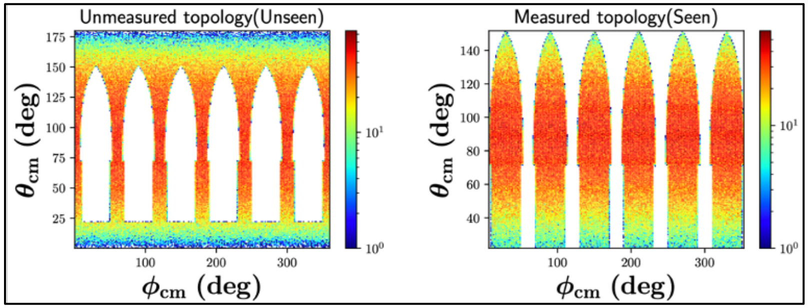
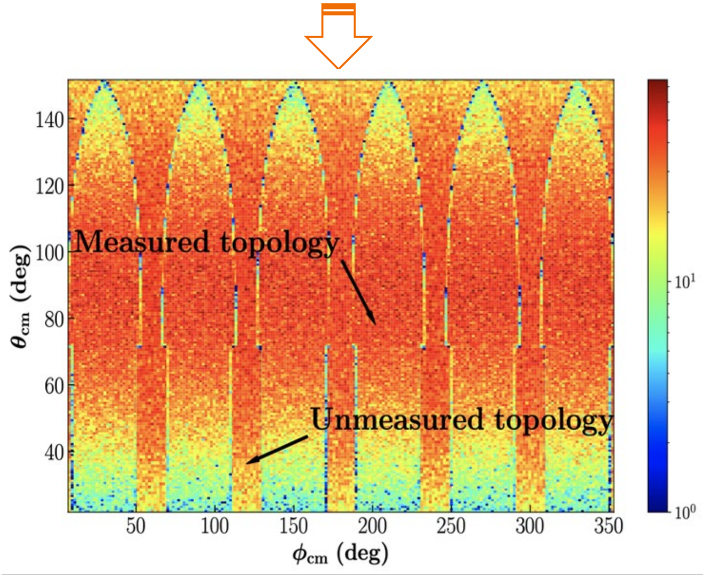
Unfolding Detector Acceptance Effects

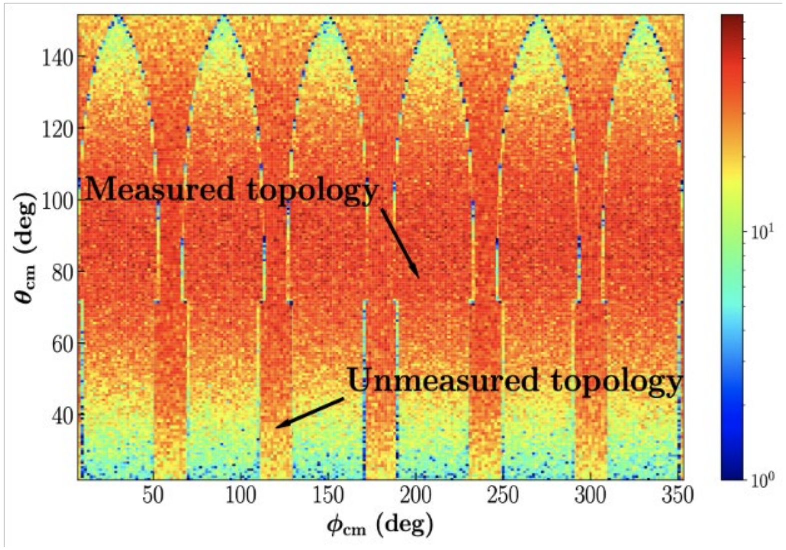
- Detector acceptance effect
  - Limited area coverage in detector
  - Particles produced in certain directions may not be detected.
- Data
  - Single-pion photoproduction reaction $\gamma p \rightarrow \pi^0 p$ in a kinematic range $E_{cm} \sim 1.34 GeV$
  - Event represented by (θ_{cm} and ϕ_{cm})
    - Direction of particle scattering in center-of-mass frame
  - Additional topological state (0 for unmeasured, 1 for measured).

