The QuantOm Event-Level Inference Framework

Daniel Lersch for the QuantOm Collaboration

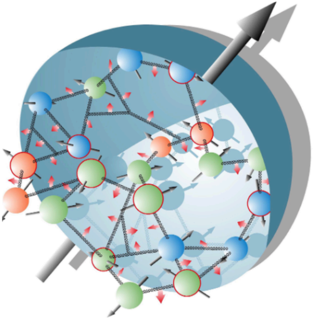
Jefferson Lab

May 11, 2023

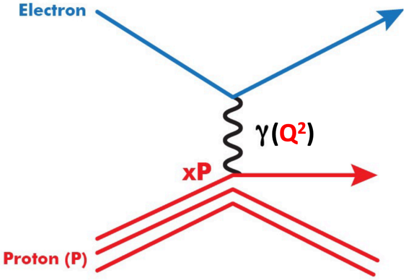
Study Quark-Gluon Structure via Scattering Events

- **Goal:** Understand Quark-Gluon system (e.g. explain nucleon mass or spin)
- **Approach:** Conduct scattering experiments ⇒ Extract Quantum Correlation Functions (QCFs)

QCD

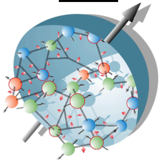


Deep Inelastic Scattering (DIS) Experiments



A “typical” Workflow

QCD



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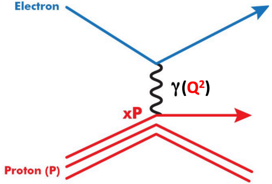
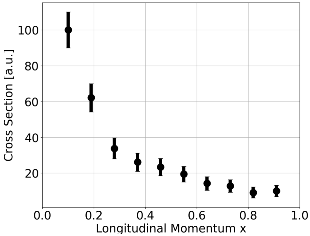


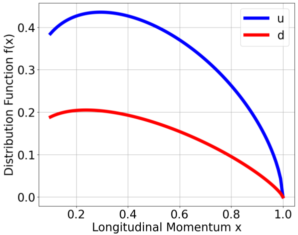
Analysis

- Event selection
- Determine observables
- Histogram observables
- Acceptance corrections
- Radiative corrections
- ....



Extract QCF

- Input from Theory
- QCD factorization
- QCD evolution
- Fit experimental data



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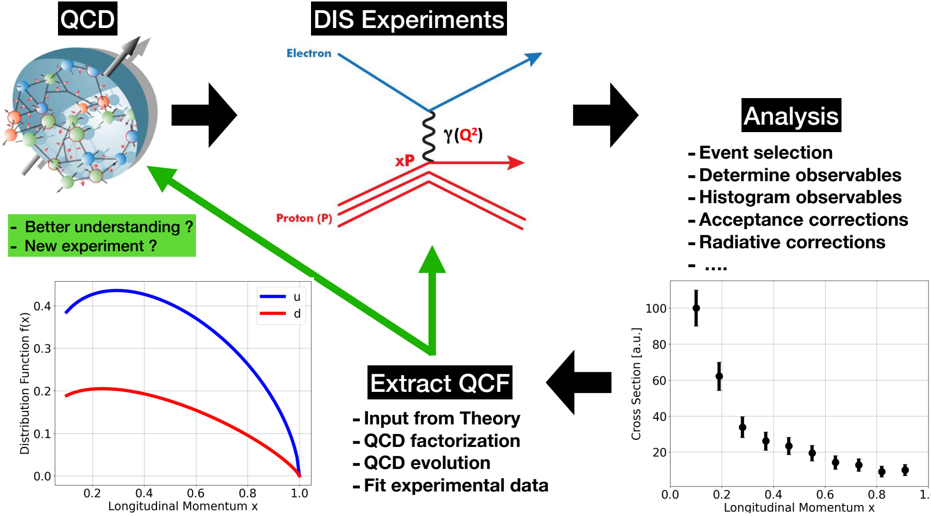

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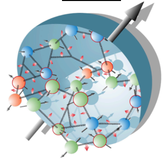

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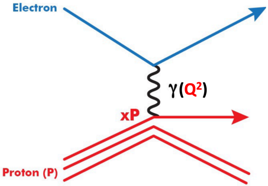

A lot of work goes in here!

