AI/ML for Experimental Physics

Motivations for ML use in experimental physics?

Techniques

Applying ML

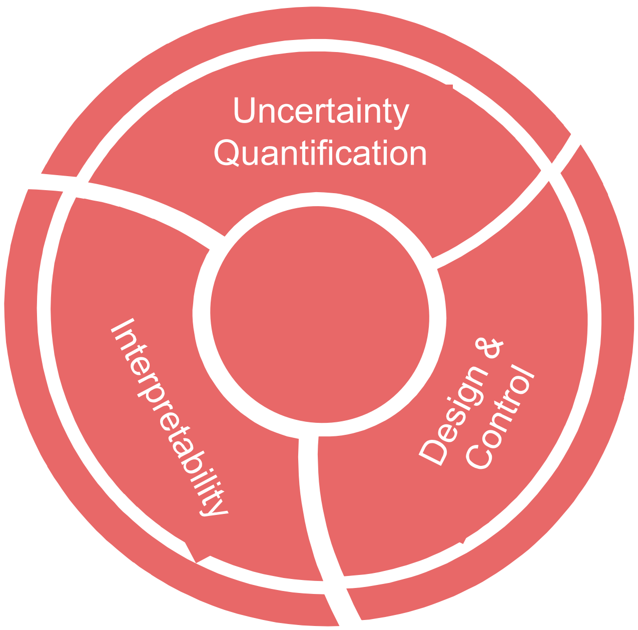
- Examples from Thomas Jefferson National Accelerator Facility (TJNAF)
- External collaborations

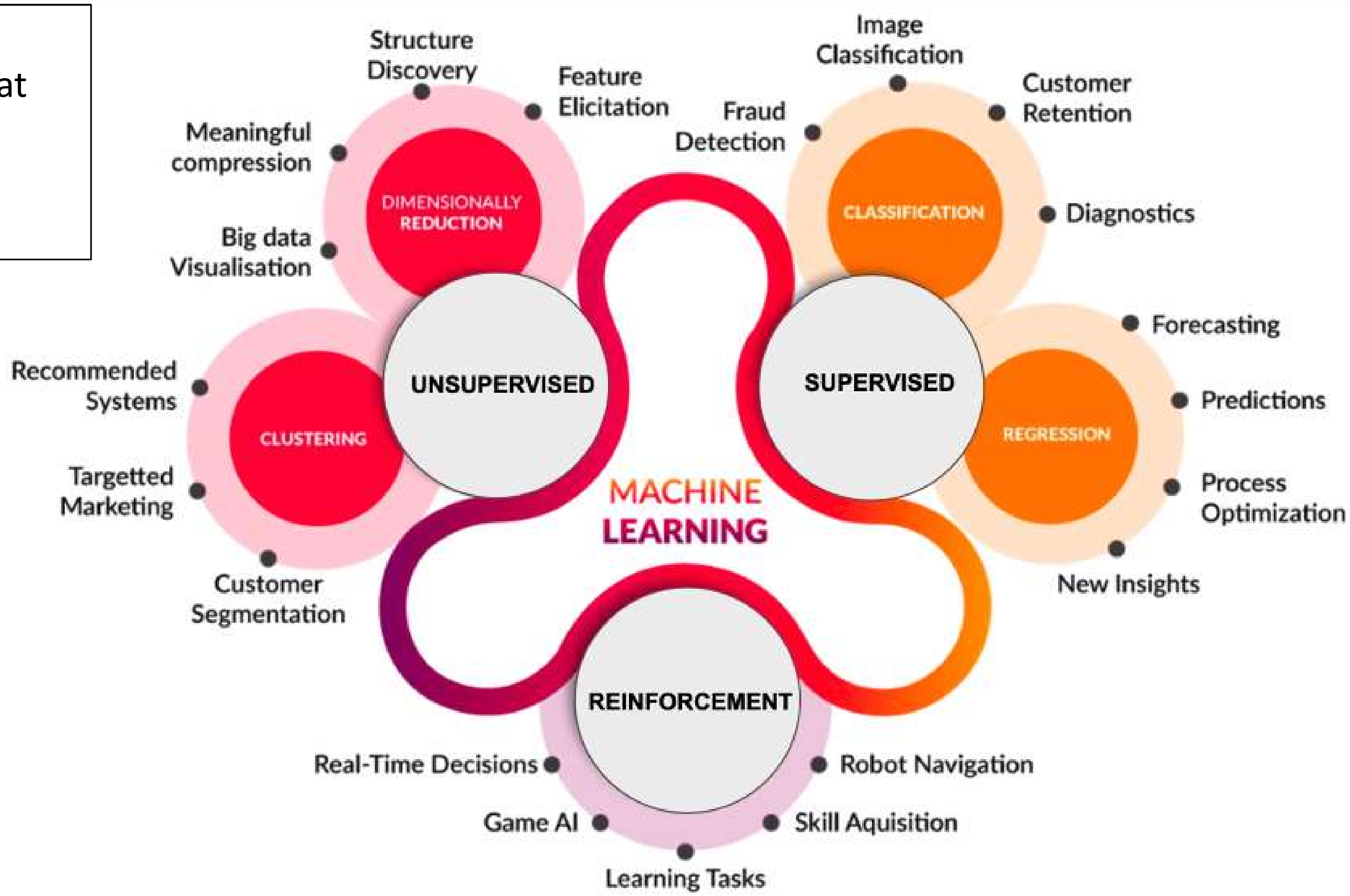
Diana McSpadden

September, 2022

Machine Learning

- Machine learning is a field focused on understanding and building methods that 'learn' a set of tasks
- Wide range of techniques
- Selection depends on the available data





Motivation

Provide world-class data science solutions to advance research

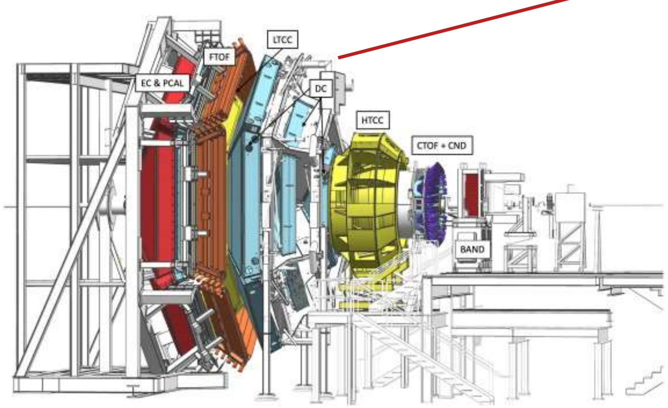
Why This Talk?