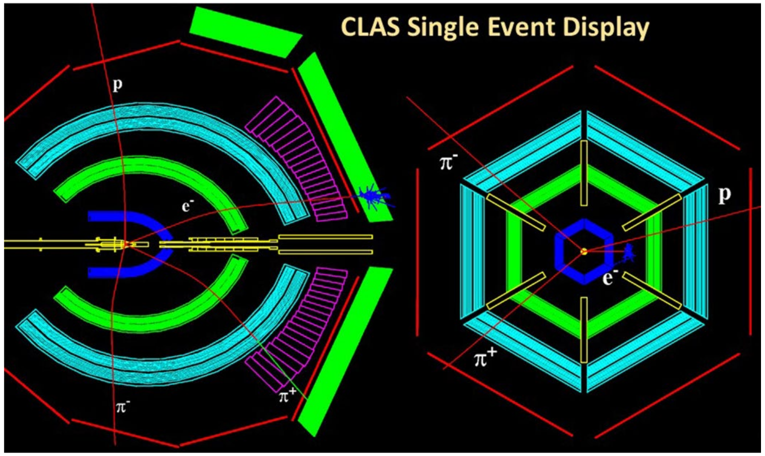




Classifier for Acceptance Effect

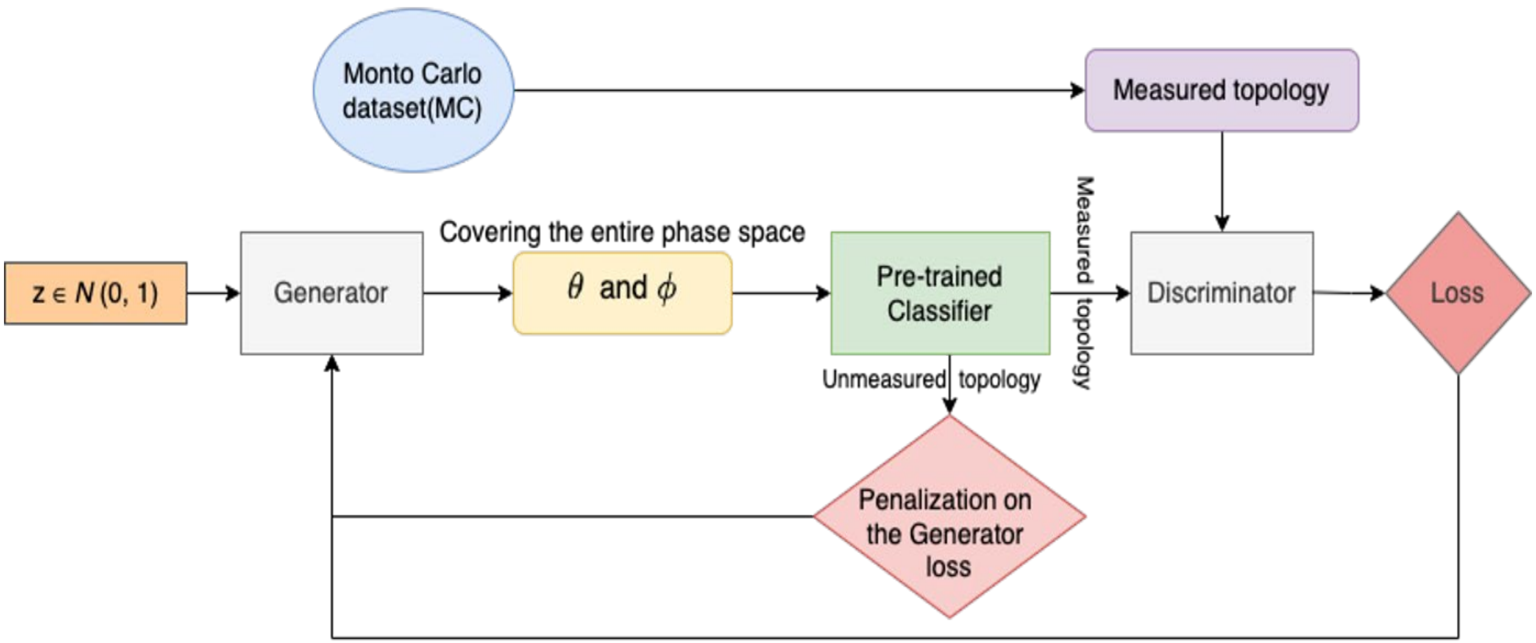
(θ_{cm}, ϕ_{cm}) → **Classifier** → **Measured or unmeasured**





GAN Architecture for Acceptance Unfolding

- Key Feature: a custom, physics-informed penalty term in the generator loss
  - Penalize discrepancies between generated and true unmeasured topology event distributions.



