AI-Driven Framework for Direct Extraction of Theoretical Parameters from Detector Data

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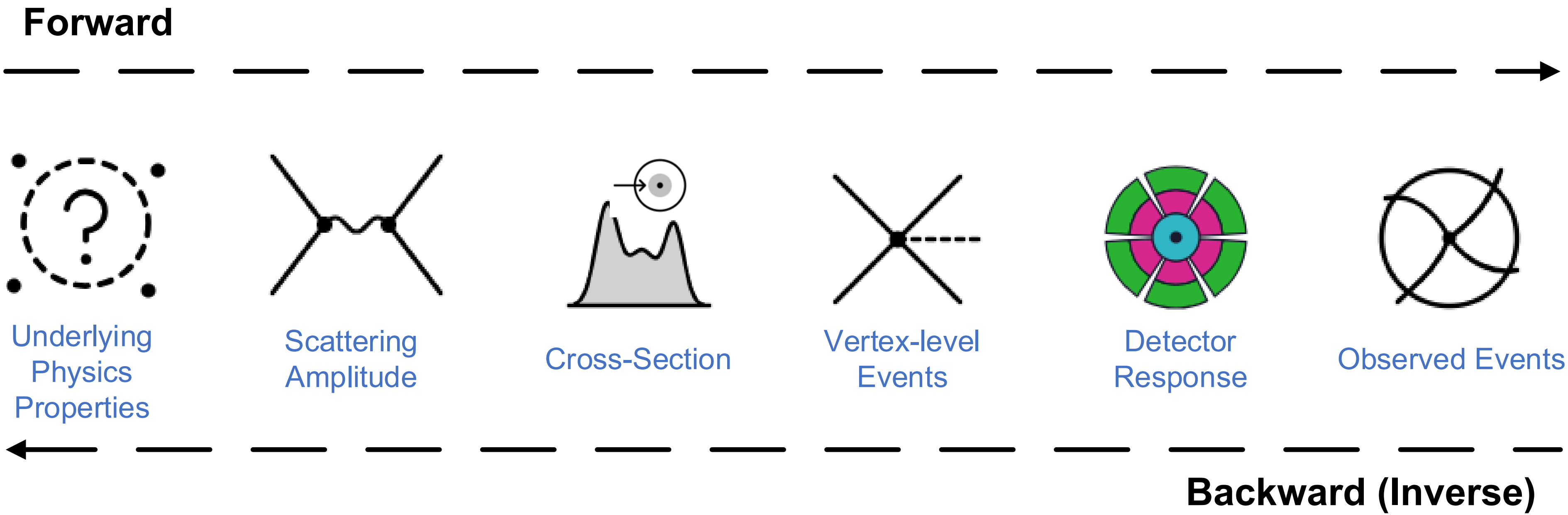
7/23/2026 @ Towards improved hadron femtography with hard exclusive reactions, edition V, UVA, 2026

Agenda

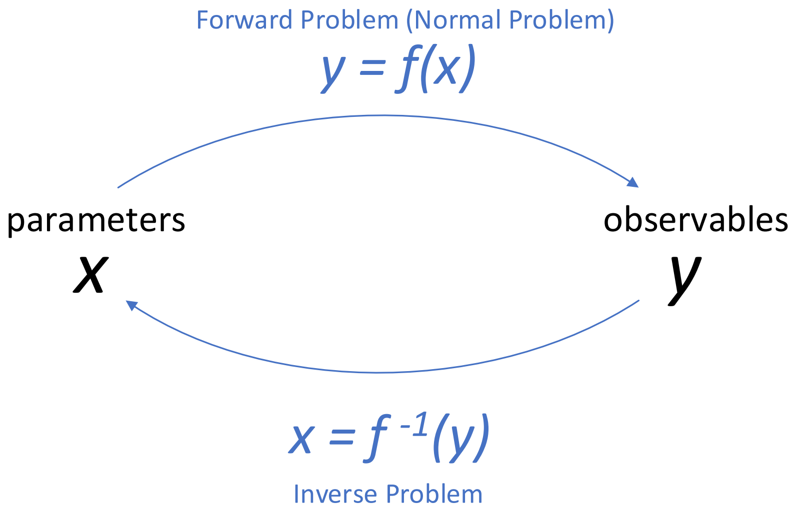
- The Inverse Problem
- Generative AI for Inverse Problem
- Model-Independent Framework
  - Reconstruct Scattering Amplitudes from Pion-Pion Scattering
  - Sampling Problem
    - QCF Parameterization
  - Unfolding Detector Effects
- Model-Dependent Framework
  - Extraction of Compton Form factors
  - Extracting TMDs from SIDIS Data
  - Out-of-Domain Problem and An Active Learning Solution
- Conclusion

Extracting Physics Properties from Observed Events

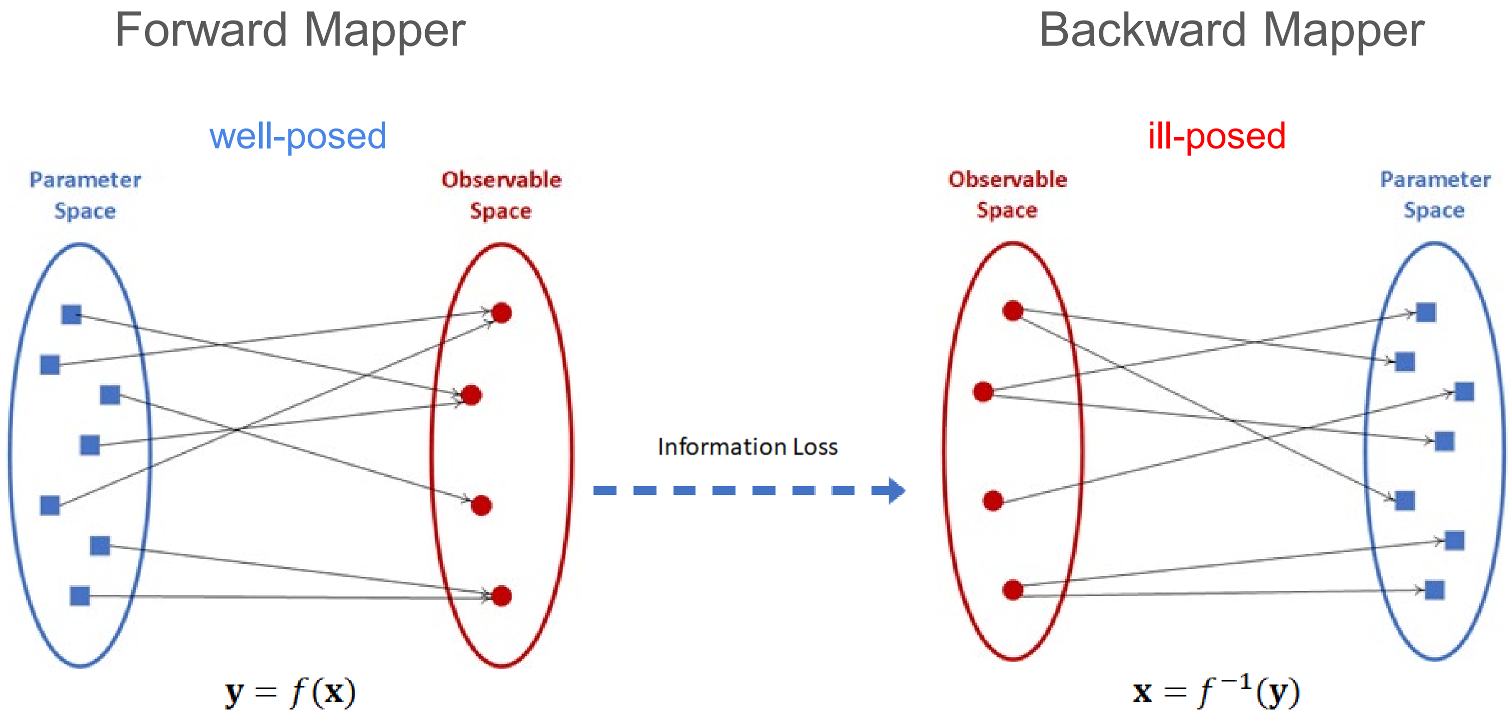


The Inverse Problem

- The Forward Problem (Normal Problem)
  - Use the model parameters to calculate the observables
- The Inverse Problem
  - Use the results of actual observables to infer the values of the parameters characterizing the system
- Challenges
  - Ill-posedness
    - Different values of the model parameters may be consistent with the observables
  - Curse of Dimensionality
    - Need to explore a huge, high-dimensional parameter space



Ill-posedness of Inverse Problems



Fundamental Idea

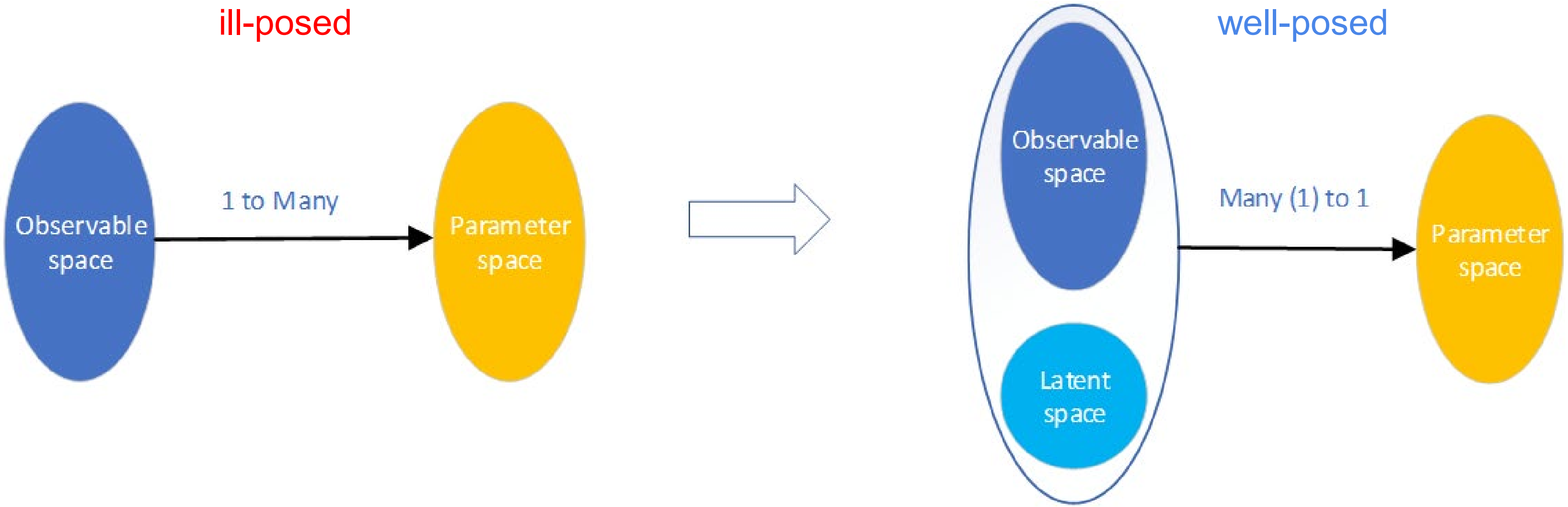
Variational Autoencoder Inverse Mapper

Inverse Problem

ill-posed

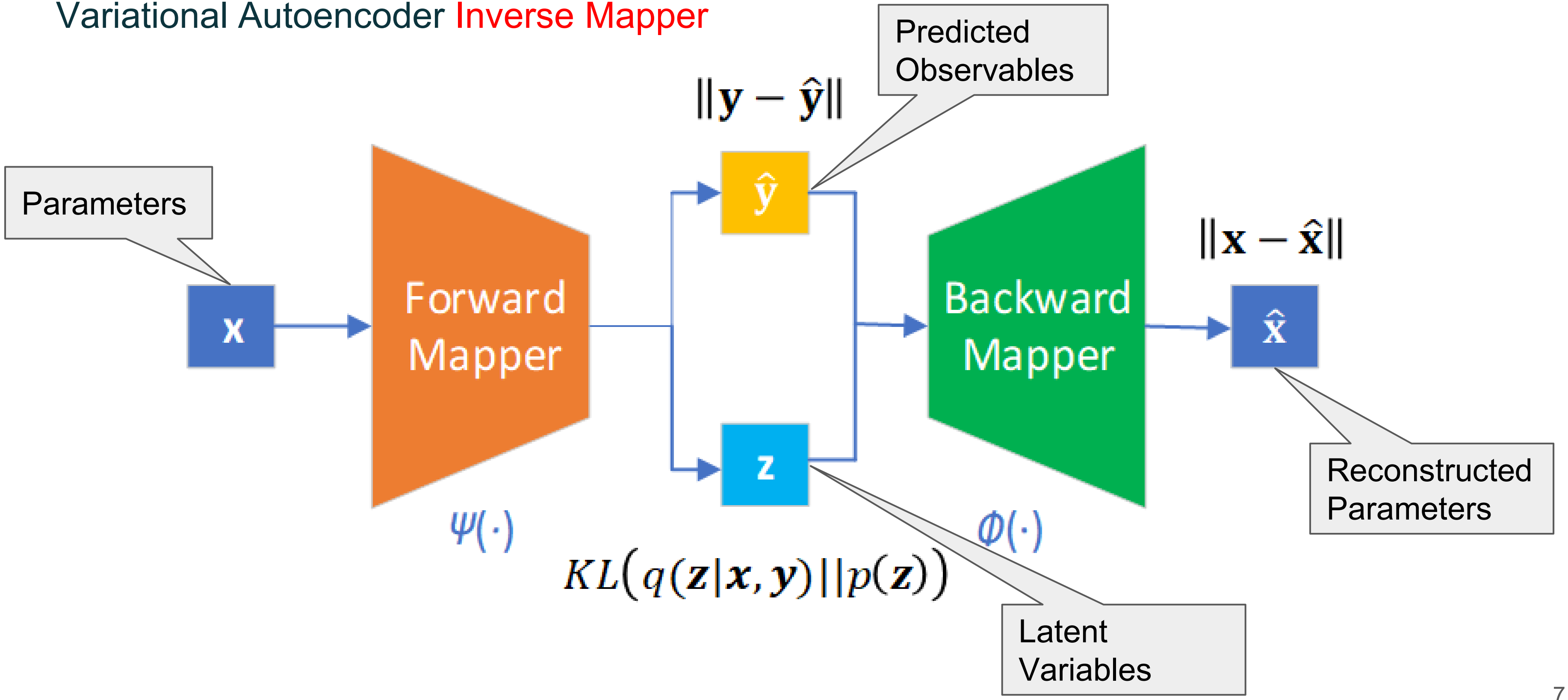
VAIM

well-posed



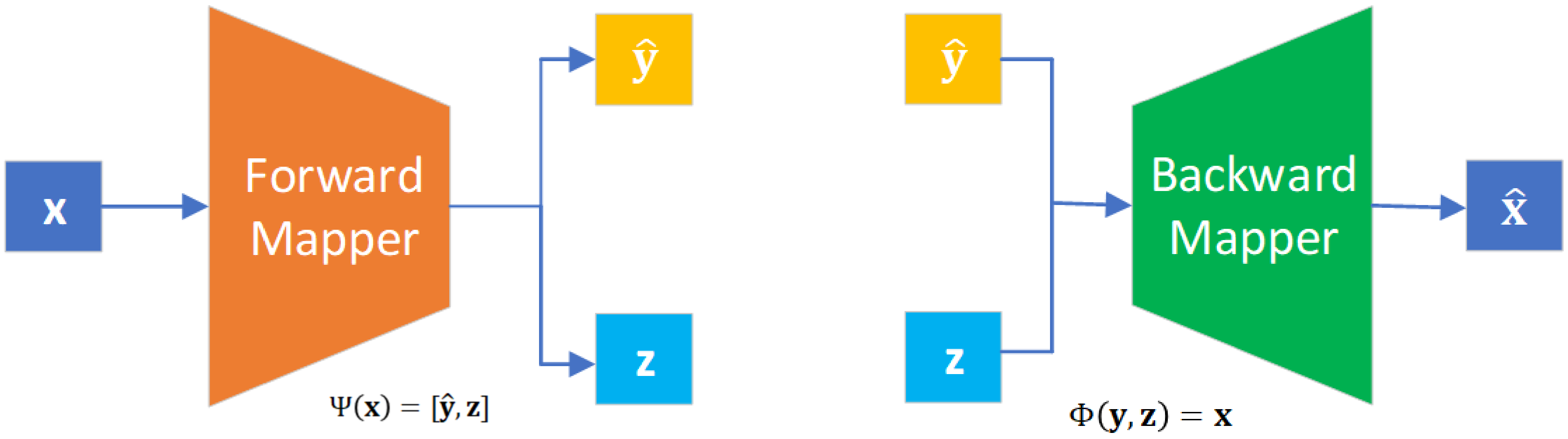
Variational Autoencoder Inverse Mapper Architecture

Variational Autoencoder Inverse Mapper



Almaeen et al., IJCNN, 2021.

