Update on DVCS Compton Form Factor fitting with PARTONS package

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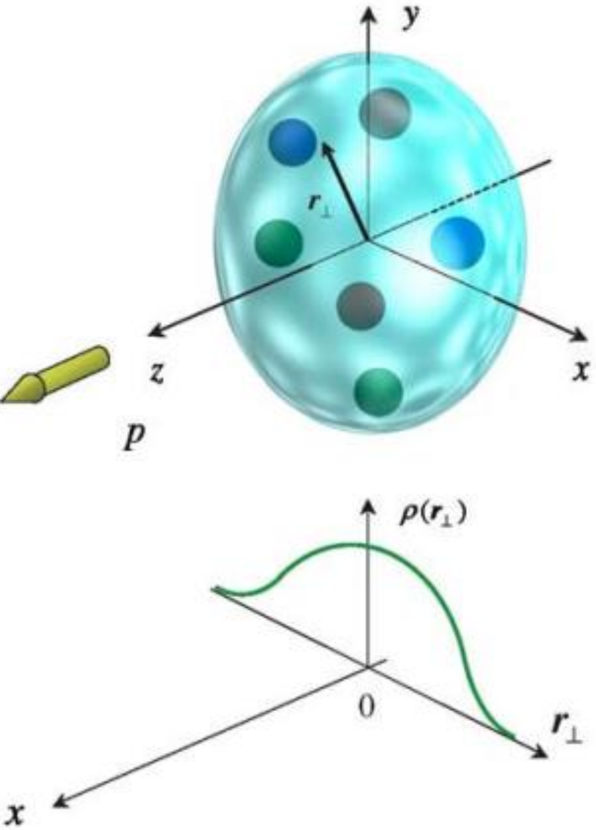
Outline

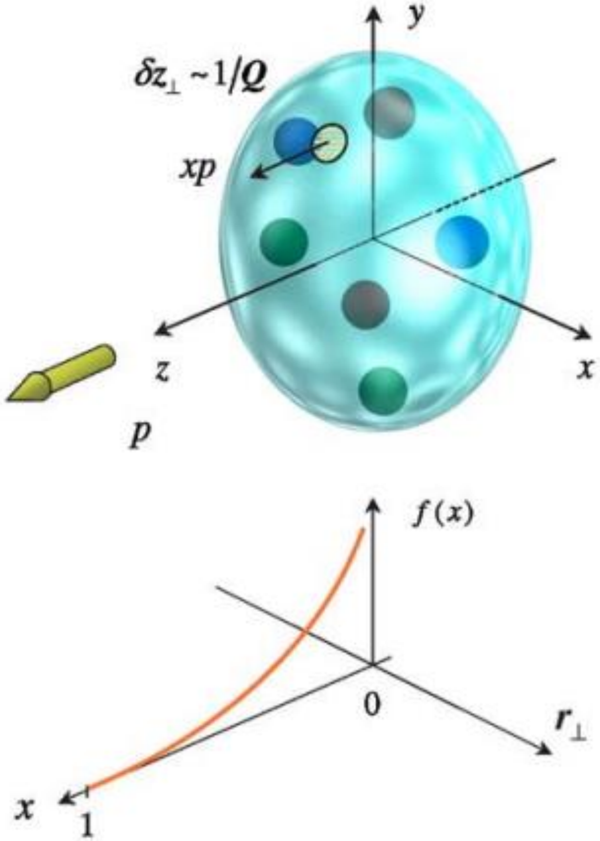
1. Motivation
2. DVCS CFF fitting strategy
3. Observable calculation studies using PARTONS
4. DVCS CFF fitting implementation and results
5. Future work

Motivation: Spatial Imaging of hadrons: Generalized Parton Distributions (GPDs)

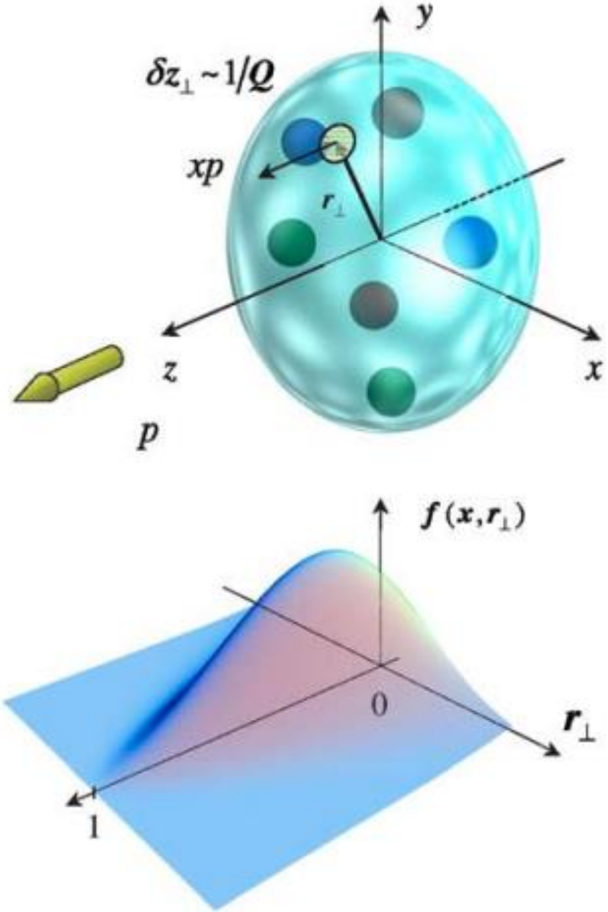
Elastic Scattering
Form Factors (FFs): Transverse charge and current density



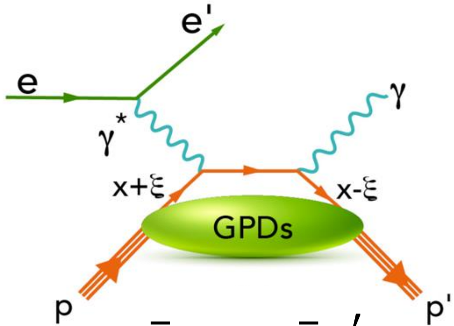
Deep Inelastic scattering
Parton Distribution Functions (PDFs): probability to find a parton i with xp longitudinal momentum



Hard Exclusive Processes
Generalized Parton Distributions: 3D image in transverse space and longitudinal momentum



Deeply Virtual Compton Scattering (DVCS)



$$e^- p \to e^- p' \gamma$$

x-internal quark momentum fraction
p-hadron momentum
x_B- Bjorken variable
$\xi \approx \frac{x_B}{2-x_B}$- skewness (longitudinal momentum transfer)

A.V. Belitsky and A.V. Radyushkin, "Unraveling hadron structure with generalized parton distributions," *Phys. Rept.* **418** (2005) 1-151

Motivation: Deeply virtual Compton scattering (DVCS) observables

DVCs GPDs ($H(x,\xi,t)$, $E(x,\xi,t)$, $\widetilde{H}(x,\xi,t)$,$\tilde{E}(x,\xi,t)$) are not observables.

The actual observables in DVCS are Compton form factors (CFFs)

$\mathcal{H},\mathcal{E},\widetilde{\mathcal{H}}\ ,\tilde{\mathcal{E}}$ given by convolution integrals at LO:

$$Re\mathcal{H}(\xi,t) + i\ Im\mathcal{H}(\xi,t) = \sum_q e_q^2 \int_{-1}^{+1} dx H_q(x,\xi,t)\left(\frac{1}{\xi - x - i\epsilon} - \frac{1}{\xi + x - i\epsilon}\right)$$

Similarly for other GPDs

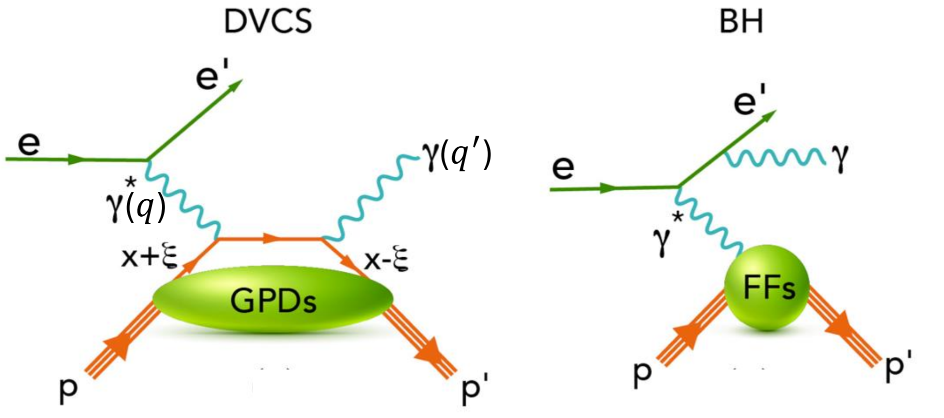
x - internal quark momentum fraction

e_q - electric charge of quark flavor q

$t = (p-p')^2\ ,\ \ \Delta = p - p',\ \ \ P = \frac{p+p'}{2}, q_M = \frac{q+q'}{2},\ \ \ Q^2 = -q^2$

$\xi = \frac{\Delta \cdot q_M}{P \cdot q_M}$.

DVCS interferes with Bethe-Heitler (BH)



CFFs $\mathcal{H}$ and $\mathcal{E}$ appear in the DVCS observables such as differential cross sections and beam and target polarization asymmetries.

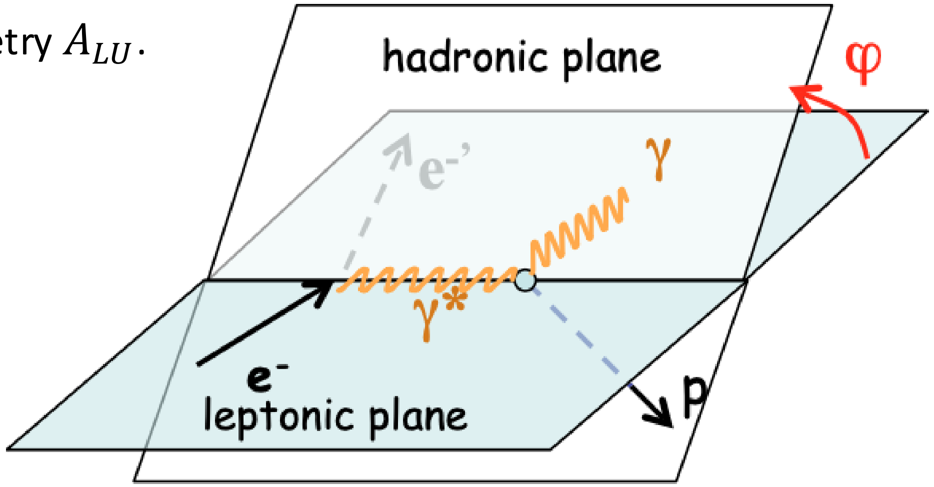
DVCS-BH interference term contains $Im\mathcal{H}$ in the beam polarization asymmetry A_{LU}.

$$A_{LU} = \frac{d^4\sigma^{\rightarrow} - d^4\sigma^{\leftarrow}}{d^4\sigma^{\rightarrow} + d^4\sigma^{\leftarrow}} \overset{\text{twist-2}}{\approx} \frac{A_{LU}^{\sin\varphi}\sin\varphi}{1 + \beta\cos\varphi}$$

$$A_{LU}^{\sin\varphi} \propto Im(F_1\mathcal{H} + \xi G_M\widetilde{\mathcal{H}} - \frac{t}{4M^2}F_2\mathcal{E})$$

F_1, G_M - Dirac and magnetic FFs

$d^4\sigma^{\rightarrow} = \frac{d^4\sigma^{\rightarrow}}{dx_B dQ^2 dt d\varphi}$ differential cross section for positive beam helicity



$Re\mathcal{H}$ appears in the differential cross section → Determine $\mathrm{Im}\mathcal{H}(\xi,t)$ and $\mathrm{Re}\mathcal{H}(\xi,t)$ from fits to BSA and the diff. cross section

Motivation: Fixed-t Dispersion Relation

The real and Imaginary $\mathcal{H}(\xi,t)$ are related via fixed-t dispersion relation (DR), where the subtraction constant $C_{\mathcal{H}}(t)$ is related to so called D-term.

$$\mathrm{Re}\mathcal{H}(\xi,t) = C_{\mathcal{H}}(t) + \frac{1}{\pi} P.V. \int_0^{+1} d\xi' \left[\frac{1}{\xi-\xi'} - \frac{1}{\xi+\xi'}\right] \mathrm{Im}\mathcal{H}(\xi',t)$$

P.V. – Cauchy's principal value of the integral

The D-term related to the proton internal force. Neglecting gluon contribution at LO:

$$C_{\mathcal{H}}(t) = 2\sum_q e_q^2 \int_{-1}^{1} dz \frac{D_{\text{term}}^q(z,t)}{1-z}$$

$$D_{\text{term}}^q(z,t) = (1-z^2) \sum_{odd\ n} d_n^q(t) C_n^{\frac{3}{2}}(z)$$

q- quark flavor, $\mathrm{z} = \mathrm{x}/\xi$, $C_n^{\alpha}(z)$- Gegenbauer polynomials

In the limit of renormalization scale $\mu \to \infty$ only $d_1^q(t)$ contributes:

$D_q(t) = \frac{4}{5} d_1^q(t) = \int_{-1}^{1} dz\, z\ \ D_{\text{term}}^q(z,t)$

Neglecting strange and heavy quark contribution

$d_1^u \approx d_1^d \approx d_1^{u+d}/2$

$C_{\mathcal{H}}(t) \approx \frac{10}{9} d_1^{u+d}(t) = \frac{25}{18} D_{u+d}(t)$

Gravitational Form Factor (GFF) describing mechanical properties of the proton

Analysis based on unconstrained ANN techniques (Eur. Phys. J. C 81 (2021), 300) report Subtraction term compatible with 0 within large uncertainties.