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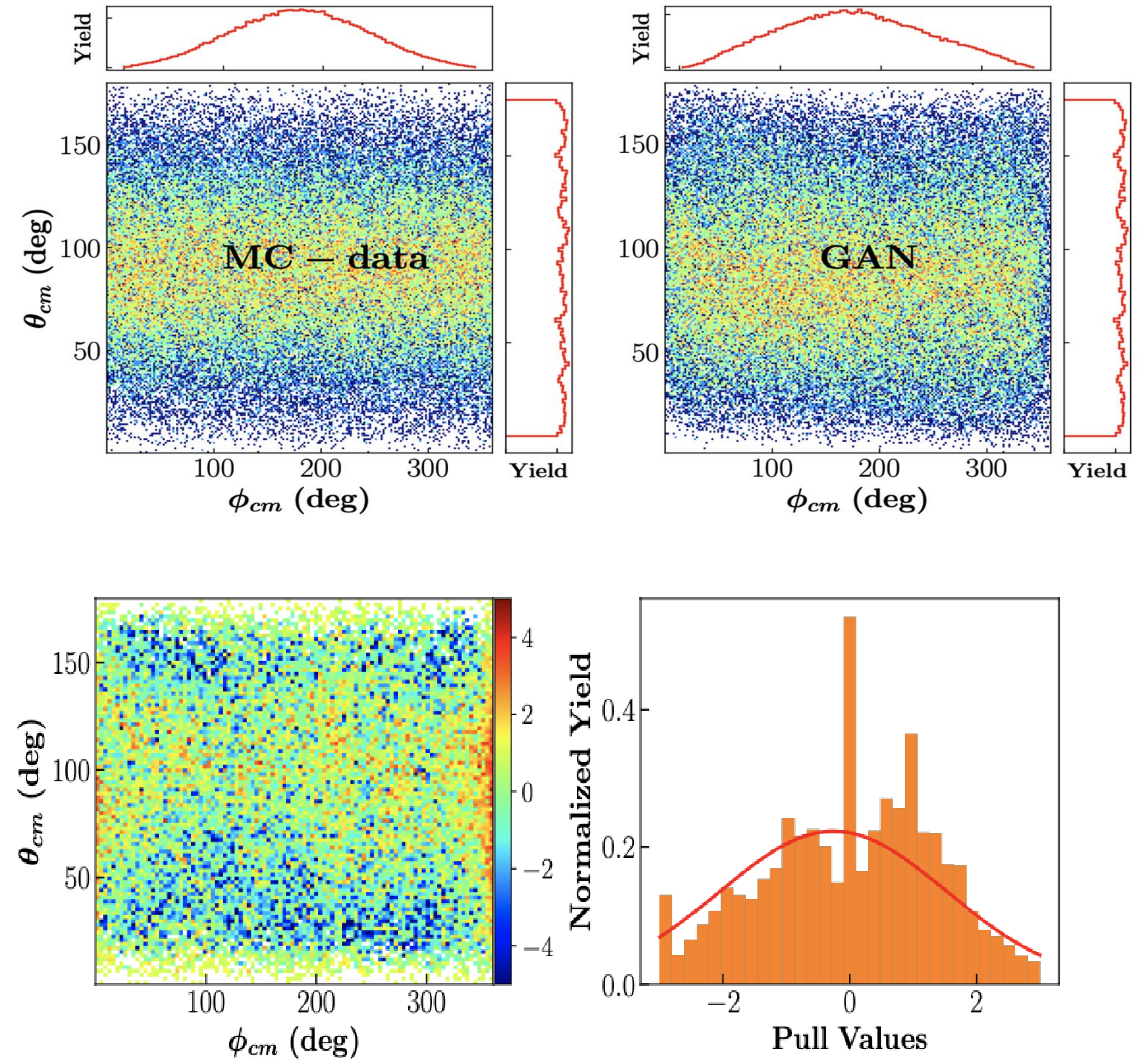
Results



Entire Phase Space

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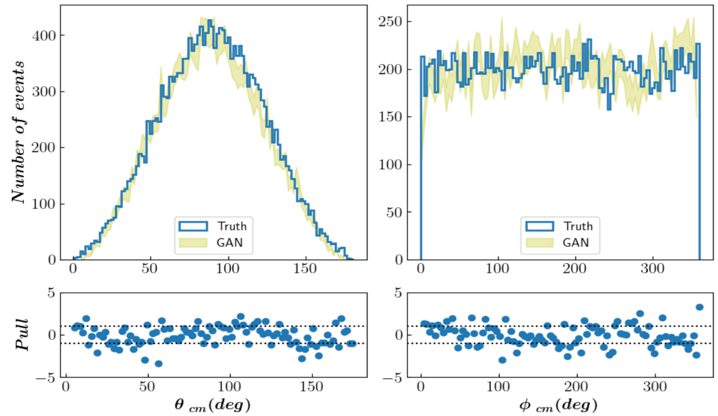
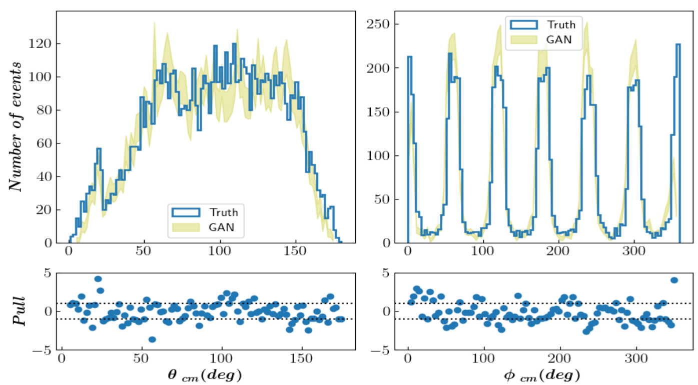
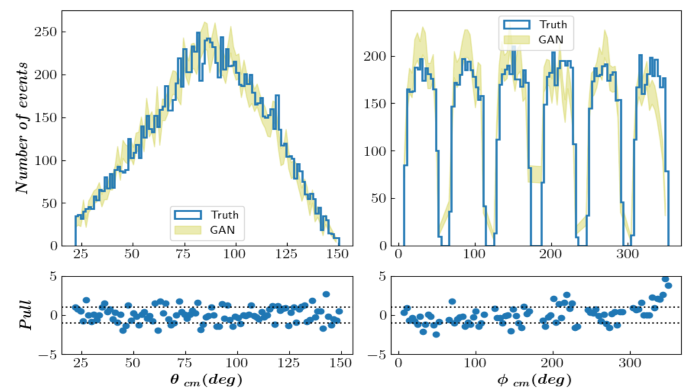
Results of Unfolding Acceptance Effect



