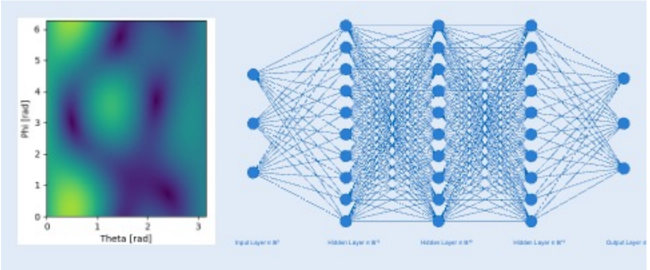
DEEP LEARNING FOR SPECTROSCOPY AND AMPLITUDE ANALYSIS

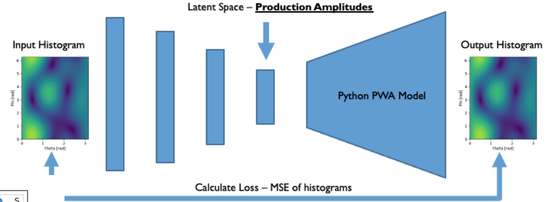
William Phelps

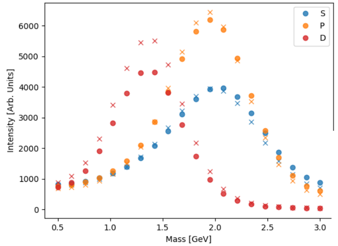
Christopher Newport University/Jefferson Lab

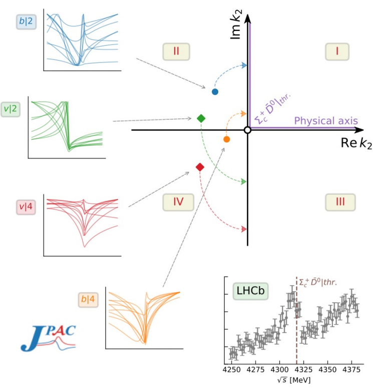
Roadmap

- Deep Learning - Partial Wave Analysis (PyPWA)
  - Uncertainty Quantification
  - Wave Selection
- Artificial Intelligence for Hadron Spectroscopy









t time

Partial Wave Analysis

PyPWA

- A python-based software framework designed to perform Partial Wave and Amplitude Analysis with the **goal of extracting resonance information from multi-particle final states.**
- In development since 2014 and has been significantly improved with each revision. Version 4.0 with PyTorch library is out (tagged release coming soon)
- Efficient amplitude analysis framework including multithreading, CUDA support, and PyTorch libraries
- Optimizers include: Minuit, Nestle, MCMC (or add your own!)
- NIM Paper almost ready to be submitted (~late 2022)

Website: https://pypwa.jlab.org
GitHub: https://github.com/JeffersonLab/PyPWA

Group Members

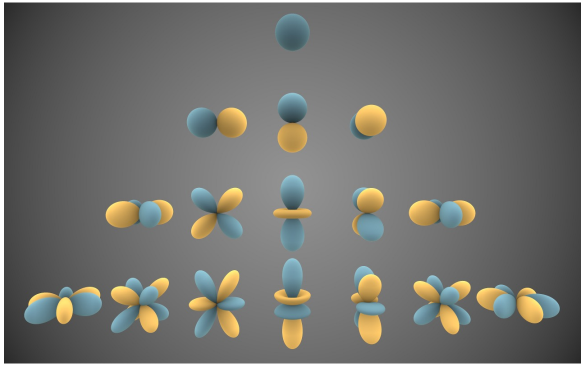
Carlos Salgado (NSU/Jlab)
Mark Jones (NSU)
Peter Hurck (Glasgow)
William Phelps (CNU/Jlab)
Nathan Kolling (CNU)

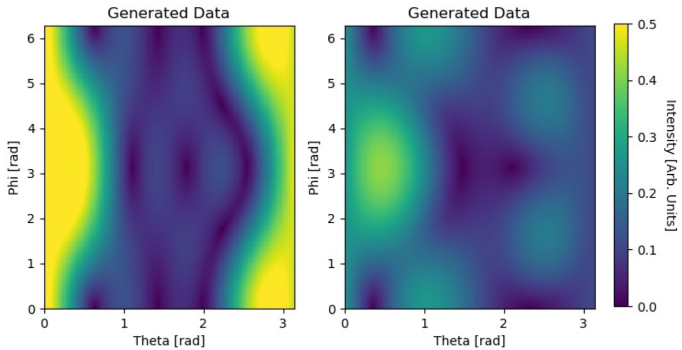
Former Group Members

Josh Pond
Stephanie Bramlett
Brandon DeMello
Michael Harris (NSU)
Andru Quiroga (CNU)
Bruna Goncalves (NSU)