By utilizing this DR, along with other phenomenological assumptions, we can extract CFFs and GFFs from experimental data.

DVCS CFF fitting strategy: Artificial Neural Networks (ANNs)

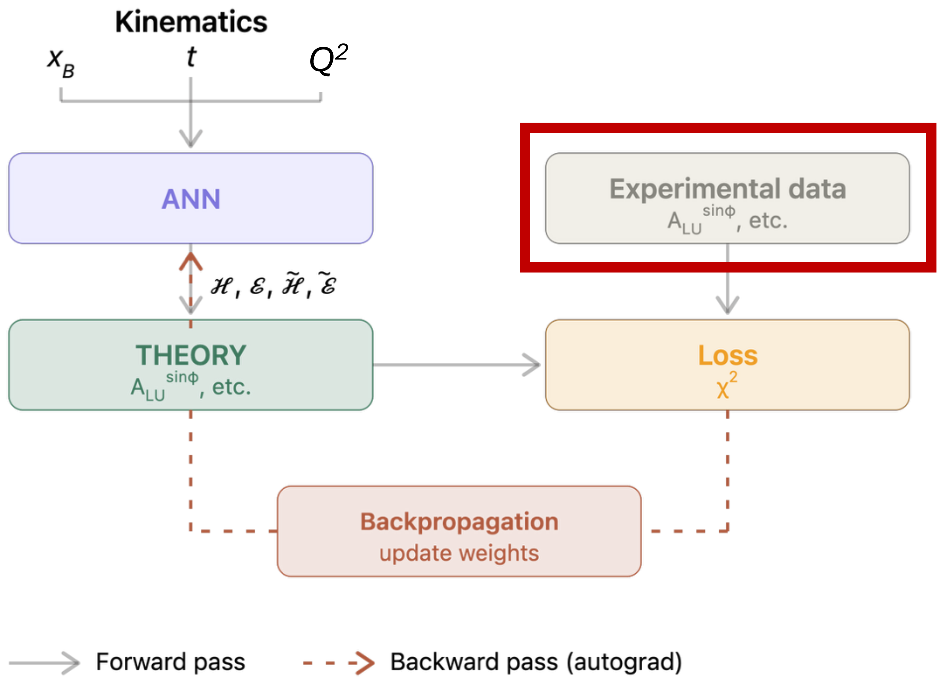
Use ANNs to describe CFF functional form model independent way.
Fit data for existing DVCS experimental observable measurements.
Use custom loss function in NN training:

$$\chi^2 = \sum_{i=1}^{n} \frac{(O_i^{theory} - O_i^{exp})^2}{(\sigma_i^{exp})^2}$$

O_i-denoting observables calculated from theory and measured from experiment
σ_i^{exp}-uncertainty from experimental measurement
n-total number of kinematic points for observable measurements

Collab	Year	Observable	E_{Beam}[GeV]	x_B	Q^2[GeV^2]	|t|[GeV^2]
CLAS	2001	$A_{LU}^{\sin(\phi)}$	4.25	0.19	1.25	0.19
CLAS	2006	$A_{UL}^{\sin(\phi)}$	5.7	0.2–0.4	1.82	0.15–0.44
CLAS	2007	A_{LU}	5.77	0.13–0.35	1.1–3	0.1–0.3
CLAS	2009	A_{LU}	4.8	0.12–0.48	1.0–2.8	0.09–1.8
CLAS	2015	$A_{LU}(\phi)$, $A_{UL}(\phi)$, $A_{LL}(\phi)$	5.93	0.18–0.4	1.6–3.2	0.1–0.45
CLAS	2015	$\sigma(\phi)$, $\Delta\sigma(\phi)$	5.75	0.1–0.58	1–4.6	0.09–0.52
CLAS	2018	$\sigma(\phi)$	5.88	0.12–0.5	1.1–4	0.1–1.6
CLAS	2023	A_{LU}	10.2	0.09–0.45	1.3–6	0.1–2.2
CLAS	2023	A_{LU}	10.6	0.09–0.62	1.1–7.2	0.1–2.8
HERMES	2001	$A_{LU}^{\sin(\phi)}$	27.6	0.11	2.6	0.27
HERMES	2006	$A_C^{\cos(\phi)}$	27.6	0.08–0.12	2.0–3.7	0.03–0.42
HERMES	2008	A_C, $A_{UT,I}$, $A_{UT,DVCS}$	27.6	0.03–0.35	1–10	<0.7
HERMES	2009	A_C, $A_{LU,I}$, $A_{LU,DVCS}$	27.6	0.05–0.24	1.2–5.75	<0.7
HERMES	2010	A_{UL}, A_{LL}	27.6	0.03–0.35	1–10	<0.7
HERMES	2011	$A_{LT,I}$, $A_{LT,BH+DVCS}$	27.6	0.03–0.35	1–10	<0.7
HERMES	2012	$A_{LU,I}$, $A_{LU,DVCS}$, A_C	27.6	0.03–0.35	1–10	<0.7
HALL A	2015	$\sigma(\phi)$, $\Delta\sigma(\phi)$	5.75	0.33–0.40	1.5–2.6	0.17–0.37

Training schematics



Setting up ANN fitting of DVCS CFFs in PARTONS in 3 steps

1. Setup ANN model training on observable data ($A_{LU}^{\sin\phi}$) that takes Kinematics as input and has desired architecture using LibTorch (C++ API for the PyTorch machine learning framework) with it's gradient based optimizers. Use Mean Squared Error as loss function:

$$MSE = \sum_{i=1}^{n} \frac{(O_i^{exp} - O_i^{pred})^2}{n}$$

O_i- denoting observable value predicted by ANN and measured from experiment

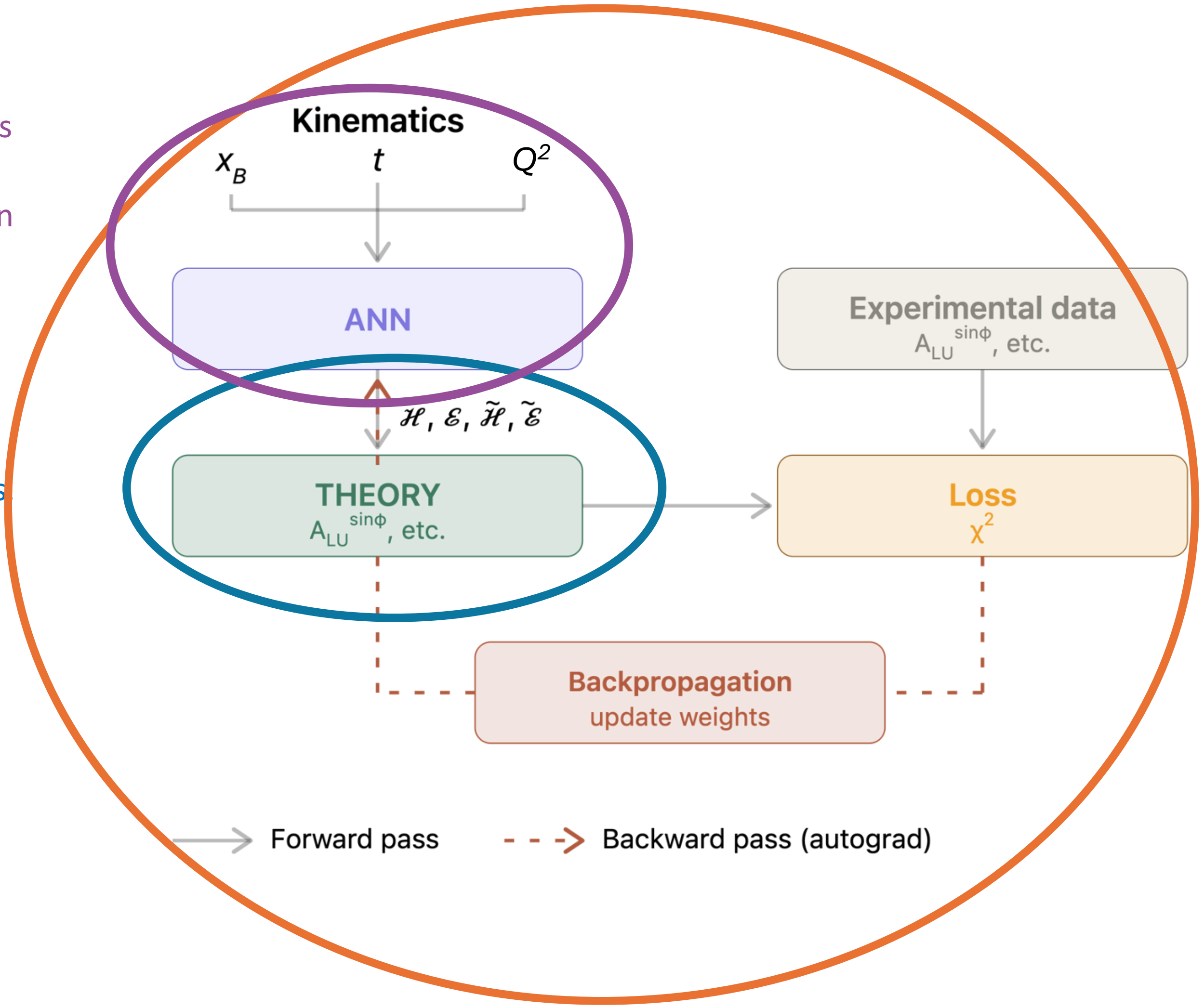
2. Use the model trained in previous step and assume it outputs DVCS CFF values Calculate observables from CFFs using PARTONS.