Entire Phase Space



Unmeasured topology



Measured topology

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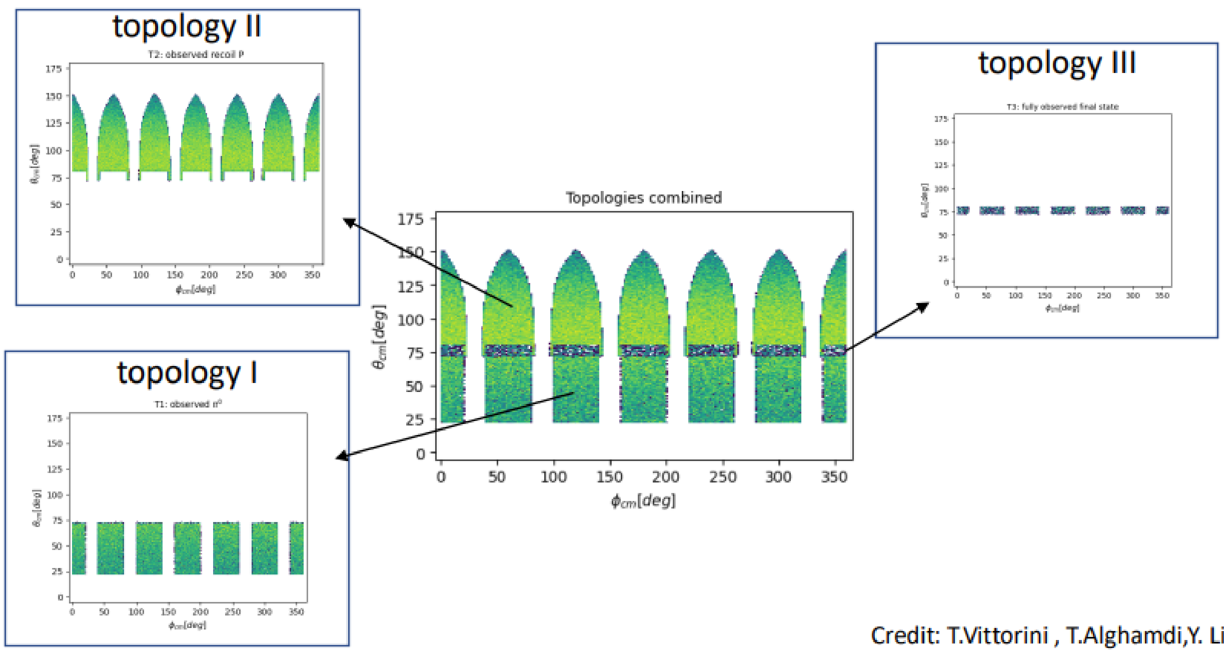
- **Conclusion and Future Work**