PWA using Neural Networks

- Generate datasets using decay amplitudes (linear combination of spherical harmonics) with the following quantum numbers
  - L = 1,2,3
  - m = 0,1
  - ϵ_R = -1,+1
  - 9 total waves ("fit parameters")





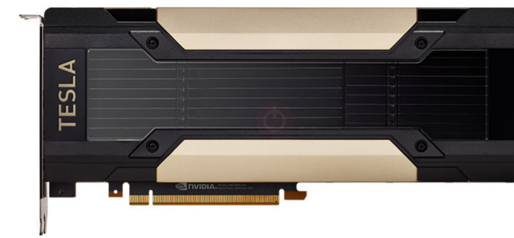
$$I(\Omega) = \sum_k \sum_{\epsilon_R} \sum_{l,|m|,l',|m'|} {}^{\epsilon_R}Y_l^{|m|}(\Omega)\; {}^{\epsilon_R}V_{l,|m|}^{k}\; {}^{\epsilon_R}V_{l',|m'|}^{k*}\; {}^{\epsilon_R}Y_{l'}^{|m'|*}(\Omega)$$

Production Amplitudes

Decay Amplitudes

Tools of the Trade

- Python 3.9 – Anaconda
  - Keras/TensorFlow – NN Libraries
  - Pandas/Numpy – Data Handling
  - Matplotlib – Visualization
  - Uproot – Native Python ROOT Library (J. Pivarski)
  - Optuna – Hyperparameter optimization library
- Institutional GPU nodes or those through Jefferson Lab
  - Either through Jupyterhub or interactively using slurm to request a node
  - Several institutions with Nvidia V100 and A100 Cards (NSU/JLAB)
  - Several machines with 4 Nvidia Titan RTX GPUs and some with 14 Nvidia T4 GPUs



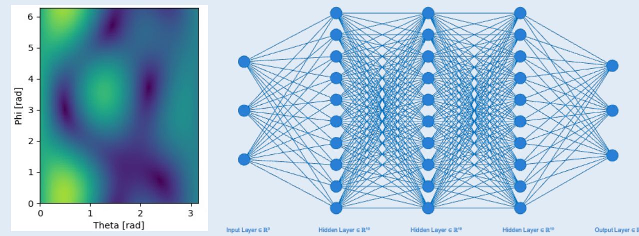
Example Training Script

```
test = pd.read_csv("TRAIN/TRAIN.csv")
labels = pd.read_csv("TRAIN/TRAIN_labels.csv")
activation = 'relu'

model = Sequential()
model.add(Dense(units=1000, activation=activation, input_shape=(3600, )))
model.add(Dense(units=1000, activation=activation))
model.add(Dense(units=1000, activation=activation))
model.add(Dense(units=2))
model.compile(optimizer=adam(lr=.001), loss='mean_squared_error', metrics=['accuracy'])

model.fit(test, labels[labels.columns[1:]], epochs=300, batch_size=256, validation_split=0.2)
```