3. Using previous two steps set up ANN fitting of DVCS CFFs in PARTONS using custom loss function:

$$\chi^2 = \sum_{i=1}^{n} \frac{(O_i^{theory} - O_i^{exp})^2}{(\sigma_i^{exp})^2}$$

O_i-denoting observables calculated from theory and measured from experiment
σ_i^{exp}-uncertainty from experimental measurement
n-total number of kinematic points for observable measurements

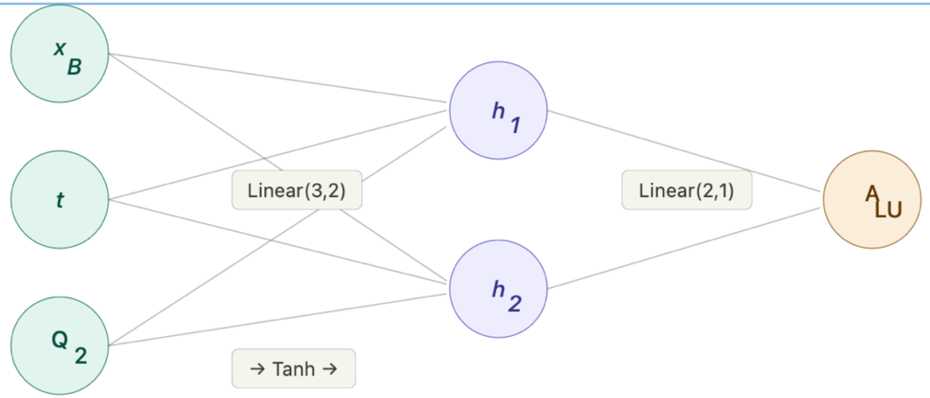
Training schematics



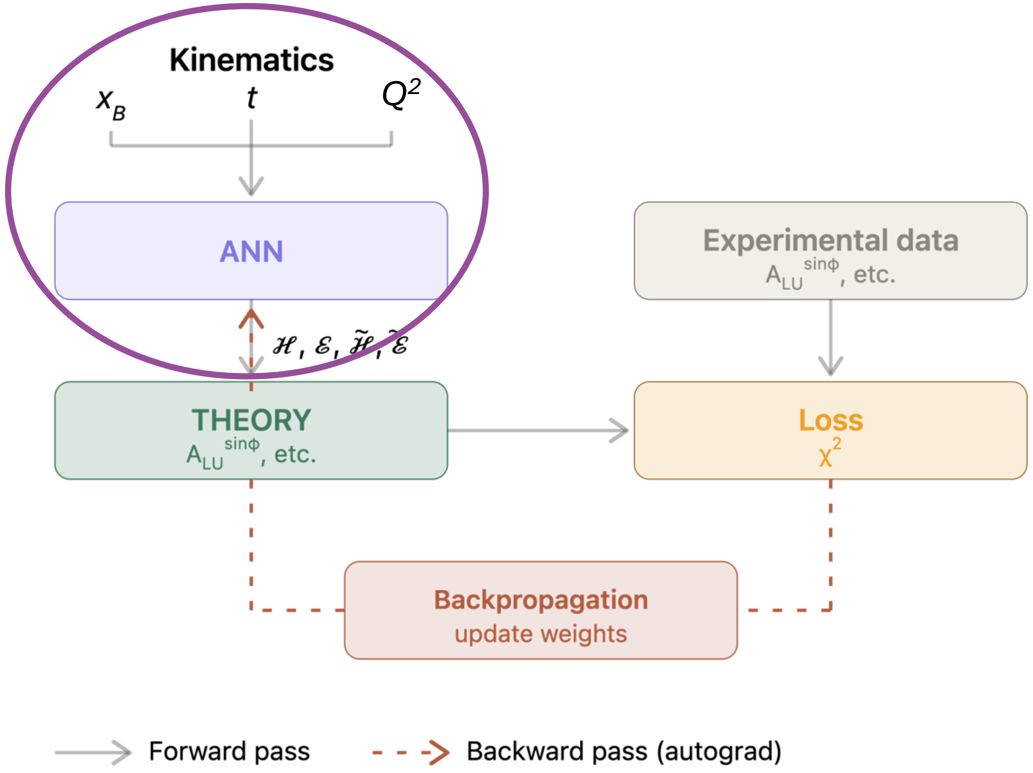
Setting up ANN fitting of DVCS CFFs in PARTONS : Step 1 - NN prediction of $A_{LU}^{\sin\phi}$ using LibTorch

CLAS 2007 DVCS (arXiv:0711.4805)

#	x_B	t	Q^2	E	ϕ	$A_{LU}^{\sin\phi}$
1	0.177	−0.138	1.560	5.770	6.000	0.204
2	0.245	−0.147	1.680	5.770	6.000	0.275
3	0.245	−0.284	1.680	5.770	6.000	0.302
4	0.245	−0.145	1.930	5.770	6.000	0.232
5	0.245	−0.281	1.930	5.770	6.000	0.281
6	0.245	−0.487	1.930	5.770	6.000	0.200
7	0.250	−0.144	2.190	5.770	6.000	0.204
8	0.250	−0.281	2.190	5.770	6.000	0.223
9	0.250	−0.488	2.190	5.770	6.000	0.213
10	0.338	−0.301	2.280	5.770	6.000	0.251
11	0.338	−0.494	2.280	5.770	6.000	0.188
12	0.340	−0.174	2.610	5.770	6.000	0.227
13	0.340	−0.297	2.610	5.770	6.000	0.282
14	0.340	−0.489	2.610	5.770	6.000	0.257
15	0.343	−0.294	2.930	5.770	6.000	0.209
16	0.343	−0.485	2.930	5.770	6.000	0.259



Training schematics



Setup ANN model training on observable data ($A_{LU}^{\sin\phi}$) that takes kinematics as input and has desired architecture using LibTorch. Use Mean Squared Error (MSE) as loss function:

$$MSE = \sum_{i=1}^{n} \frac{(O_i^{exp} - O_i^{pred})^2}{n}$$

O_i- denoting observable value predicted by ANN and measured from experiment

Training strategy for small data (15 points)

- Train for many epochs (20000), use MinMax scaling
- Use L2 regularization
- Learning rate of 10^{-4}
- Early stopping based on validation loss, random shuffle and 30% train/test split

Setting up ANN fitting of DVCS CFFs in PARTONS : Step 1 - NN prediction of $A_{LU}^{\sin\phi}$ using LibTorch

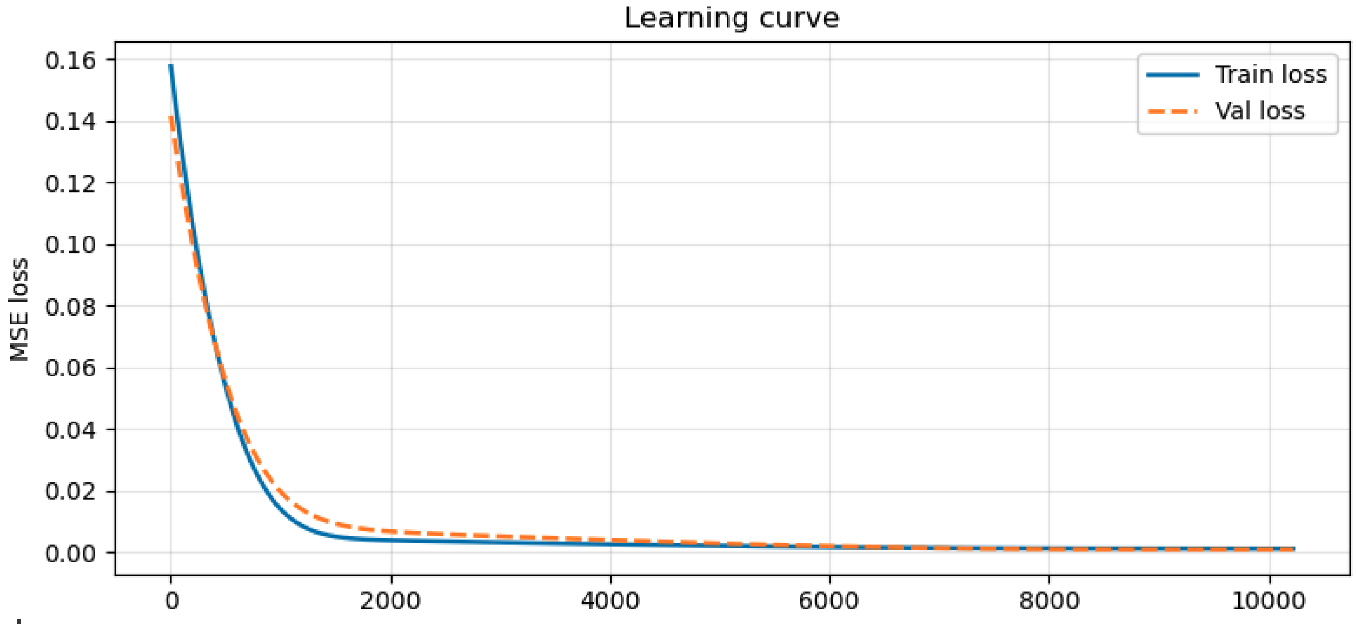
Training succeeded.

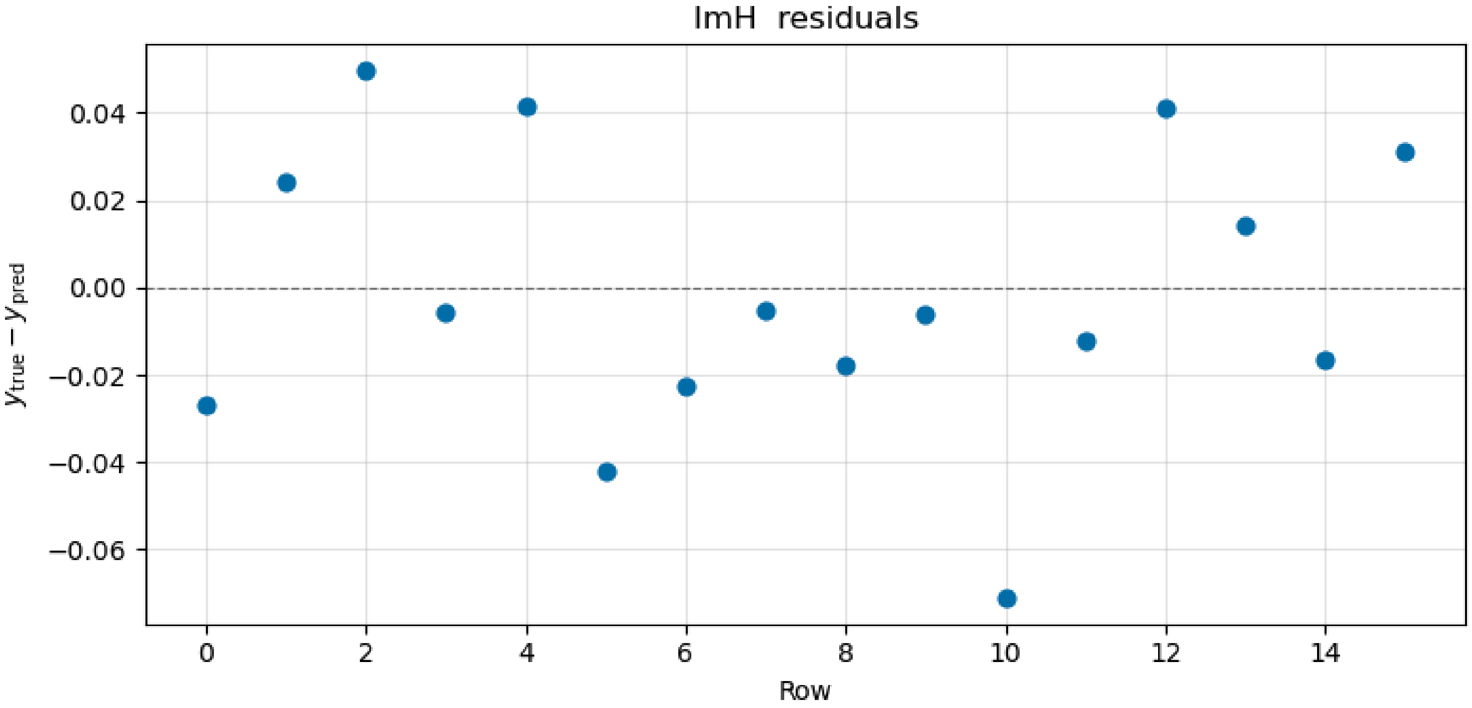
Model evaluation metrics:

Mean Squared Error (MSE) =0.001

Root Mean Squared Error (RMSE) ≈0.032

Predictions are off from true values by ~16%



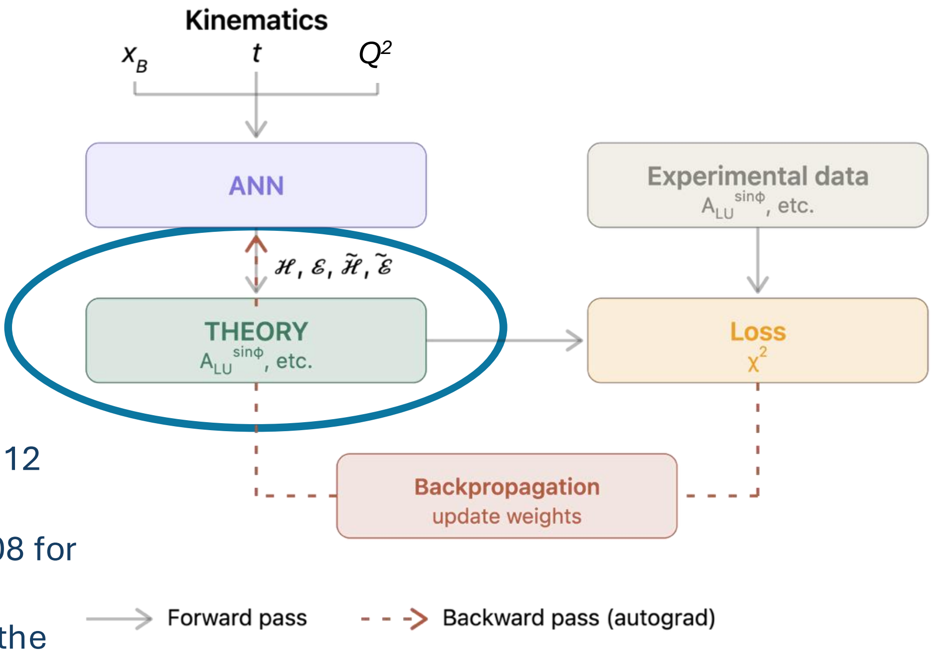


Setting up ANN fitting of DVCS CFFs in PARTONS : Step 2 - Use the ANN model trained via LibTorch in previous step and assume it outputs DVCS CFF values. Calculate observables from CFFs.

