Uncertainty Aware Machine Learning Models for Particle Physics Applications

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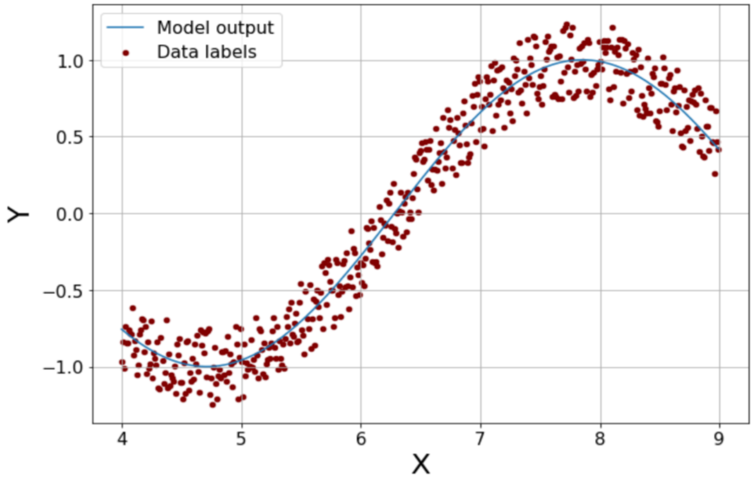
Uncertainty Quantification in Machine Learning

- Deterministic transformation functions

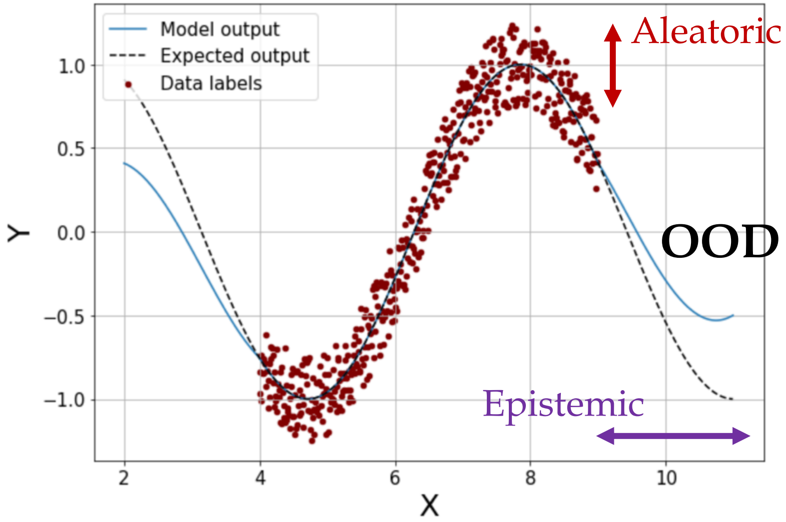
Input(s) → ML model → Output(s)

- Decision making based on predictions from ML models
  - Uncertainty Quantification is required to make an informed decision

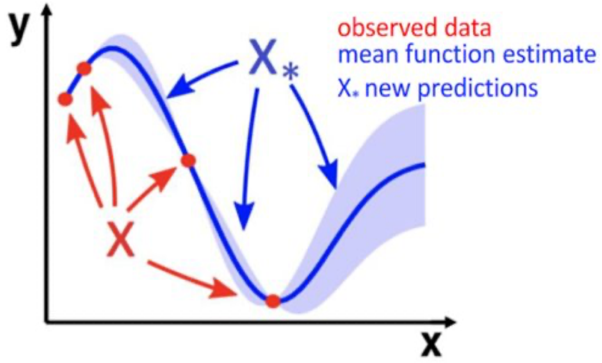


Uncertainty Types: Aleatoric vs Epistemic uncertainties

- Aleatoric → Data uncertainties
- Epistemic → Model or Out of training distribution uncertainty (OOD)



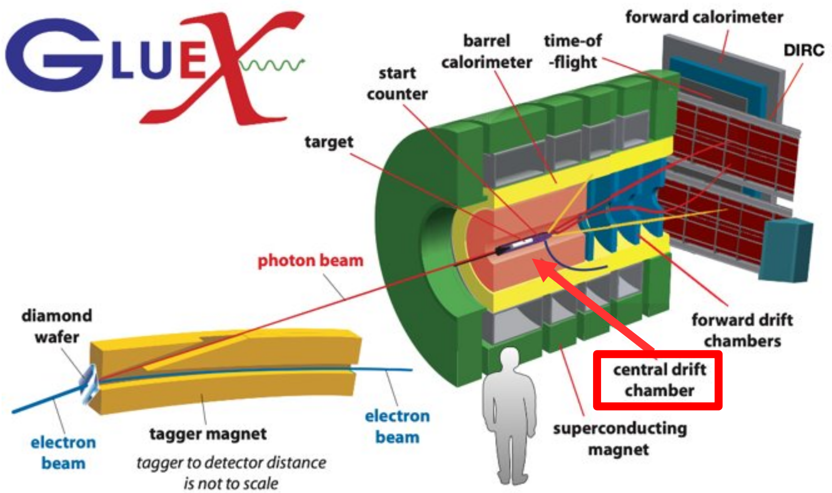
Gaussian Process (GP) provide robust uncertainty quantification