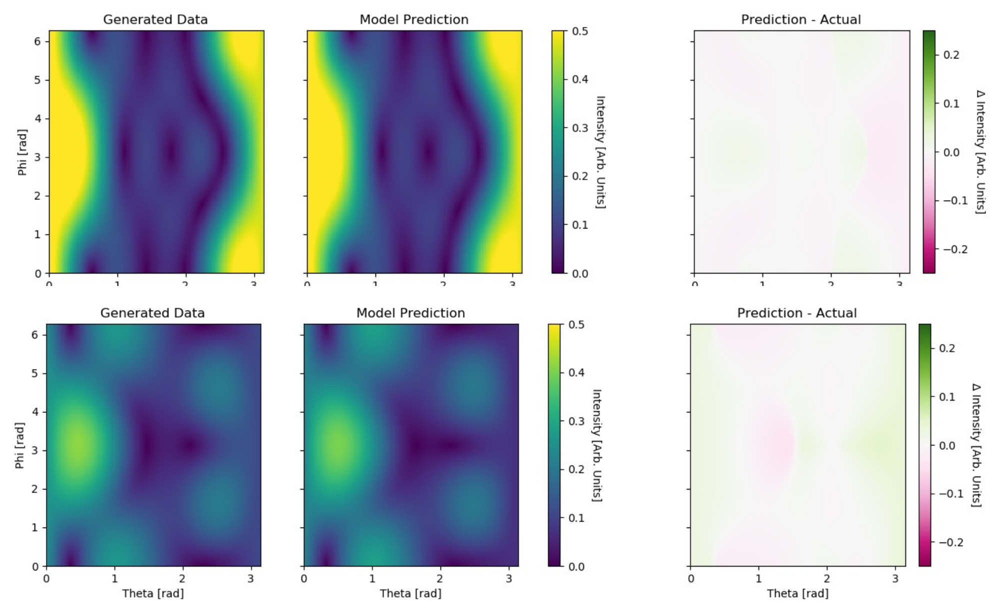
First Results

- We compare the intensity function and compare it to the model prediction
- Model Architecture:
  - 128x128 2D histogram as input
  - 9x128 Dense Layers – RELU activation
  - 9 production amplitudes as output
- In order to deal with the vast amounts of data we used generators to generate data for each epoch on the fly