For ANN fitting of DVCS CFFs, we need to calculate observables from CFFs to estimate loss function at each step of training.
This is done using PARTONS: PARtonic Tomography Of Nucleon Software:

- official website https://3d-partons.github.io/partons/development.html
- C++ based package developed by a team of physicists primarily from CEA Saclay (France) and collaborating institutions.
- provides a necessary bridge between GPD models and experimental data
- many physics processes (DVCS, Double DVCS, timelike Compton scattering (TCS), Deeply Virtual Meson Production (DVMP) and exclusive diphoton photoproduction (GAM2)).
- We plan to use it also for DDVCS impact studies
- We are implementing DVCS CFF fitting framework which can later also be expanded into fitting GPDs and doing

Belitsky–Müller–Ji 2012 formulation arxiv:hep-ph/0112108 for the BH amplitude ; arxiv:1212.6674 for the DVCS amplitude and interference.

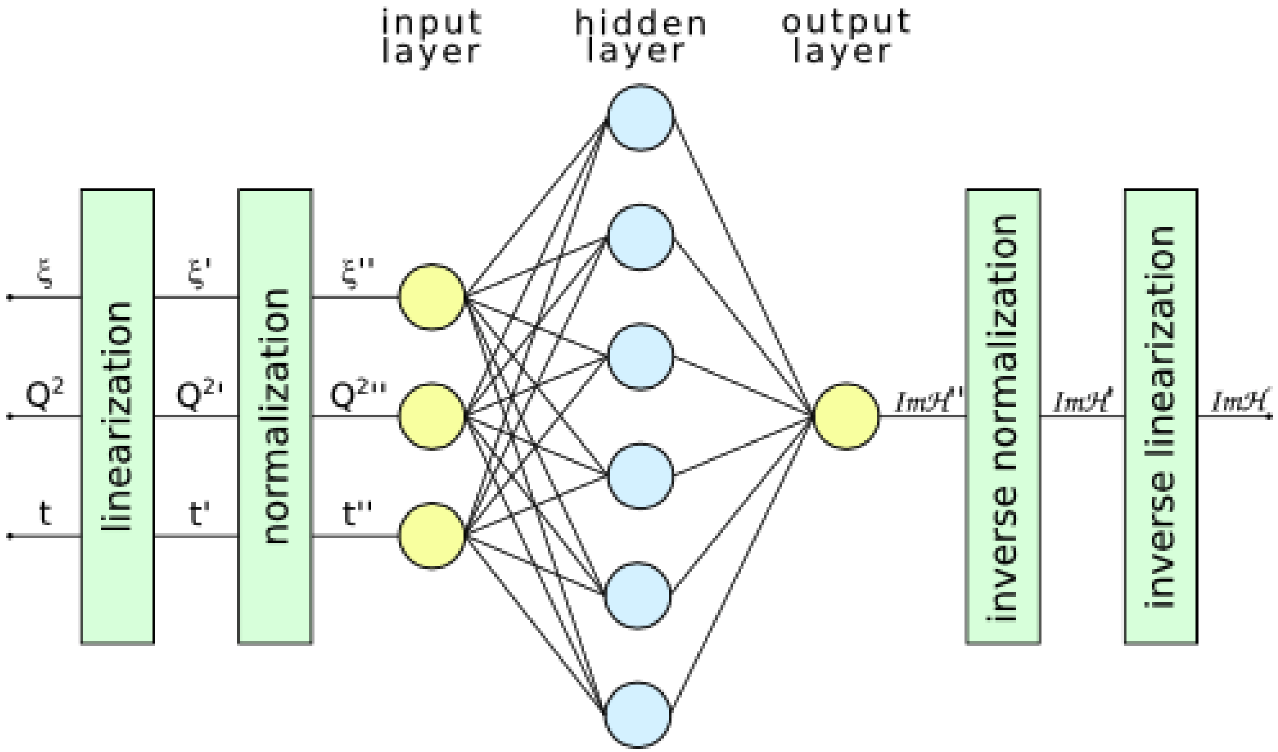


DVCS CFF ANN fitting with PARTONS has been done previously and corresponding parametrizations were saved in PARTONS.

We have used this to calculate $A_{LU}^{\sin\phi}$ and compare with data.

Fitting details:

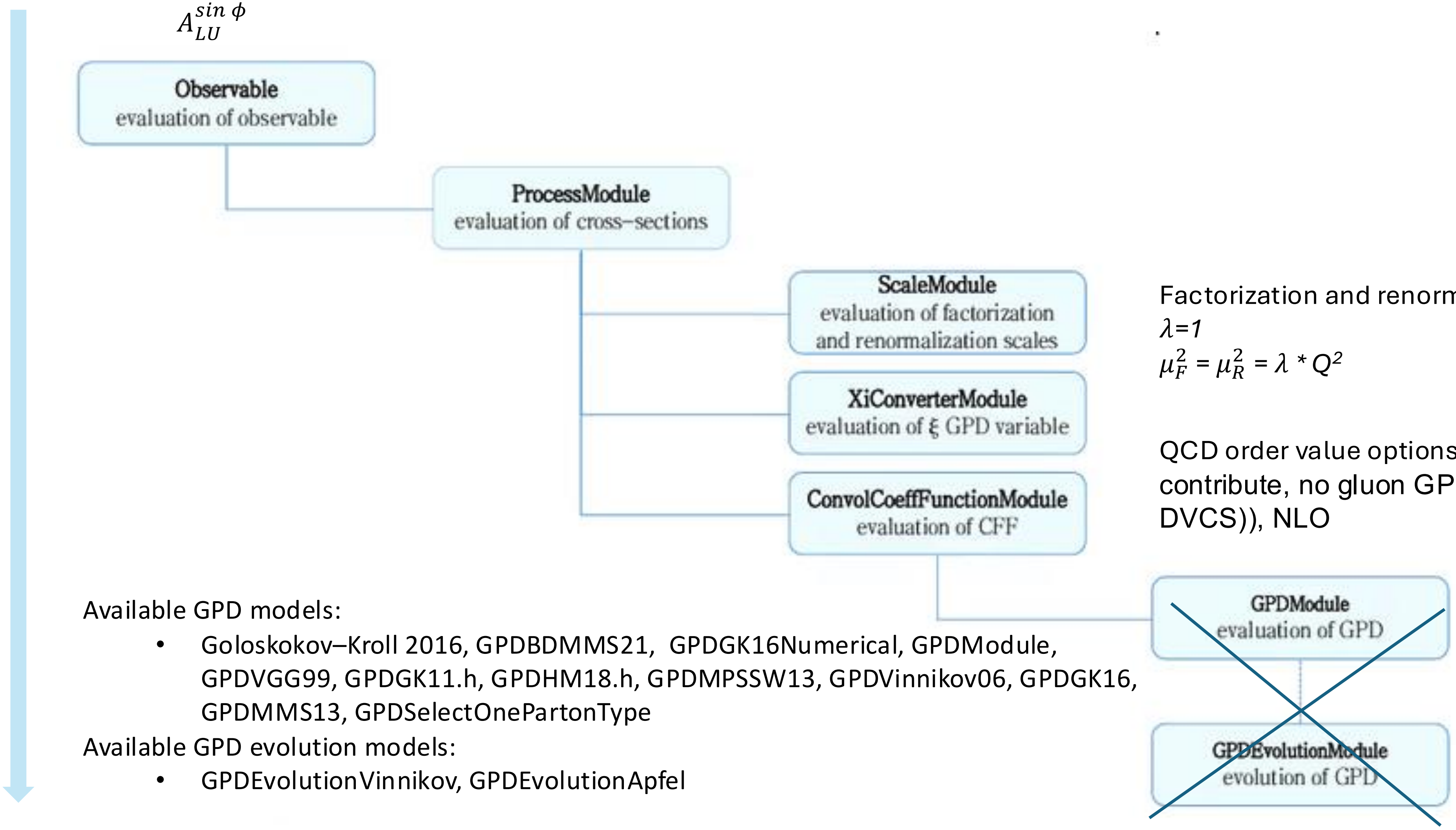
- Re$\mathcal{H}$, Im$\mathcal{H}$ treated independent (8 independent NNs))
- Training uses the genetic algorithm (backpropagation not straightforward)
- Regularization is done via early stopping
- Use replica Monte Carlo technique to propagate experimental uncertainties into the extracted CFFs:
  - One "central" fit + 100 replica fits = 101 total.



Observable calculation studies using PARTONS

PARTONS observable computation schematics

$A_{LU}^{\sin \phi}$



Factorization and renormalization scales
λ=1
$\mu_F^2 = \mu_R^2 = \lambda * Q^2$

QCD order value options LO (Only quark GPDs contribute, no gluon GPD contribution (in DVCS)), NLO

Available GPD models:

- Goloskokov–Kroll 2016, GPDBDMMS21, GPDGK16Numerical, GPDModule, GPDVGG99, GPDGK11.h, GPDHM18.h, GPDMPSSW13, GPDVinnikov06, GPDGK16, GPDMMS13, GPDSelectOnePartonType

Available GPD evolution models:

- GPDEvolutionVinnikov, GPDEvolutionApfel

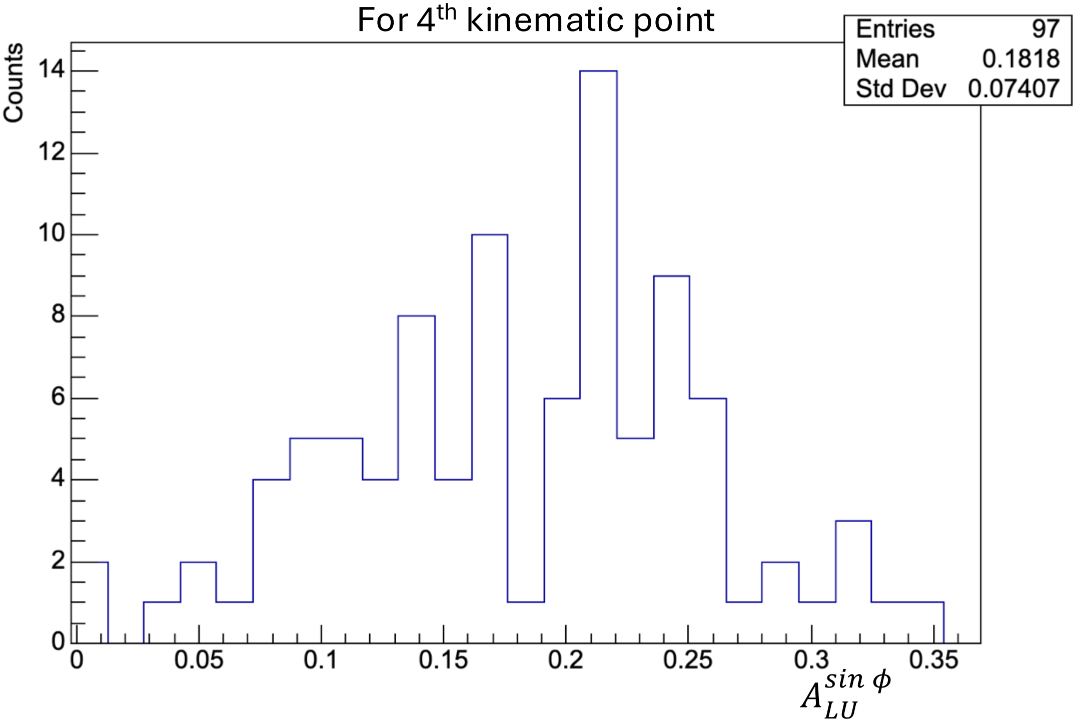
Current analysis
Instead of GPD → convolution → CFF
Neural Network → CFF via DVCSCFFNN module in PARTONS