Forward Mapper and Backward Mapper



Learn posterior distribution

$p(\mathbf{z}|\mathbf{x},\mathbf{y})$

Learn likelihood distribution

$p(\mathbf{x},\mathbf{y}|\mathbf{z})$

Almaeen et al., IJCNN, 2021.

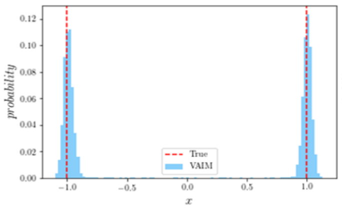
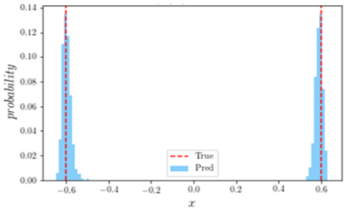
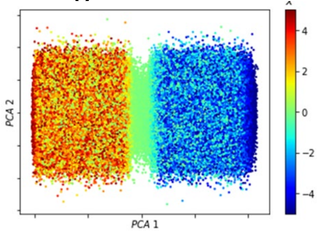
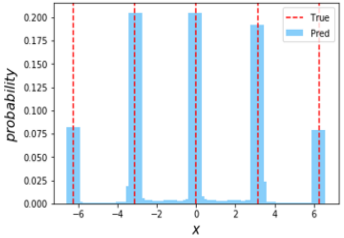
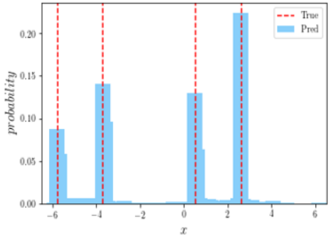
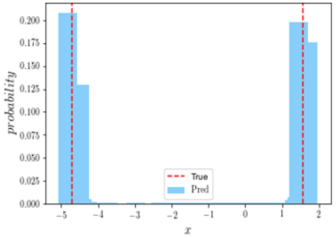
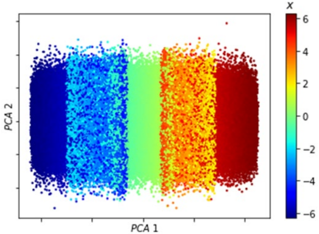
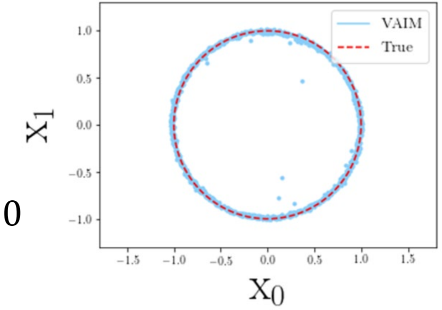
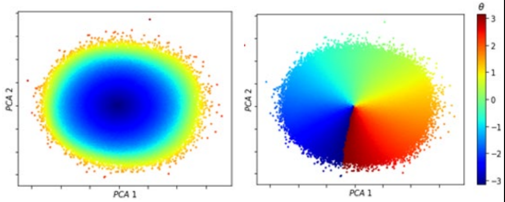
Math behind Variational Autoencoder Inverse Mapper

- Approximate
  - True posterior distribution $p(\mathbf{z}|\mathbf{x},\mathbf{y})$
- Variational Inference
  - Learn an approximate distribution $q(\mathbf{z}|\mathbf{x},\mathbf{y})$ such that
    $q(\mathbf{z}|\mathbf{x},\mathbf{y}) \sim p(\mathbf{z}|\mathbf{x},\mathbf{y})$
  - Minimize the Kullback-Leibler (KL) divergence
    $$\min KL(q(\mathbf{z}|\mathbf{x},\mathbf{y})||p(\mathbf{z}|\mathbf{x},\mathbf{y}))$$
- Variational Autoencoder Theory
  $$\min KL(q(\mathbf{z}|\mathbf{x},\mathbf{y})||p(\mathbf{z}|\mathbf{x},\mathbf{y}))$$
  equivalent to
  $$\min \|\mathbf{y}-\hat{\mathbf{y}}\|_2^2 + \|\mathbf{x}-\hat{\mathbf{x}}\|_2^2 + KL(q(\mathbf{z} \mid \mathbf{x},\mathbf{y}) \mid\mid p(\mathbf{z}))$$
  - True prior distribution $p(\mathbf{z})$
    - Select tractable distribution easy to generate
      - Gaussian
      - Uniform

Almaeen et al., IJCNN, 2021.

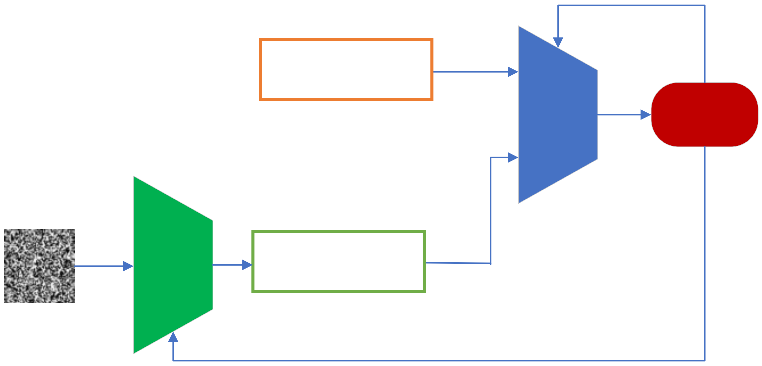
VAIM on Toy Inverse Problems

Almaeen et al., IJCNN, 2021.

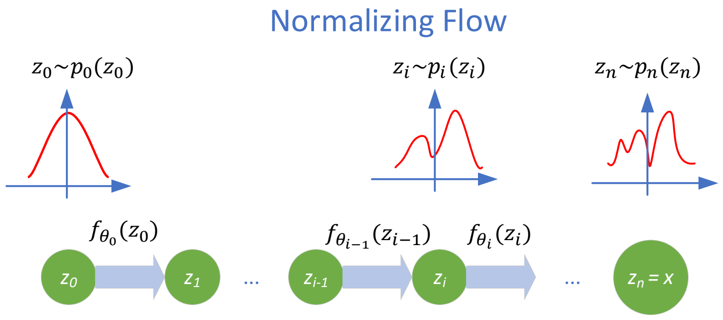
	Multiple Solutions	Latent Space Distribution
$f(x) = x^2$	 Parameter x distribution for $f(x) = 1.0$  Parameter x distribution for $f(x) = 0.36$	Sign Information 
$f(x) = \sin(x)$ $x \in [-2\pi, 2\pi]$	 $f(x) = 1.0$  $f(x) = -0.5$  $f(x) = 0.0$	Period Information 
$f(x_0, x_1)$ $= {x_0}^2 + {x_1}^2$	$f(x_0, x_1) = 1.0$  	Radius and Polar Angle Information 

Generative AI for Inverse Problem

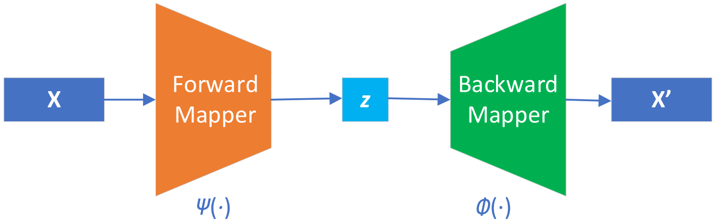
- **Generative Adversarial Networks (GANs)**



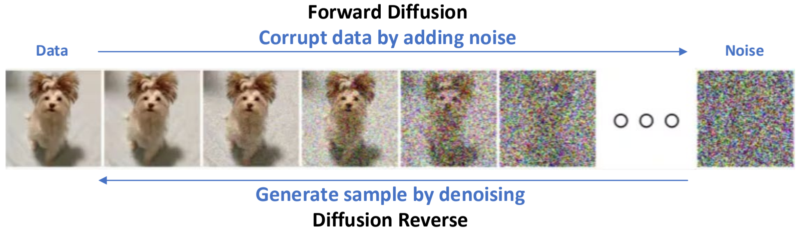
- **Normalizing Flow (NF)**



- **Variational Autoencoder (VAE)**



- **Diffusion Models (DM)**



Conditional diffusion: posterior sampling by denoising

- Forward: corrupt θ_0 with Gaussian noise over T steps
- Reverse: $\epsilon_\phi(\theta_t, y, t)$ denoises step by step, conditioned on y
- Train on noise prediction; sample from noise to obtain $\theta_0 \sim p(\theta \mid y)$

Machine Learning for Inverse Problems

- Classical Methods
    - Regularization (L2, Sparsity)
    - Bayesian Inference
    - Optimization-based inversion

Limitations:

- Rely on strong priors
- Application-specific tuning

- Generative AI
    - Invertible Neural Networks
    - Variational Autoencoder Inverse Mapper
    - Normalizing Flows
    - Diffusion Models

Advantages

- Learn full posterior $p(\theta|y)$
- From point estimation to distribution

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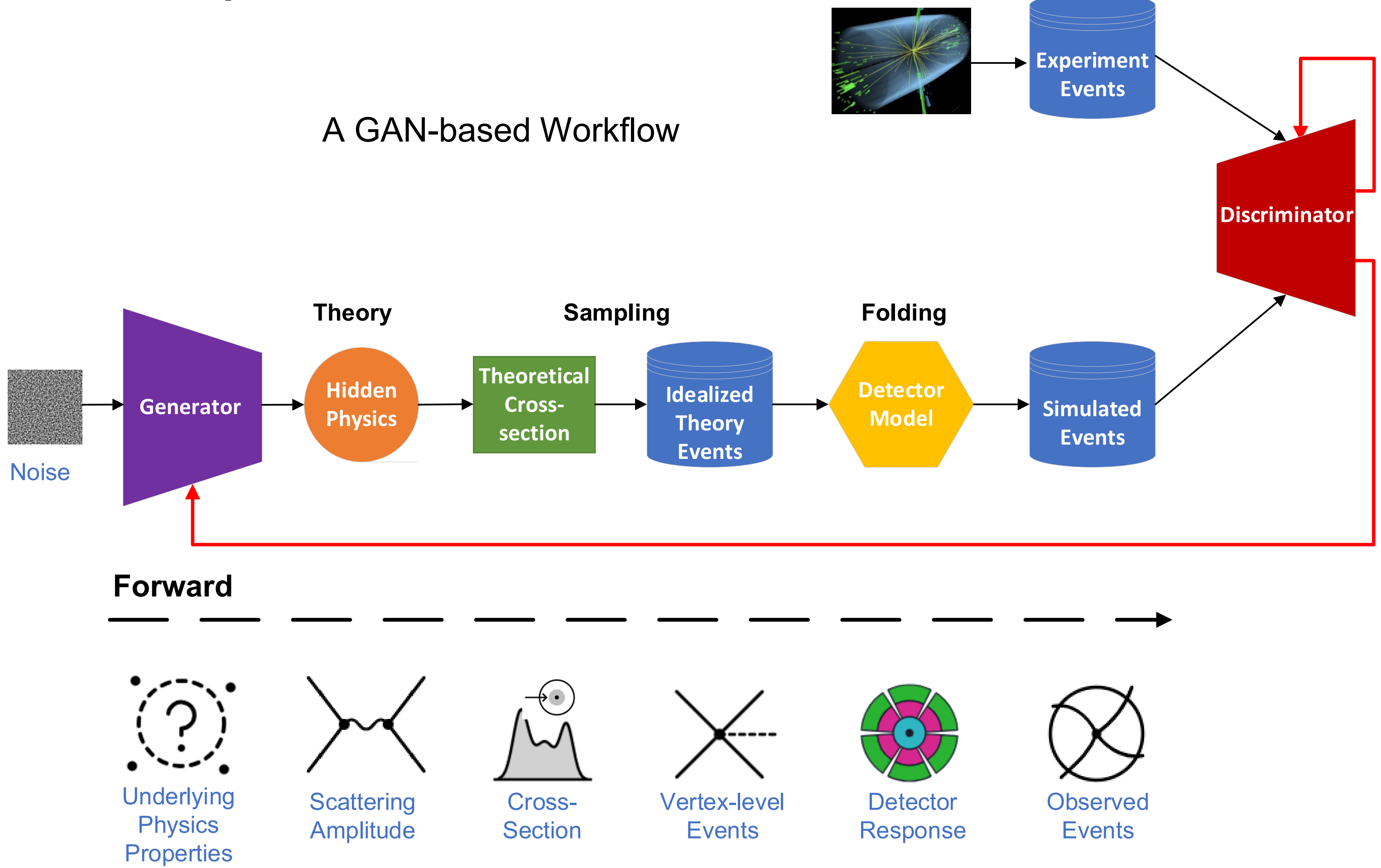
A Model-Independent Framework



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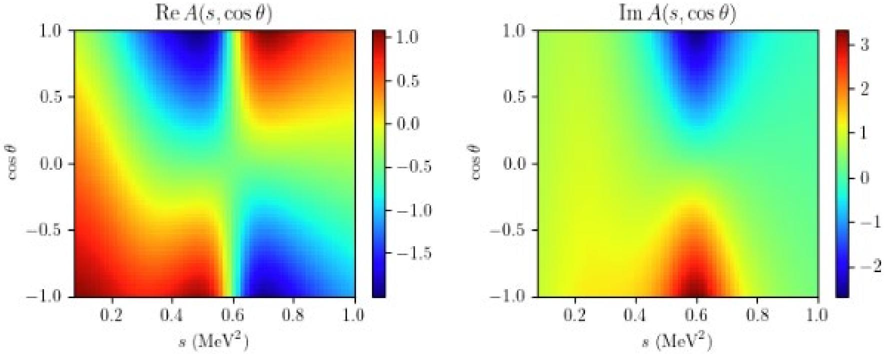
Reconstruct Scattering Amplitudes from Pion-Pion Scattering

- $\pi^+\pi^-$ elastic scattering
  - Elastic 2 → 2 of spinless particles

Collaboration with Gloria Montaña, Adam Szczepaniakj, Marco Battaglieri, Alessandro Pilloni, Jitao Xu, Derek Glazier, and others in AIDAPT Collaboration

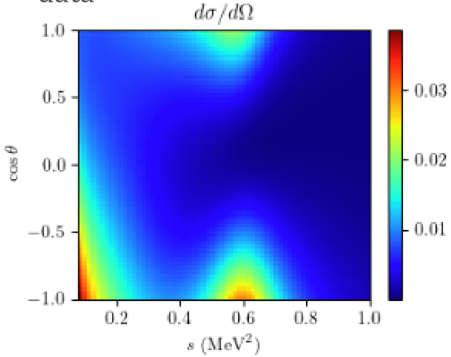
- Simplified Model
  - Partial-wave decomposition of the amplitude truncated to $n=1$ $\mathcal{A}(s,\cos\theta)=\sum_{l=0}^{n=1}(2l+1)f_l(s)P_l(\cos\theta)$
  - Breit-Wigner type partial waves $f_l=\frac{m_l\Gamma_l}{m_l^2-s-im_l\Gamma_l}$