Outline

- Traditional application of Gaussian Process (GP):
  - Uncertainty aware experiment control at GlueX with GP
- Scaling limitations of GP and UQ for Deep Neural Networks (DNN):
  - Uncertainty aware anomaly prediction at SNS
  - Uncertainty aware particle identification for SoLID
  - Uncertainty aware surrogate model for FNAL booster
- Conclusion

Gaussian Process (GP) for Calibration of the Central Drift Chamber (CDC)



- Requires two calibrations: **gain** and drift time-to-distance
  - **Gain Correction Factor (GCF)** [variation +/- 15%]
- Has **one** control: **operating voltage**
- CDC is gas filled, sensitive to
  - Atmospheric pressure
  - Temperature
- Experimental conditions change, i.e. beam current
  - model uses high voltage board current as a proxy for beam current

Motivation: Online calibration to save time and computing resources required for post calibration

Conventional

Calibrate: calibration values **iteratively** produced after the experiment

No Control: CDC operating voltage is ***fixed*** at 2125 V

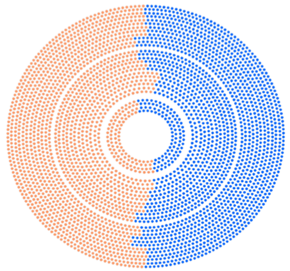
Online and ML

Online. calibration and Control: Stabilize detector response to changing environmental/experimental conditions by ***adjusting*** CDC HV

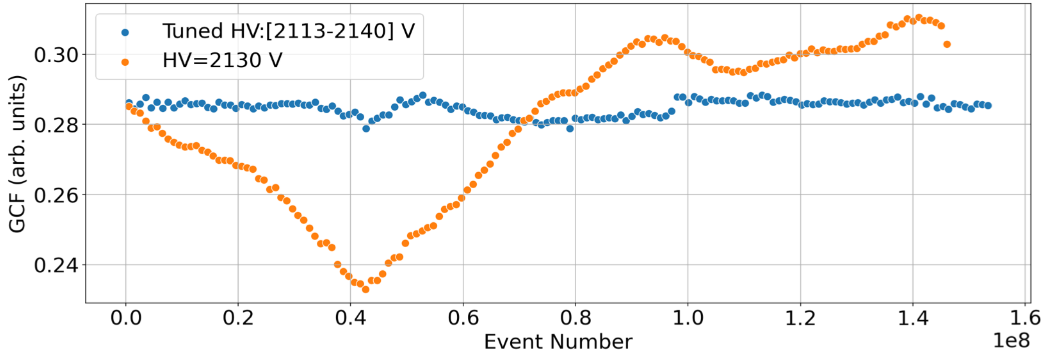
GP for Calibration of the Central Drift Chamber (CDC)

Cosmic Ray Experiment

- Sorted the CDC into **2 halves**
- Leave one side at a **fixed HV (conventional)**
- Let the **ML control the other**
- **Autonomously** adjust HV every 5 min



Conventional in orange
ML-tuned in blue



Experimental Control Requires Uncertainty Quantification

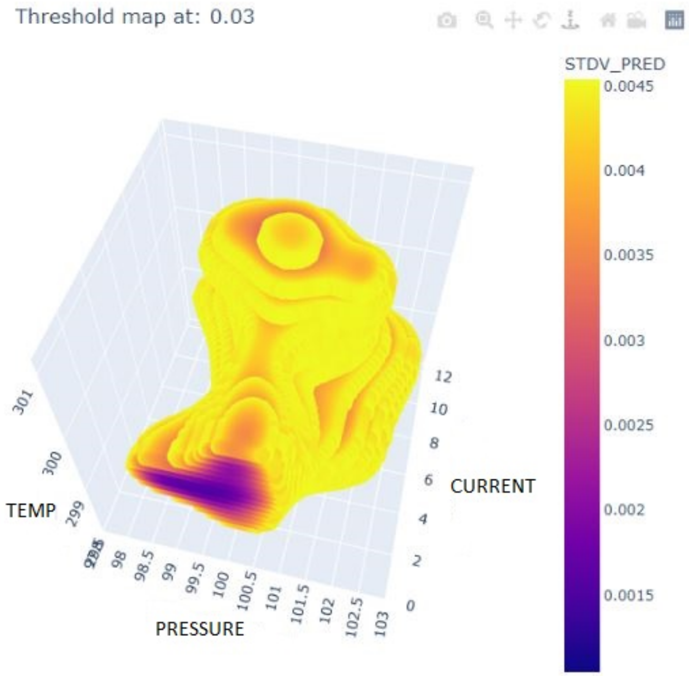
- Training data rarely has complete coverage: 601 runs, 2 run periods
- Do experts trust model predictions?