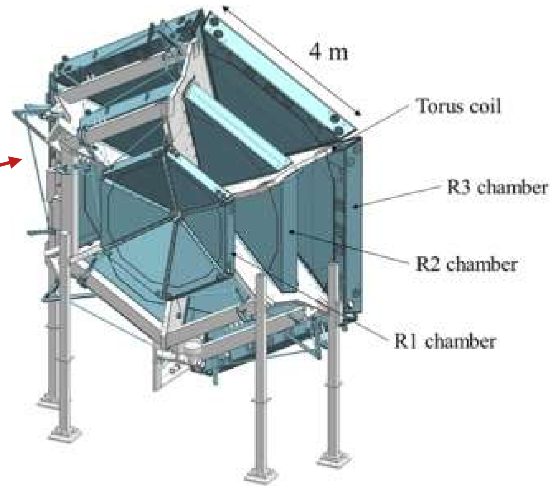
- Interested in the variety of applications of machine learning in experimental physics
- ML to augment or replace current processes that are temporally or computationally expensive
- ML used to address previously unaddressed or inadequately addressed problems

Hall-B: CLAS12 Tracking

From Gagik Gavalian

CEBAF Large Acceptance Spectrometer (CLAS12) located in Hall-B

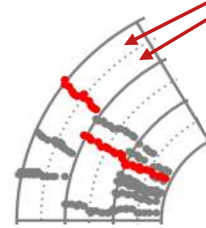




CLAS12 Drift Chamber:

- 6 drift chambers
  - each composed of **3 chambers**
    (one from each region: R1, R2, R3)
    (beam enters from the smallest region)
- Each sector has **2 superlayers** of wires

combinations of **clusters** form **track candidates**



Track candidates then processed further by time-based tracking

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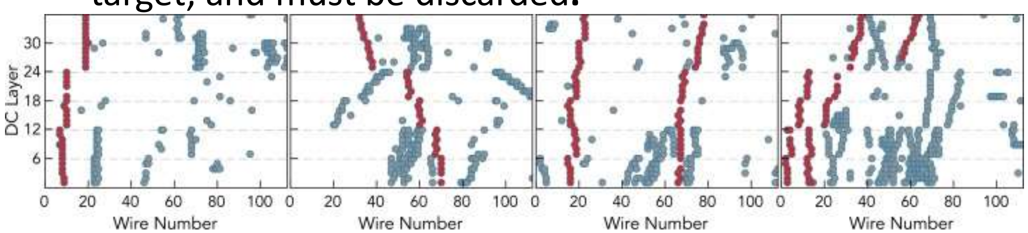
From Gagik Gavalian

Motivation: Tracking is computationally intensive

(takes a really long time)

Traditional

- Relies on fitting tracks with Kalman-Filter
  - Time-to-complete not guaranteed.
- All clusters evaluated with all other clusters to form track candidates
- Many later determined **not be a valid track**
  - though time was spent on fitting them
- Even after fitting, some tracks are not traced to the target, and must be discarded**.**



ML for particle track identification

- Reduction in track candidates to fit can lead to speed up of the fitting code (in theory)
  - Time to inference guaranteed
- CLAS12 Tracking: Identify clusters from individual hits in Drift Chambers, construct track candidates **using 5 or 6 layer** combinations
  - **Considerations**:
    - Inefficiencies and dead channels in drift chambers can lead to lost tracks
    - Traditional tracking algorithm considers **5 segment** combinations and recovers tracks
    - If track candidate detection is replaced with AI, a method must be developed to address the missing layer **issue.**

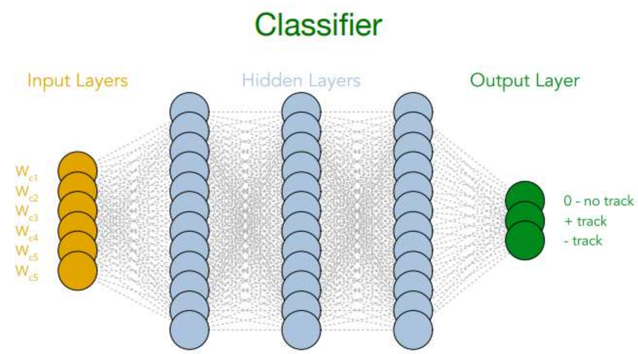
From Gagik Gavalian

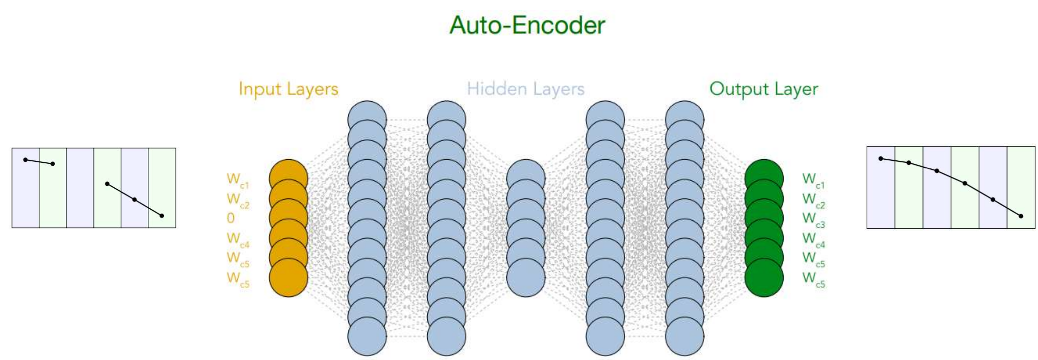
ML Technique

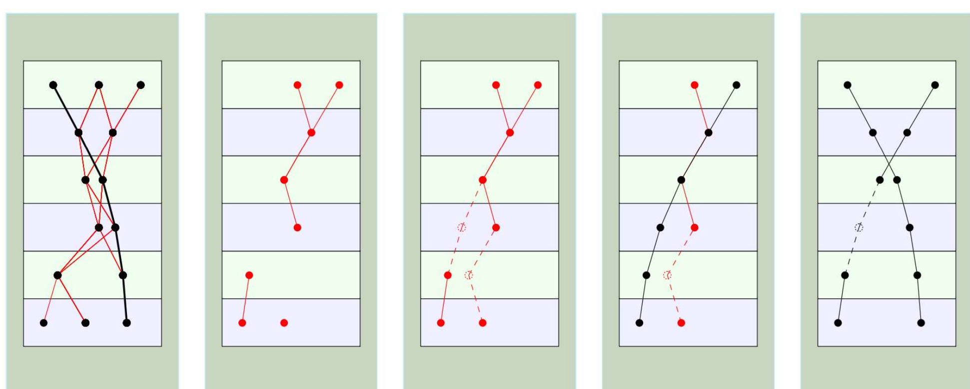
https://doi.org/10.1016/j.cpc.2022.108360

Combined Neural Networks

- Multi-layer perceptron (MLP) classifier – to identify best track candidates composed of 6 segments
- MLP Auto-encoder to fix corruption/inefficiencies by predicting the position of missing segments