Input Histogram



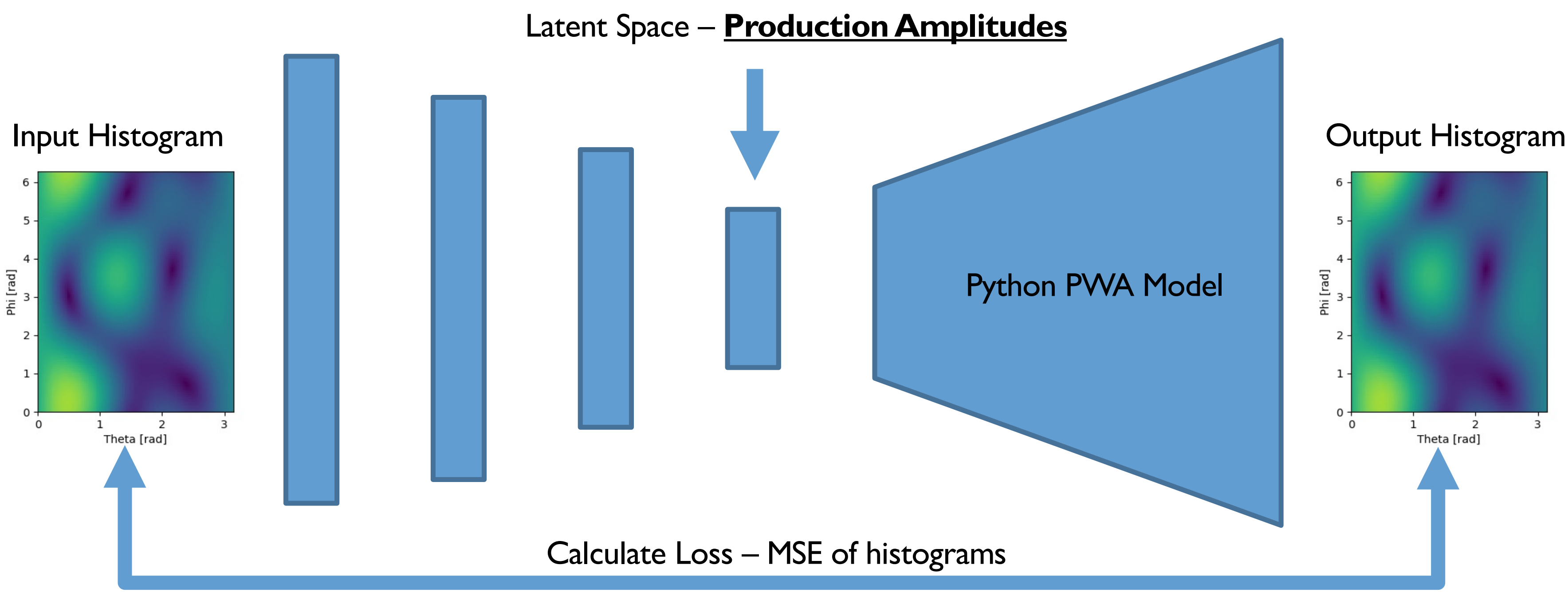
Output - Production Amplitudes



Useful Tools: Generators, Complex Valued Deep Learning

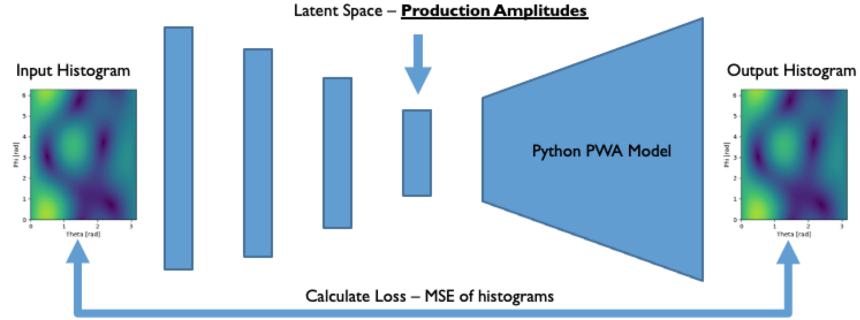
Autoencoder for PWA

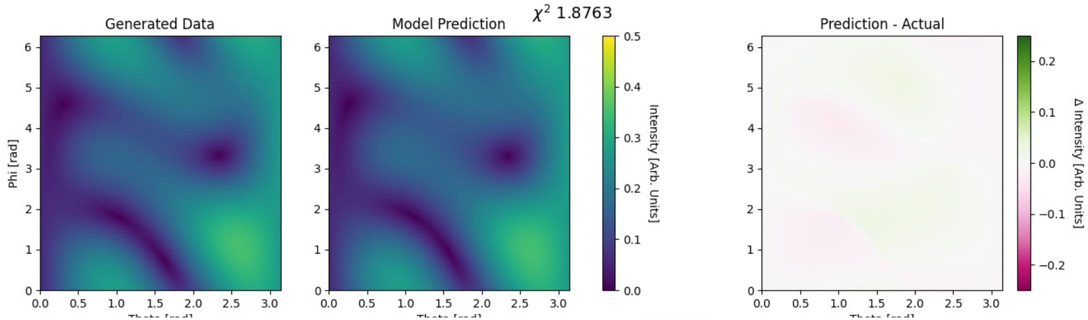
Unsupervised learning!