Uncertainty Surface Mesh:

- Threshold of standard deviation, visualize feature space
- **Uncertainty > threshold**

  Approach-1: use prediction for the closest point on the surface

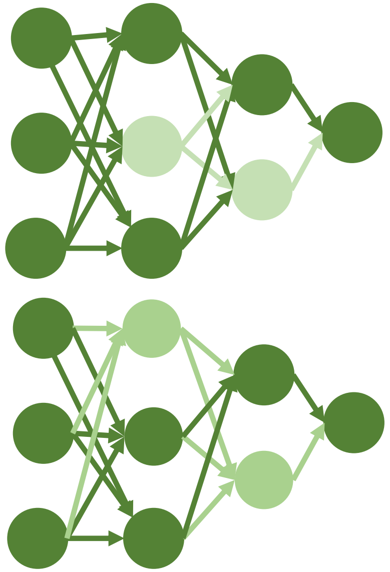
  Approach-2: return CDC to traditional high voltage setting, 2125 V and collect more data to train



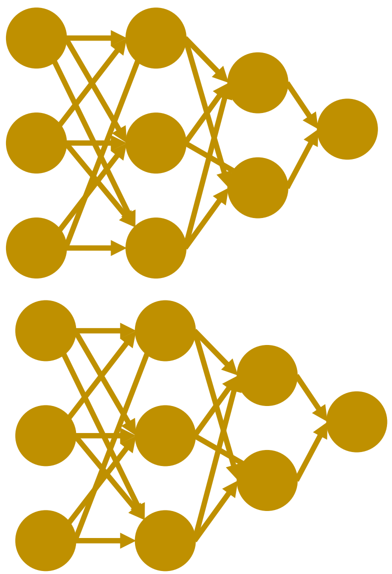
Large data sets with higher dimensions and GP

- **GP provides robust UQ but scales poorly with increase in data samples (O(n^3))**
- For large datasets and/or in large feature space, **GP approximation** is required
- Deep Neural Networks (DNN) are very expressive and scales with size of dataset
- DNN can deal with different types of data including images, text, and timeseries
- What about UQ for DNN?

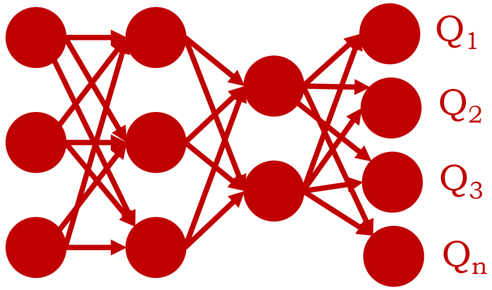
UQ in Deep Learning



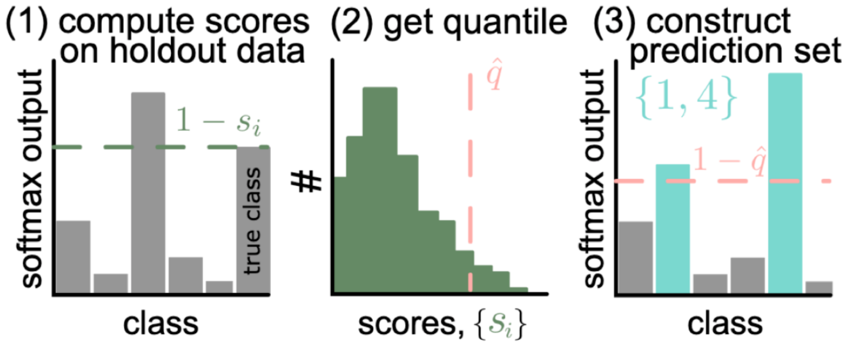
(a) MC Dropout



(b) Ensemble



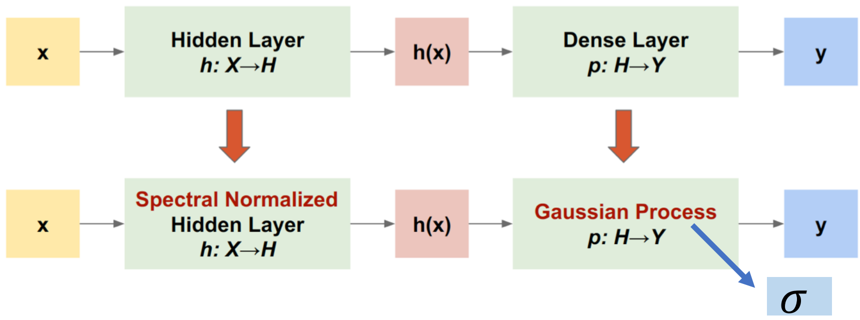
(c) Quantile Regression



https://arxiv.org/abs/2107.07511

(d) Conformal Predictions

GP takes into account distance between input samples explicitly



Spectral Neural Gaussian Process

- Distance preservation via Spectral Norm on each hidden layer
  - Reduced expressivity, harder to learn
- Distance preservation via bi-lipschitz