6 SL Tracks

Pseudo Track Generation

5 SL Tracks

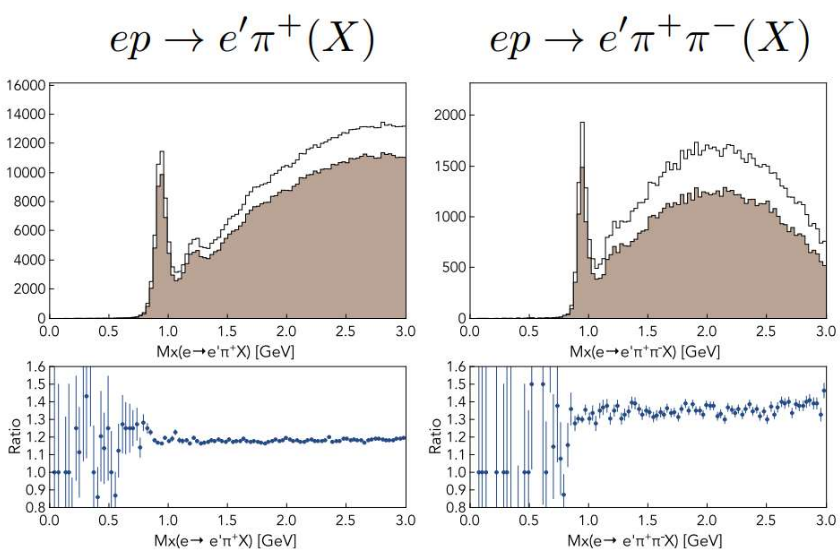
2 good tracks Reconstructed

Jefferson Lab

Hall-B: CLAS12 Tracking

From Gagik Gavalian

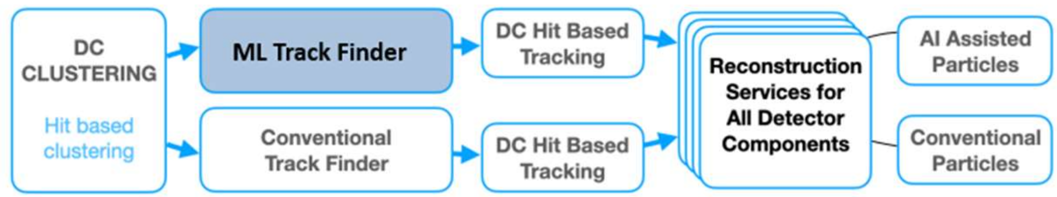
Results:



RG-A [45 nA]

Brown is traditional White is ML

- Reconstruction software can process in parallel conventional and ML-assisted tracking

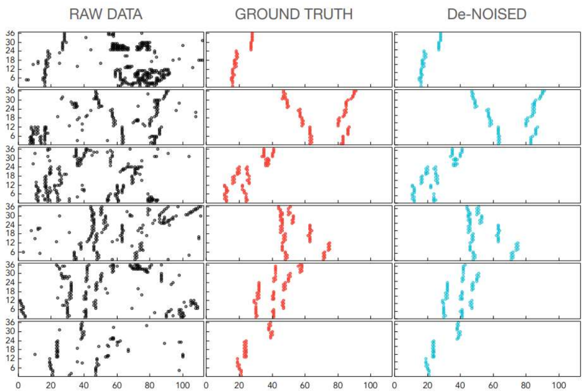


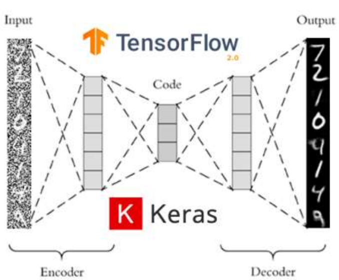
- Improved track finding efficiency by 12% - 15%
- Tracking code speedup ~35%
- **Physics impact**:
  - Two particle final state reaction gain ~20%
  - Three particle final state missing mass shows **35% increase in statistics** of the missing proton

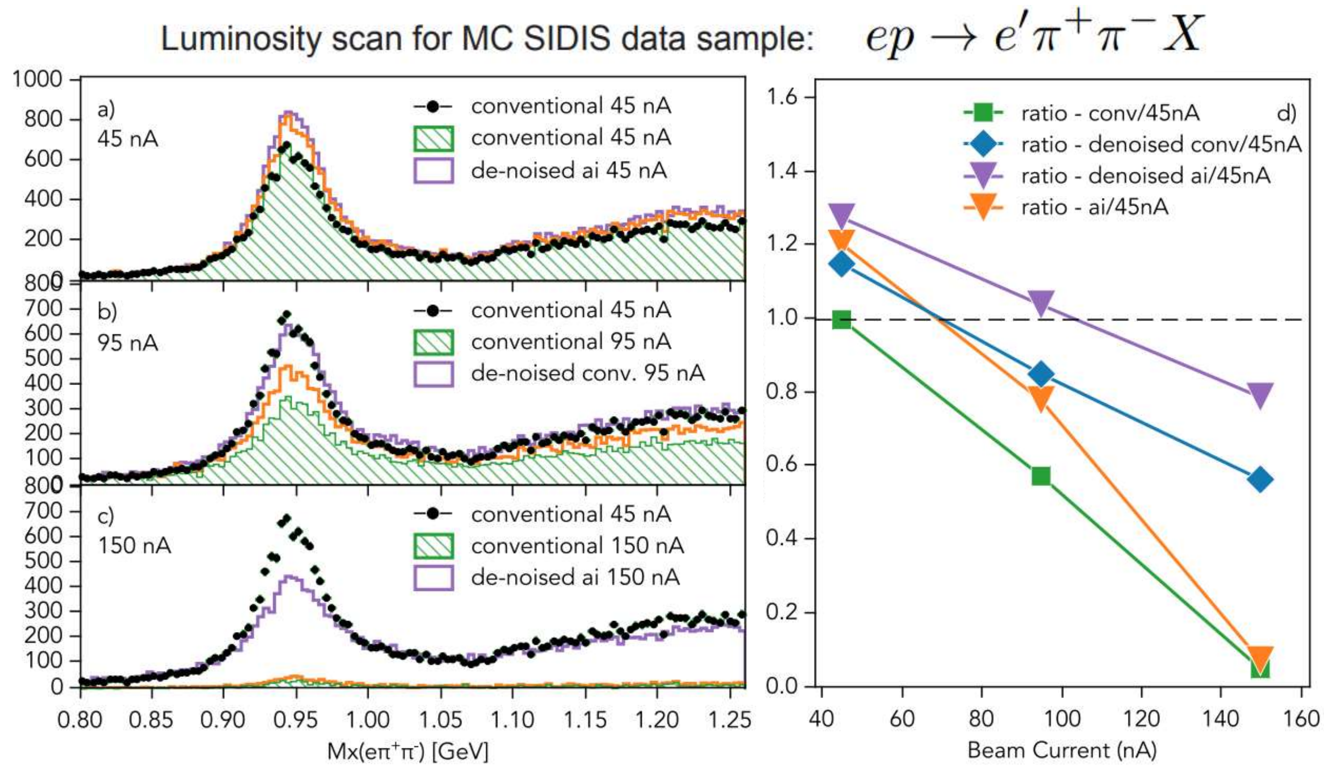
<u>**CLAS Collaboration meeting slides**</u>

Can We Make This Even Better? Especially at higher luminosity?

- Autoencoder was trained to clean raw data samples and leave only hit belonging to a track.
- As luminosity increases, noise in the raw data increases == combinatorics cause problems for traditional algorithms.