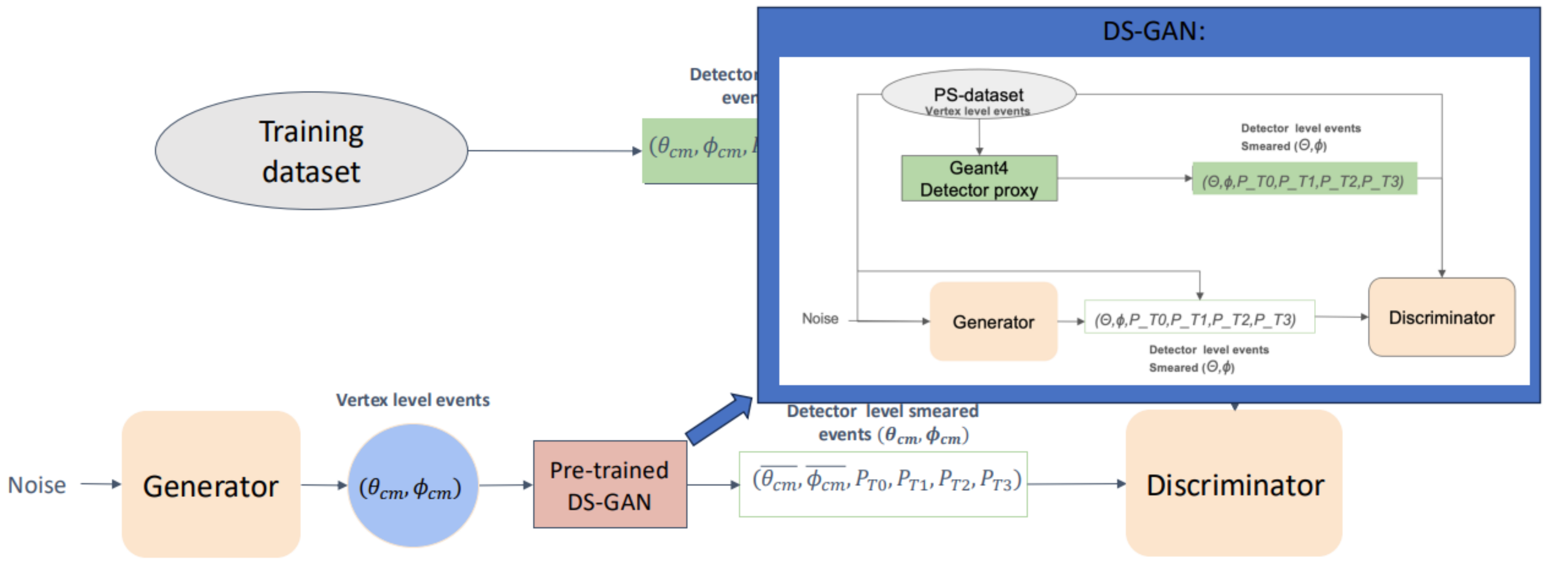
Generative AI for Multiple Topologies

- Build a single ML model to generate in the full phase space
    - According to the correct distributions