$\mathcal{A}(s,\cos\theta)=f_0(s)+3f_1(s)\cos\theta$

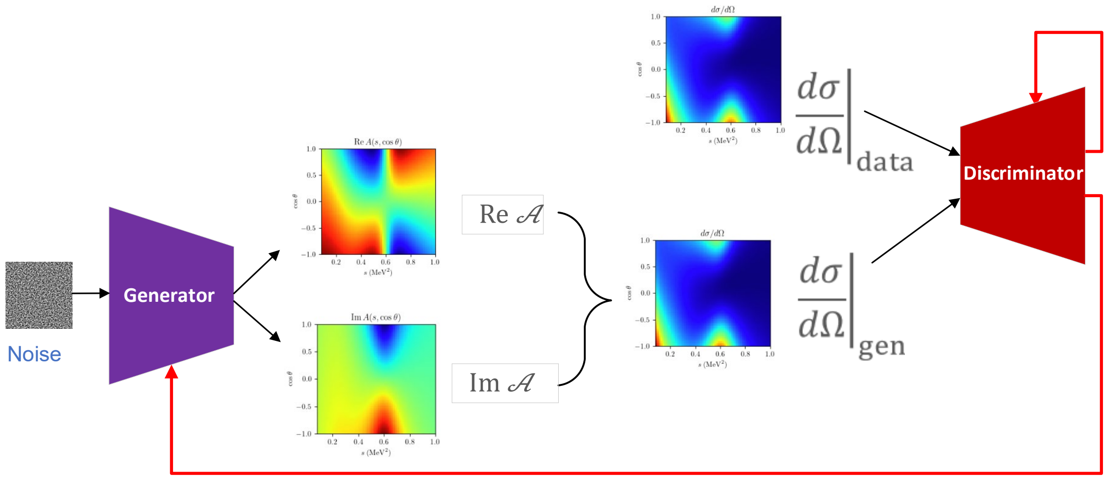


- Differential cross section

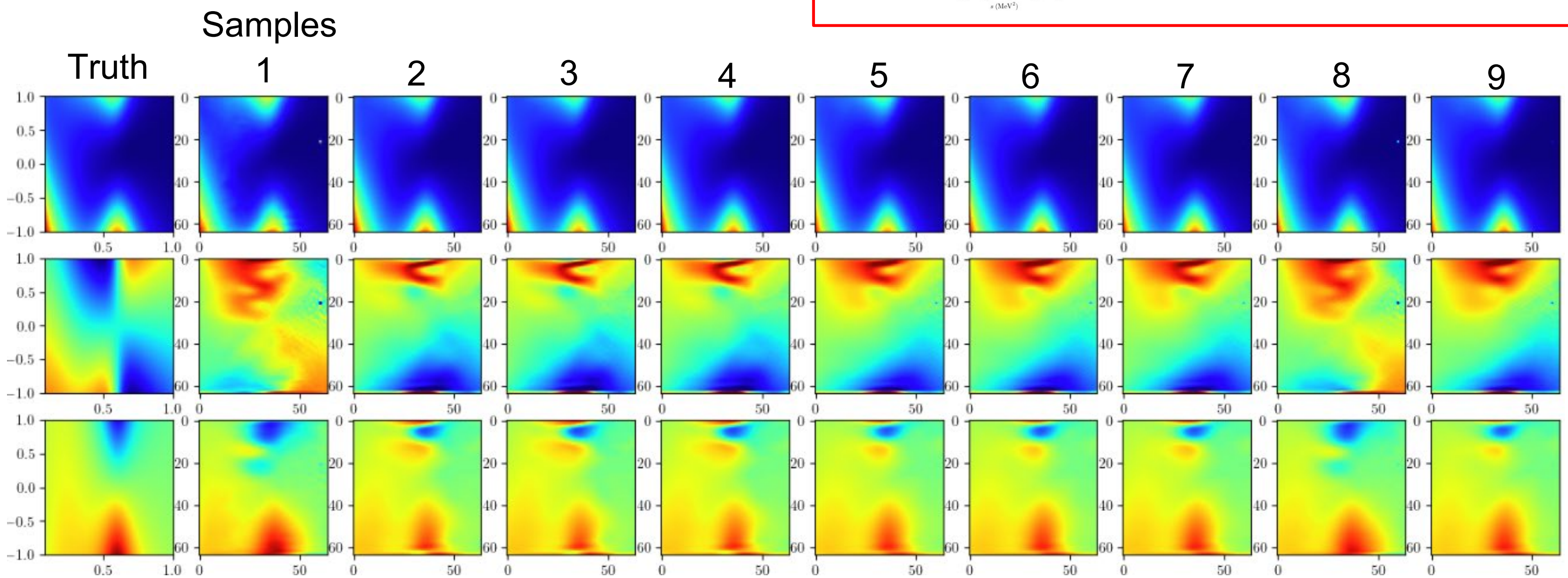
$$\left.\frac{d\sigma}{d\Omega}\right|_{\text{data}} \quad \frac{d\sigma}{d\Omega}=\frac{1}{64\pi^2}\frac{1}{s}|\mathcal{A}(s,\cos\theta)|^2$$



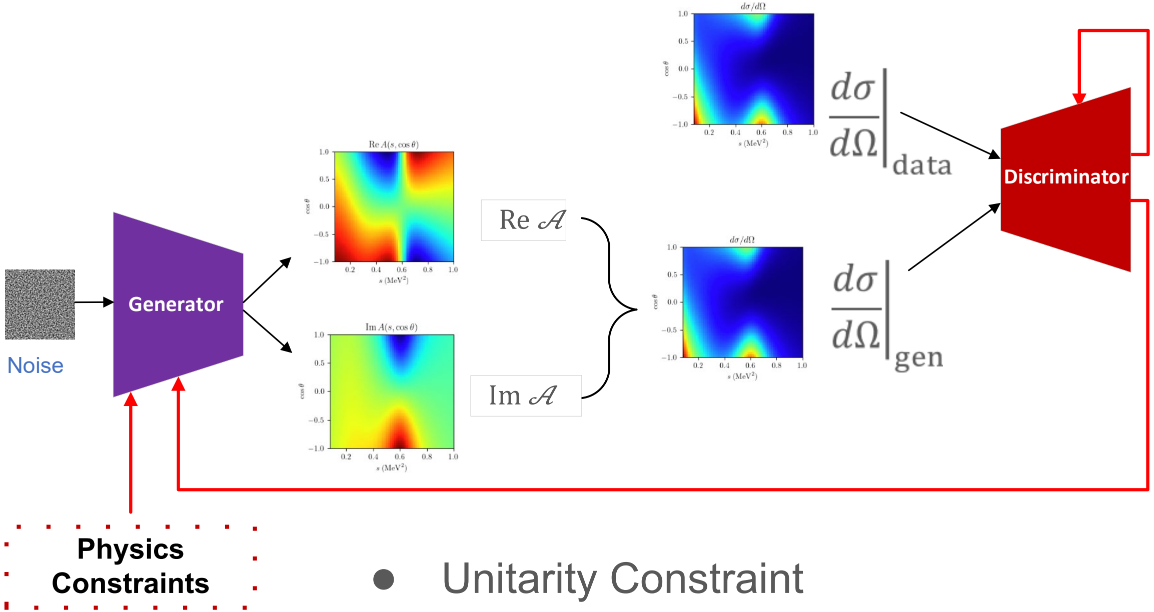
GAN Framework



- Preliminary Results

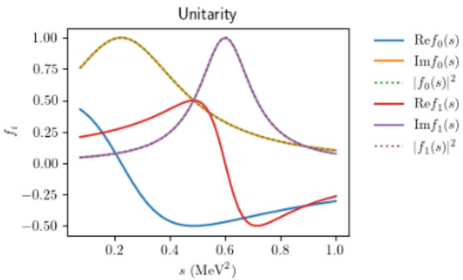


GAN Framework with Physics Constraints



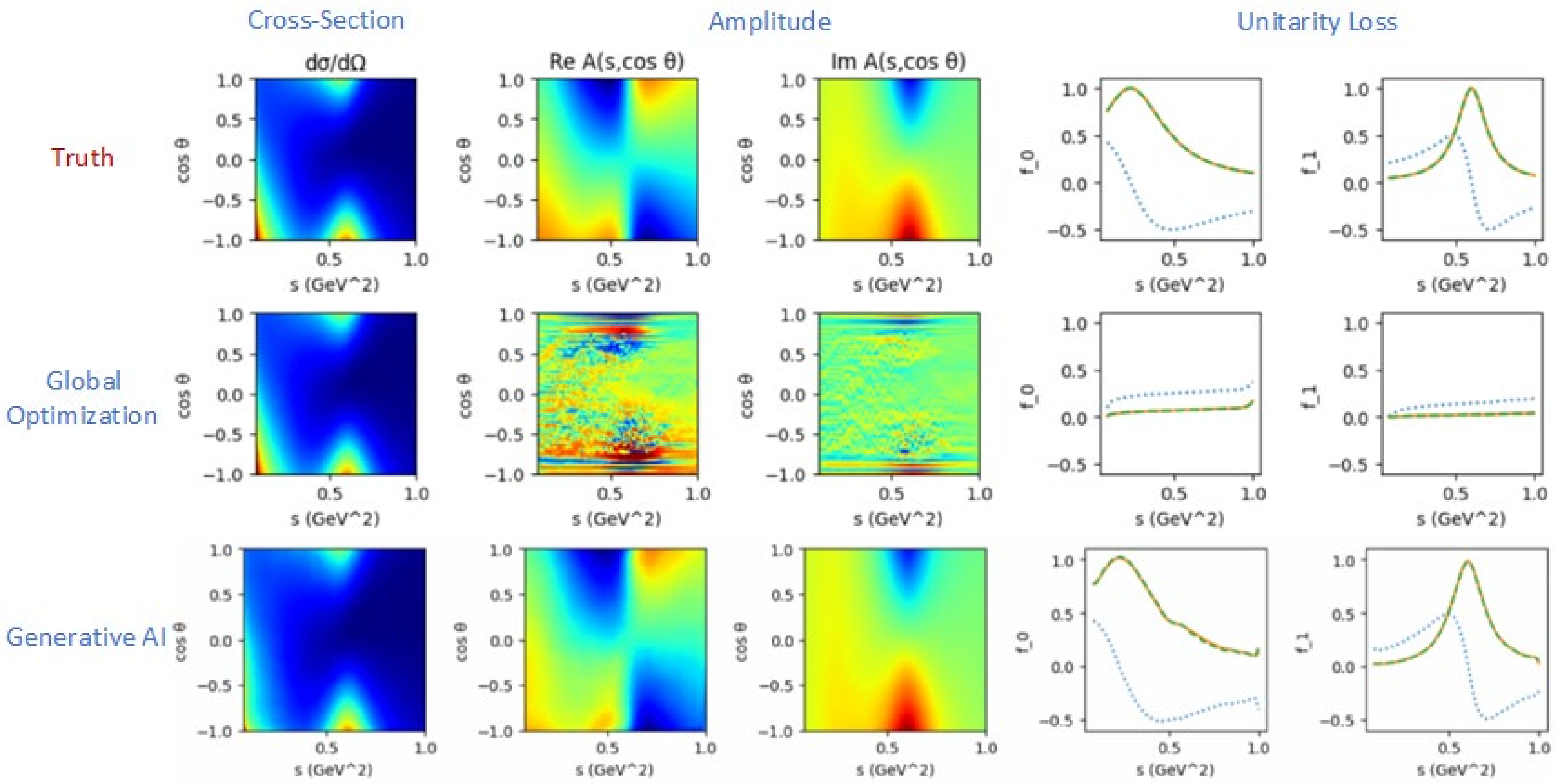
$$\mathcal{L} = \mathcal{L}_{\text{GAN}} + \mathcal{L}_{\text{Unitarity}} + \mathcal{L}_{\text{Phase Shift}}$$

- Unitarity Constraint
  - Comparing the modulus squared of the integral of the scattering amplitude over angular variables to the imaginary part



- Phase Shift Constraint
  - The positive derivative of the phase shift

Results (With Unitary Constraints)



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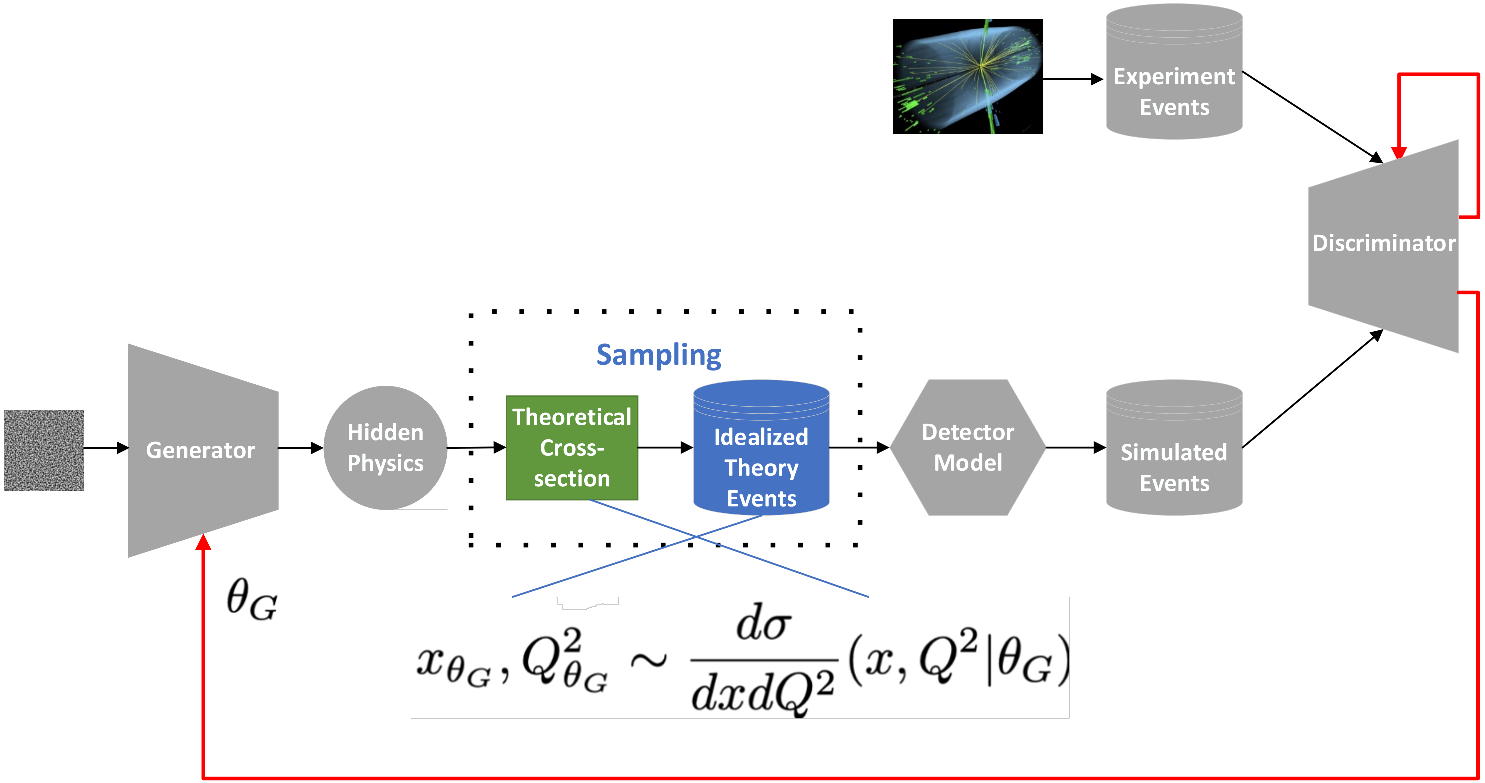
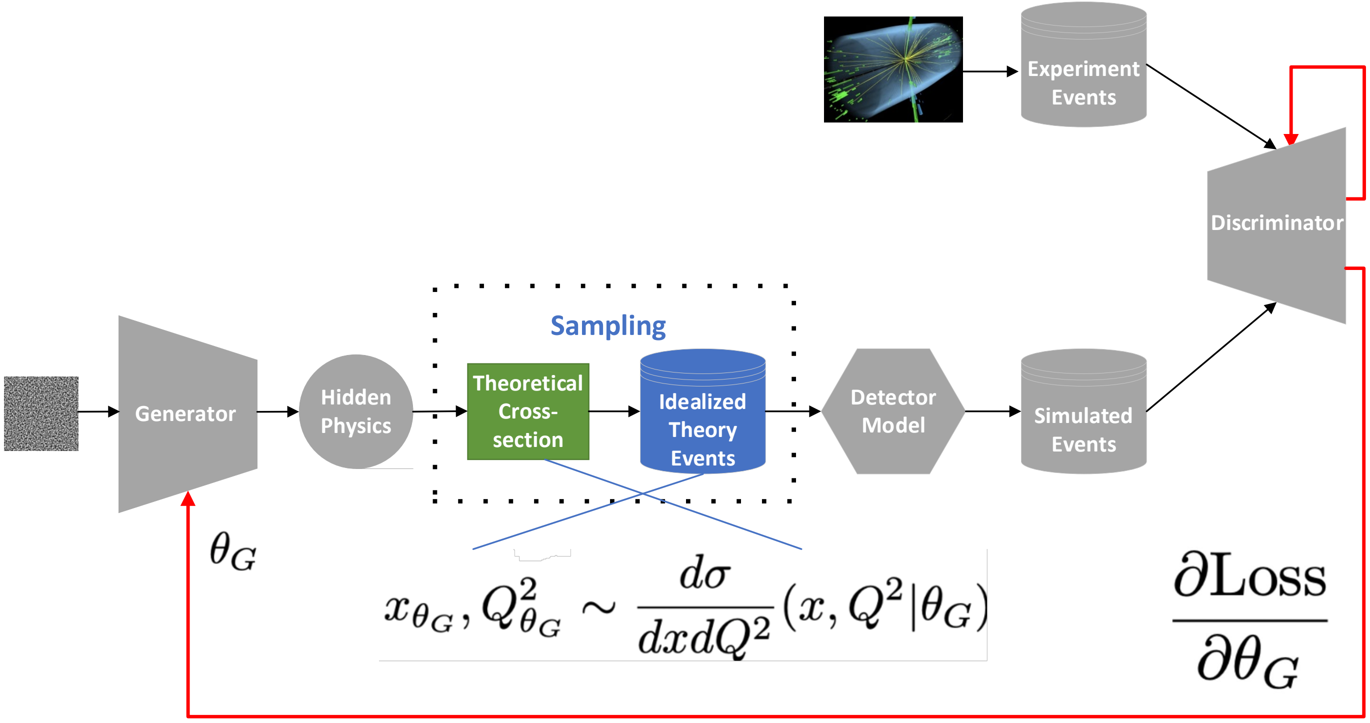
The Issue of Sampling