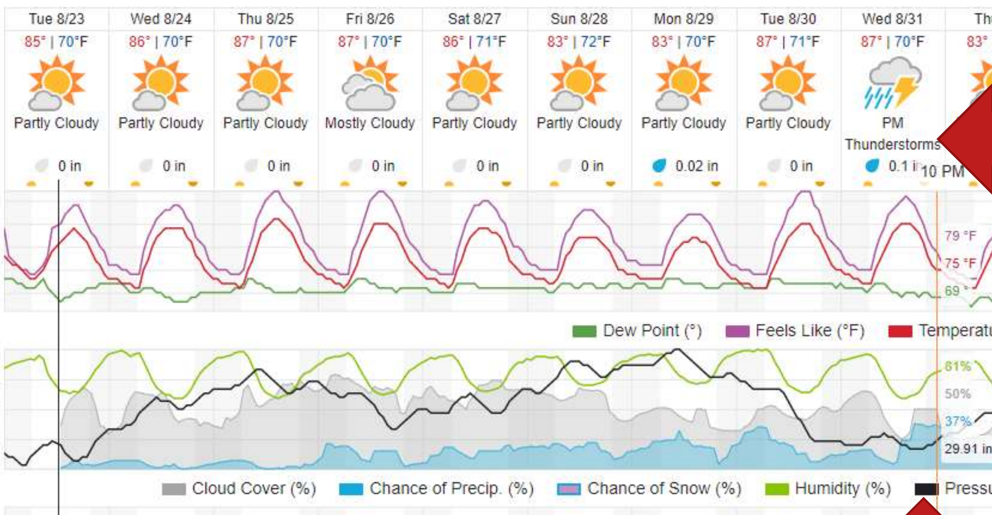


[CLAS Collaboration meeting slides]

Uncertainty Quantification (UQ)

Prediction: It will rain in Newport News, Virginia in 2022.

P(rain | where=Newport News, when=2022) = 100%, 99.999….% confidence



Wunderground says 37% chance of evening rain.

It will rain on my parking spot in at 17:15 in 8 days

P(rain | where=parking spot, when= **17:15 in 8 days**):

= 37% chance in the PM,

so…..**maybe 30% at 15:17, maybe 60% confidence**

JUST BRING AN UMBRELLA

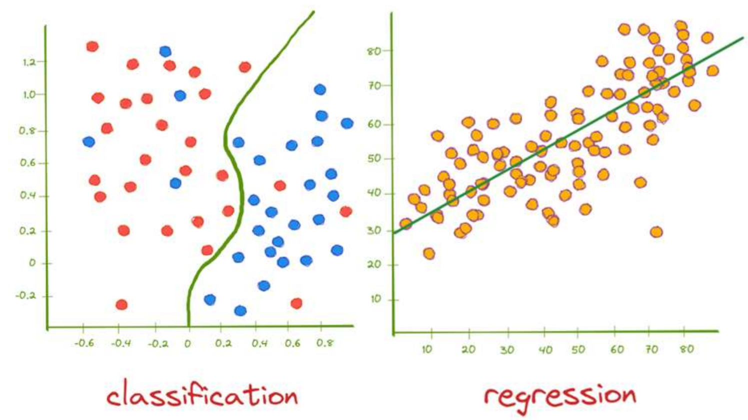

craiyon.com generated images for "bring umbrella due to uncertain rain outside my office"

Uncertainty Quantification (UQ) in ML for Experimental Physics

When might we be concerned with uncertainty quantification?

- Provides valuable information (about the model, about the data)
- High risk
- Significantly different actions taken based on the prediction and the uncertainty
- **Uncertainty quantification identified as an important topic at the recent series of DOE workshops for Advanced Research Directions in AI for Science and Security** (https://www.anl.gov/cels/advanced-research-directions-on-ai-for-science-and-security)

- It is critical to quantify the uncertainties in safety, optimization, and control applications
- Classification: Output label along with **confidence**
- Regression: Output mean along with **variance**

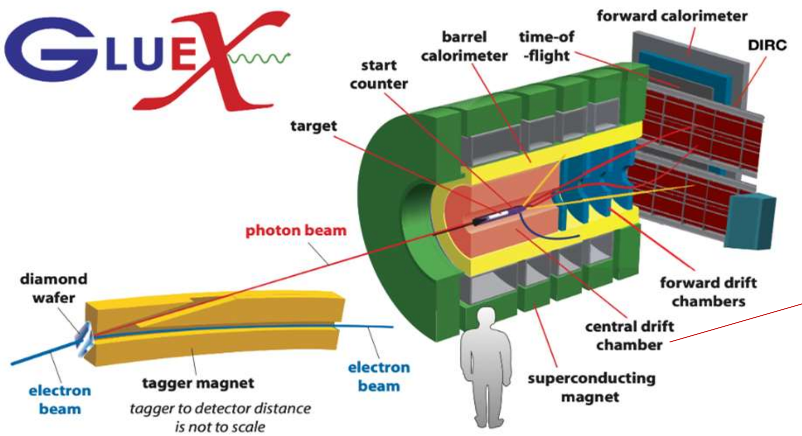


label + confidence

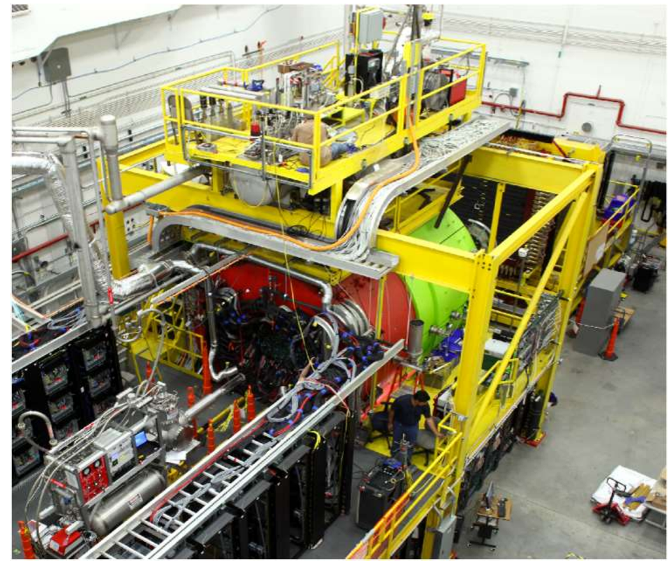
mean + variance

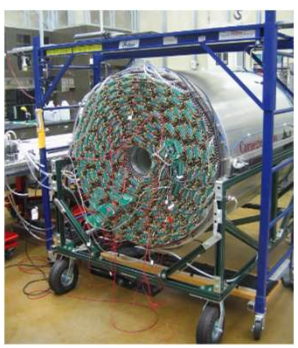
Hall-D: GlueX Central Drift Chamber (CDC) Calibration and Control

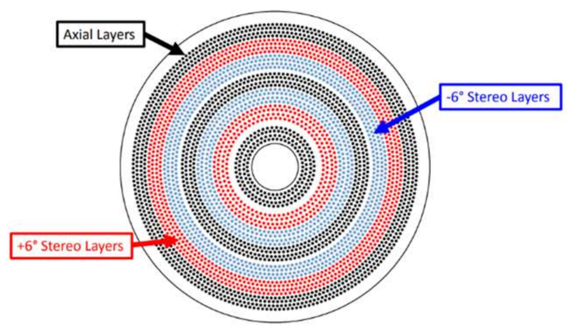
GlueX detector located in Hall-D



The CDC measures drift time and deposited charge and is used for particle identification