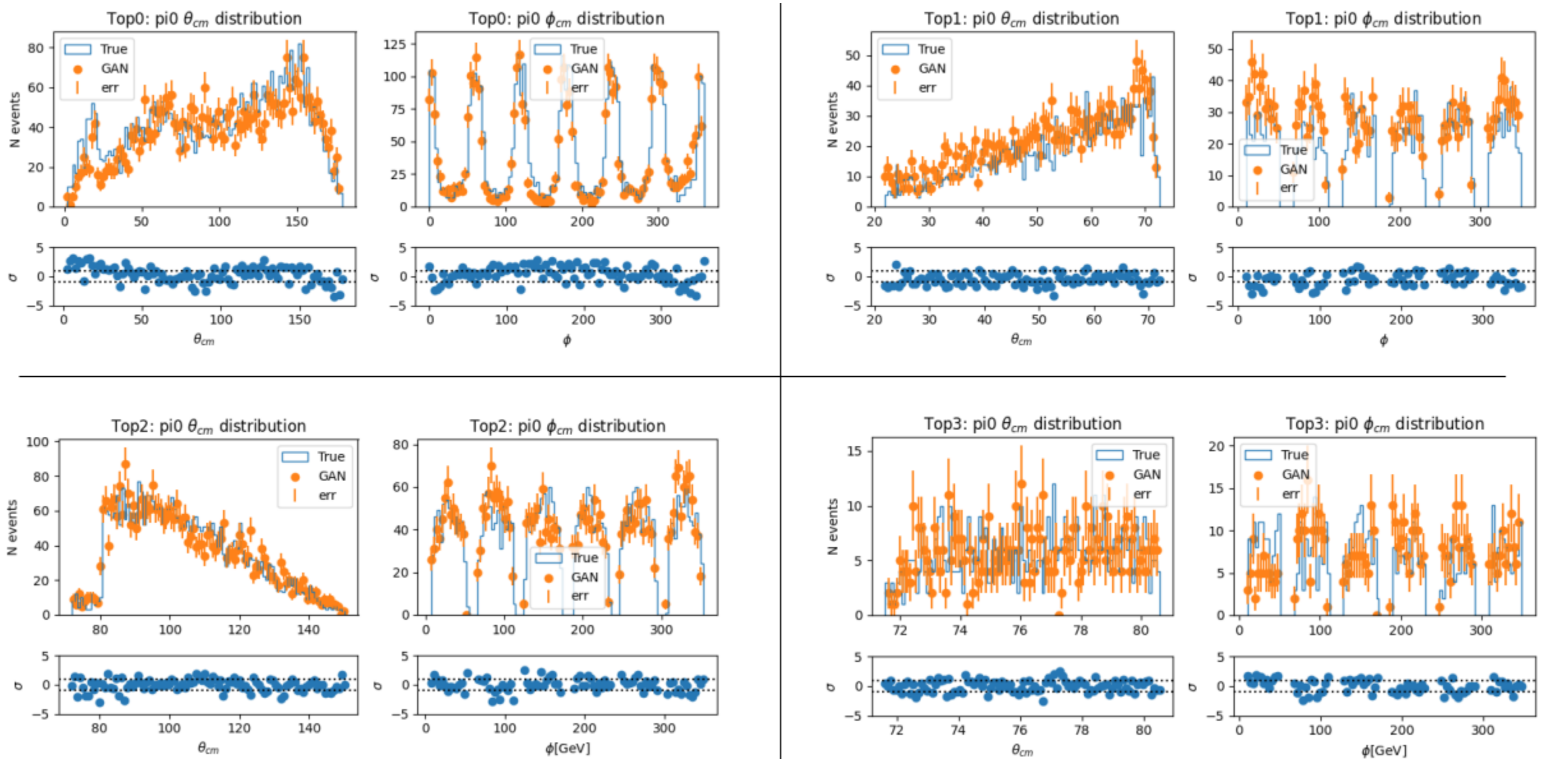


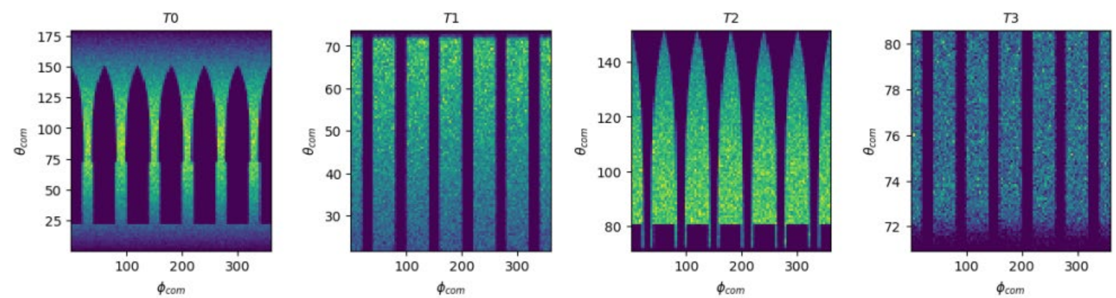
Credit: T.Vittorini , T.Alghamdi,Y. Li

GAN Architecture for Multiple Topologies Simulation

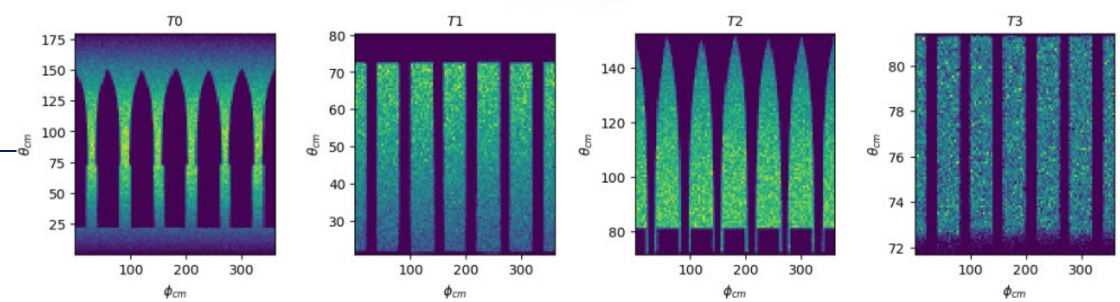


Results





Generated:



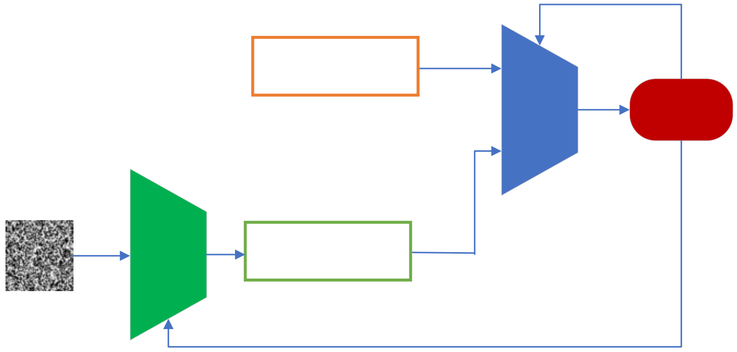
Tommaso Vittorini et al., GANs towards data smearing and acceptance corrections

Agenda

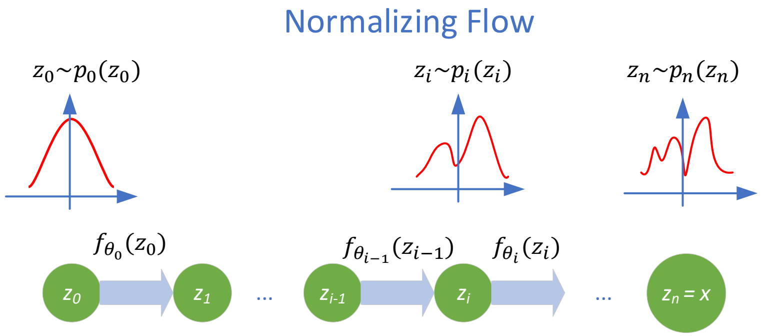
- **Initial Attempt in Exclusive Electron-Proton Scattering**
  - FAT-GAN
  - Conditional GAN
- **Unfolding Smearing Effects**
  - Electron-Proton Scattering
  - CLAS Exclusive 2π photoproduction
- **Unfolding Acceptance Effects**
  - Single-pion photoproduction reaction
- **Multiple Topologies**
- **Conclusion and Future Work**

Generative AI

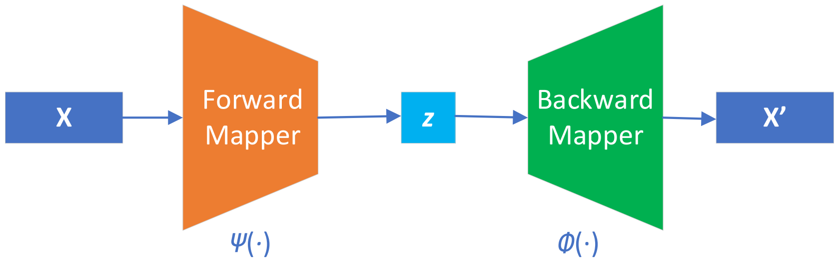
- **Generative Adversarial Networks (GANs)**