Observable calculations with Partons using ANN parametrization of DVCS CFFs by EPJ C79 (2019) 614

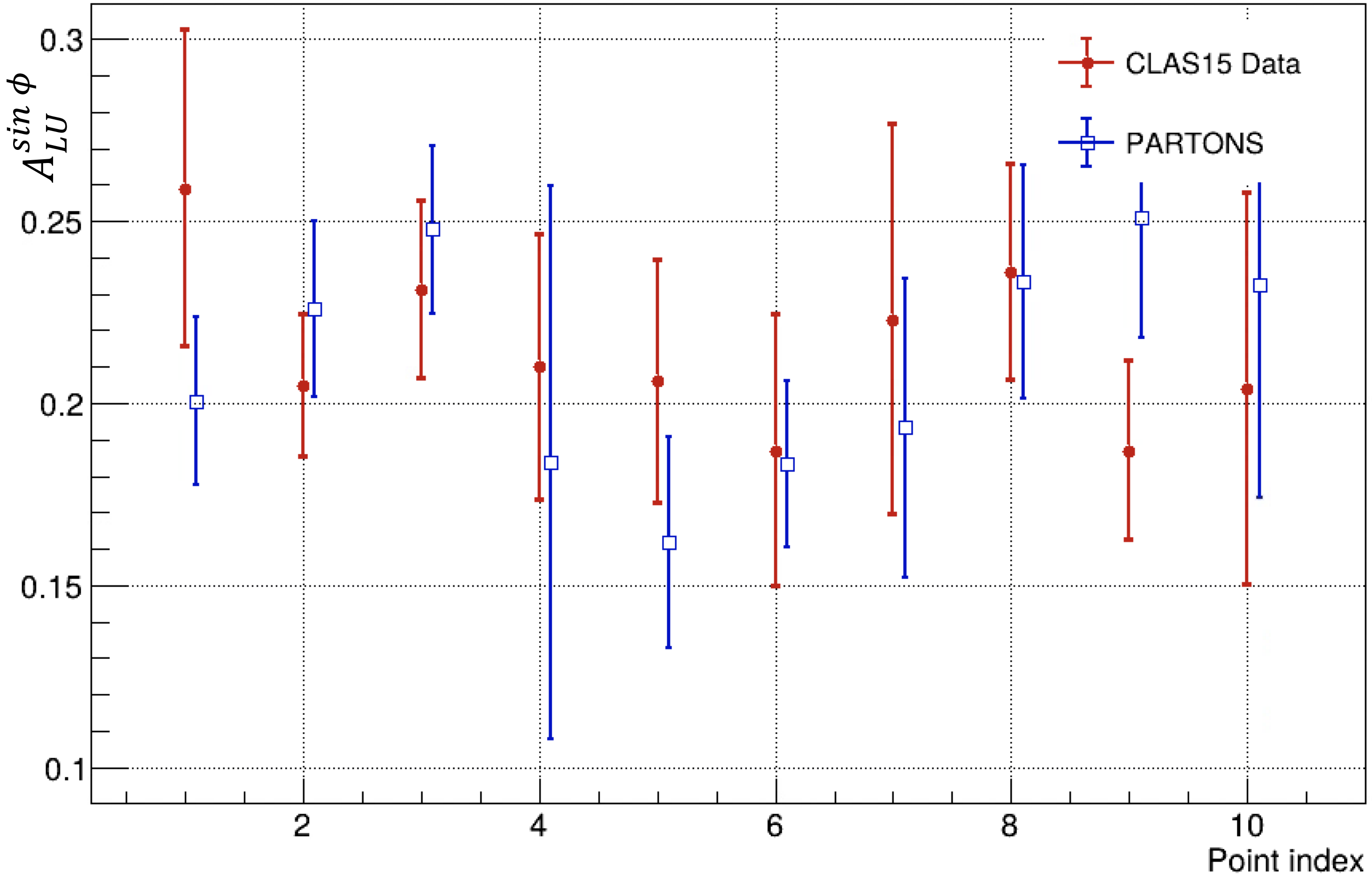
CLAS 2015 DVCS Data at Ebeam= 5.932 GeV (arXiv:1501.07052, harmonics fit by Kresimir Kumerički)

#	Q^2	x_B	$-t$	$A_{LU}^{\sin\phi}$	stat	syst
1	1.554	0.181	0.129	0.259	0.042	0.012
2	1.979	0.247	0.136	0.205	0.017	0.010
3	2.048	0.259	0.228	0.231	0.022	0.011
4	1.943	0.258	0.457	0.210	0.030	0.021
5	2.362	0.255	0.138	0.206	0.027	0.020
6	2.448	0.265	0.229	0.187	0.031	0.021
7	2.458	0.265	0.443	0.223	0.038	0.038
8	2.670	0.337	0.240	0.236	0.026	0.015
9	2.665	0.350	0.456	0.187	0.021	0.013
10	3.314	0.442	0.507	0.204	0.041	0.035

$A_{LU}^{sin\,\phi}$ for given kinematic point from 101 replicas
For 4th kinematic point

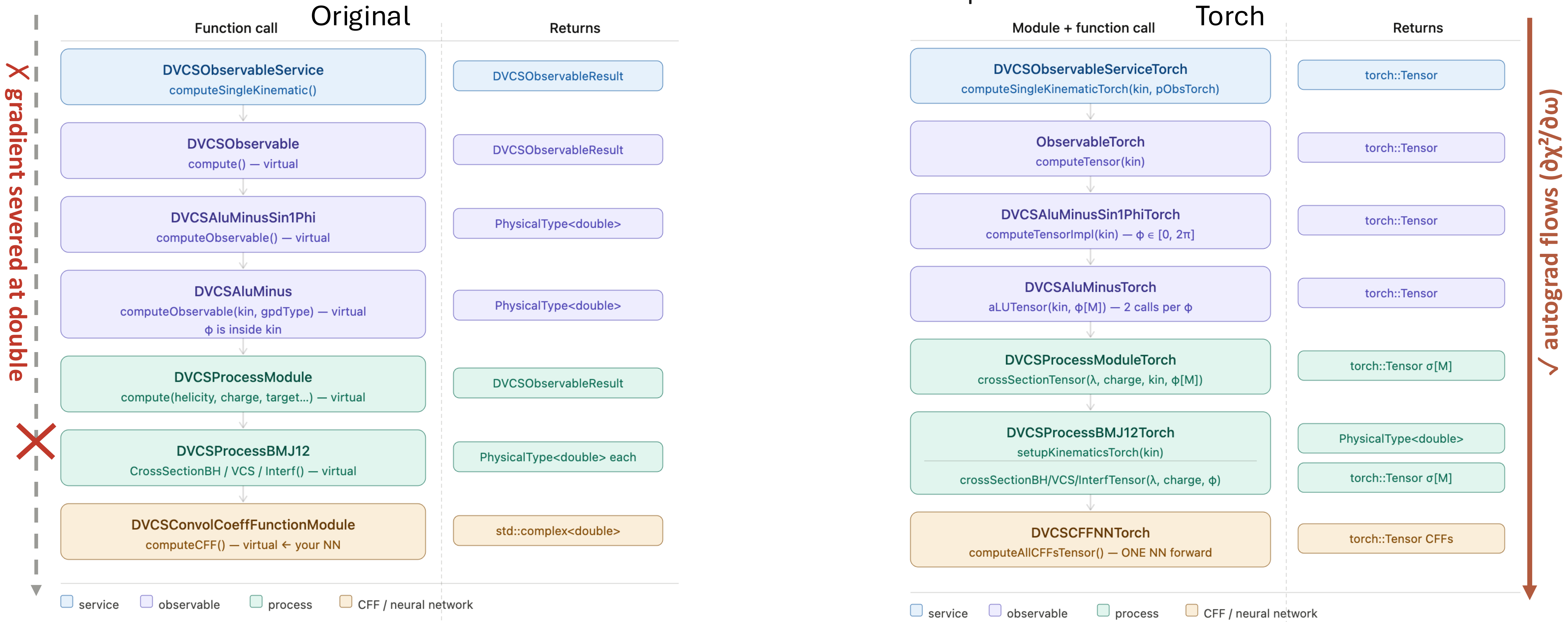


$A_{LU}^{\sin\phi}$ harmonic values calculated in PARTONS via ANN parametrization of DVCS CFFs (EPJ C79 (2019) 614) agree with data



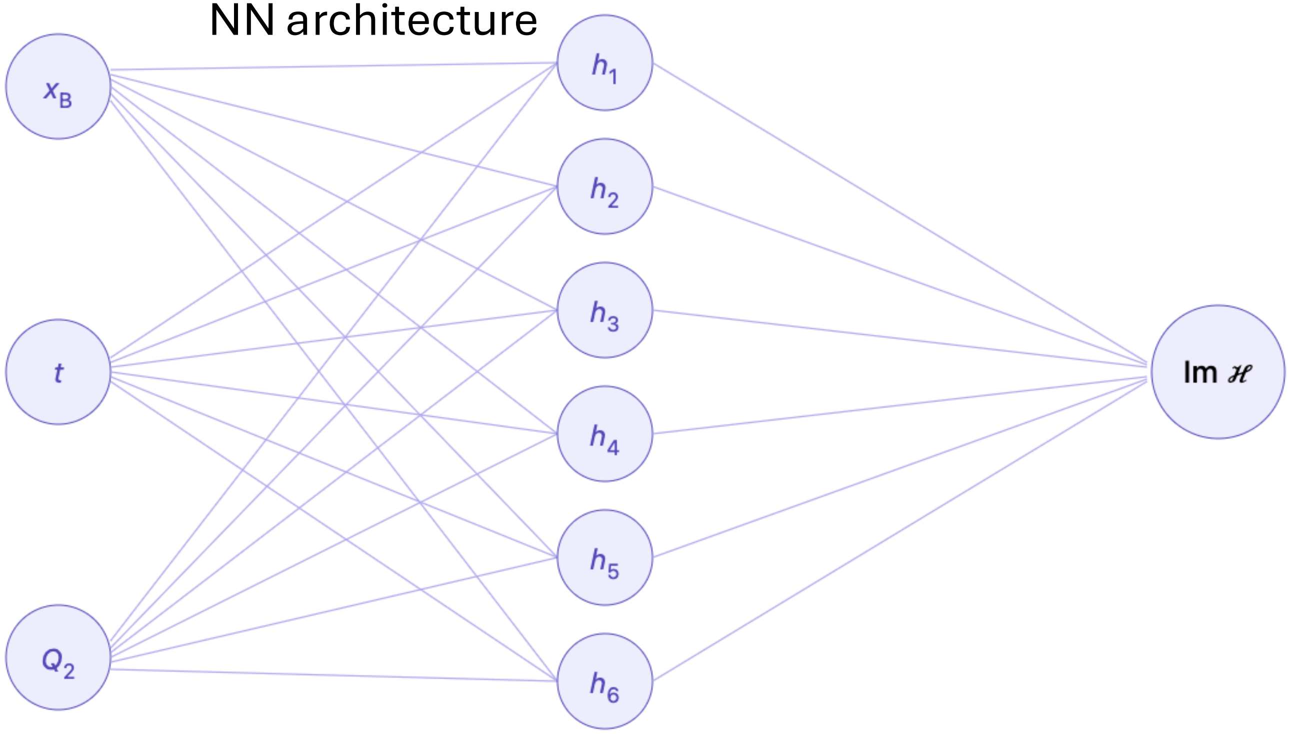
- We have used corresponding DVCSCFFNN module that calculates DVCS CFFs using DVCS CFF NN parametrization model from (EPJ C79 (2019) 614), to implement new module DVCSCFFNNTorch for DVCS CFFs evaluated from a Libtorch trained NN.
- We then use DVCSCFFNNTorch to calculate observables using DVCS CFFs evaluated from a Libtorch trained NN from step 1 to accomplish step 2.