(Apologies for this oversimplified representation)

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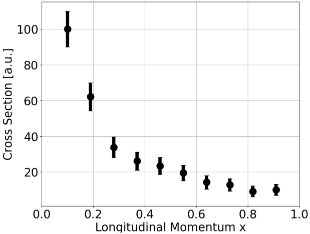
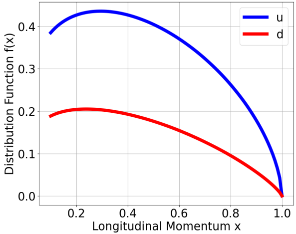
- **Histogram observables**
- **Acceptance corrections**
- **Radiative corrections**
- **....**



Extract QCF

- **Input from Theory**
- **QCD factorization**
- **QCD evolution**
- **Fit experimental data**



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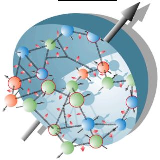

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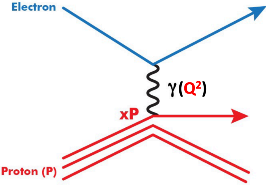

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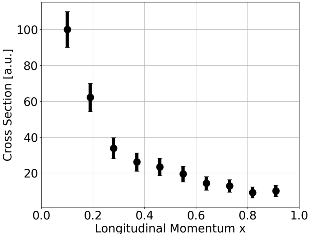

- **Possible information loss**
- **Handling correlations ?**
- **Binning / smearing effects ?**
- **Need to re-iterate with different binning ?**
- **...**

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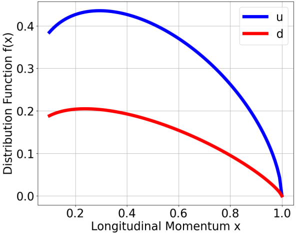
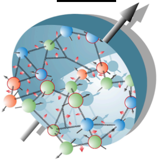


From Histograms to Event-Level Analysis

QCD



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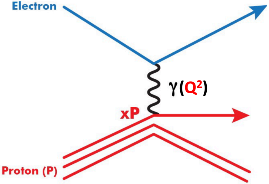
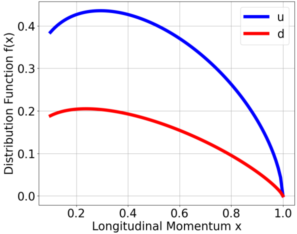


Event-Level Analysis

Combine:
- **Theory**
- **Experiment**
- **Math + Statistics**
- **AI / ML**
- **High performance computing**



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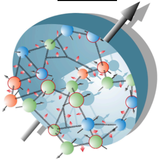

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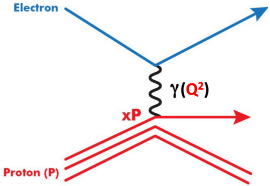

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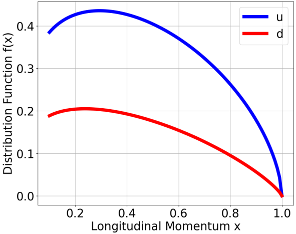
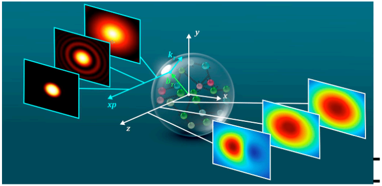


3D Imaging



- **Utilize all information in data**
- **Fully explore feature space**

The **QUA**ntum chromodynamics **N**uclear **TOM**ography Collaboration (**QuantOm**)

- Part of the **Sci**entific **D**iscovery through **A**dvanced **Computing** (**SciDAC**) program