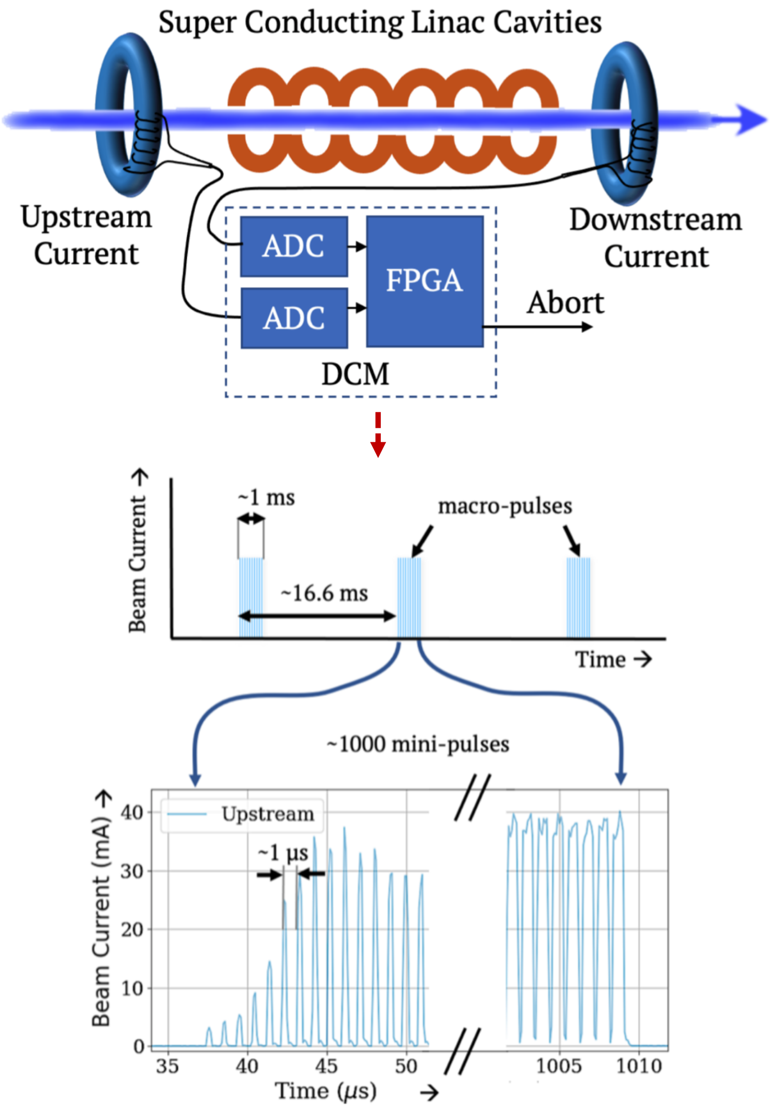
$$L_1 \times ||x_1 - x_2|| \leq ||h_{x_1} - h_{x_2}|| \leq L_2 \times ||x_1 - x_2||$$

L_1 and L_2 are hyper-parameters, h_{x_1}, h_{x_2} are hidden layer outputs corresponding to inputs x_1, x_2 respectively

Anomaly Prediction at SNS Accelerator

- Accelerators are complex multi-system machine
- Failure in any equipment can cause errant beams
- Fault prediction is beneficial in many ways including reduced downtime

Goal: To predict errant beam pulses (with uncertainty quantification) before they occur to avoid potential damage to the equipment(s) and reduce the downtime



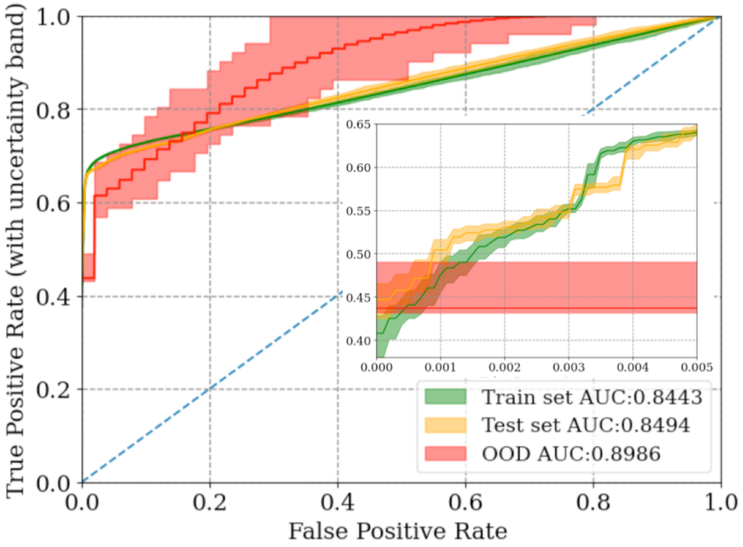
Dataset:

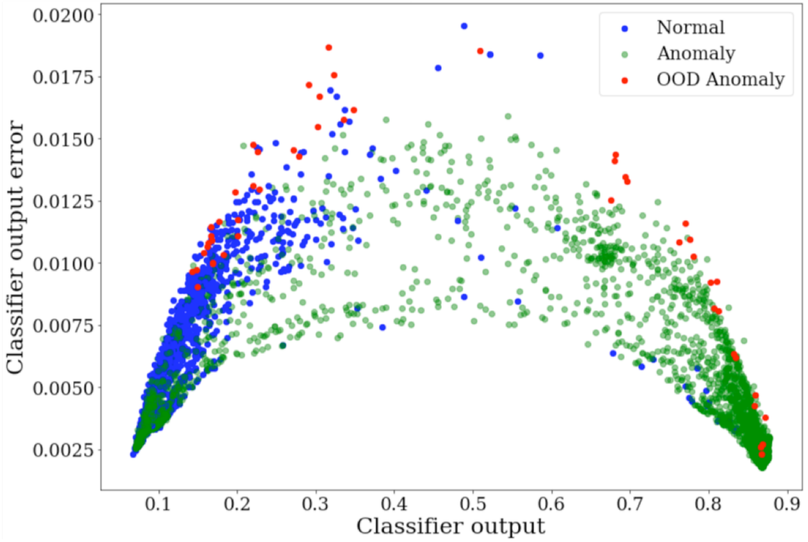
- We used the macro-pulse before an errant beam pulse (and labeled it as anomaly) and macro-pulses from the normal operation (and labeled them as normal) for our studies
- Our hypothesis: there is a sign about upcoming anomaly in macro-pulses even before it happens
- We also need to forecast the fault within a **short time window** to be actionable

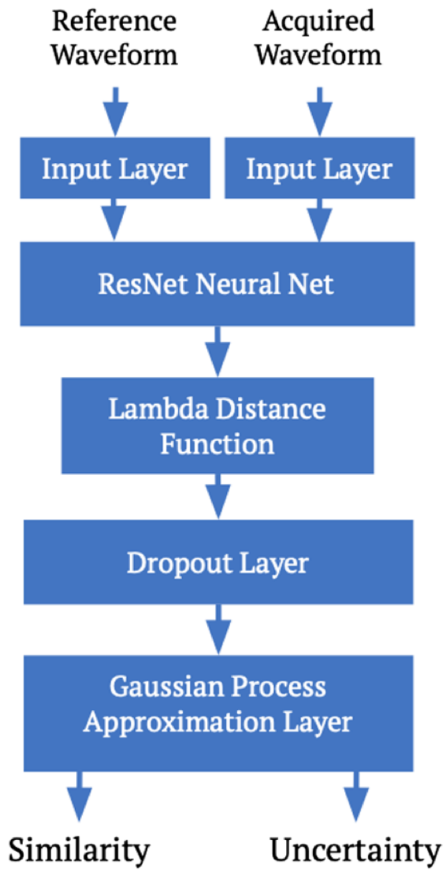
Uncertainty Aware Siamese Model and Results

- We use Siamese Model to predict similarities with normal reference waveforms
- Attached GP approximation layer at the end to provide UQ
- The ROC curves bands are produced by smearing the predictions with uncertainty
- To evaluate the OOD uncertainty robustness
  - Introduced a different anomaly type (not included in training)
  - The model predicts OOD anomaly reasonably well with higher uncertainty

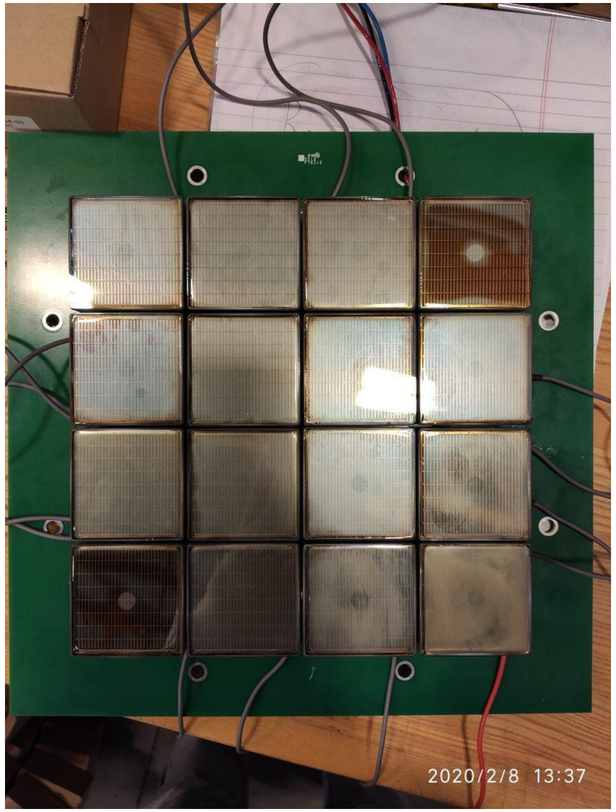
Maximize TPR at FPR < 0.5%







Uncertainty Aware PID for SoLID



Cherenkov Readout:

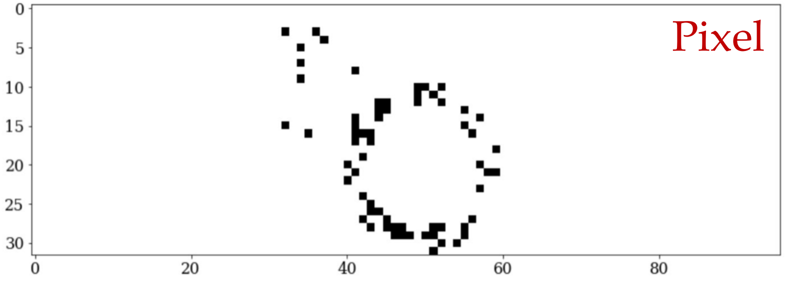
each 5cmx5cm MAPMT can have

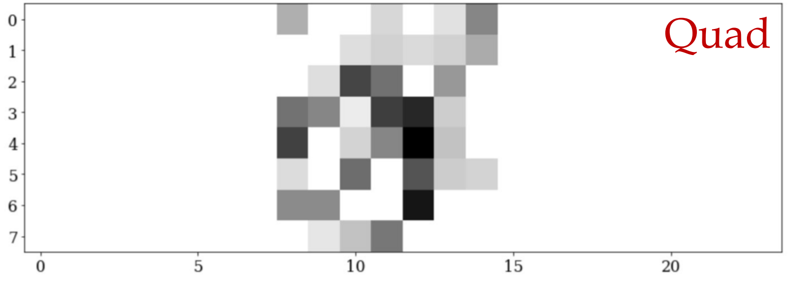
- 1 pmt sum output with Number of photoelectrons (Npe)
- 4 2.5cm x 2.5cm quad sum output with Npe
- 64 6mm x 6mm pixels with 0/1
- Cost increase with more readout channels and increasing resolution

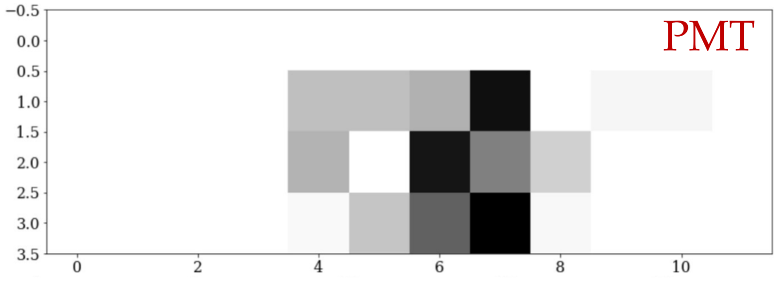
Goal: Use ML to understand what level of readout is needed to achieve desired performance

Dataset:

- Readout hits on the sensors from PMT having the lowest to Pixel readout having the highest resolution

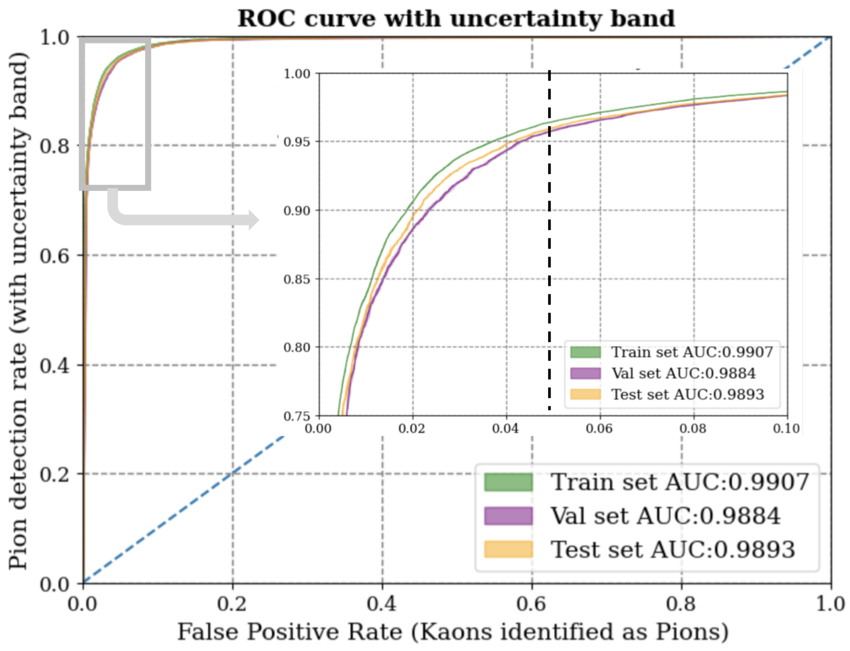






Uncertainty Aware PID for SoLID

- Pion vs Kaon
- The PID data is converted to images
- The deep learning model is designed using conv2D layers to learn the patterns
- GP approximation layer to provide UQ
- Simulation data is used with higher background noise to mimic the realistic scenario