Setting up ANN fitting of DVCS CFFs in PARTONS : Step 3-Implementing differentiable observable chain via Torch tensors that mirrors the scalar PARTONS path

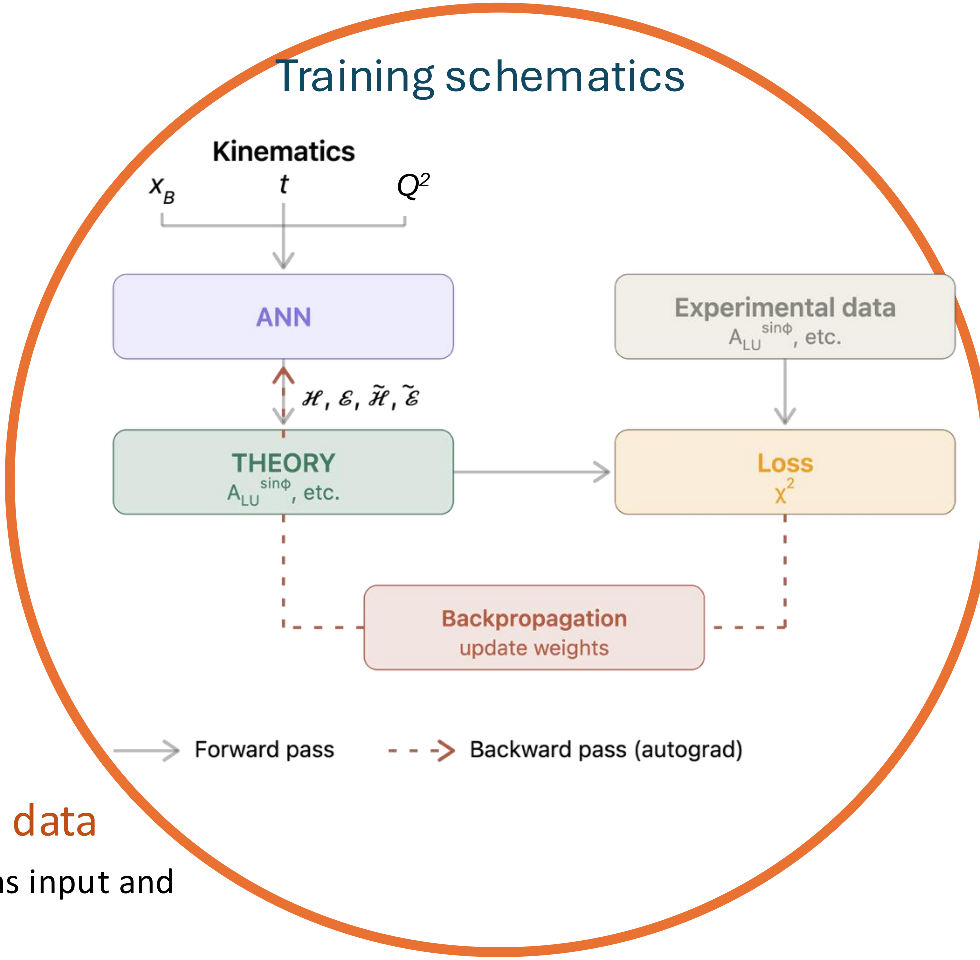


- We use Autograd (automatic differentiation) mechanism in LibTorch that automatically computes $\partial\chi^2/\partial\omega$ for updating NN weights (ω) during training- possible if every operation between the NN weights and the $\chi^2 = \sum_{i=1}^{n} \frac{(O_i^{theory} - O_i^{exp})^2}{(\sigma_i^{exp})^2}$ custom loss is expressed in torch tensor operations
- Each class in Torch chain can be called in original chain as it has a scalar virtual method that PARTONS calls, and that method wraps the tensor method without gradient propagation (NoGradGuard + .item()).
- Have tested Torch path by calculating observable for the same kinematic point from both paths and making sure they agree.

NN architecture



Training schematics



NN parametrization of DVCS CFFs via training on observable data

Setup ANN model training on observable data ($\boldsymbol{A_{LU}^{sin\,\phi}}$) that takes kinematics as input and outputs $Im\mathcal{H}$ and has desired architecture. Use custom loss function:

$$\chi^2 = \sum_{i=1}^{n} \frac{(O_i^{theory} - O_i^{exp})^2}{(\sigma_i^{exp})^2}$$

O_i-denoting observables calculated from theory and measured from experiment
σ_i^{exp}-uncertainty from experimental measurement
n-total number of kinematic points for observable measurement
Training strategy for small data (15 points)

- Train for many epochs (10000), use MinMax scaling, activation function hyperbolic tangent
- Adam optimizer with L2 regularization (weight decay 10^{-3}) and learning rate of 10^{-2}
- Early stopping based on validation loss (patience 200), random shuffle and 30% train/test split

DVCS CFF ANN fitting results in PARTONS

CLAS 2007 DVCS data
(arXiv:0711.4805)

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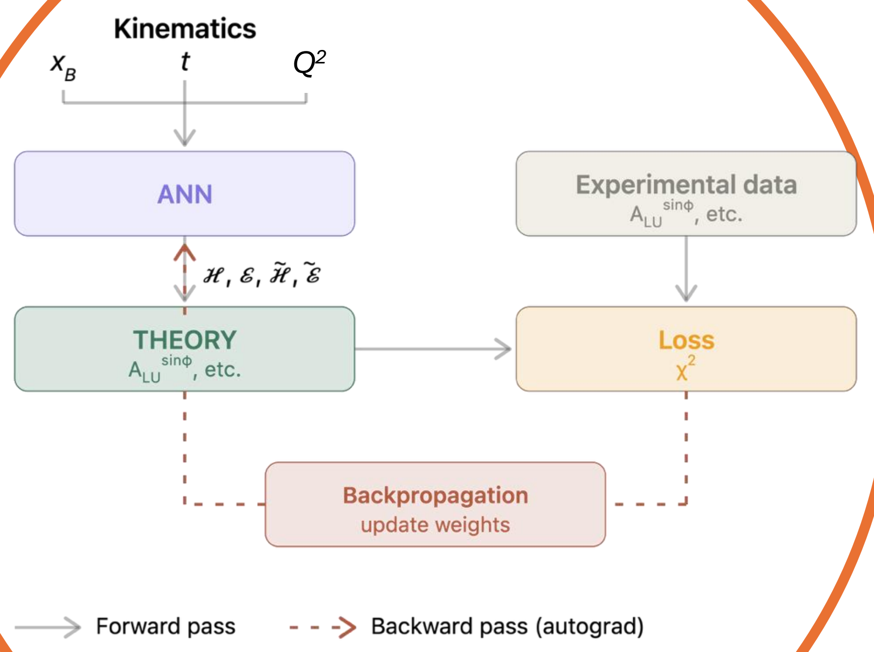
Training schematics

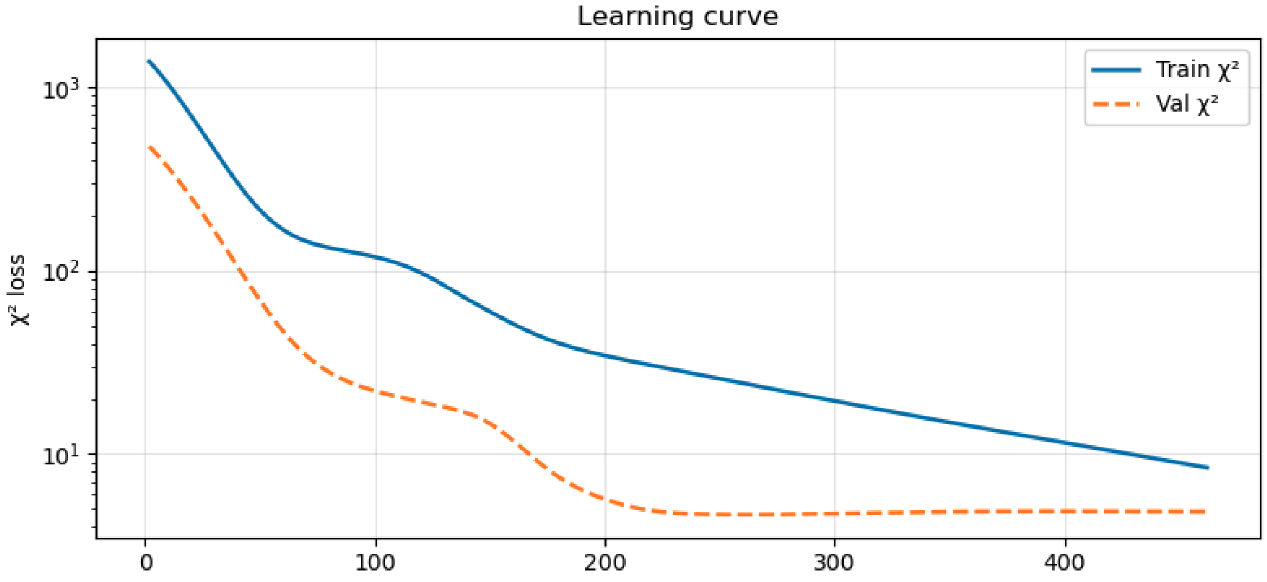


DVCS CFF ANN fitting results in PARTONS

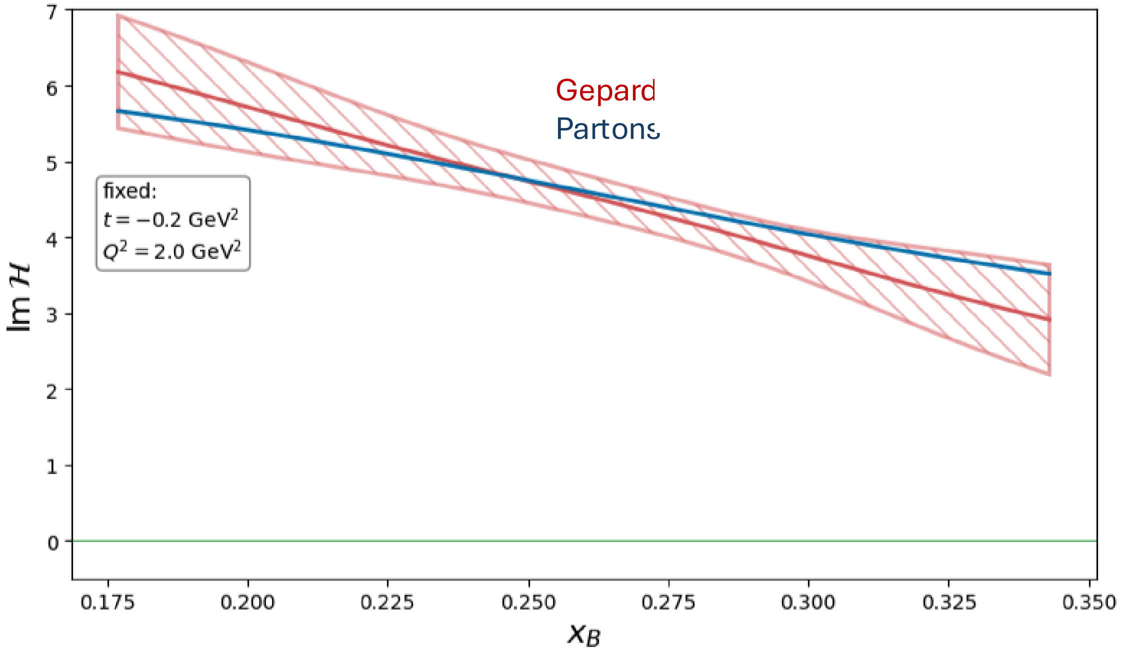
Model evaluation metrics look good

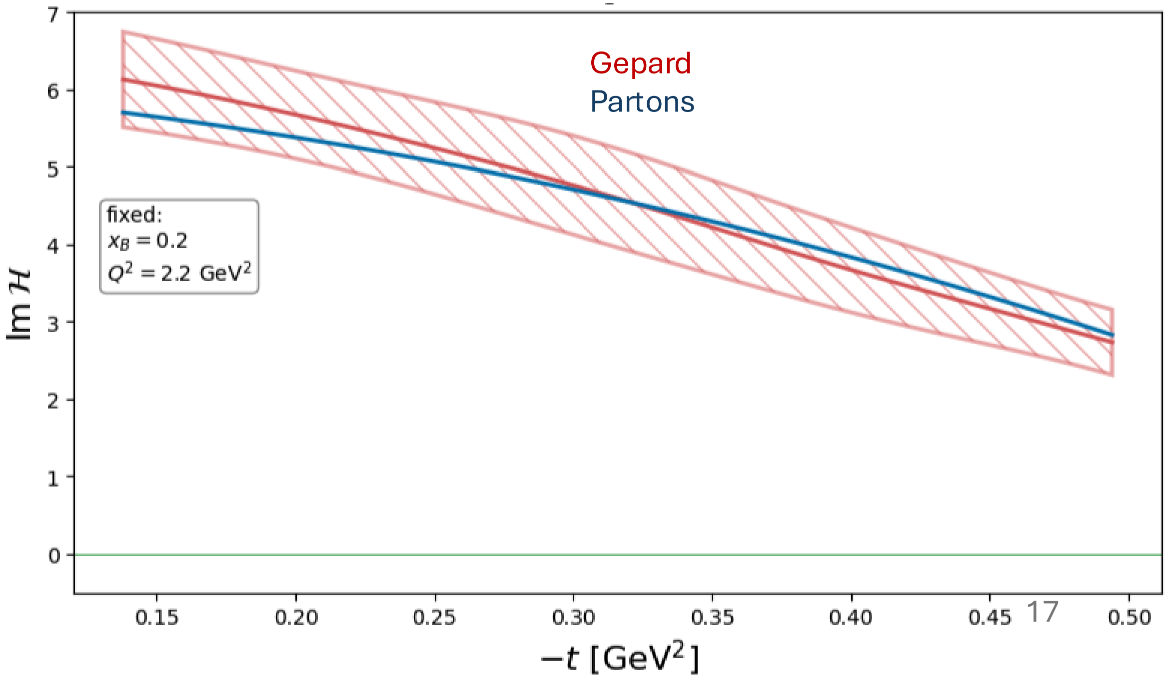
MSE=0.0006
RMSE ≈0.0235
$\chi^2 = 13.2117$

Per epoch training speed is ~0.2 s for 16 points.
Average training 2000 epochs ~7 m.