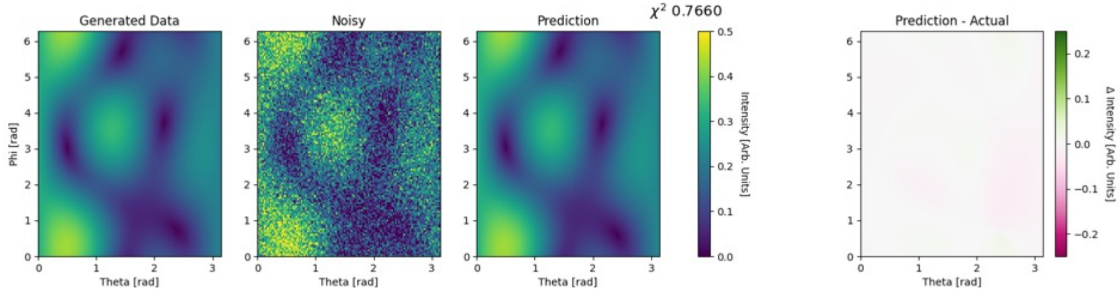


Autoencoders for PyPWA

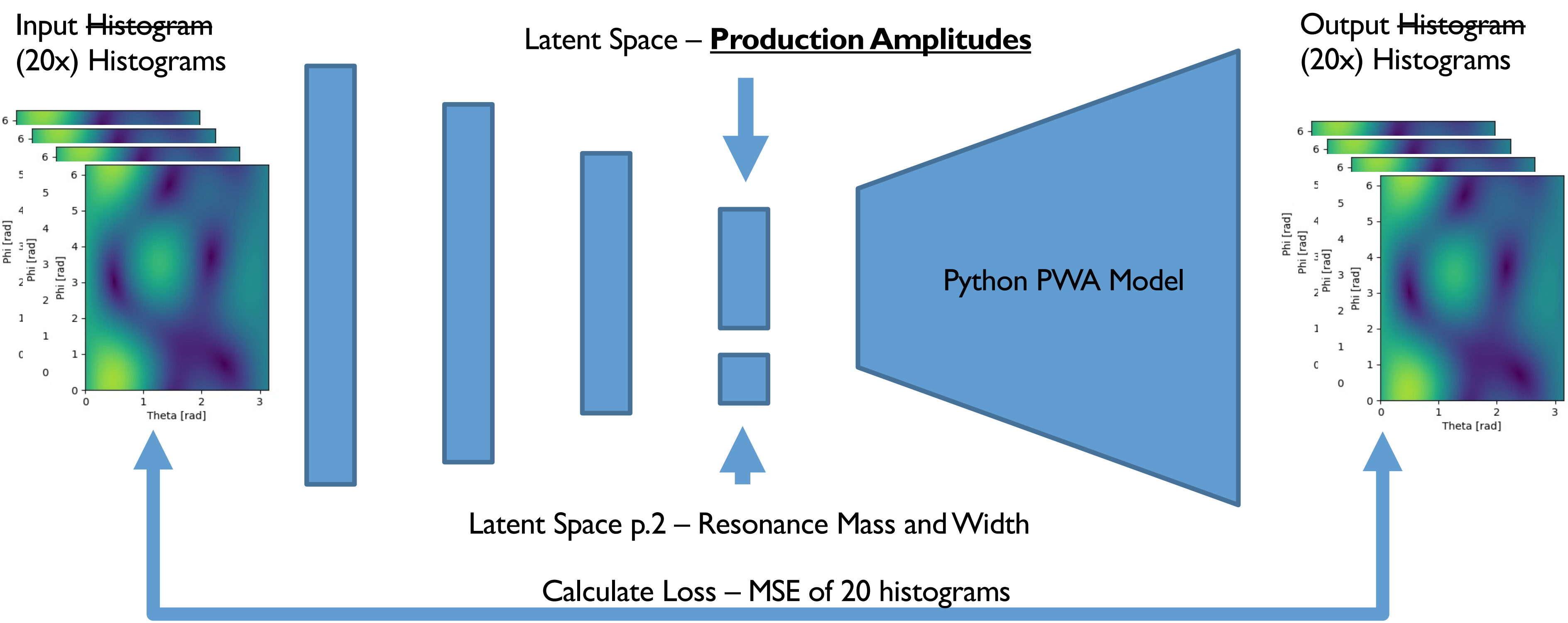
- Encoder portion is a standard MLP, but without labels!
- Decoder is a PyPWA model that takes in production amplitudes and produces a histogram
- Autoencoders *dramatically* improved the accuracy!
- Even works well for noisy data