$$x_{\theta_G}, Q^2_{\theta_G} \sim \frac{d\sigma}{dx dQ^2}(x, Q^2 | \theta_G)$$

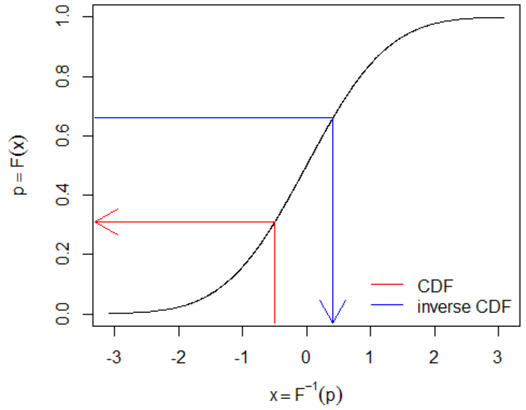
A Critical Obstacle in Backpropagation: Gradient over Sampling



$$\frac{\partial x_{\theta_G}}{\partial \theta_G}, \frac{\partial Q^2_{\theta_G}}{\partial \theta_G}$$ Gradient?

Problems of Classical Sampling Algorithms

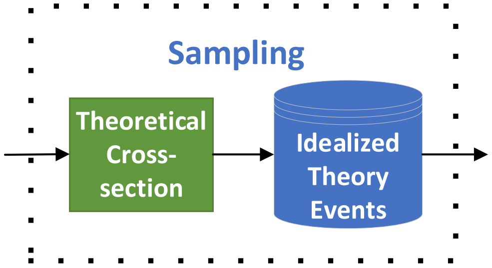
- Inverse CDF
  - Can provide meaningful gradient
  - Only works in 1D



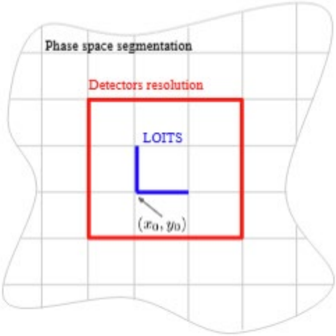
- Markov Chain Monte Carlo (Gaussian proposal function)
  - Random walk
  - Can work in higher dimensionality
  - No useful gradient

Two Possible Solutions

- Build a Surrogate Model
  - Neural Network
  - Approximate the sampling process
  - Differentiable
  - Easy to incorporate in the event-based analysis workflow



- Make the Sampling Method Differentiable (LOITS - by Nobuo Sato)
  - Partition space into grid cells
  - Compute the distribution value at each grid point
  - Sample each grid cell
    - Compute marginal distribution in each dimension
    - 1D inverse CDF in each dimension
    - Assemble the samples (Approximate)
    - MCMC Correction (Precise)
      - $\text{Ratio} = \dfrac{p(prop)p_{LOITS}(curr)}{p(curr)p_{LOITS}(prop)}$



Alghamdi et al., ITCAI, 2025.

Braga et al., arXiv:2507.15768, 2025.

QCF Proxy Model

- **Measurable observables**
  - $\boldsymbol{\sigma_p^o}$ and $\boldsymbol{\sigma_n^o}$
    - Cross-section distributions from proton and neutron targets, respectively.
    - Driven by underlying quark distributions $\boldsymbol{u(x;p)}$and $\boldsymbol{d(x;p)}$, which act as proxies for QCFs.
- **Forward model**

$$\boldsymbol{\sigma_1(x;p) = 4u(x;p) + d(x;p)}$$
$$\boldsymbol{\sigma_2(x;p) = u(x;p) + 4d(x;p)}$$
$$\boldsymbol{u(x;p) = N_u x^{a_u}(1-x)^{b_u}}$$
$$\boldsymbol{d(x;p) = N_d x^{a_d}(1-x)^{b_d}}$$

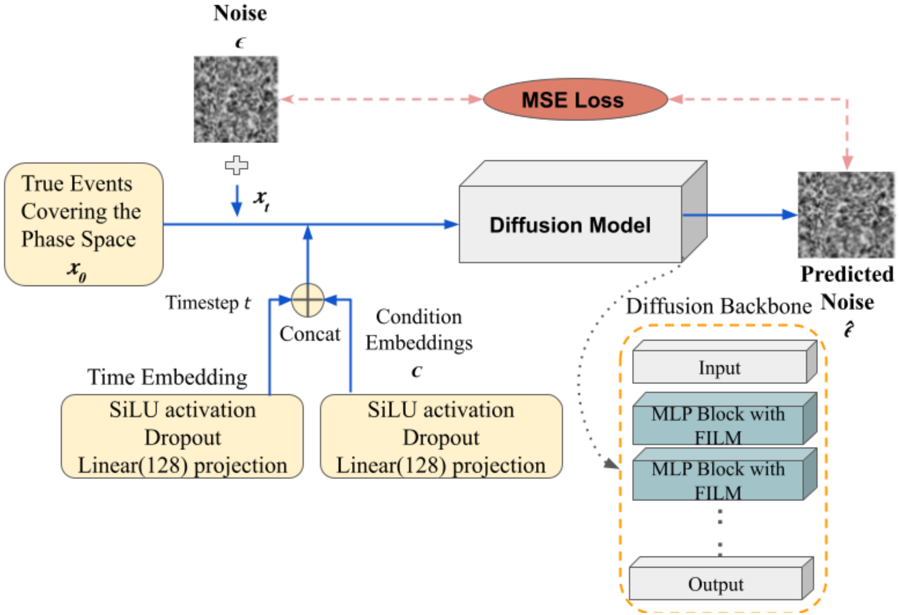
- **Inverse problem**
  - Given event-level samples $\boldsymbol{\sigma_p^o}$ and $\boldsymbol{\sigma_n^o}$, infer QCF parameters

$$p = \{\boldsymbol{N_u}, a_{\boldsymbol{u}}, b_{\boldsymbol{u}}, \boldsymbol{N_d}, a_{\boldsymbol{d}}, b_{\boldsymbol{d}}\}$$

Alghamdi et al., ITCAI, 2025.

Surrogate for Sampling

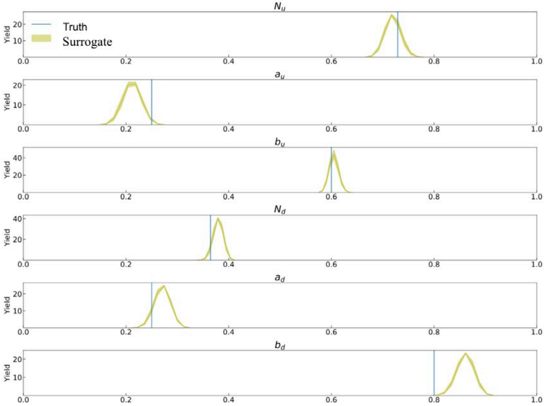
- Conditional Diffusion Model
  - Denoising Network
    - 6 MLP blocks (256 hidden units)
    - FiLM (Feature-wise Linear Modulation) conditioning
  - Noise schedule
    - T = 1,000 steps
    - $\beta_{min} = 10^{-4}$
    - $\beta_{max} = 0.02$
  - Training
    - MSE loss between predicted and true noise
    - Trained on 20M parameter-event pairs



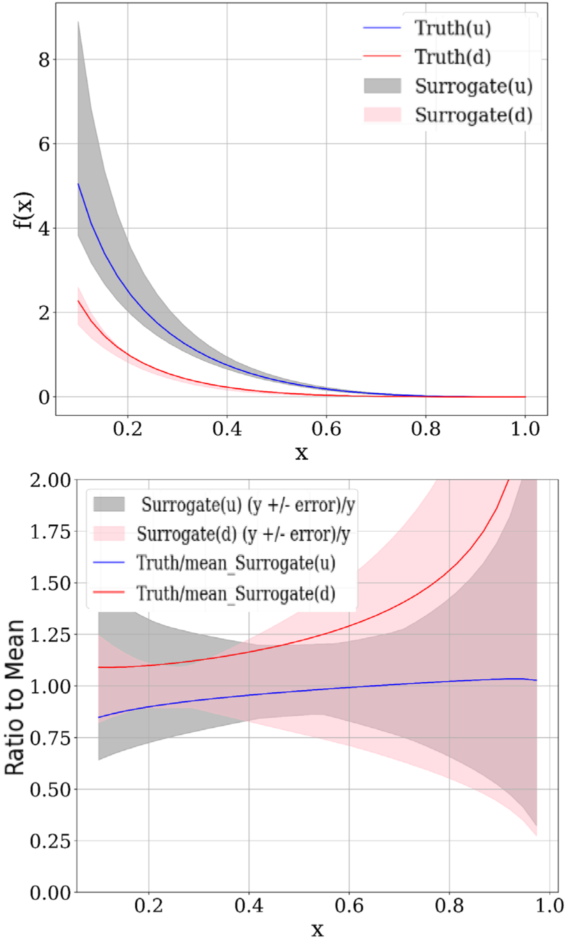
Alghamdi et al., ITCAI, 2025.

QCF Inference

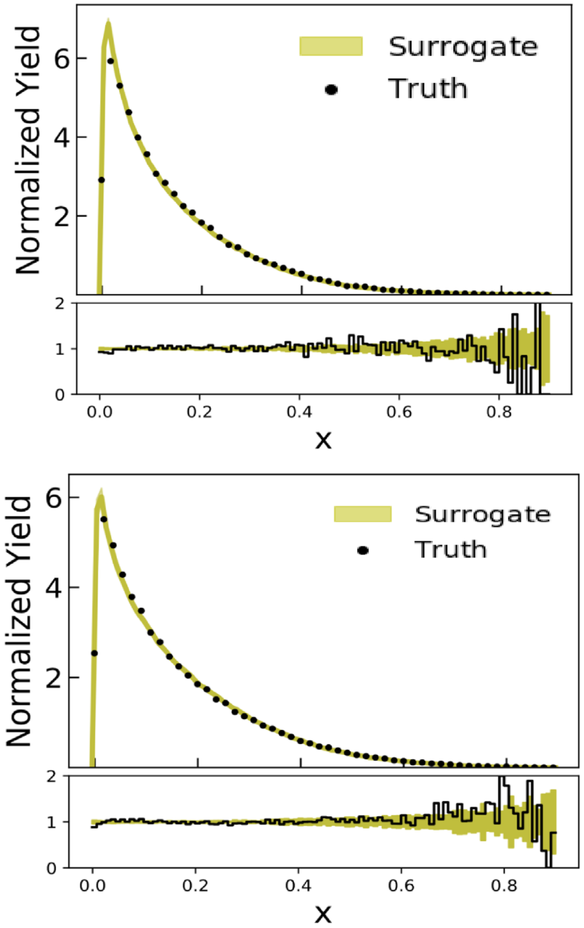
QCF Parameters Inference



Reconstructed QCF



Reconstructed Cross-section



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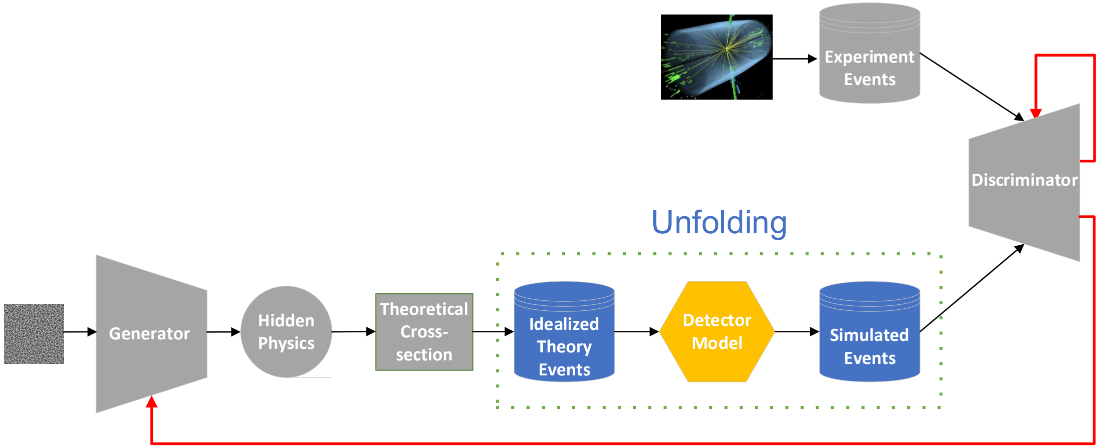
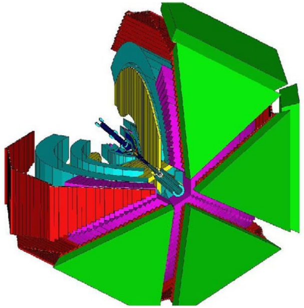
Unfolding Detector Effects





- **Smearing**
  - Finite resolution of the detector
  - Distortion of measured distribution
- **Acceptance**
  - Detector's inability to cover the full space
  - Lost sections of detected distributions
- **Inefficiency**
  - Detector's failure to register certain particles
  - Missing data