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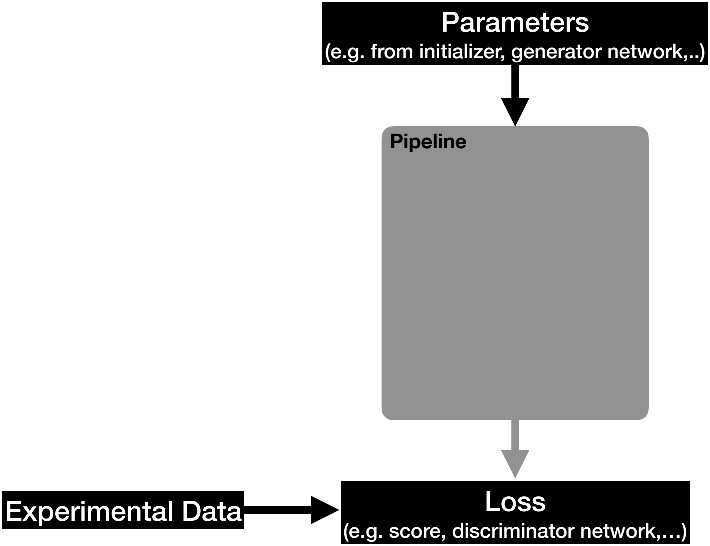
- Interdisciplinary research
  - Applied mathematics
  - Computer and Data science
  - Theoretical and experimental nuclear physics
  - High performance computing
- Utilize various research institutions
  - Jefferson Lab
  - Argonne National Laboratory
  - Virginia Tech
  - Old Dominion University

The QuantOm Event-Level Workflow



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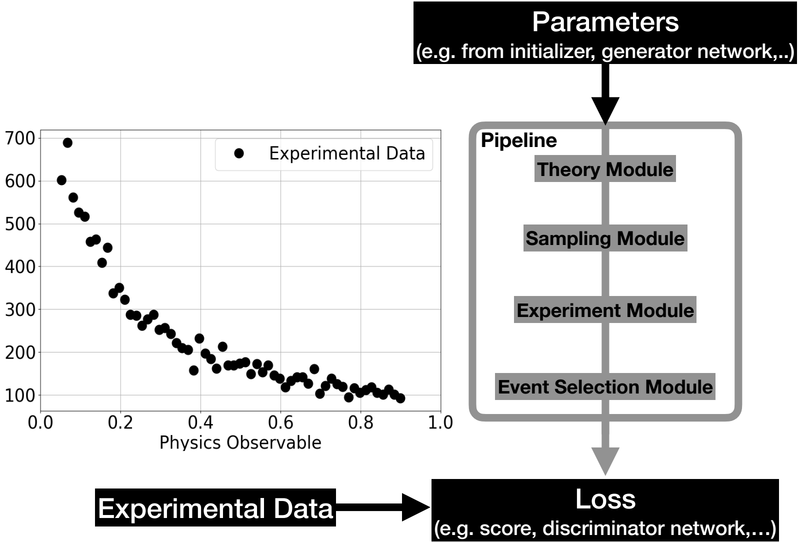
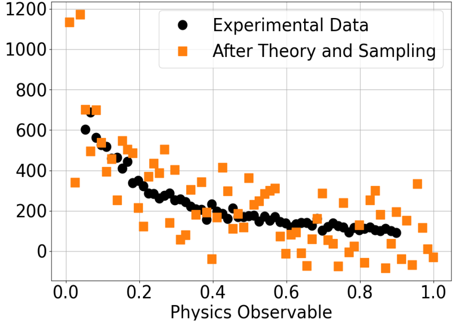


NOTE: Plots shown here are used for visualization only and not part of the workflow

The QuantOm Event-Level Workflow

Parameters
(initializer, generator network,..)

Translate parameters to physics events
- Convert parameters to parton density functions (PDFs)
- Include higher order and radiative effects (i.e. full theory of the process)
- Sample ideal events from PDFs (e.g via MCMC)



Pipeline
- Theory Module
- Sampling Module
- Experiment Module
- Event Selection Module

Experimental Data → **Loss**
(e.g. score, discriminator network,...)