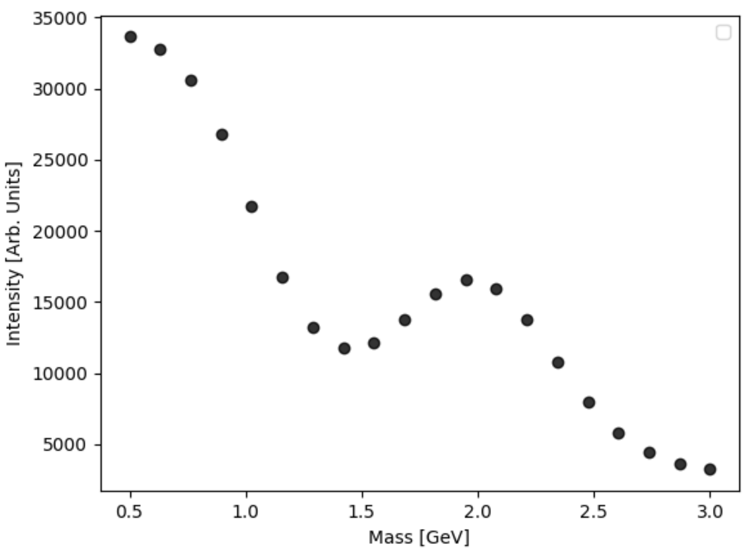


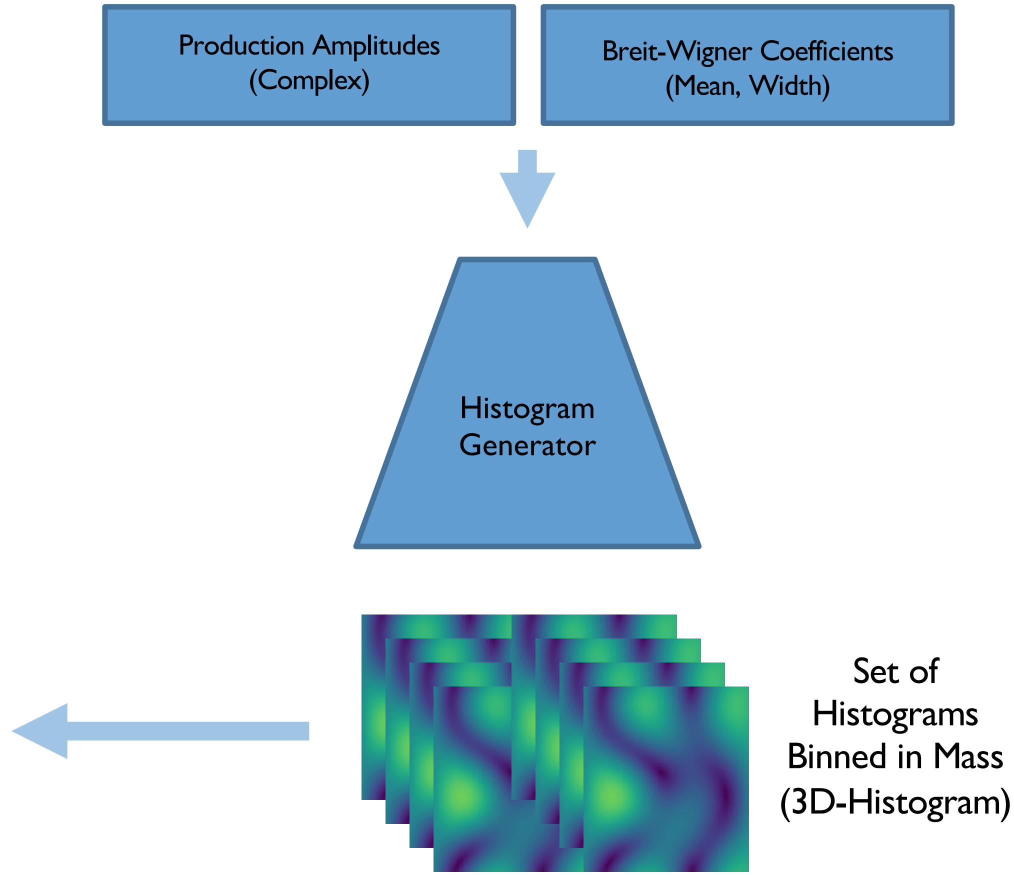
Mass Dependent Autoencoder work for PWA



The Mass-Dependent Generator

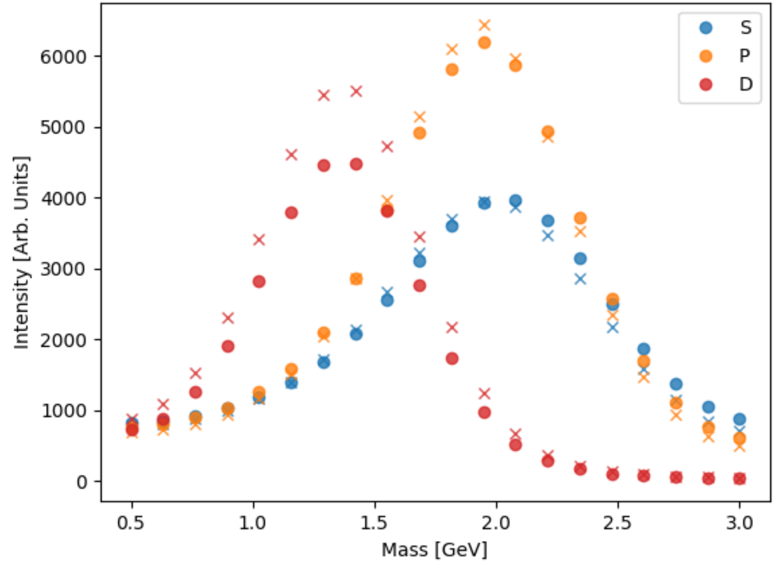
Randomly Generated Event
(Currently One Resonance per Wave)