Unfolding Detector Effects

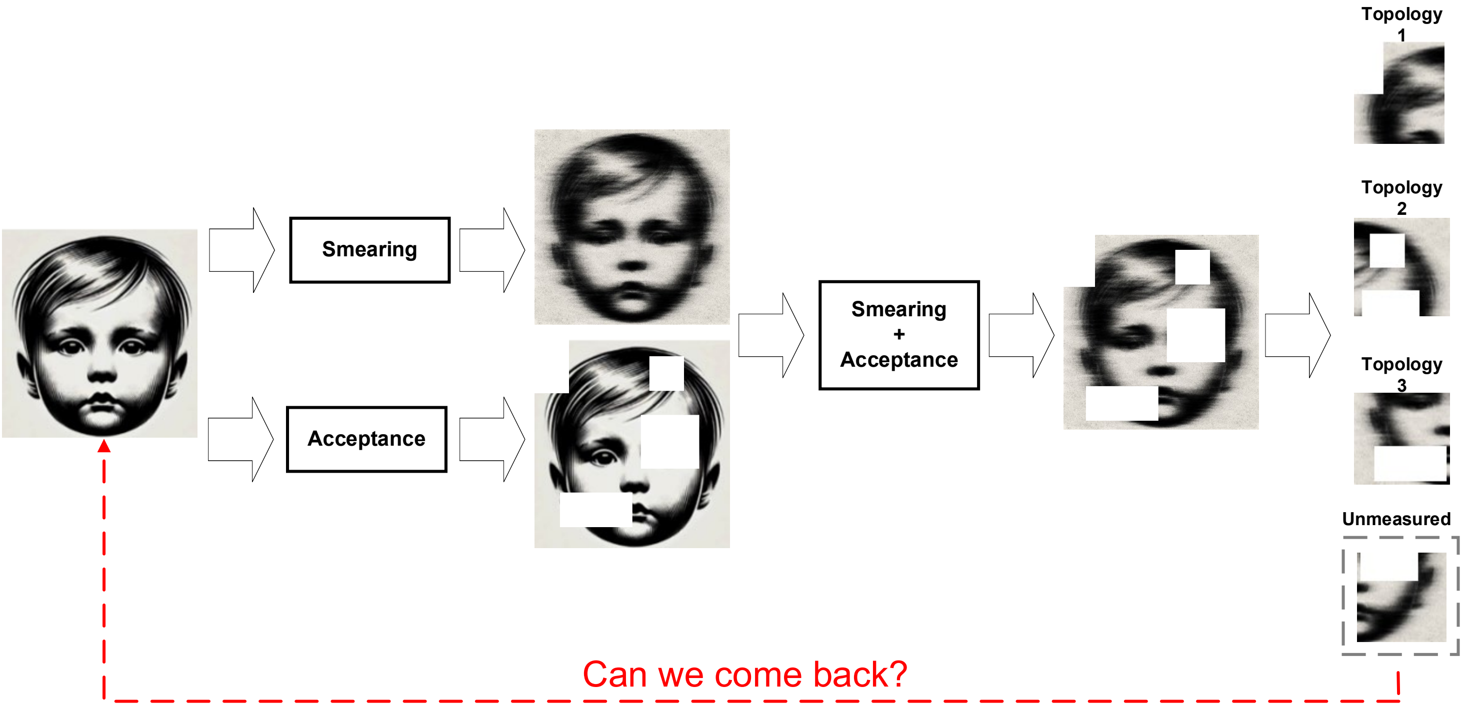
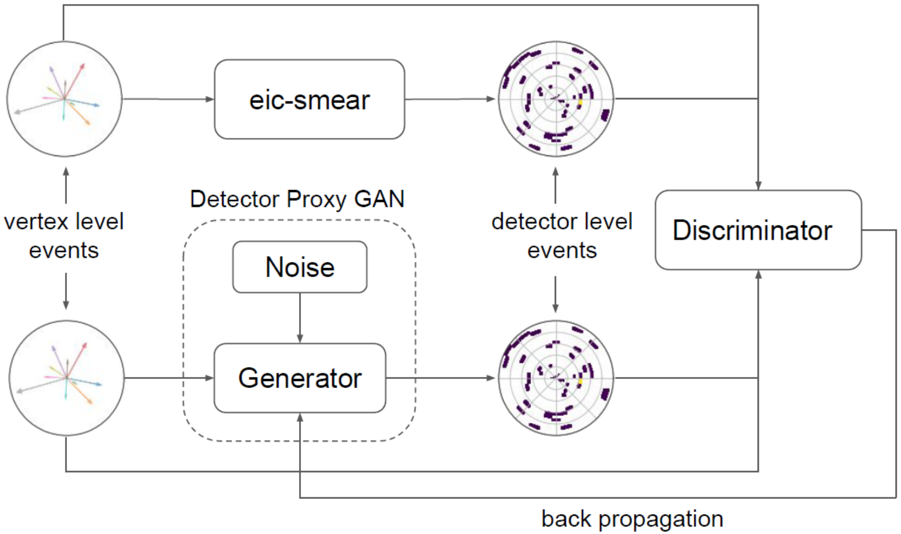


Image credit to Marco Battaglieri

Detector Surrogate

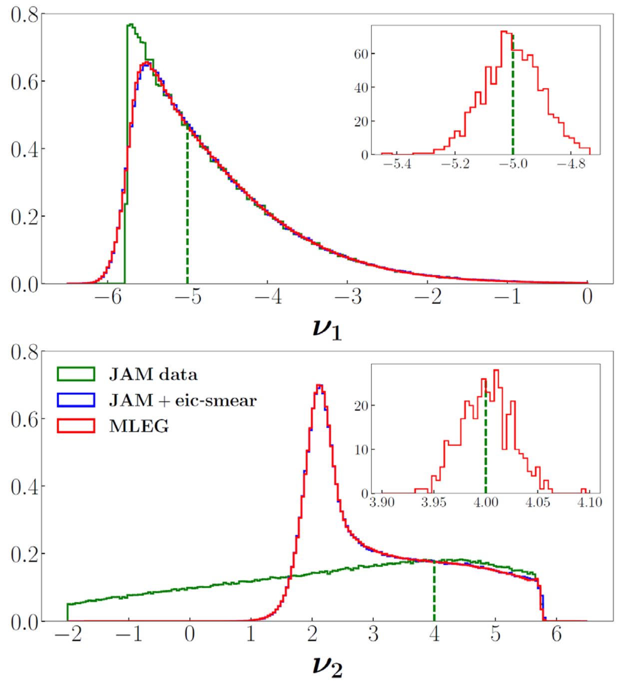
- **Detector Proxy GAN**
  - Conditional GAN
  - Training samples
    - From guessed vertex-level samples and corresponding detector-level samples using a detector simulator



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

Detector Surrogate for Electron-Proton Scattering

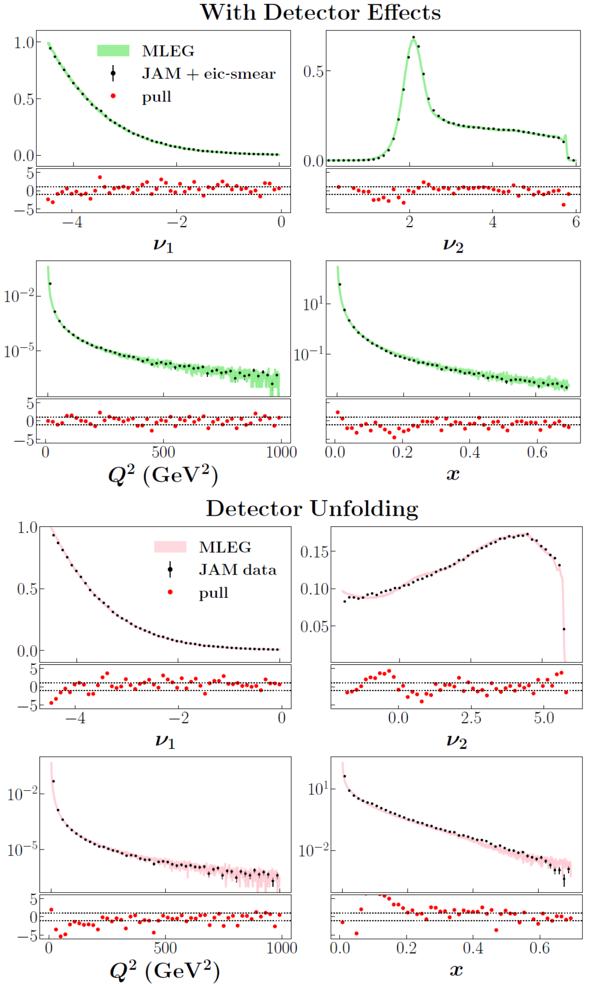
- **Detector Surrogate**
  - Conditional GAN Architecture
  - Translate vertex-level events to detector level events
  - Trained by detector parametrization provided by the eic-smear.
- **Vertex-level events**
  - JAM global QCD analysis
- **Detector-level events**
  - Simulated by EIC-smear
  - Vertex-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

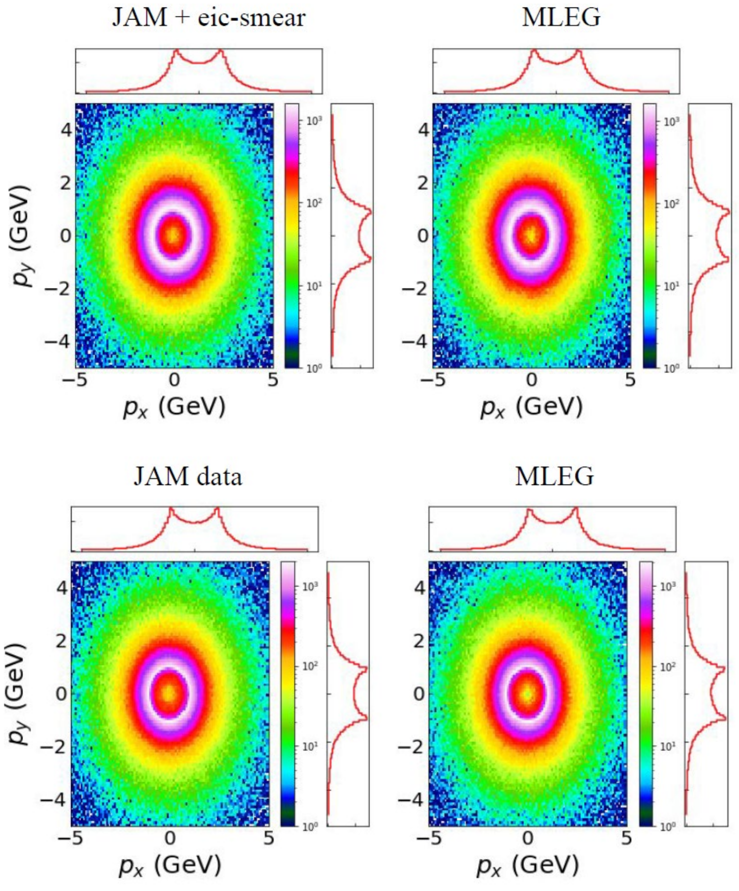


Comparison of training features at the vertex level (generated, green histograms) and detector level (smeared, blue histograms) with the MLEG generated synthetic data (red histograms). The insets illustrate the local smearing effect at the points indicated by the green vertical dashed lines.

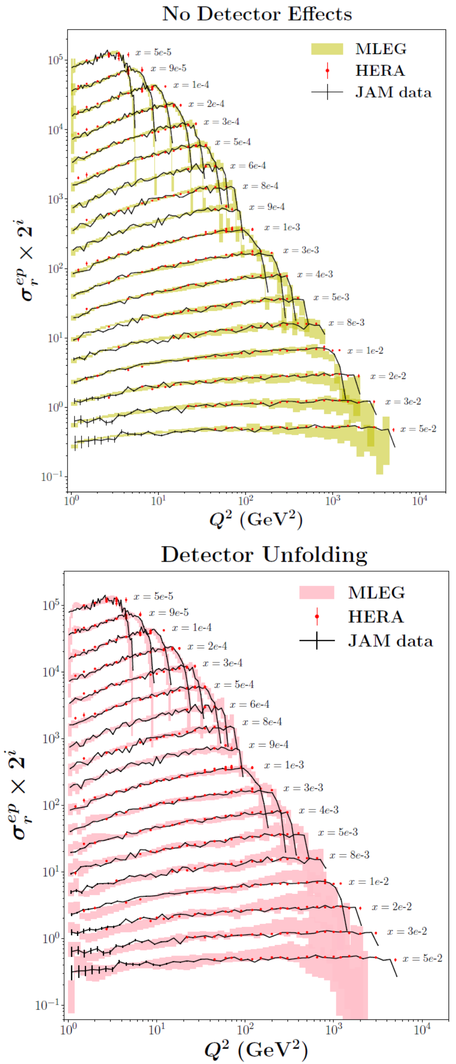
Alanazi et al., Phys. Rev. D 106, 096002, 2022

Unfolding Results



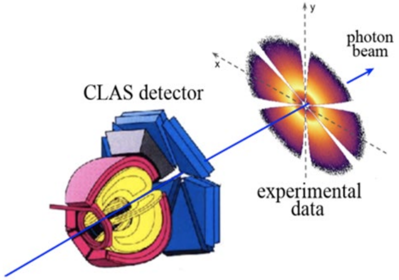


HERA



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

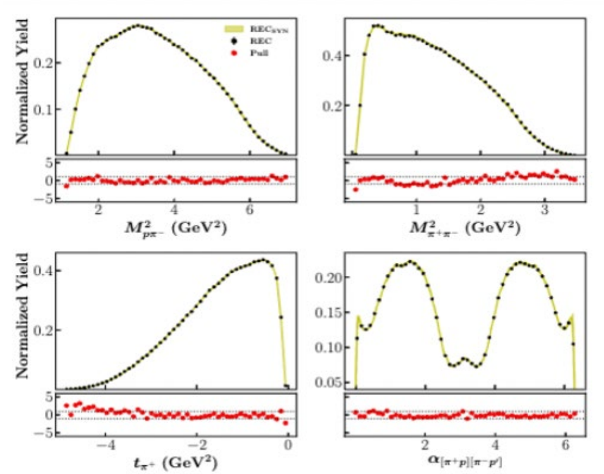
Detector Effect for CLAS Exclusive 2π photoproduction



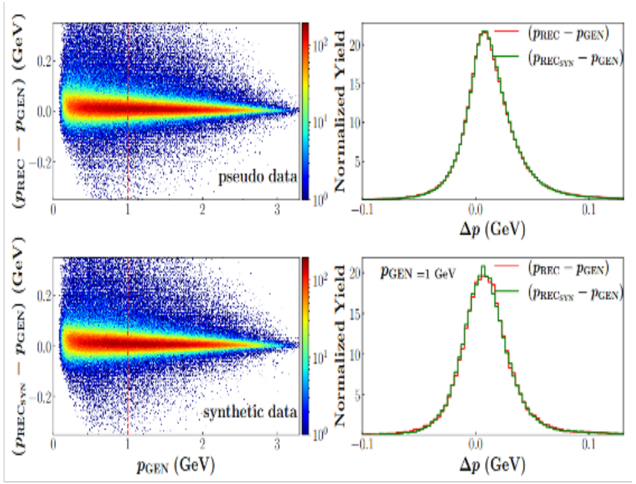
- Detector Simulation GAN (DS-GAN): Simulate the smearing detector effects

MC-Phase Space Events

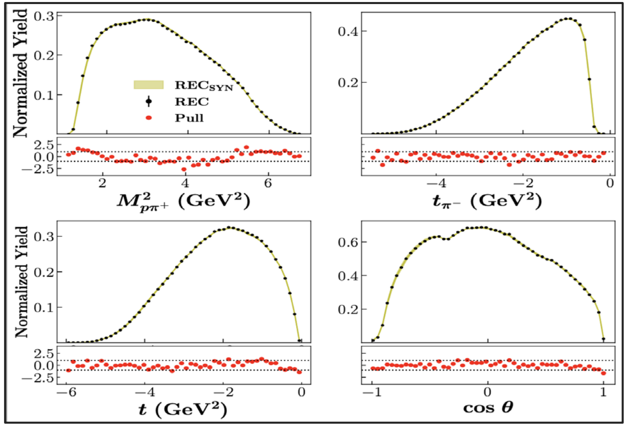
Vertex-level → **DS-GAN** → **Detector-level**



MC REC events vs DS-GAN synthetic events



CLAS Resolution



Derived Variables (not used in training)