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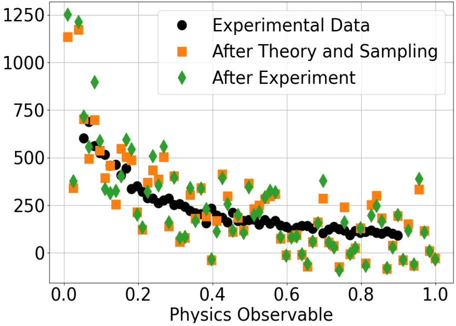
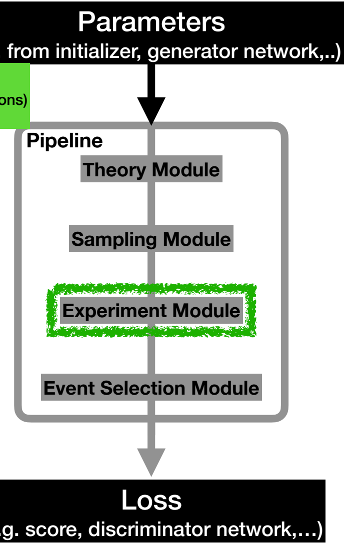
The QuantOm Event-Level Workflow

Apply experimental effects (e.g. resolution)

- Use all available information about experiment (e.g. simulations)
- Use surrogate for detector (e.g. matrix, ML model,...)





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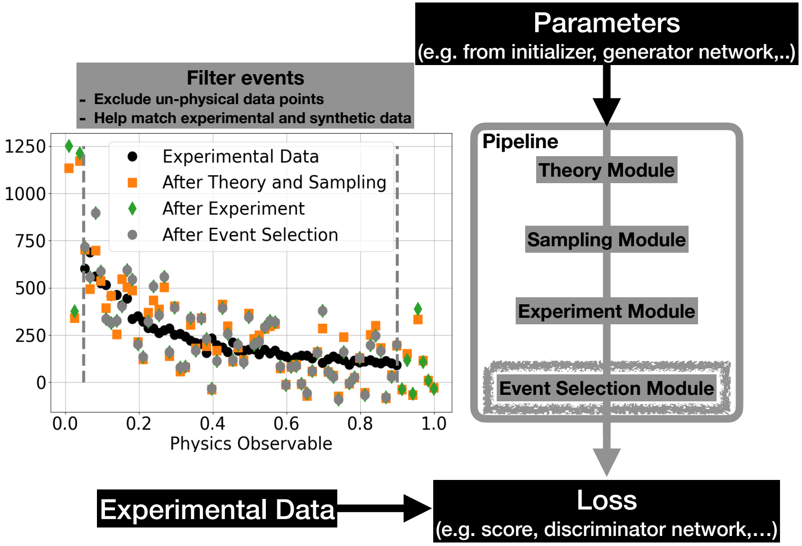

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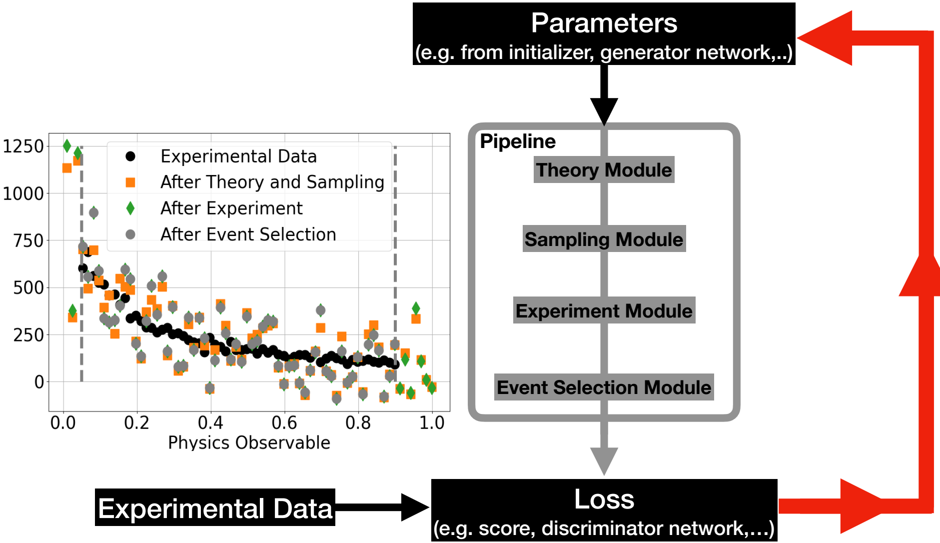