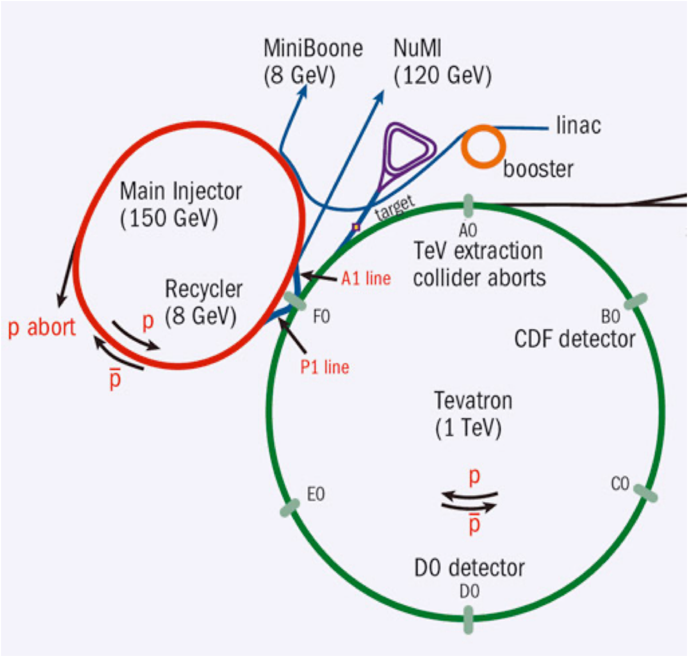


- DNN based PID model has shown much better performance than traditional cuts
- *Next Step: Evaluate the UQ robustness by introducing third/ noise particle*

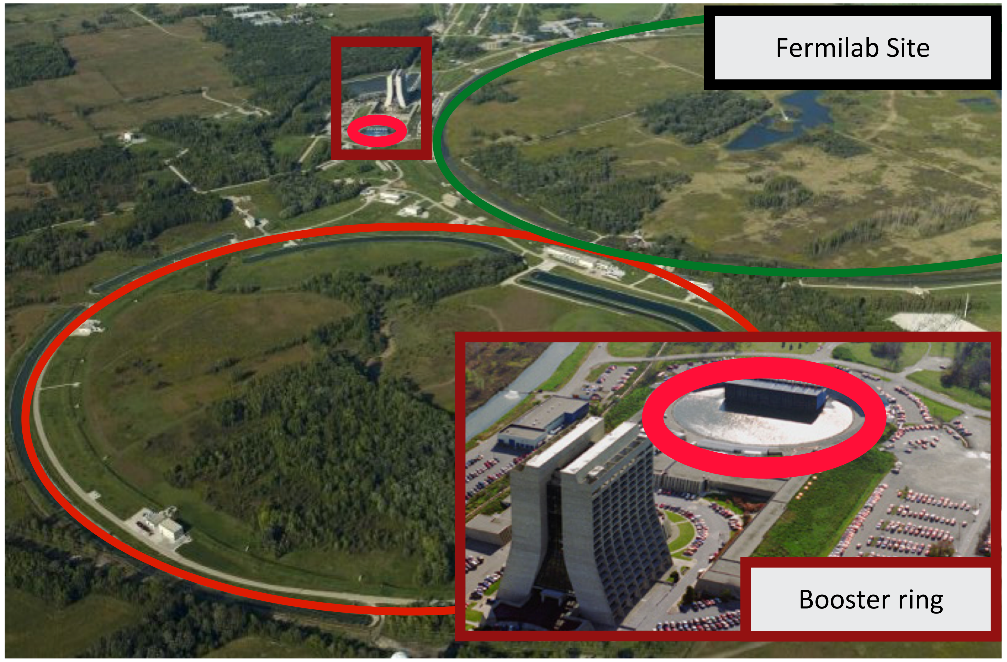
True prediction rate at False Positive rate of 5%

Section	PMT	Quad	Pixel	Npe cut
P 2.5 GeV theta 8.0 degree (most difficult for pion acceptance)	0.978	0.991	0.994	0.5
P 7.5 GeV theta 14.0 degree (most difficult for kaon rejection)	0.991	0.995	0.997	0.6

Uncertainty Aware Surrogate Model for FNAL Booster



Courtesy: Christian Herwig



The Booster accelerates 400 MeV beam to 8GeV with the help of booster cavities and Combined-function bending and focusing electromagnets known as gradient magnets.

These magnets are powered by the gradient magnet power supply (GMPS)

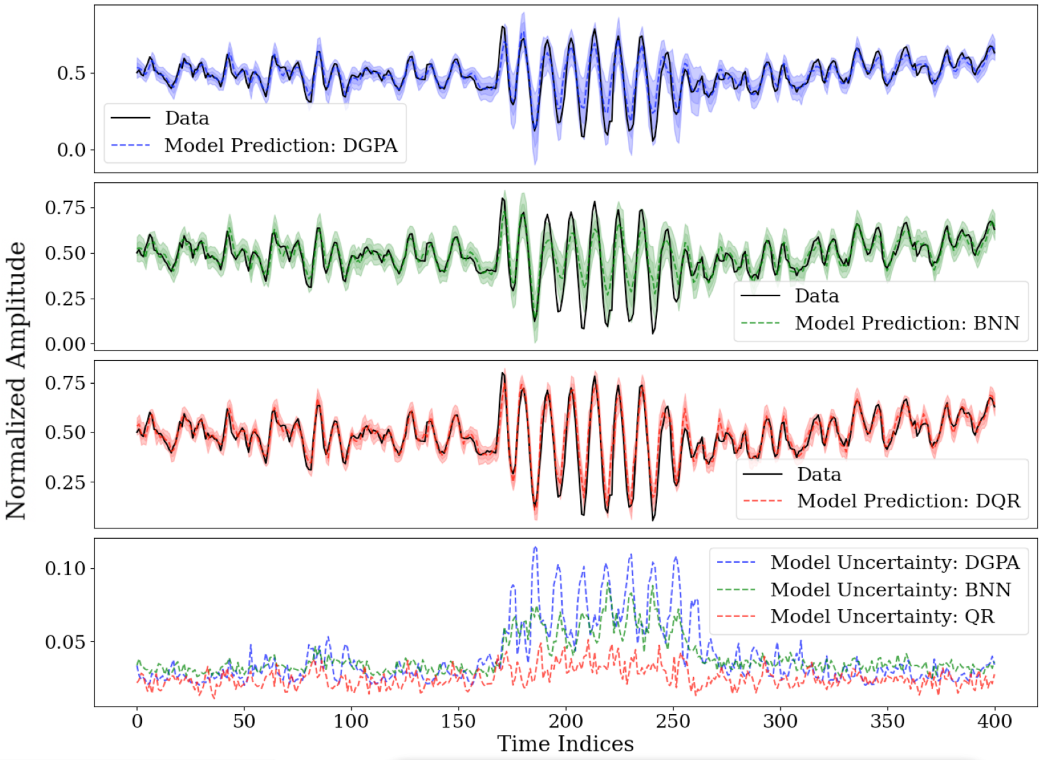
Fluctuations in GMPS electrical current due to neighboring electrical loads and thus fluctuations of the magnetic field in the Booster gradient magnets