- Requires two calibrations: **chamber gain** and drift time-to-distance
  - **Gain Correction Factor (GCF)**: gain calibrations have the most variation **+/- 15%**
- Has **one** control: **operating voltage**

Hall-D: GlueX Central Drift Chamber (CDC) Calibration and Control

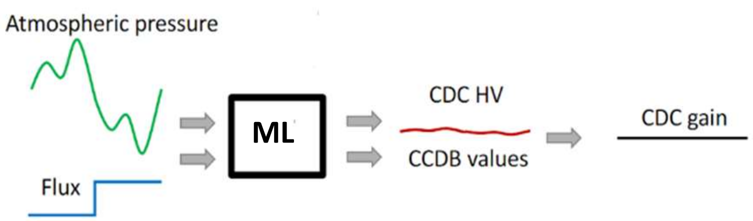
Motivation: Conventional vs. Online, ML Calibration Paradigms

Conventional

- **Control**: CDC operating voltage ***fixed*** at 2125 V
- **Calibrate**: calibration values **iteratively,** produced after the experiment
  - **~2 hour runs**

Online and ML

- **Control**: Stabilize detector response to changing environmental/experimental conditions by ***adjusting*** CDC HV
- **Calibrate**: **online** calibration values produced during the experiment

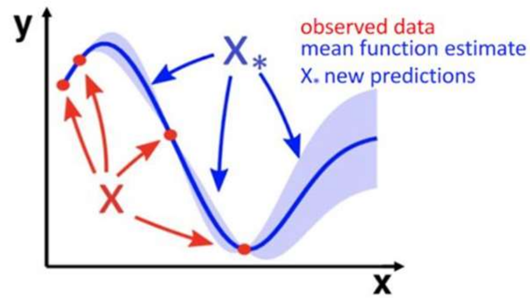


Hall-D: GlueX Central Drift Chamber (CDC) Calibration and Control

ML Technique

Gaussian Process (GP)

- 3 features:
  - **atmospheric pressure** within the hall
  - **temperature** within CDC
  - **CDC high voltage board current** -> a measure of intensity of the electron beam current within the CDC
- 1 target: the traditional Gain Correction Factor (**GCF**)
- GP calculates PDF over admissible functions that fit the data
- GP provides the standard deviation
  - we can exploit for uncertainty quantification (UQ)
- We used a basic GP kernel:
  - Radial Basis Function + White Noise
  - Tested isotropic and anisotropic kernels



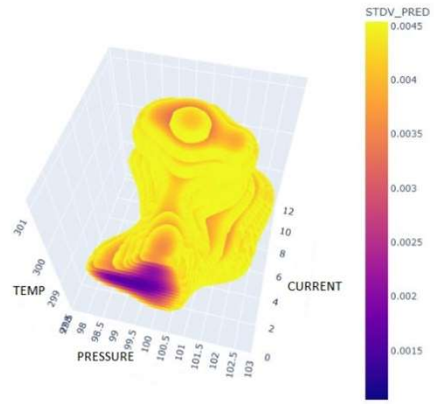
Do not set the CDC HV to a value for which we are uncertain

Hall-D: GlueX Central Drift Chamber (CDC) Calibration and Control

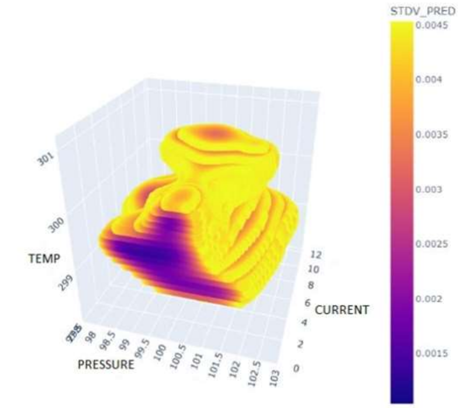
Considering UQ for control decisions

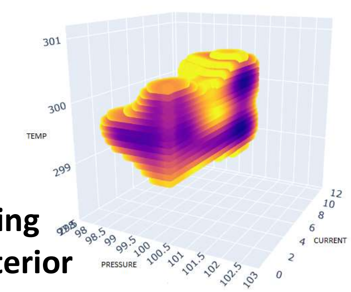
- We do **not** want to adjust high voltage to an "uncertain" value
- Gaussian Process provides uncertainty quantification
- Only apply a new calibration if the uncertainty is within the 3% of ideal gain correction factor otherwise, we extract to the “nearest” prediction within tolerance
- This method implemented in the Charged Pion Polarizability (CPP) experiment

Few low current training runs



Added low current training runs





With low current training runs, displaying the interior of certainty “surface”

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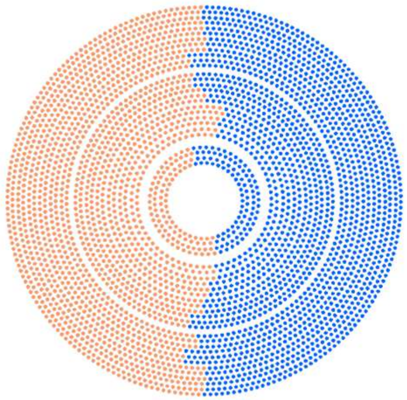
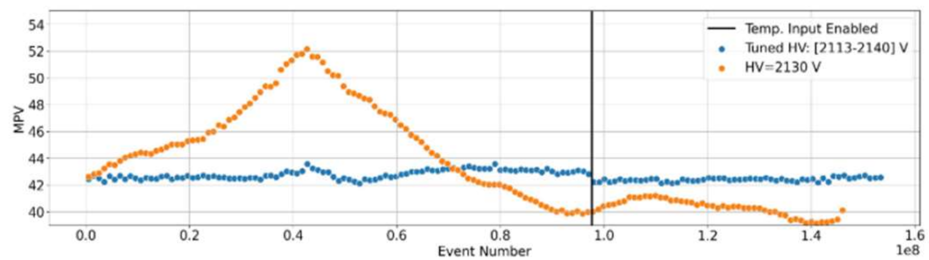
Hall-D: GlueX Central Drift Chamber (CDC) Calibration and Control

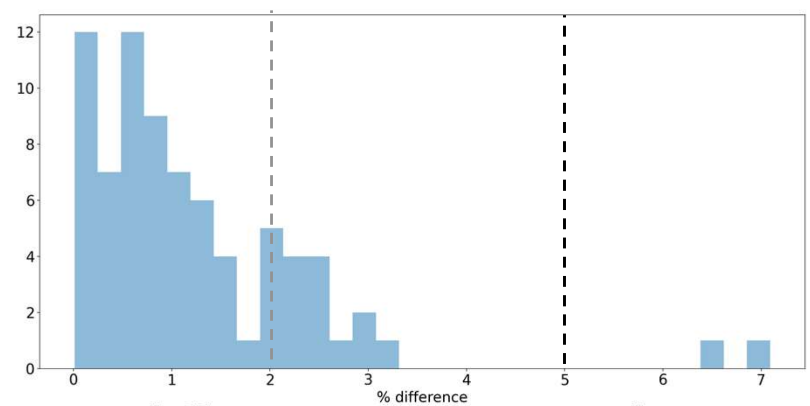
Verification Results:
Cosmic Rays
(no beam)