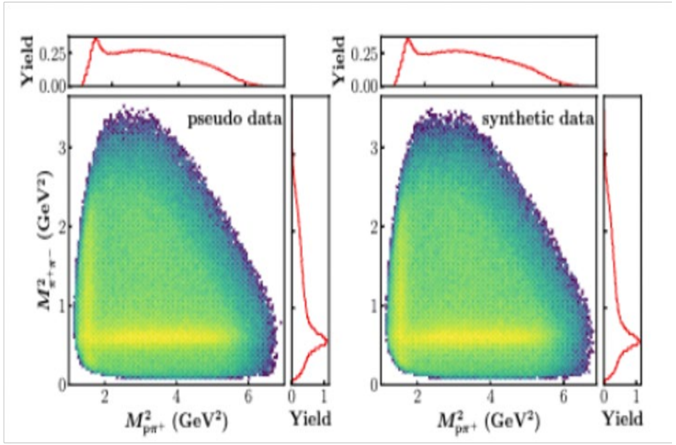
Alghamdi et al., Phys. Rev. D 108, 094030, 2023

Unfolding Detector Effect for CLAS Exclusive 2π photoproduction

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

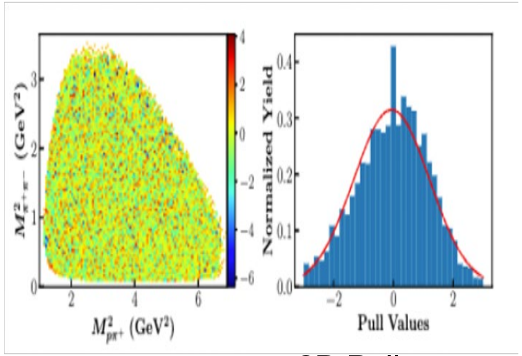
MC-Realistic Events

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



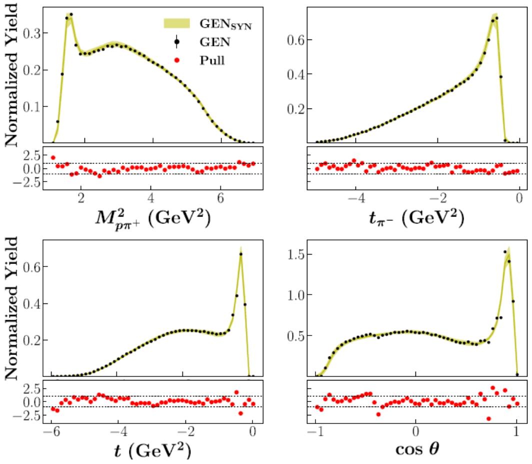
RE-MC GEN events

UNF-GAN SYN events

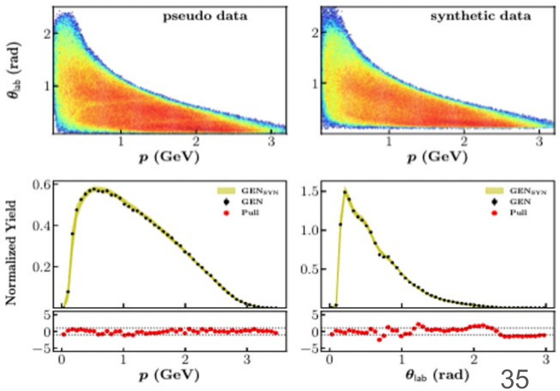


2D Pull

Derived Variables



CM Frame

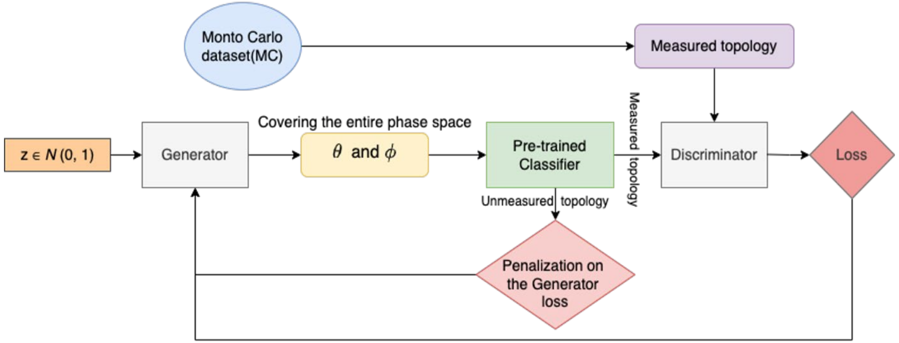


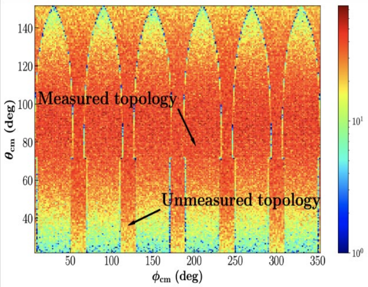
Lab Frame

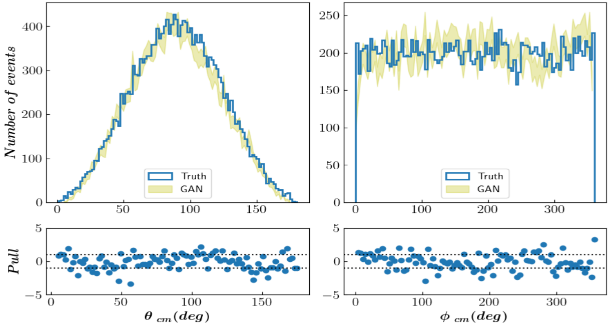
Alghamdi et al., Phys. Rev. D 108, 094030, 2023

GAN Architecture for Acceptance Unfolding

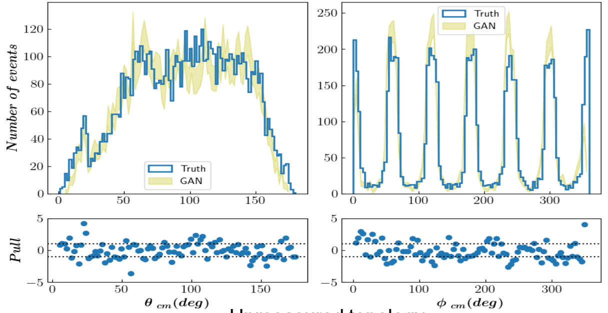
- Key Feature: a custom, physics-informed penalty term in the generator loss
  - Penalize discrepancies between generated and true unmeasured topology event distributions.



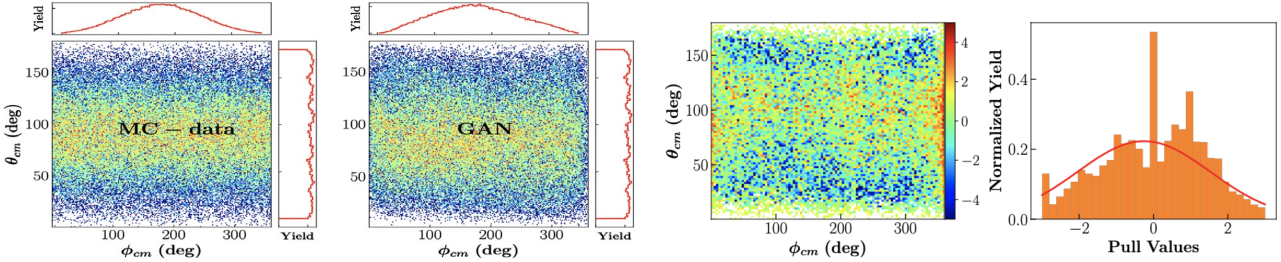




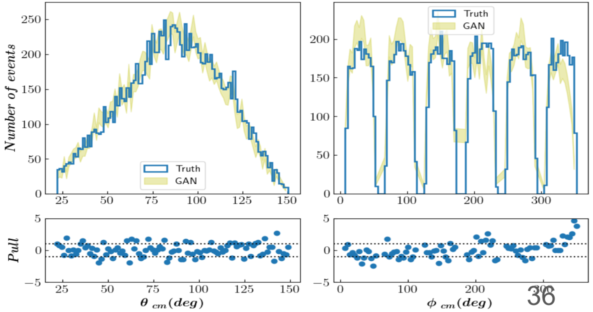
Entire Phase Space



Unmeasured topology



Entire Phase Space

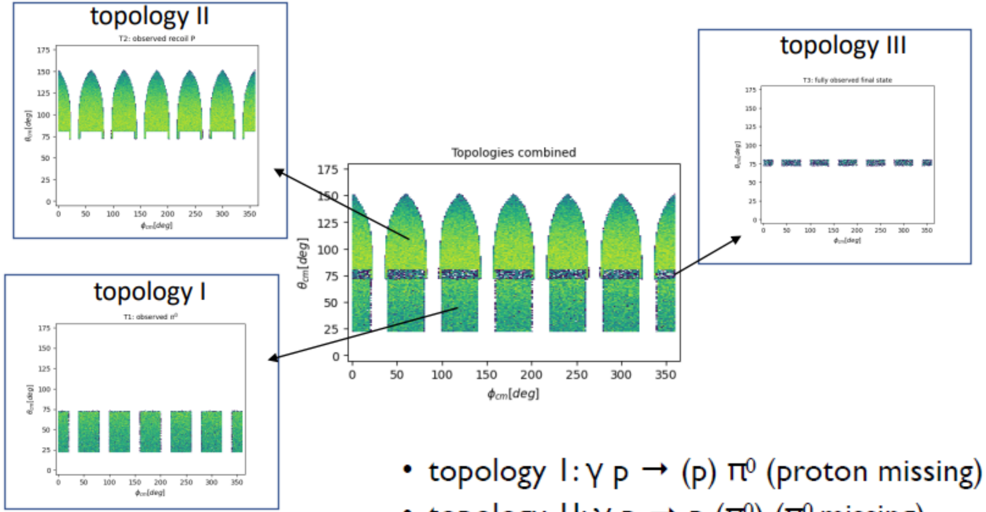


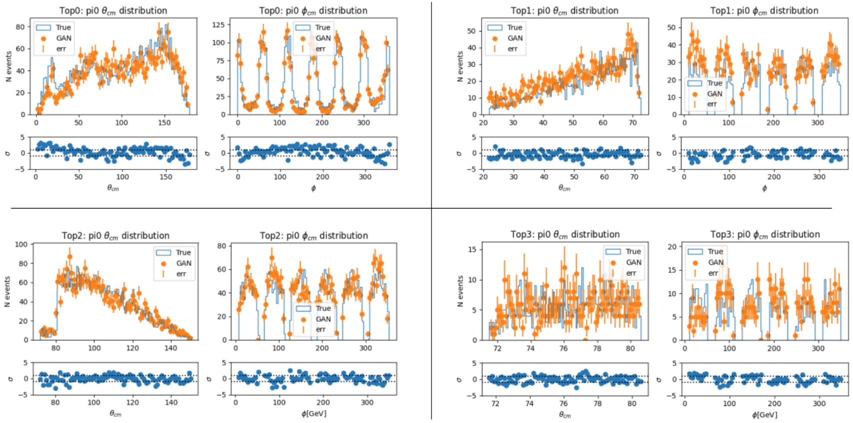
Measured topology

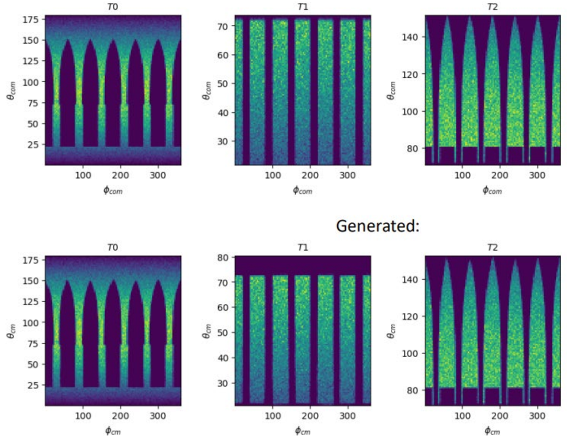
Alghamdi et al., ITCAI, 2024

Generative AI for Multiple Topologies

- Build a single ML model to generate in the full phase space
  - Combine vertex-level data from different experiments
  - Extend as much as possible the measured phase space
  - Minimize model dependency







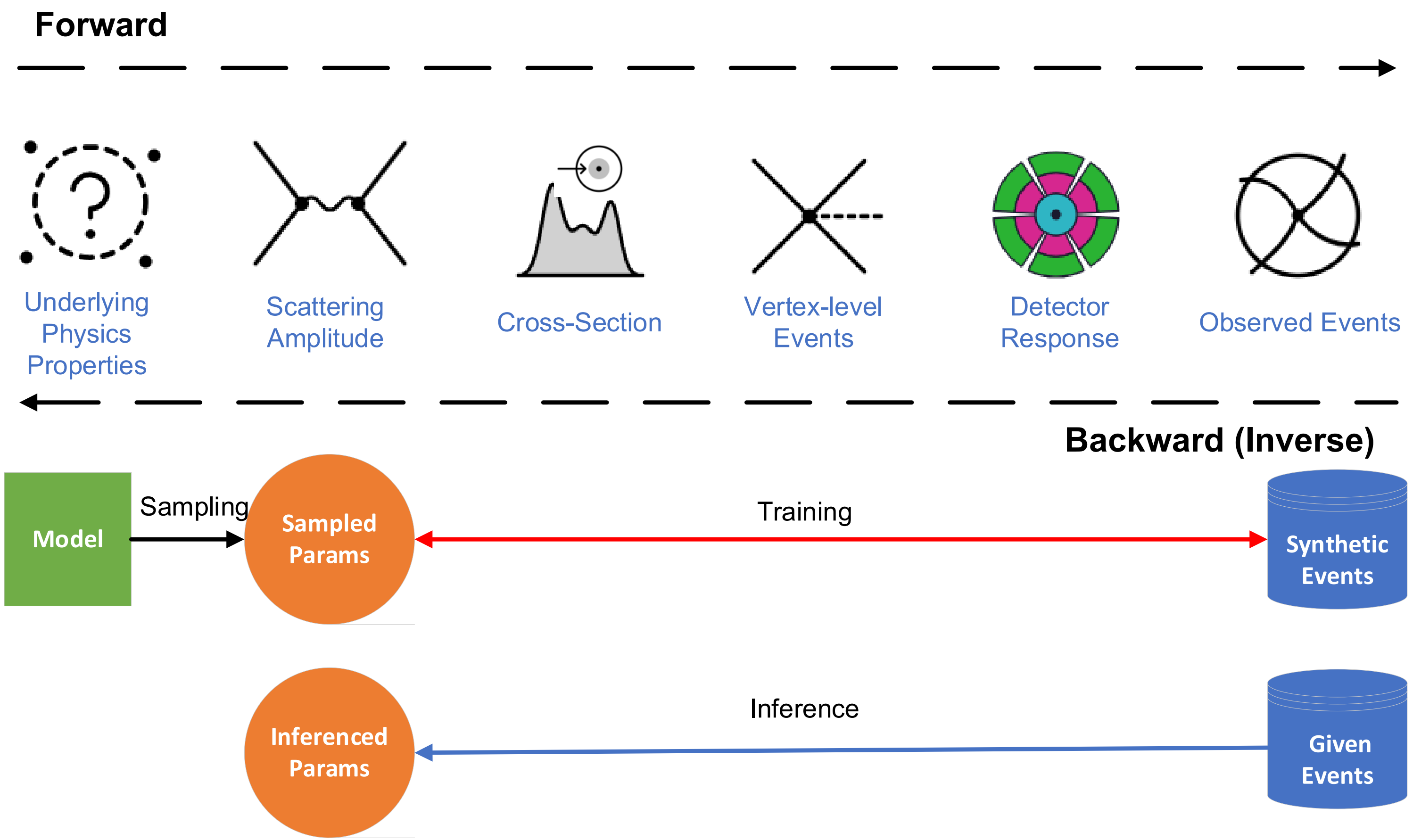
- topology I: $\gamma\, p \rightarrow (p)\, \pi^0$ (proton missing)
- topology II: $\gamma\, p \rightarrow p\, (\pi^0)$ (π^0 missing)
- topology III: $\gamma\, p \rightarrow p\, \pi^0$ (all detected)
- topology 0: unmeasured

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

Agenda

- The Inverse Problem
- Generative AI for Inverse Problem
- Model-Independent Framework
  - Reconstruct Scattering Amplitudes from Pion-Pion Scattering
  - Sampling Problem
    - QCF Parameterization
  - Unfolding Detector Effects
- Model-Dependent Framework
  - Extraction of Compton Form factors
  - Extracting TMDs from SIDIS Data
  - Out-of-Domain Problem and An Active Learning Solution
- Conclusion