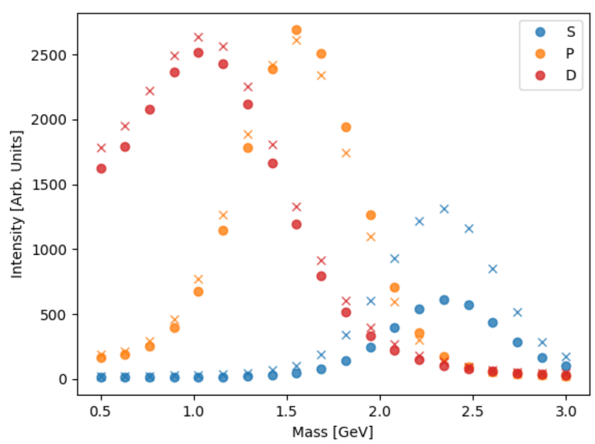


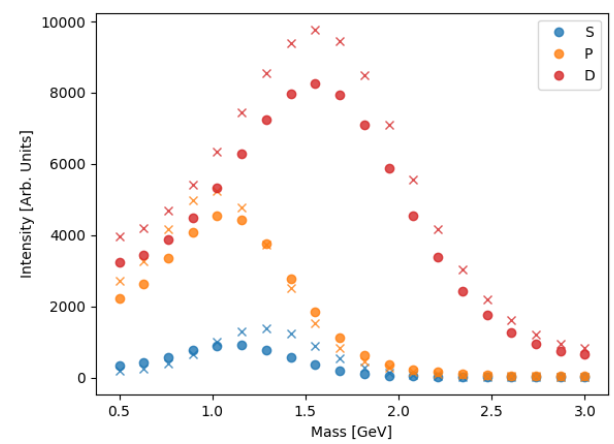
Results

- With a CONV3D input to our autoencoder we see a good agreement with the generated data and inference from our neural networks
- Shown on the right are three different tests with randomly generated data/resonances



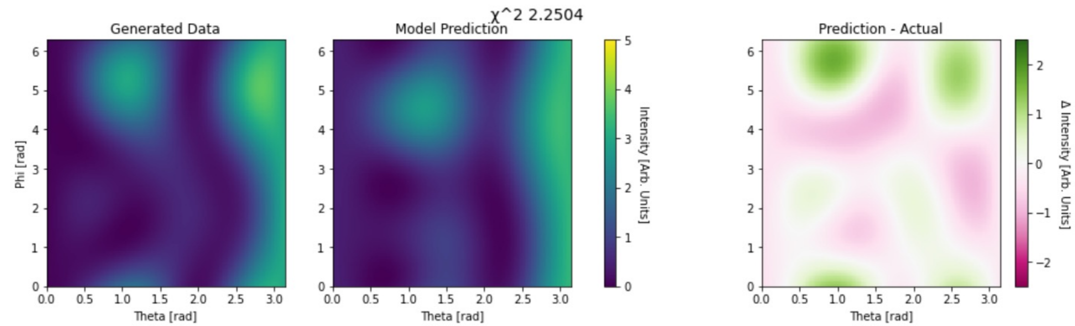
Crosses – Generated
Circles – Inference

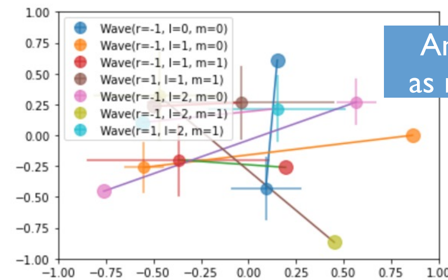




Uncertainty Quantification - VAE

- For uncertainty quantification we are using Variational Autoencoders (VAE) with some success
- Traditional (hybrid) autoencoder performs better for now
- Future work could involve some constraints to resolve ambiguities and allow better fits





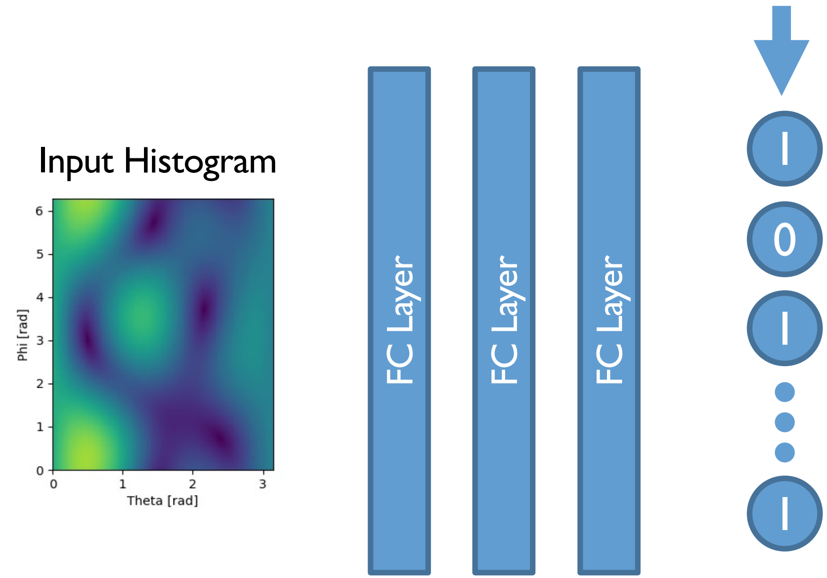
Ambiguities appear as rotations/sign flips

	X_0	X_1	X_2	X_3	X_4	X_5	X_6	Y_0	Y_1	Y_2	Y_3	Y_4	Y_5	Y_6
True	0.15	0.86	0.19	-0.50	-0.76	0.45	-0.56	0.61	0.00	-0.26	0.24	-0.45	-0.87	0.10
Pred	0.09	-0.55	-0.37	-0.04	0.57	-0.47	0.15	-0.43	-0.26	-0.20	0.26	0.27	0.32	0.22