Conventional ML controlled

Preliminary Results:
Charged Pion Polarizability (CPP)
(beam on)



$\%$ difference $\mathbf{GCF_{traditional}}$ and $\mathbf{GCF_{ML}}$

Jefferson Lab

Different methods for UQ in DL

- Unfortunately, majority UQ methods for DL do not account for

out-of-distribution (OOD) uncertainty

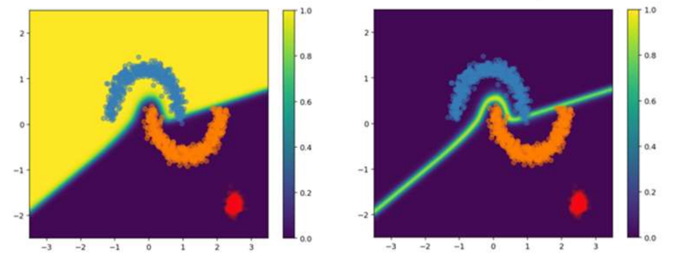
- This is critical in optimization or control problems
- For example, different methods yield vastly different uncertainty estimation
  - Deterministic - standard neural network for classification

Class Probability

Deterministic Model

(Normalized) Predictive Uncertainty

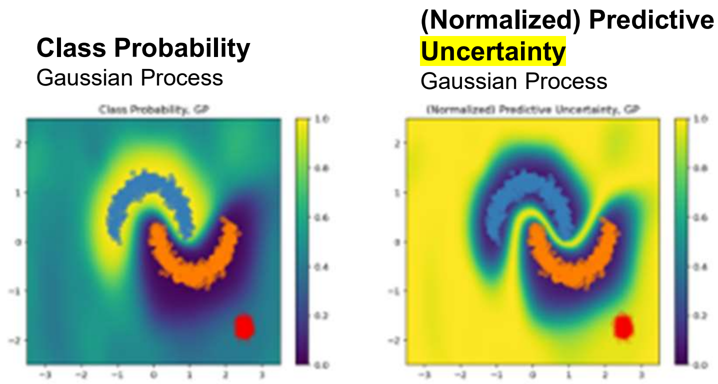
Deterministic Model

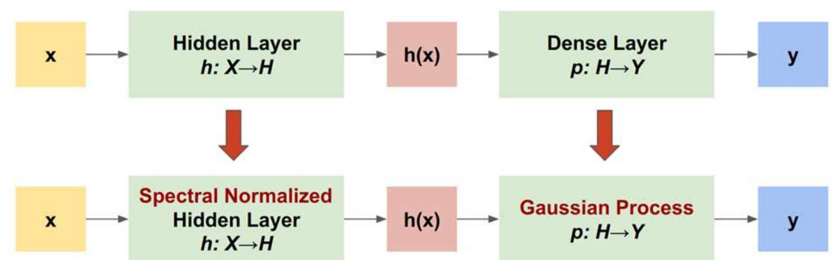


Gaussian Process (GP) for UQ in DL

- GP transforms the input space into a higher dimensional space with the help of a kernel
- The inferences are based on the distance measured between different input samples
- This allows GP to intrinsically provide uncertainty estimates including OOD
- Recent work from Google Research presented a way to introduce Gaussian Process approximation within a neural network: https://arxiv.org/pdf/2006.10108.pdf
- This allows highly expressive deep networks and provides uncertainty estimation

Gaussian Process



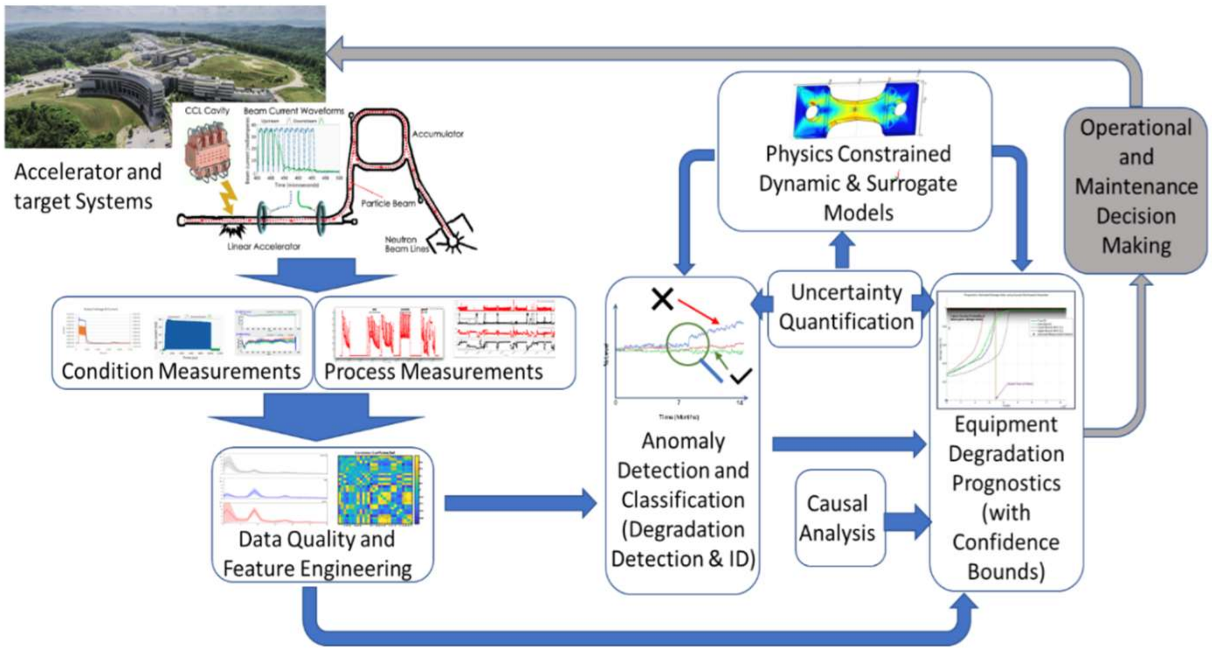


Spectral Neural Gaussian Process

ORNL: Spallation Neutron Source Accelerator Anomaly Detection

Spallation Neutron Source located at Oak Ridge National Lab

- **Predict errant beam pulses** as well as equipment degradation
- Continuous data collection is done by **Differential Current Monitor (DCM)**, Beam Position Monitor (BPM), etc.
- **Goal**: Errant beam prediction on one pulse **before it happens**