A Model-Dependent Framework (End-to-End)



DM for Amplitude Reconstruction

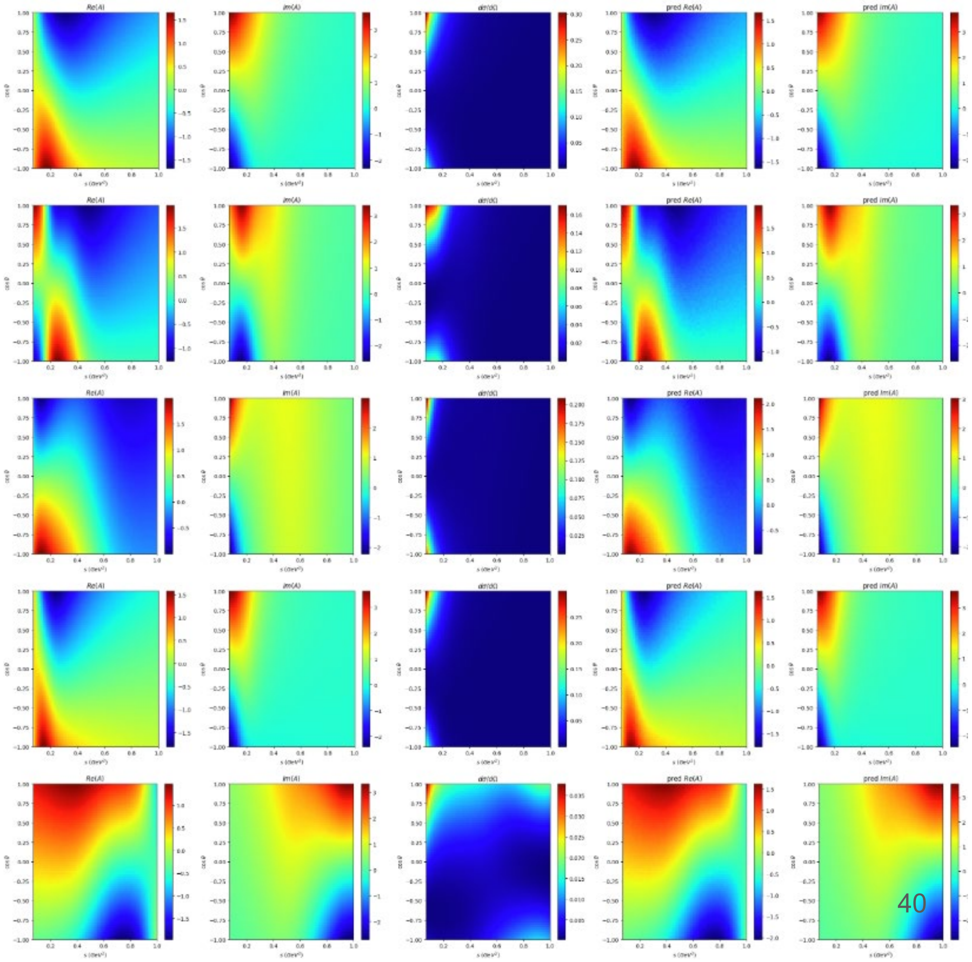
- $\pi^+\pi^-$ elastic scattering
  - Elastic 2 → 2 of spinless particles
- Simplified Model
  - Partial-wave decomposition of the amplitude truncated to $n = 1$ $\mathcal{A}(s, \cos\theta) = \sum_{l=0}^{n=1}(2l+1) f_l(s) P_l(\cos\theta)$
  - Breit-Wigner type partial waves $f_l = \frac{m_l \Gamma_l}{m_l^2 - s - i m_l \Gamma_l}$

$\mathcal{A}(s, \cos\theta) = f_0(s) + 3f_1(s)\cos\theta$

Truth

Cross-Section

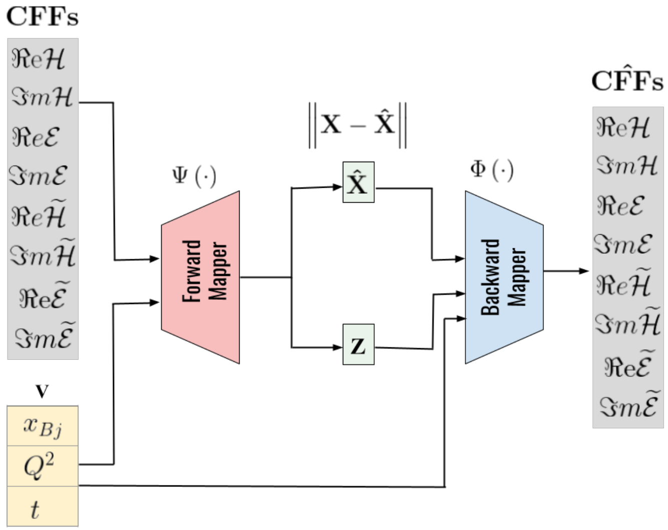
Reconstructed



Extraction of Compton Form factors

- Generalized Parton Distributions (GPDs)
  - Multi-dimensional descriptions of proton structure
- Deeply virtual exclusive scattering processes
  - Golden channel for the extraction of information on partonic 3D dynamics in the nucleon
- Compton Form Factors (CFFs)
  - 2D Slices of GPDs
  - Measured in DVCS
  - Contain potentially new information on hadronic structure
- Extraction of 8 CFFs from a single polarization observable
  - An inverse problem of extracting 8 unknowns from a single equation: $Re(H), Im(H), Re(\widetilde{H}), Im(\widetilde{H}), Re(E), Im(E), Re(\tilde{E}), Im(\tilde{E})$
  - Quantification of information extracted from experiments

Almaeen et al., EPJC, 2025



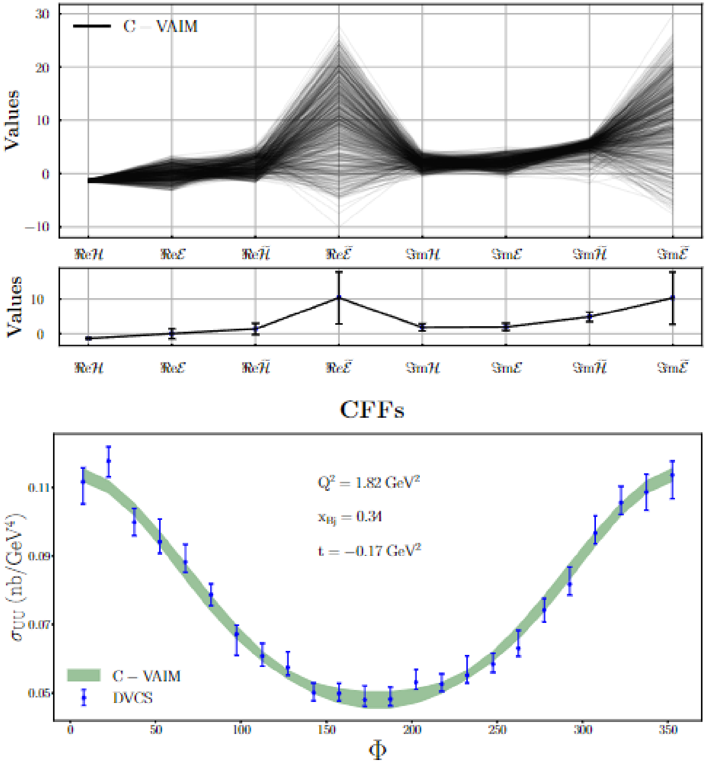
Training Data:
Kinematics values

Bin	x_{bj}	t (GeV^2)	Q^2 (GeV^2)
1	0.343	-0.172	1.820
2	0.368	-0.232	1.933
3	0.375	-0.278	1.964
4	0.379	-0.323	1.986
5	0.381	-0.371	1.999

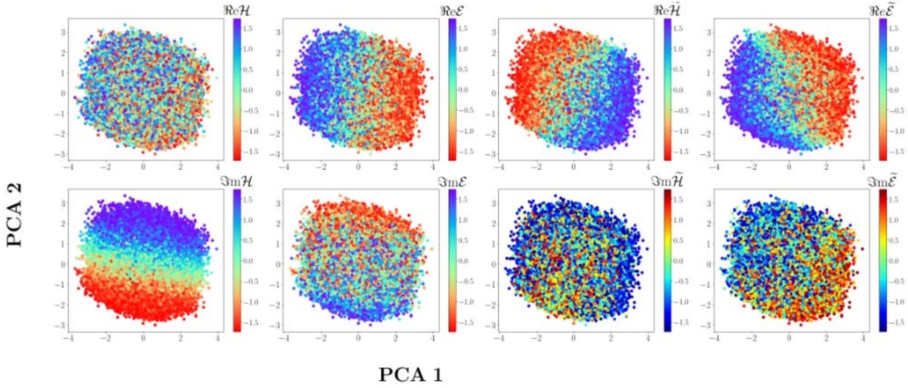
Generate uniformly distributed CFFs

- $ReH \in [-4, 4]$
- $ReE \in [-4, 4]$
- $Re\widetilde{H} \in [-10, 10]$
- $Re\tilde{E} \in [-10, 30]$
- $ImH \in [-1, 5]$
- $ImE \in [-1, 5]$
- $Im\widetilde{H} \in [-1, 20]$
- $Im\tilde{E} \in [-10, 30]$

Prediction of CFFs



- Predicted CFFs from VAIM-CFF
  - $X_{Bj} = 0.343$
  - $t = -0.172$ GeV^2
  - $Q^2 = 1.820$ GeV^2

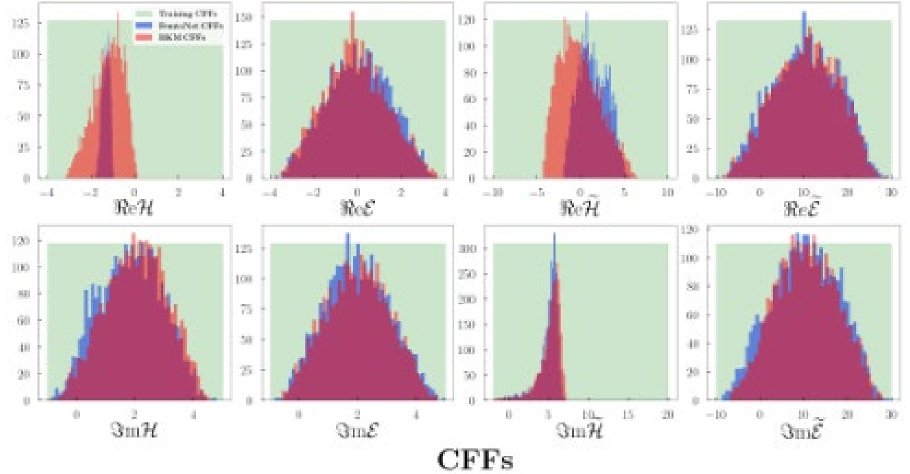


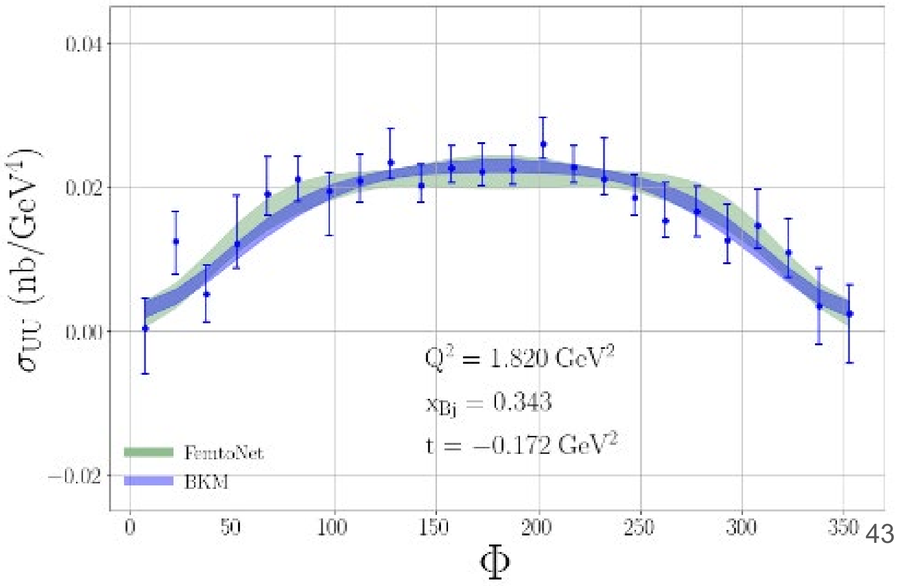
Latent Space Analysis

Almaeen et al., EPJC, 2025

Training C-VAIM on Different Cross-section Formulations

- Two Cross-section Formulations
  - FemtoNet (UVA)
  - BKM (Belitksy, Kirchner, Mueller)
- Kinematics
  - $X_{Bj} = 0.35$
  - $t = 0.172$
  - $Q^2 = 1.9\ GeV^2$
  - $Eb = 5.75\ GeV$

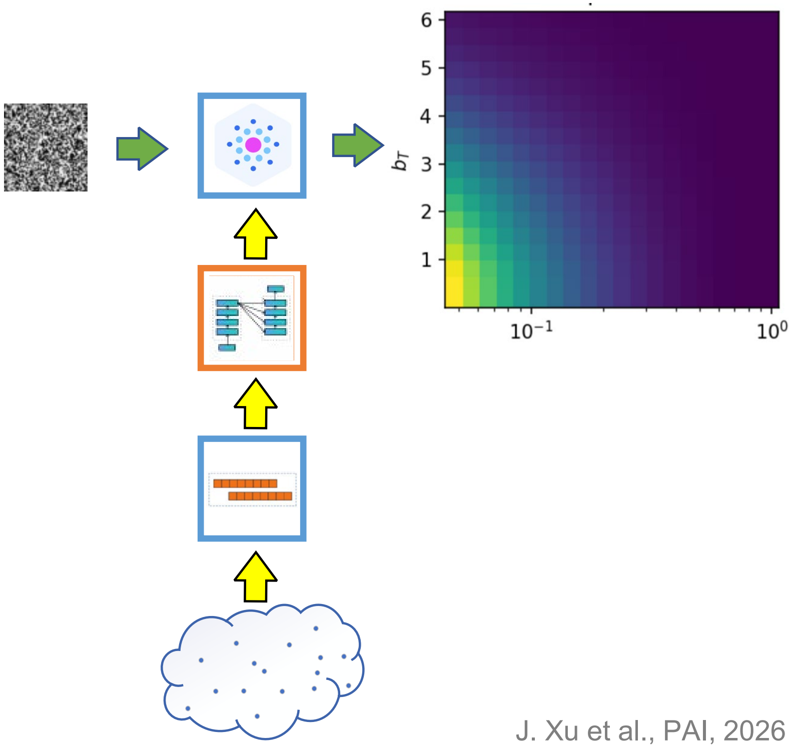




Almaeen et al., EPJC, 2025

Extracting TMDs from SIDIS Data

- **Infer Transverse Momentum Dependent (TMD) PDFs from experimental data**
- **Input: SIDIS events:** (x, Q^2, z, q_T, ϕ)
- **Challenge: Inverse problem through a complex physics pipeline**
  - High dimensional
  - Nonlinear transformations
  - Limited experimental statistics
- **Conditional Diffusion for TMD Inference**
  - Learn $p(TMD \mid events)$
  - Generates full posterior distribution
- **Event-to-TMD Pipeline**
  - Diffusion backbone:
    - 2D U-Net on TMD images (20×30 grid)
  - Conditioning:
    - PointNet-style encoder for variable-size event sets
    - Transformer → fixed embedding
  - Integration:
    - Event embedding injected into diffusion steps