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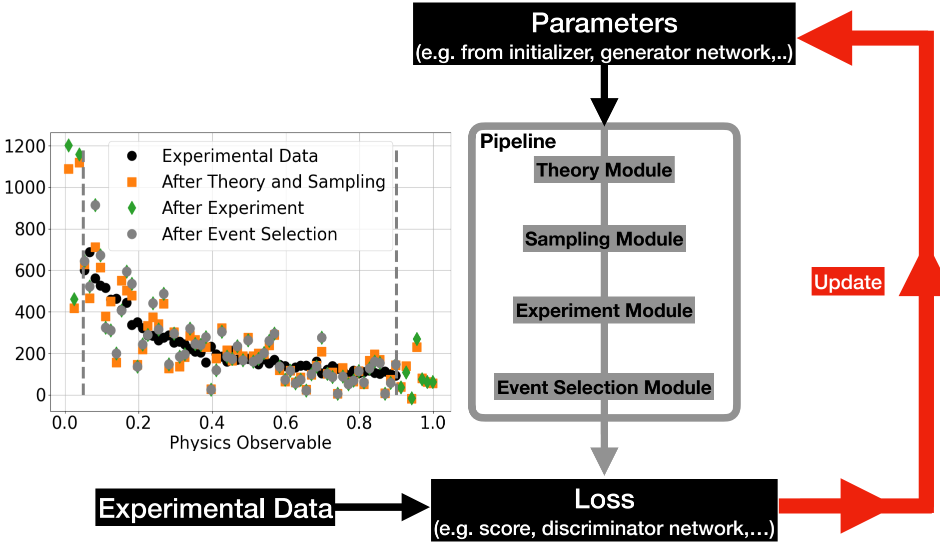

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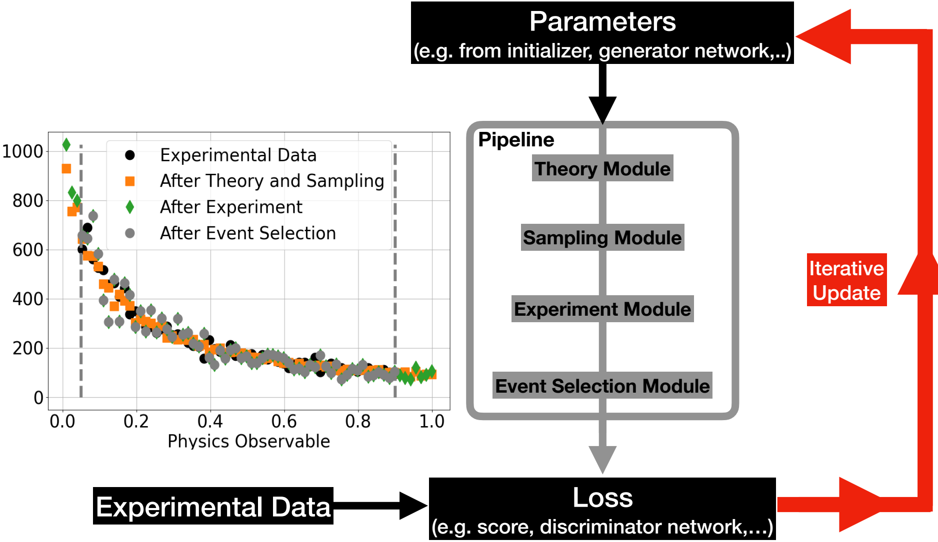

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Features of the Workflow

- Operates on the event-level
  - No information lost in histograming process
  - Access to entire feature space
  - Perform real-time analysis
  - Identify rare events
- Flexible
  - Change / update / add individual modules
  - Customize entire pipeline
- Fit multiple experiments simultaneously
  - Combine available data (more statistics / better feature space coverage)
  - Each experiment has its own dedicated module