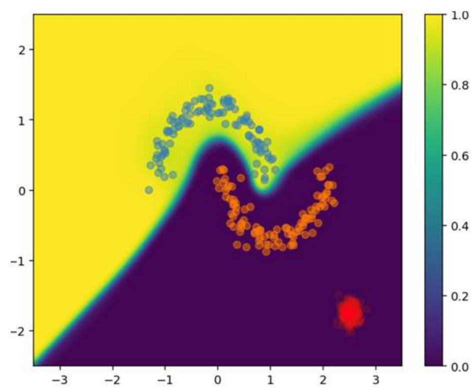


ORNL: Spallation Neutron Source Accelerator Anomaly Detection

Traditional classification models vs Siamese model

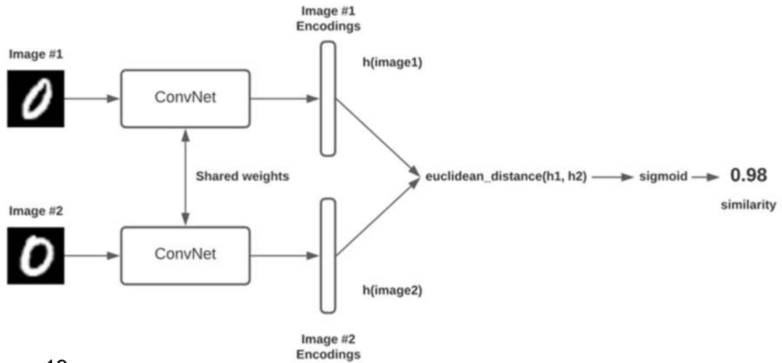
Traditional

- Traditional DL classification **models fails to identify unseen anomalies (OOD)**



Siamese model

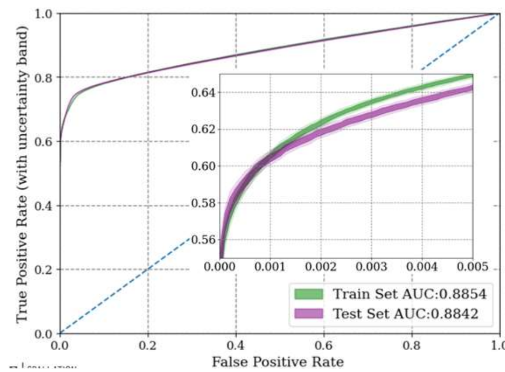
- **Similarity based** models can correctly classify unseen anomalies, e.g. a Siamese model
- Siamese model does not explicitly model the classification but **focuses on the similarities**
  - learns **twin embedding models** to transform inputs into a latent space
  - **Distance measures are applied at latent space** to compute the similarity

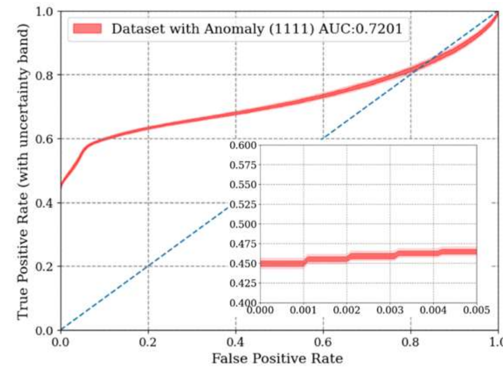


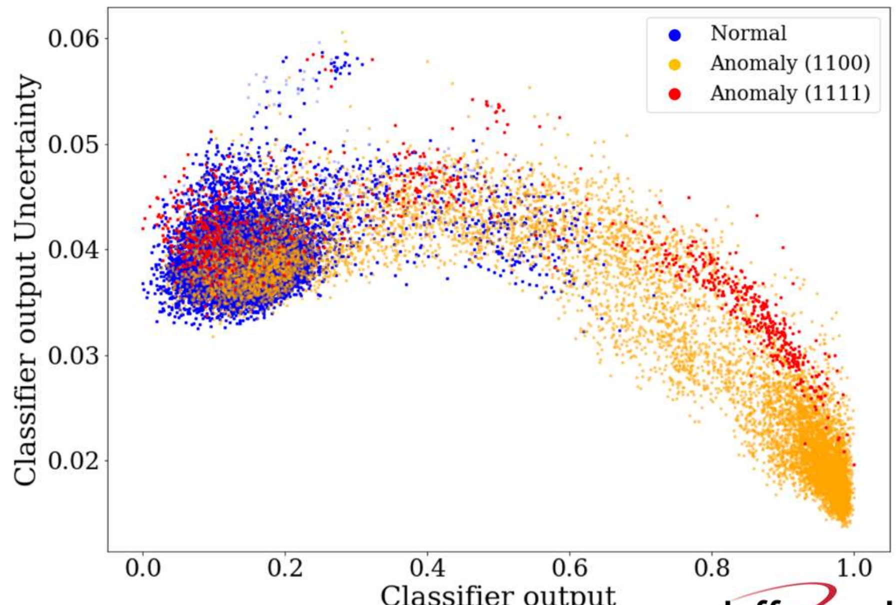
ORNL: Spallation Neutron Source Accelerator Anomaly Detection

Uncertainty aware Siamese model

- We enhanced a Siamese model of normal and errant beam pulses by adding GP layer providing an uncertainty estimate
- Results from the similarity model showed an ~4x improvement in performance over previously published results
- The ROC curves shows nearly the same level of performance (not optimized)
- We introduced an out-of-domain anomaly, labelled 1111 (red), the UQ-based model correctly identified the anomaly and indicated high uncertainty (as expected)





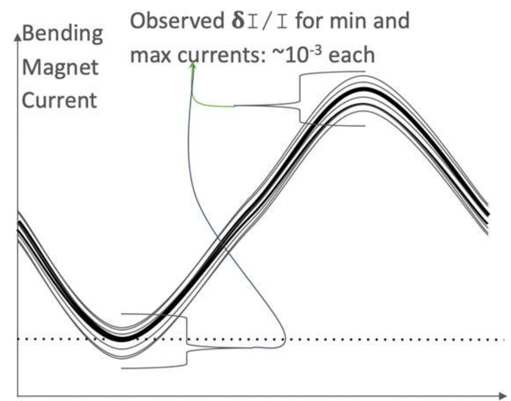


Fermilab: Reinforcement Learning for Booster Control Policy

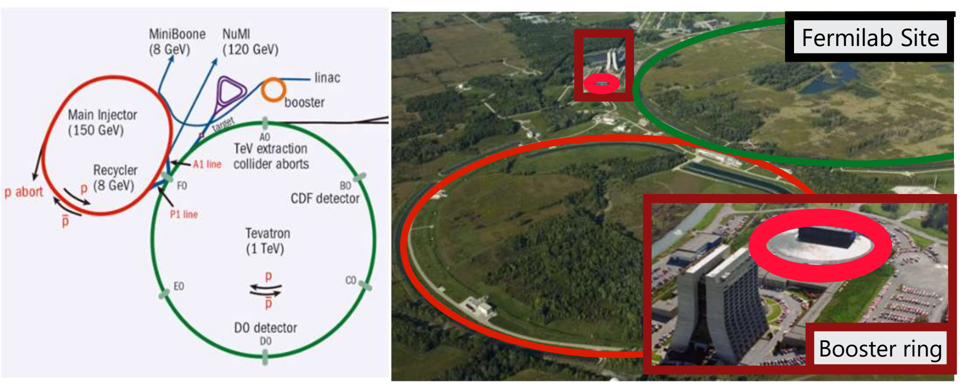
Problem definition

- Reduce beam losses in the FNAL Booster
  - Machine Learning (ML) model to provide an optimal set of actions for accelerator controls
- The beam is accelerated with the help of booster cavities and combined-function bending and focusing electromagnets known as gradient magnets powered by the **gradient magnet power supply (GMPS) –** regulated by the **GMPS regulator**