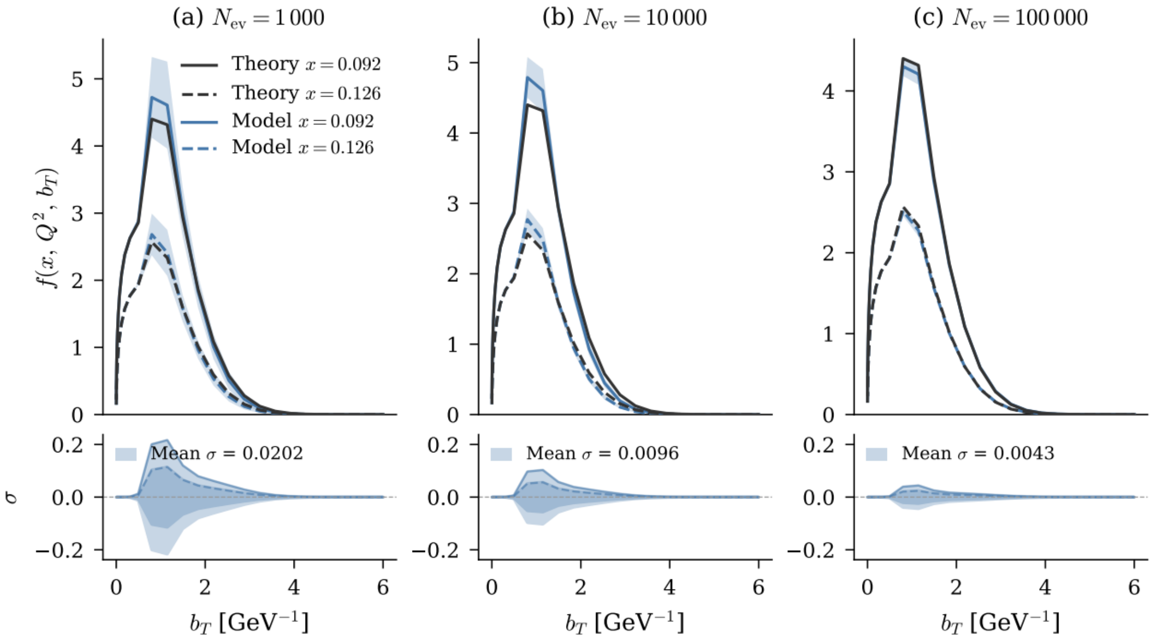


J. Xu et al., PAI, 2026

Results

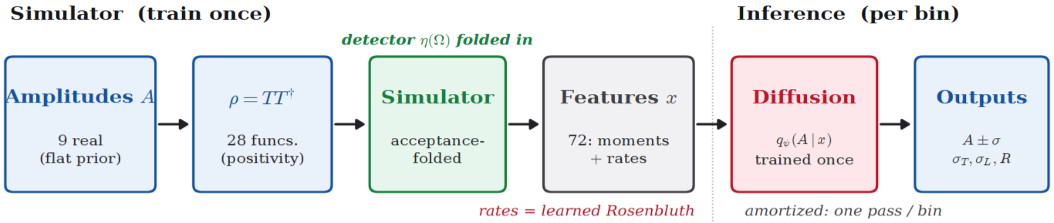
Performance vs Number of Events

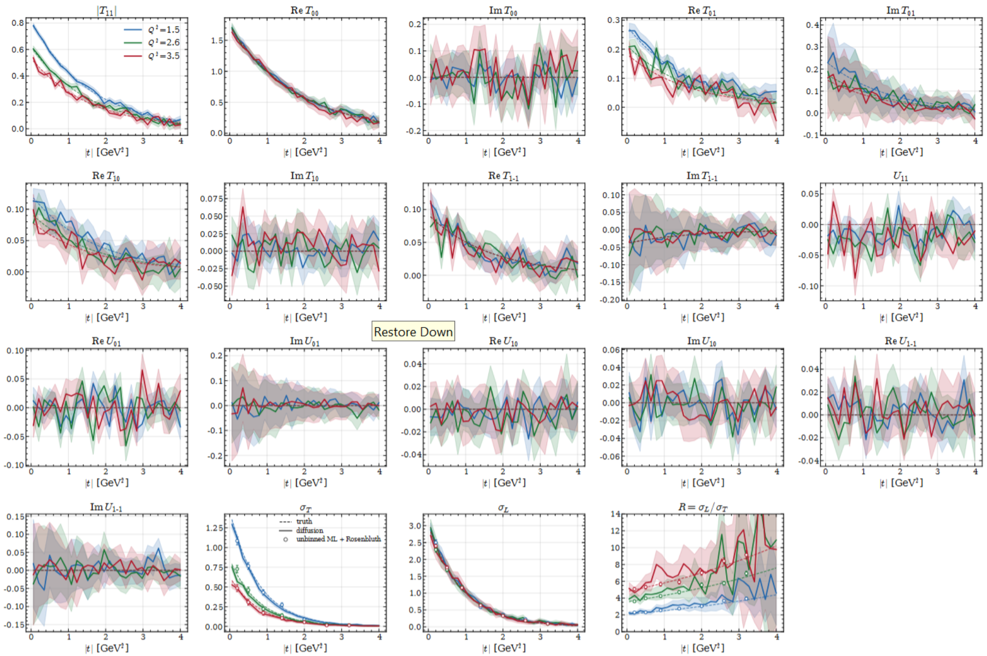
- $N_{ev} = 1{,}000$:
  - Captures shape, high uncertainty
- $N_{ev} = 10{,}000$:
  - Accurate reconstruction, reduced variance
- $N_{ev} = 100{,}000$:
  - Near-perfect recovery, very low uncertainty
- **Uncertainty scales as** $\sim 1/\sqrt{N_{ev}}$



J. Xu et al., PAI, 2026

Helicity-amplitude Extraction



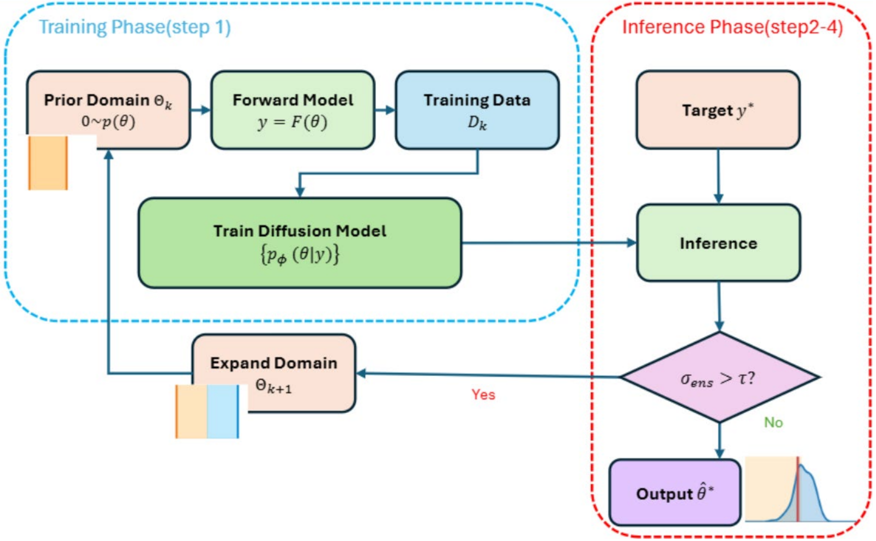


Collaboration with B. Singh (main developer), H. Avakian, S. Bhattacharya, V. Burkert, L. Elouadrhiri, D.I. Glazier, V. Kubarovsky, R.G. Milner, and Y. Wang

Preliminary (unpublished) work

Helicity-amplitude extraction and its kinematic dependence: the 16 amplitude parameters (nine natural-parity, seven unnatural-parity) and the derived σ_T , σ_L, R vs. |t|(to 4 GeV^2) for three Q^2 rings, extracted (solid line ± total-uncertainty band) versus the injected truth(dashed).

A Hidden Problem



- Out-of-domain Inference
  - Training
    - Assumption: known parameter domain Θ_0
  - Reality
    - True parameters θ^* may be outside of training range $\theta^* \notin \Theta_0$
  - Consequence
    - Confident but wrong predictions in diffusion model-based inference
    - No built-in warning signals
- Active-learning Solution
  - Detect Model Failure → Expand domain → Retrain
    - Generative AI
      - For posterior sampling
    - Active learning
      - For domain refinement
  - Learn correct parameter region even with incomplete priors

Active Learning Loop

Step 1: Initial guess. Select an initial parameter domain Θ_0 based on physical guess and generate a dataset on the initial training region

$$D_0 = \{(\theta_i, \mathcal{F}(\theta_i)) : \theta_i \in \Theta_0\}$$

Train the diffusion model on D_0

Step 2: Inference on target data. Given the control observable y^*, perform reverse diffusion to obtain inferred parameter samples

$$\tilde{\theta} \sim p_\phi(\tilde{\theta} | y^*)$$

Compute $\Sigma_{\tilde{\theta}}$

Step 3: Uncertainty-triggered domain update. If $Tr(\Sigma_{\tilde{\theta}}) > \tau$, expand domain

$$\Theta_{k+1} = Expand(\Theta_k, \tilde{\theta})$$

Generate synthetic samples

$$D_{k+1} = \left\{\left(\theta_j, \mathcal{F}(\theta_j)\right) : \theta_j \in \Theta_{k+1}\right\}$$

Fine-tune the diffusion model on the augmented dataset D_{k+1}.

Step 4: Iteration. Repeat steps 2-3 until $Tr(\Sigma_{\tilde{\theta}}) \le \tau$

The posterior has contracted to a well-supported region containing θ^*.

QCF Parameterization

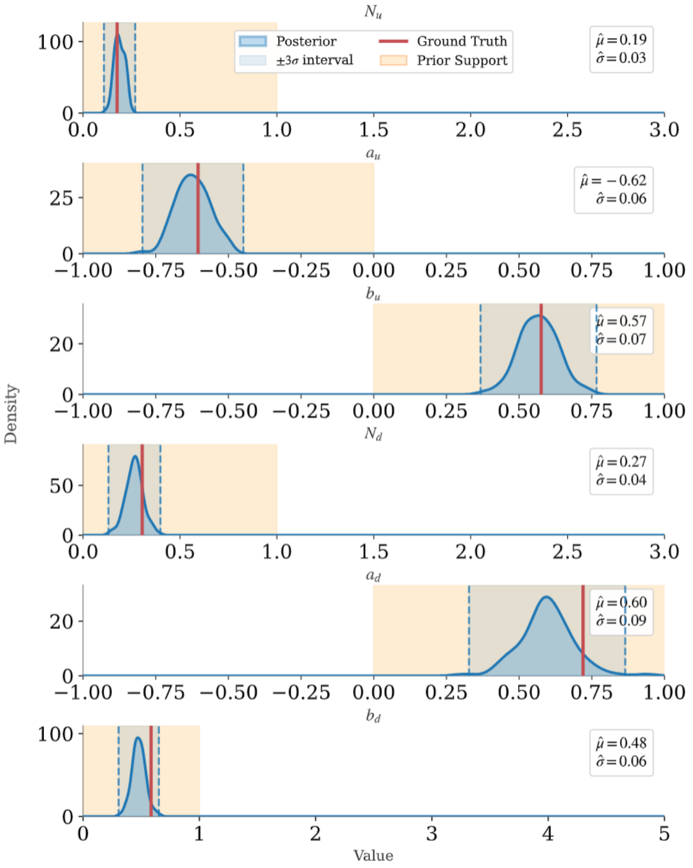
- **Measurable observables**
  - σ_p^o and σ_n^o
    - Cross-section distributions from proton and neutron targets, respectively.
    - Driven by underlying quark distributions $u(x;p)$and $d(x;p)$, which act as proxies for QCFs.
- **Forward model**

$$\sigma_1(x;p) = 4u(x;p) + d(x;p)$$
$$\sigma_2(x;p) = u(x;p) + 4d(x;p)$$
$$u(x;p) = N_u x^{a_u}(1-x)^{b_u}$$
$$d(x;p) = N_d x^{a_d}(1-x)^{b_d}$$

- **Inverse problem**
  - Given event-level samples σ_p^o and σ_n^o , infer QCF parameters

$$p = \{N_u, a_u, b_u, N_d, a_d, b_d\}$$

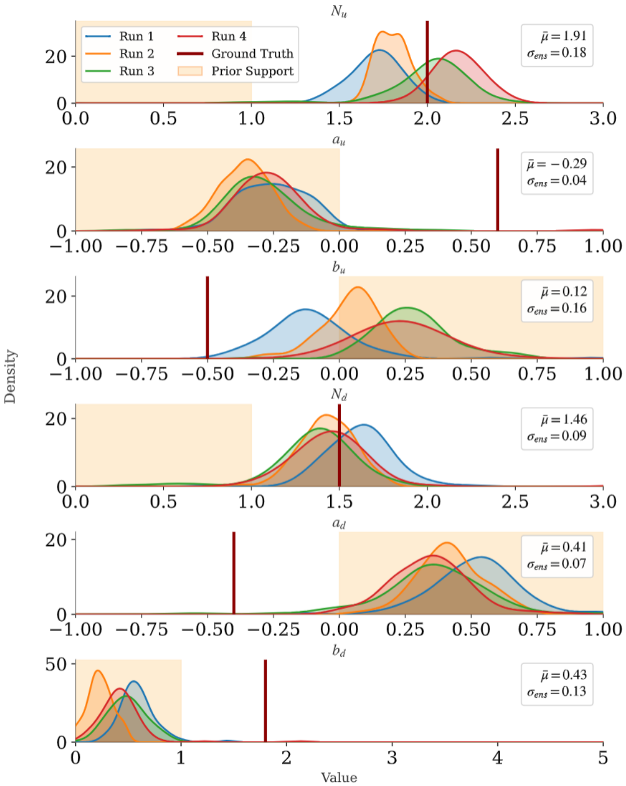
In domain predictions



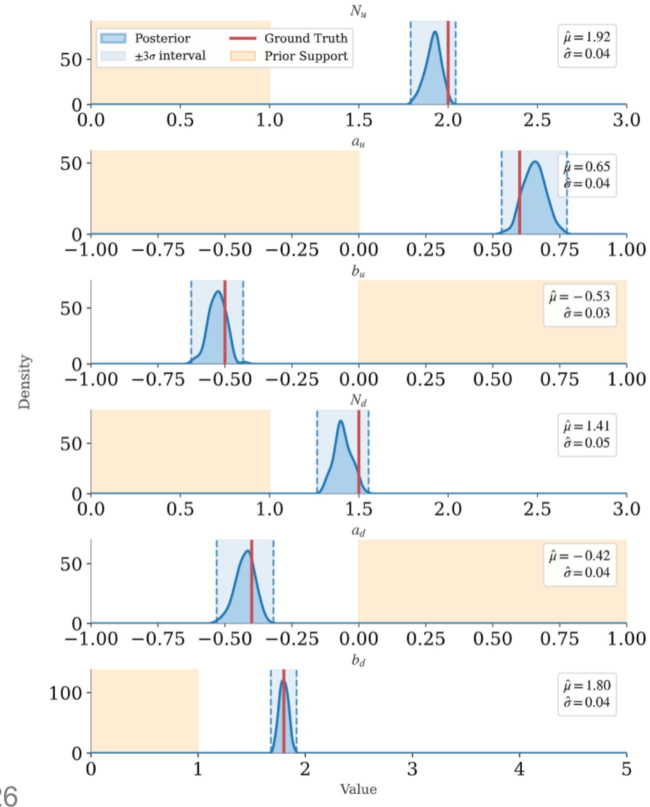
J. Xu et al., IJCAI, 2026

Incomplete Prior for QCF Parameterization

Out–of–domain Inferences



After Active Learning



J. Xu et al., IJCAI, 2026

Summary

- Generative AI for Inverse Problem
- Model-Independent Framework
  - Does not rely on a particular physics model
  - Gradient problem
  - Detector response unfolding
- Model-Dependent Framework
  - Need some assumption of a physics model
    - Parameterization
  - Out-of-Domain Problem
    - Active Learning

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Acknowledgements

- DOE SciDAC Program
- DOE Research on Artificial Intelligence and Machine Learning Applied to Nuclear Science and Technology Program
- Center for Nuclear Femtography (CNF)
- A(I)DAPT Collaboration

  A(i)DAPT
  AI for Data Analysis and PreservaTion
- EXCLAIM Collaboration
- QuantOm Collaboration