Loop Closure Test

- Would like to...
  - ... understand the workflow
  - ... evaluate the performance
  - ... identify potential problems

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- Run tests on toy data set
  - Known "QCF" $\Rightarrow$ (what we are trying to find in a real analysis, e.g. PDF)
  - Simplified theory, sampling and experiment modules
  - Two observables $\Rightarrow$ (mimic what is usually histogramed, e.g. cross sections)
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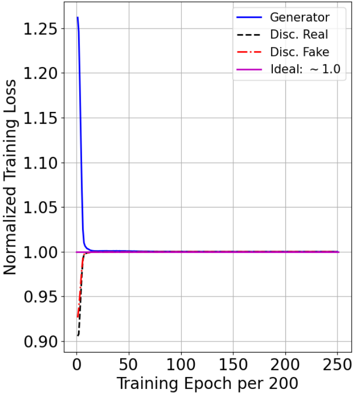
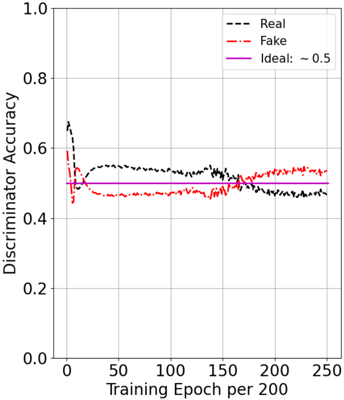
- Use GAN workflow
  1. Generator predicts parameters
  2. Parameters are translated to fake events with two observables
  3. Discriminator tries to distinguish between fake and toy data events

First Results from Loop Closure Test

GAN Convergence

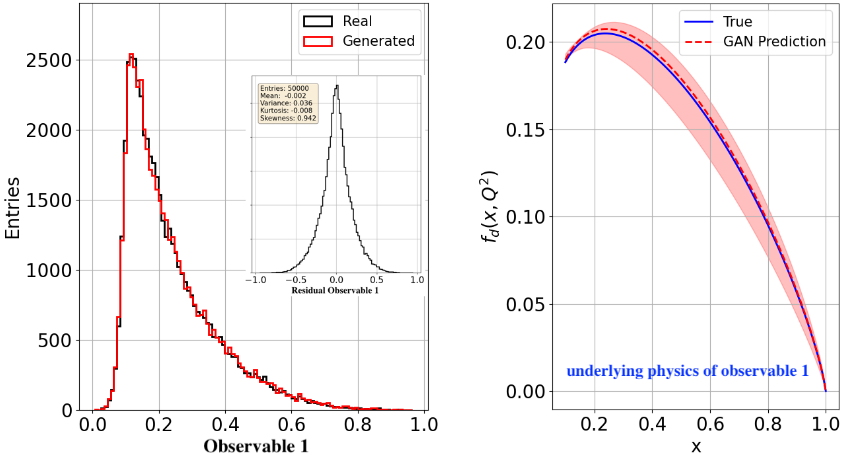




- Trained one GAN workflow on toy data set
- Used best guess settings for first tests
- **Ideally**
  - Generator and discriminator losses converge to same value
  - Discriminator accuracy is 0.5 for fake and real events

First Results from Loop Closure Test

GAN Predictions



- **Left:** Reproduce observables presented in toy data
- **Right:** True "QCF" and GAN prediction

Summary and Outlook

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  - Modular
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  - Uncertainty quantification
    (Statistical uncertainty vs. Neural net uncertainty vs. Module uncertainty,..)
  - Scalability (Distributed training with 2,4,8,... GPUs)
  - Neural network independent workflow developed in parallel
  - Hyper parameter optimization (HPO)
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  - Identify bugs and bottle-necks in workflow
- Analyze measured data from experiment
  - How to handle possible background in data ?
    (⇒ Background studies on toy data currently ongoing)
  - Use "realistic" experiment module (⇒ ML surrogate)