PARTONS fit results are in agreement with Gepard results





Future work

- PARTONS package is powerful tool for studies of DVCS and DDVCS and many other physics processes.
- Have implemented DVCS CFF fitting using PARTONS for one observable ($A_{\mathrm{LU}}^{\sin\varphi}$) and checked against Gepard DVCS CFF fitting framework. Next:
  - Add replica fitting
  - Extend fitting to more observables
  - Implement speedup via vectorization
  - Consider using Python wrapper of PARTONS

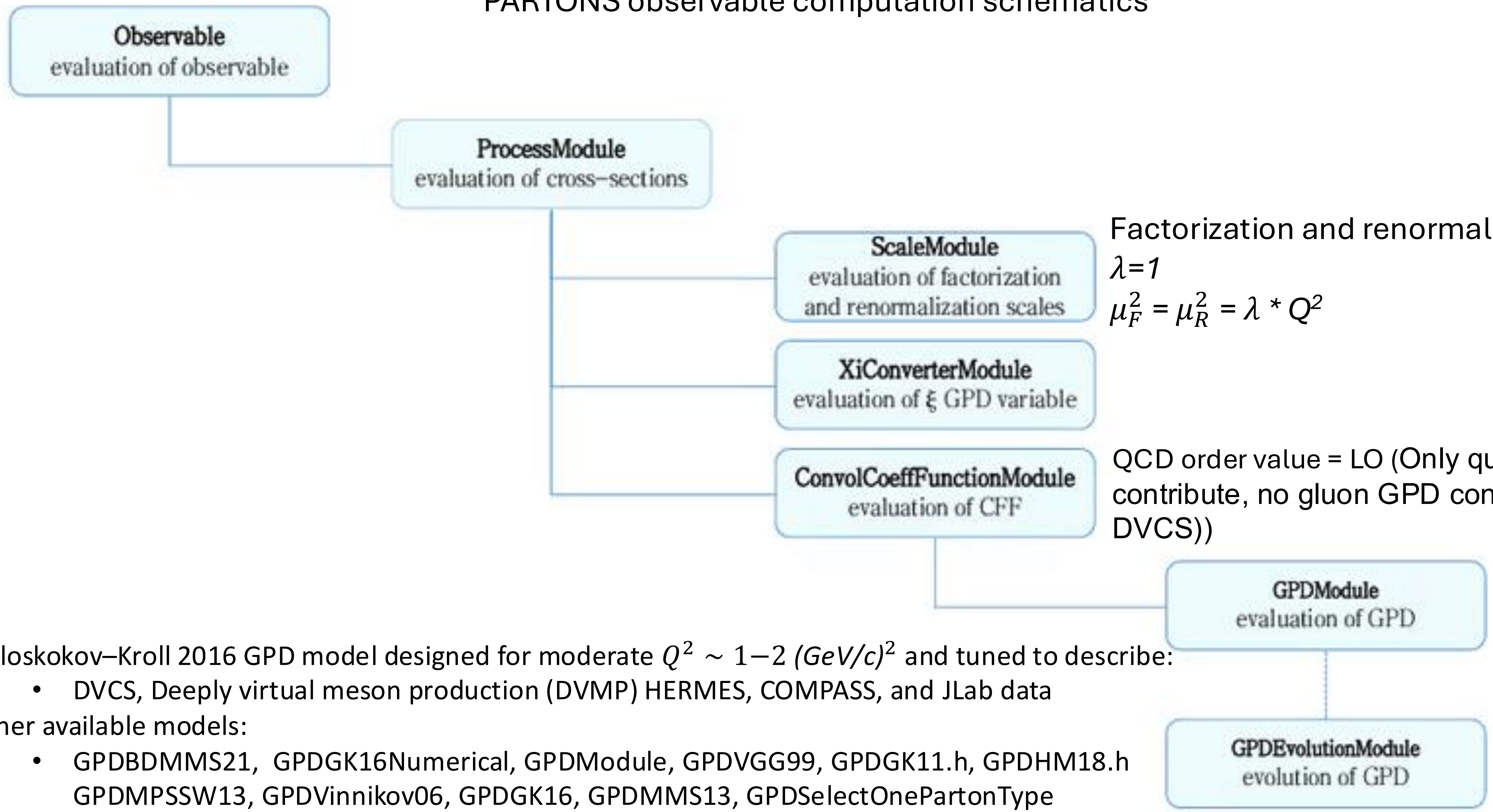
- Use CFF parametrization to estimate D-term and learn about mechanical properties of proton.
- Expand analysis to GPD fitting and DDVCS impact studies.

Acknowledgement

I would like to thank members of CEA Saclay (France) research center and collaborating institutions, in particular Cédric Mezrag, Maxime Defurne, Paweł Sznajder and Valerio Bertone for assisting me with PARTONS analysis.

Observable calculation studies using PARTONS

PARTONS observable computation schematics



Factorization and renormalization scales

λ=1

$\mu_F^2 = \mu_R^2 = \lambda * Q^2$

QCD order value = LO (Only quark GPDs contribute, no gluon GPD contribution (in DVCS))

Goloskokov–Kroll 2016 GPD model designed for moderate $Q^2 \sim 1{-}2$ $(GeV/c)^2$ and tuned to describe:

- DVCS, Deeply virtual meson production (DVMP) HERMES, COMPASS, and JLab data

Other available models:

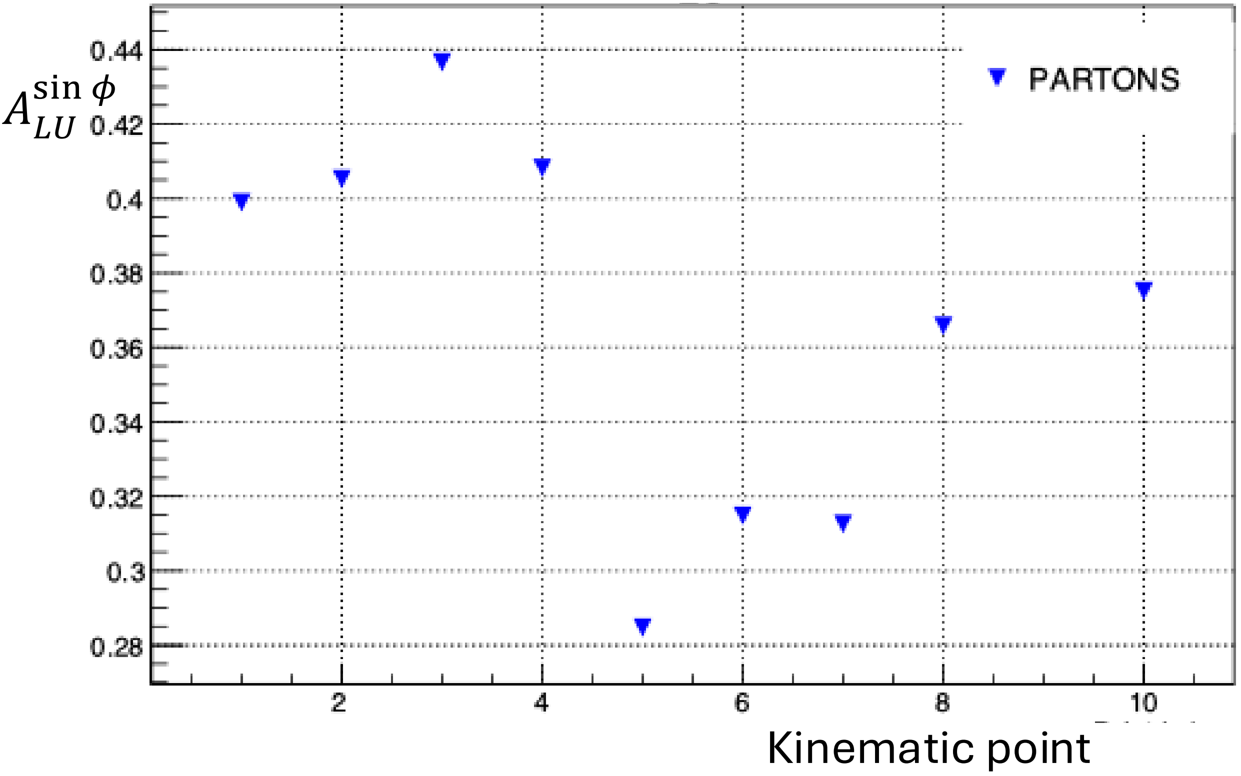
- GPDBDMMS21, GPDGK16Numerical, GPDModule, GPDVGG99, GPDGK11.h, GPDHM18.h GPDMPSSW13, GPDVinnikov06, GPDGK16, GPDMMS13, GPDSelectOnePartonType

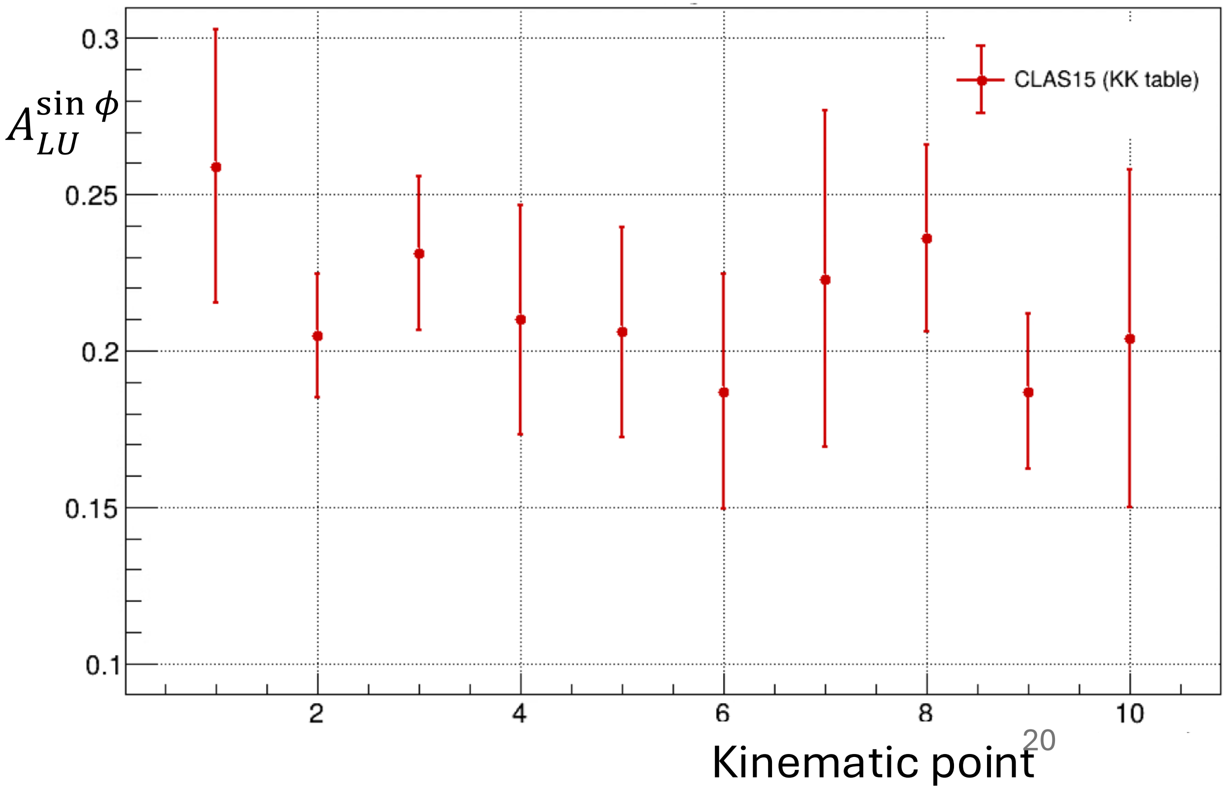
Calculation for $sin(\phi)$ first harmonic using Goloskokov–Kroll 2016 GPD model doesn't agree with data

Important part of DVCS CFF ANN fitting is calculation of observables using PARTONS package.