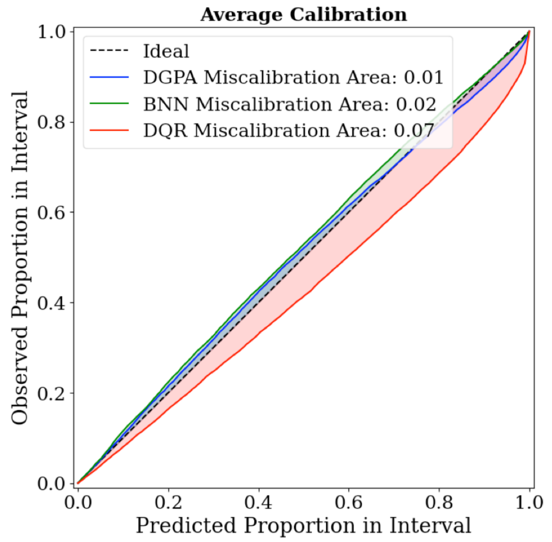
A GMPS regulator is required to stabilize the accelerating magnetic field

Problem definition:
Develop a surrogate model of the GMPS that can be leveraged to train a modern control system such as reinforcement learning agent to stabilize the GMPS power supply

Uncertainty Aware Surrogate Model for FNAL Booster

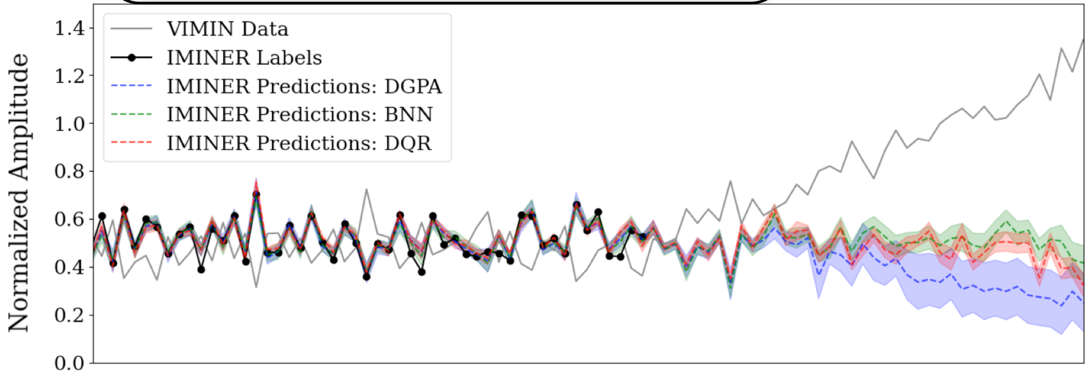
- Surrogate model is developed using ResNet Conv1D blocks followed by fully connected layers
  - **UQ is important to know which areas are not well modeled by the surrogate model**
- We evaluated three different methods of UQ for DNN regression
  - DQR provide robust UQ in-distribution but not on OOD
  - BNN method does a better job at estimating OOD uncertainty
  - GP approximation model provide the best OOD estimation and is calibrated by design





In distribution data

The high frequency with higher fluctuation in amplitude are removed from training to make it OOD



One of the input variable is monotonically increased manually to make it go OOD

https://arxiv.org/pdf/2109.10254.pdf

Conclusion

- GP provides robust uncertainty quantifications for both in-distribution and OOD samples
- Presented application of GP to autonomously calibrate CDC in GlueX detector
- With larger datasets and higher dimension, GP does not scale; approximation required
- DNN can handle large multi-model datasets with ease
- GP can be attached to DNN models to provide UQ
- Distance between input samples need to be preserved through hidden layers
- Presented uncertainty aware anomaly prediction for SNS accelerator with GP approximation
- Presented comparison of PID in SoLID with different readout resolutions
- Presented uncertainty aware surrogate model for FNAL booster

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