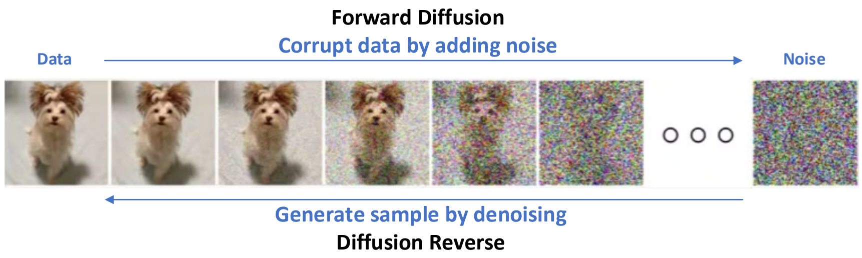
- **Normalizing Flow (NF)**



- **Variational Autoencoder (VAE)**



- **Diffusion Models (DM)**



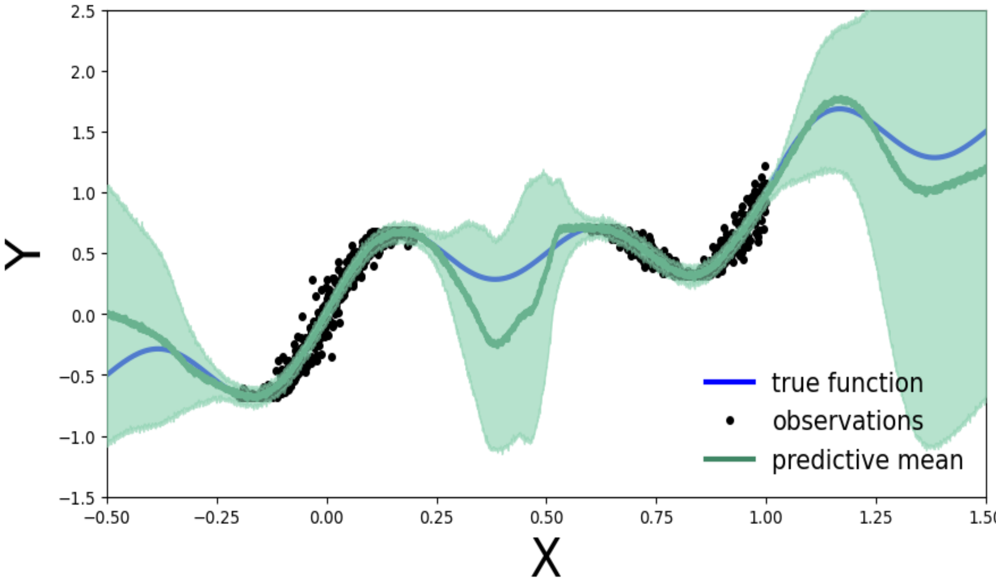
A Comparison of GANs, VAEs, NFs, and DMs

Model	Training Stability	Scalability	Inference Speed	Fidelity	Expressivity
DMs	High	Moderate-High	Slow (many denoising steps) Fast (with distillation)	High	High
GANs	Unstable	High	Very Fast (single forward pass)	High (but prone to mode collapse)	High
VAEs	Moderate - High	High	Very Fast (single pass)	Moderate	Moderate
NFs	Moderate (stability depends on architecture constraints)	Moderate	Fast (direct sampling, but deep layers slow down)	High	Moderate

Tareq et al., 2025

Uncertainty Quantification in Generative AI

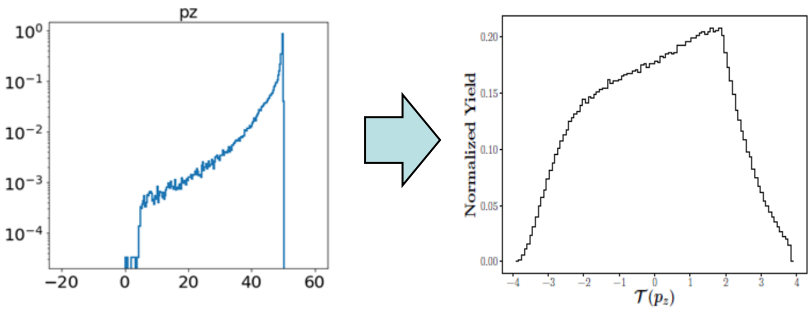
- **Aleatory Uncertainty (Stochastic Uncertainty)**
  - Inherent random effects
  - Not related to the number of data samples
  - Not reducible with increasing number of data samples
- **Epistemic Uncertainty (Systematic Uncertainty)**
  - Uncertainty due to lack of knowledge
  - Reducible with more data samples
- **Generative AI Model**
  - When to say “I don’t know”?