As a first step calculate $A_{LU}^{\sin\phi}$ harmonic using PARTONS and compare to experimental values from DVCS measured with CLAS in 2015, at E_{beam}= 5.932 GeV (arXiv:1501.07052, harmonics fit by by Kresimir Kumerički) using DVCSProcessGV08 module based on Guichon–Vanderhaeghen formalism.

$A_{LU}^{\sin\phi}$ harmonic values calculated in PARTONS via Goloskokov–Kroll 2016 GPD model don't agree with data





Setting up ANN fitting of DVCS CFFs in PARTONS : Step 3 - Changing integration method

1. Instead of adaptive Dexp ϕ integrator use a fixed node Gauss–Legendre (GL) (implemented)

Implemented module MathIntegratorModuleTorch similar to MathIntegratorModule:

- uses NumA's integrator configuration/types (Dexp, GL, etc.)
- reimplements the actual integration in Torch using batched tensor operation over all nodes

Verified for xB=0.2, t=−0.2 GeV^2 Q^2=2 GeV^2, E=GeV with identical NN weights

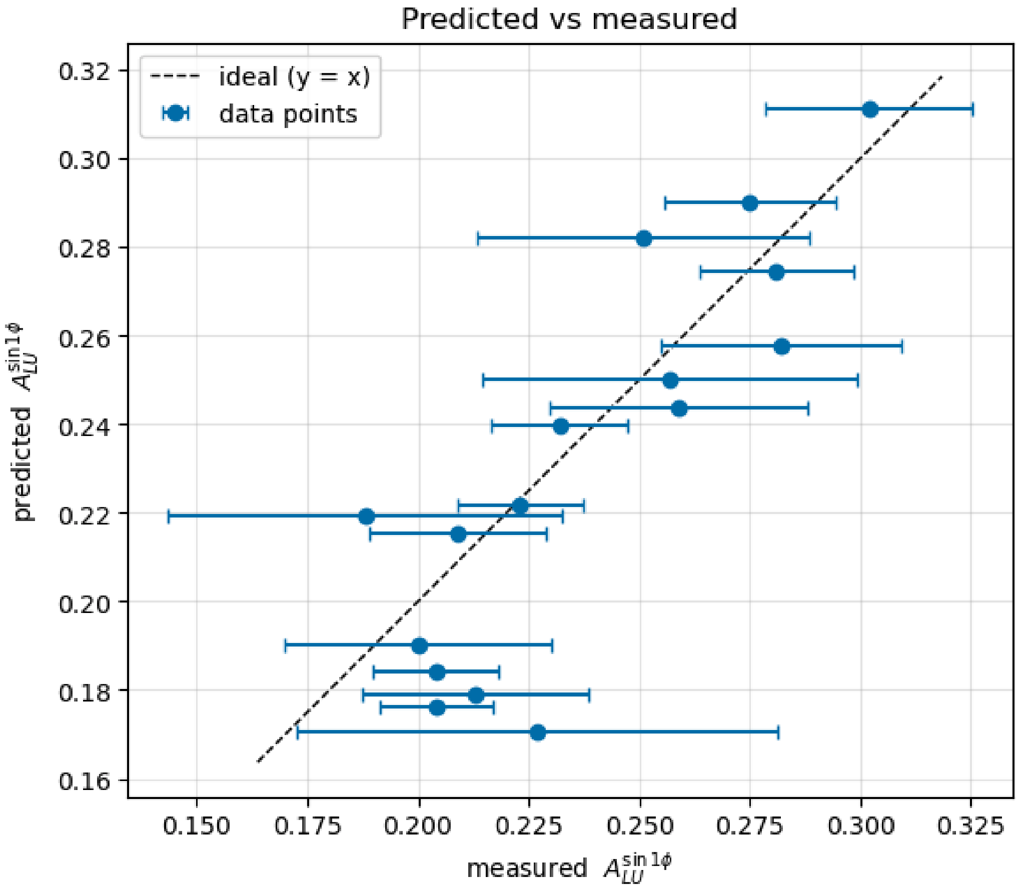
Path	Quadrature	$A_{LU}^{\sin\phi}$
observ_calc() — base PARTONS scalar	DEXP adaptive	−0.00895582
observ_calc_torch() — torch tensor path	GL-10	−0.00895585
observ_calc_torch_scalar() — torch scalar virtuals	GL-10	−0.00895585

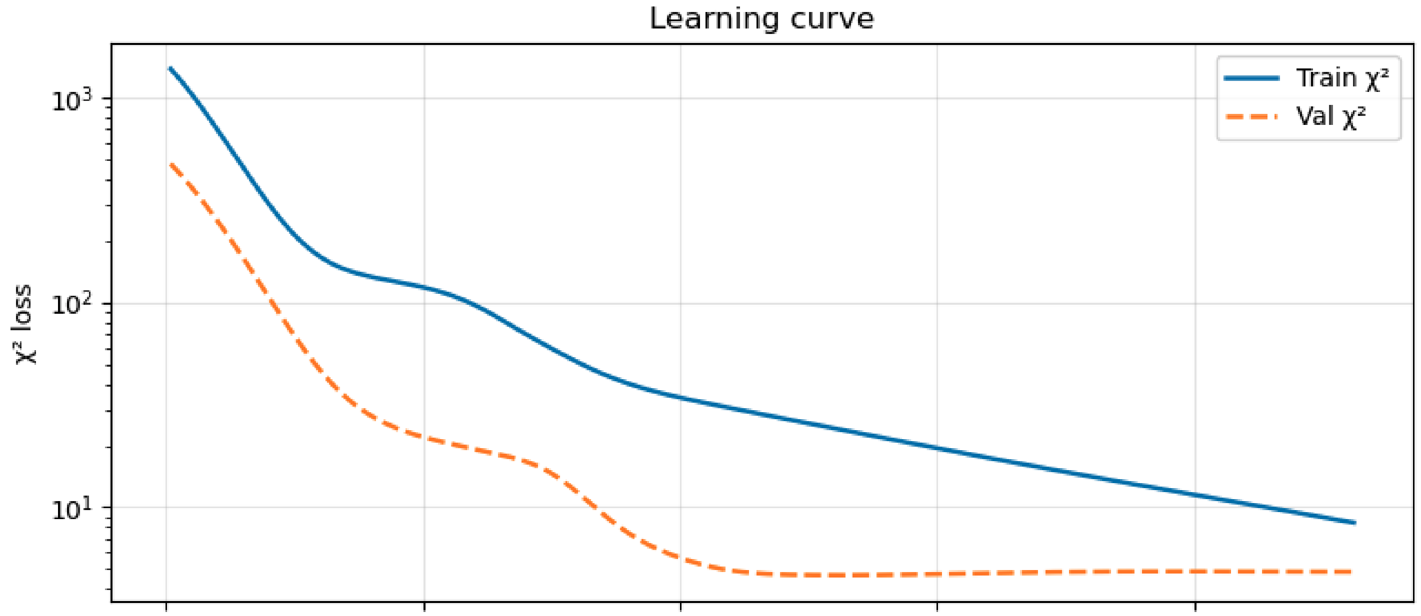
The GL-10 result matches the scalar DEXP path to ~5 significant figures ($\Delta \approx 3\times10^{-8}$ absolute difference, ~3.4×10^{-6} fractional difference)

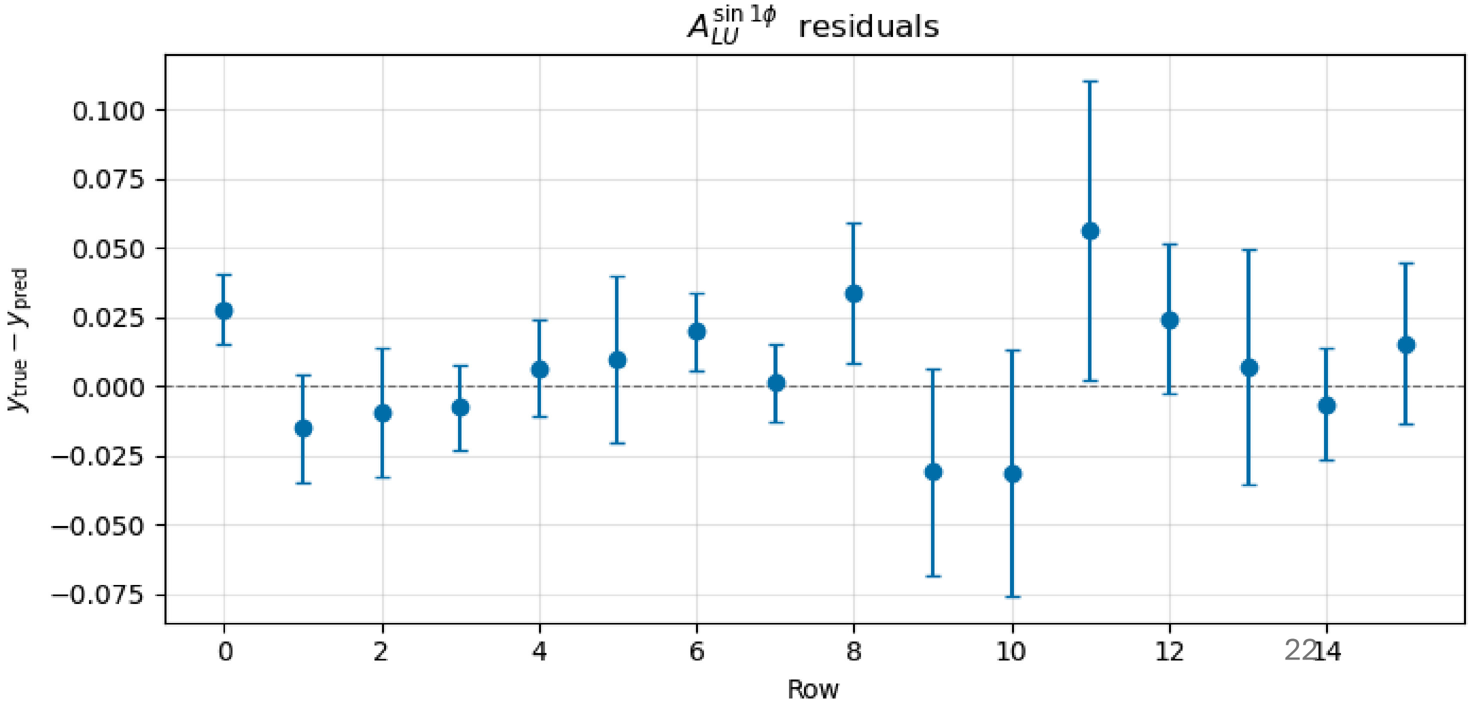
Setting up ANN fitting of DVCS CFFs in PARTONS : Step 1 - NN prediction of $A_{LU}^{sin\,\phi}$ using LibTorch

Model evaluation metrics

MSE = 0.000554217   R² = 0.516098   χ² = 13.2117







Setting up ANN fitting of DVCS CFFs in PARTONS : Step 1 - NN prediction of $A_{LU}^{\sin\phi}$ using LibTorch