Wave Selection DNN

- One of the problems that is regularly seen in PWA is choosing the right waves to use in your fit
- We simplified the regression problem we have posed in earlier slides to create a tool that could be used to select which waves are present
- Multi-label classification

Output: Wave Selection



Preliminary results:
79% accuracy in selecting the right set of waves (Lmax=2)
96.3% wave/"digit"-wise accuracy

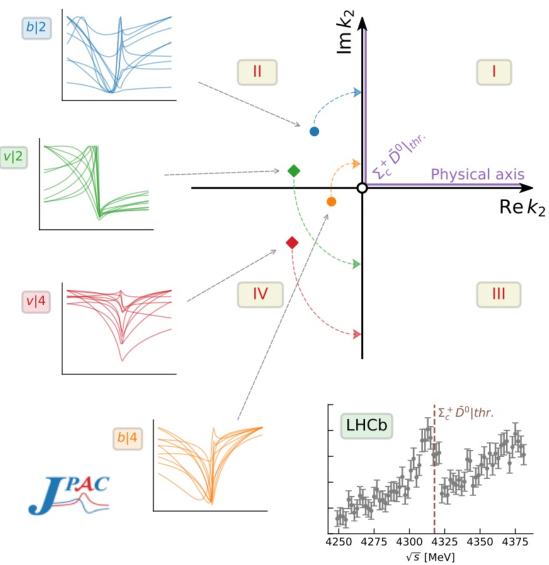
Artificial Intelligence in Spectroscopy

- Recent results from the JPAC
- Bottom-up approach providing a model-independent way to analyze resonances
- Many papers on Deep Learning in the hadron spectroscopy
- Unfortunately, I could not mention all of the ongoing work but I encourage you to look at recent publications such as the JPAC results shown with the DOI below

JLAB-THY-21-3518

Deep Learning Exotic Hadrons

L. Ng,[1,*] Ł. Bibrzycki,[2,†] J. Nys,[3,‡] C. Fernández-Ramírez,[4,5,§] A. Pilloni,[6,7,8,¶]
V. Mathieu,[9,10] A. J. Rasmusson,[11] and A. P. Szczepaniak[11,12,13]
(Joint Physics Analysis Center)
[1]*Department of Physics, Florida State University, Tallahassee, FL 32306, USA*
[2]*Pedagogical University of Krakow, 30-084 Kraków, Poland*
[3]*Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*
[4]*Departamento de Física Interdisciplinar, Universidad Nacional de Educación a Distancia (UNED), Madrid E-28040, Spain*
[5]*Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Ciudad de México 04510, Mexico*
[6]*Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra, Università degli Studi di Messina, Messina, I-98166, Italy*
[7]*INFN Sezione di Catania, Catania, I-95123, Italy*
[8]*INFN Sezione di Roma, Roma, I-00185, Italy*
[9]*Departament de Física Quàntica i Astrofísica and Institut de Ciències del Cosmos, Universitat de Barcelona, Martí i Franquès 1, E08028, Spain*
[10]*Departamento de Física Teórica, Universidad Complutense de Madrid and IPARCOS, E-28040 Madrid, Spain*
[11]*Department of Physics, Indiana University, Bloomington, IN 47405, USA*
[12]*Theory Center, Thomas Jefferson National Accelerator Facility, Newport News, VA 23606, USA*
[13]*Center for Exploration of Energy and Matter, Indiana University, Bloomington, IN 47403, USA*
(Dated: May 18, 2022)



DOI: 10.1103/PhysRevD.105.L091501

Summary

- We have been able perform PWA "fits" with neural networks
- Autoencoders dramatically improved the performance
- Variational autoencoders were tried with some degree of success for uncertainty quantification
- Future work includes continued work on hyperparameter optimization, uncertainty quantification, wave selection, and symbolic regression for PWA
- There is much deep learning work ongoing in the community! See recent JPAC results!

Many thanks to the EPSCI and Data Science group at JLab!
David Lawrence, Thomas Britton, Malachi Schram, Kishansingh Rajput

Summary

Backup

Wave Selection DNN

- Binary Classifier Ensemble/"Expert" Models
- Literature shows empirical evidence of increased performance
- https://doi.org/10.1016/j.patcog.2011.01.017

Preliminary results:
96% accuracy in selecting the right set of waves (Lmax=2)
99.4% wave/"digit"-wise accuracy