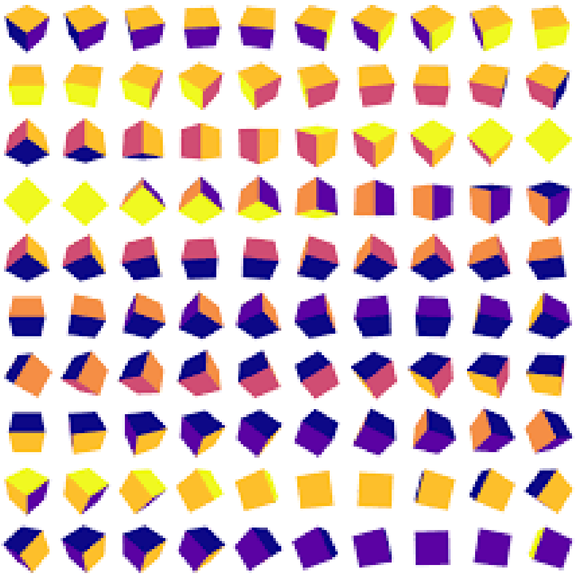
Challenges: Plug physics into generative AI

- **Change of Variables**

$$\mathcal{T}(p_z) = \log(E_\mathrm{b} - p_z)$$



- **Data Augmentation**
  - **Symmetry**

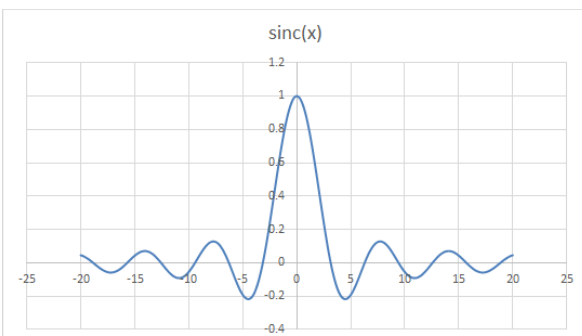


Challenges: Plug physics into AI (cont.)

- **Architectural Design**
  - Equivariance under group transformation enforced by convolutional layers

$$
\begin{tikzcd}
L_{V_1}(\mathcal{X}_1) \arrow[r, "\mathbb{T}_g"] \arrow[d, "\phi"] & L_{V_1}(\mathcal{X}_1) \arrow[d, "\phi"] \\
L_{V_2}(\mathcal{X}_2) \arrow[r, "\mathbb{T}'_g"] & L_{V_2}(\mathcal{X}_2)
\end{tikzcd}
$$

- **Output Transformation**

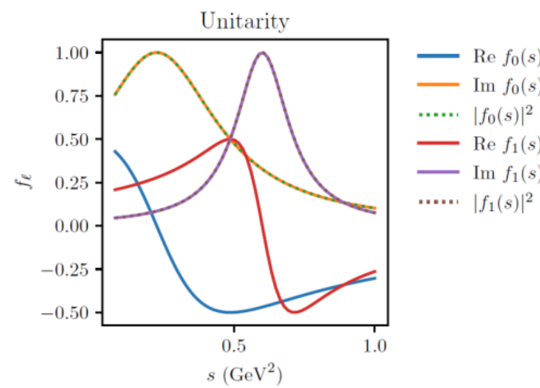


- **Loss function penalties**
  - Encode inconsistency of models inside the loss function as a penalty term

$$\mathbf{J}(\mathbf{w}) = Loss(y, \hat{y}) + \lambda ||\mathbf{w}||_2^2 + \gamma \Omega(\hat{y}, \Phi)$$

Unitarity of the partial waves

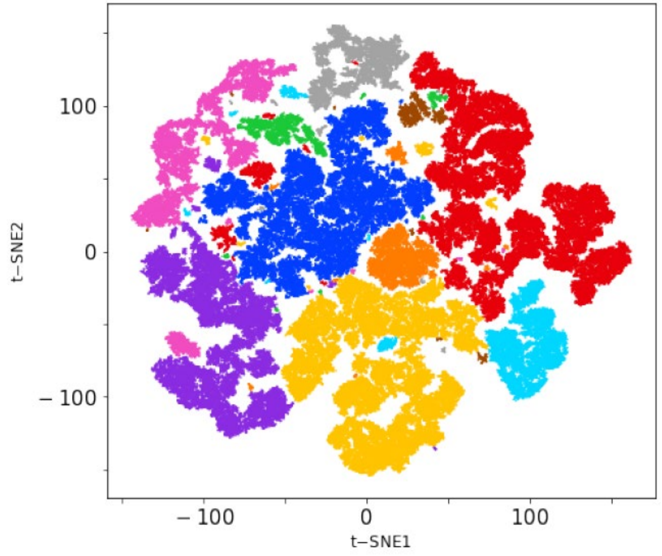
$$\mathrm{Im}\ f_\ell(s) = |f_\ell(s)|^2$$



Gloria Montana, Physics-constrained GAN for amplitude extraction

Summary

- **Development of ML-based event generator is still in its ~~infant~~ toddler stage**
  - Many Challenges in GAN
  - Normalizing Flow or Diffusion Models have further advantages
  - Incorporating physics into Machine Learning models is the KEY
- **Current/Future Research**
  - Uncertainty Quantification
  - Unfolding Detector Acceptance + Smearing + Inefficiency Effect
  - Extracting Physics from ML
    - Extract Amplitude (Collaboration with Gloria)
    - Extract Resonance (Collaboration with Marco)



Acknowledgements

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