High-current, high-power electrical loads near GMPS vary in time, causing unwanted fluctuations

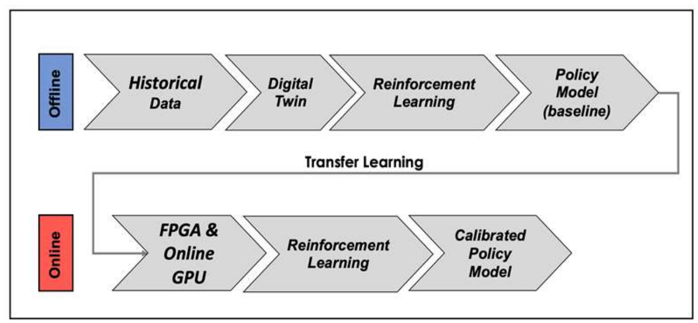


FNAL Accelerator Complex:



Courtesy: Christian Herwig

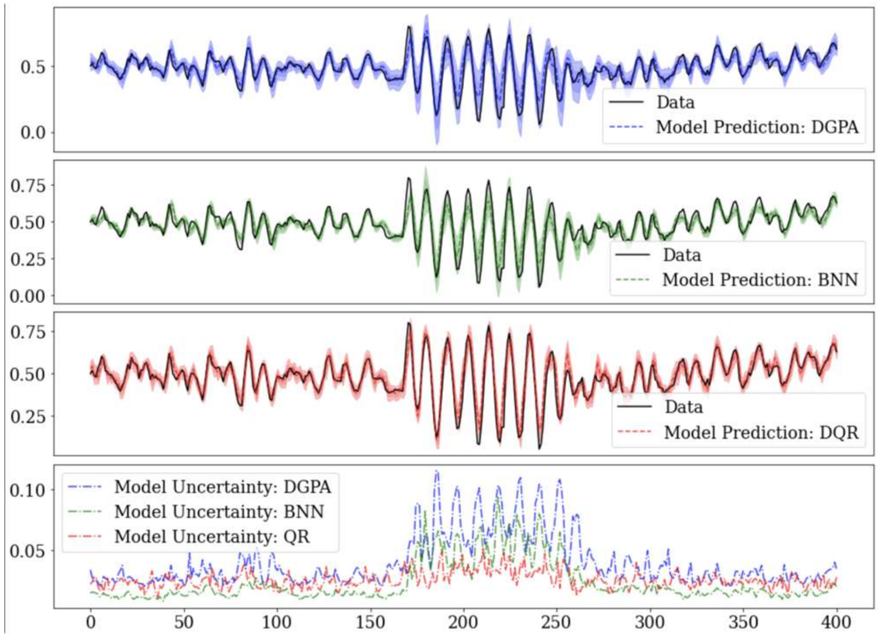
- Use of RL to improve the existing PID-based regulator
- Policy model is focused on controlling the regulator to reduce the error

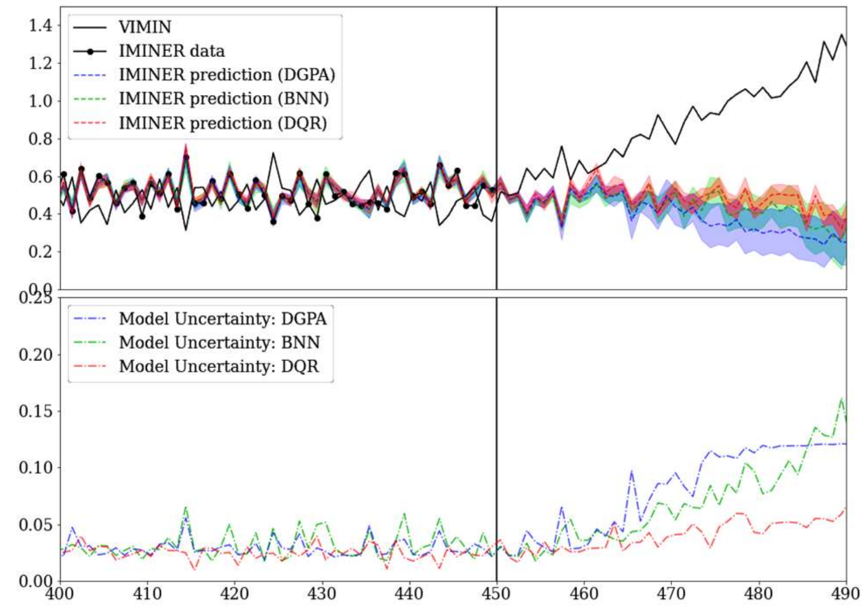


Fermilab: Reinforcement Learning for Booster Control Policy

Uncertainty quantification for surrogate models in risk-averse control research

- **Quantile regression (DQR)** method has great performance in the training distribution and is calibrated by definition, however, they do **not** perform well for **out-of-distribution** (OOD) estimation
- **Bayesian Neural Net (BNN)** models do a better job to estimate OOD **but require calibration**
- **GP approximation (DGPA)** model provides the **best OOD estimation and is calibrated by design**





References

- ML for CLAS12 Tracking:
  - https://inspirehep.net/literature/2062921
  - https://inspirehep.net/literature/1950708
  - https://arxiv.org/abs/2205.02616
  - https://arxiv.org/abs/2202.06869
  - https://arxiv.org/abs/2009.05144
- DOE Laboratory Workshop Series:
  - https://www.anl.gov/cels/advanced-research-directions-on-ai-for-science-and-security
- Spectral Normal Gaussian Process from Google Research
  - https://arxiv.org/pdf/2006.10108.pdf
- Craiyon.com: AI model drawing images from any prompt
  - https://www.craiyon.com/
- Gpflow:
  - https://www.gpflow.org/
- Gaussian Process in Deep Learning
  - https://arxiv.org/pdf/2006.10108.pdf
- GlueX Central Drift Chamber ML Control
  - https://misportal.jlab.org/ul/publications/view_pub.cfm?pub_id=17072 (video presentation from the 2022 SandiaMLDL workshop
- Uncertainty aware anomaly detection to predict errant beam pulses in the SNS accelerator
  - https://arxiv.org/abs/2110.12006
- Developing Robust Digital Twins and Reinforcement Learning for Accelerator Control Systems at the Fermilab Booster
  - https://doi.org/10.48550/arXiv.2105.12847
- Conference Slidedeck: Developing Robust Digital Twins and Reinforcement Learning for Accelerator Control Systems at the Fermilab Booster
  - https://www.osti.gov/biblio/1825276/
- Real-time artificial intelligence for accelerator control: A study at the Fermilab Booster:
  - https://journals.aps.org/prab/abstract/10.1103/PhysRevAccelBeams.24.104601
- ORNL SNS Accelerator:
  - https://neutrons.ornl.gov/sns

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