Machine Learning for Improving Accelerator and Target Performance

Uncertainty Aware Anomaly Detection to Predict Errant Beam Pulses and GradCAM Analysis

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On behalf of Errant Beam Prediction Task Force (Jefferson Lab and ORNL)

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

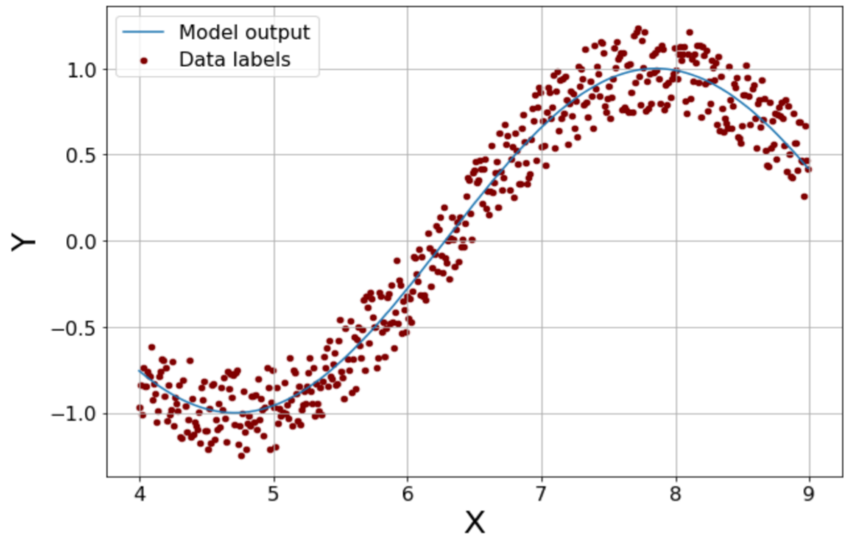
JLab is managed by Jefferson Sc. Assoc., LLC for the US Department of Energy

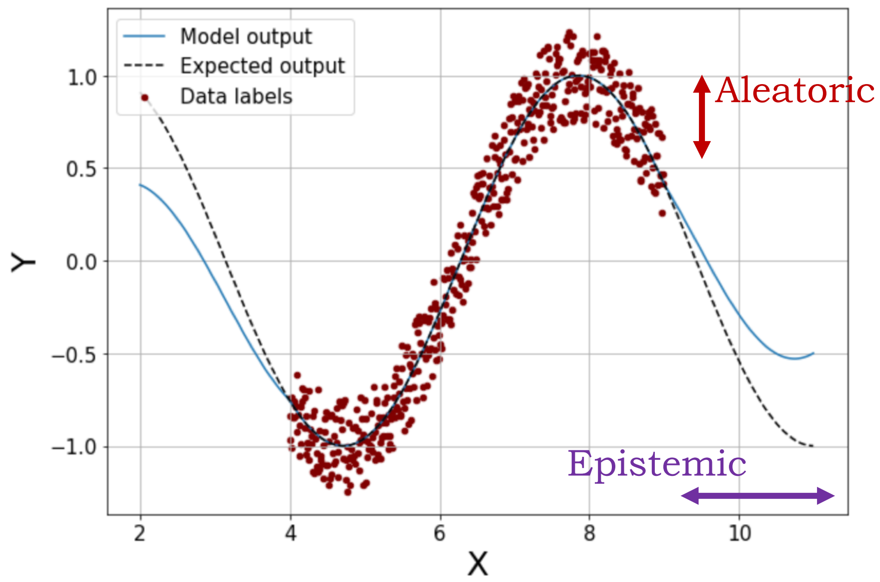
Outline

- Uncertainty Quantification in Deep Learning
- Errant Beam Prediction at SNS Accelerator
  - Introduction
  - Data Processing
  - Siamese Model
  - Uncertainty Aware Siamese Classifier
  - Equipment Fault Classification
  - Online Deployment
  - Future Roadmap
- Uncertainty Aware Booster Surrogate for FNAL
  - Uncertainty Aware Deep Regression with single inference

Uncertainty Quantification

- Deep Learning (DL) models are deterministic transformation functions from an input to the output
- DL models are very powerful and expressive
- It is important to know the confidence associated with each prediction from a DL models for decision making

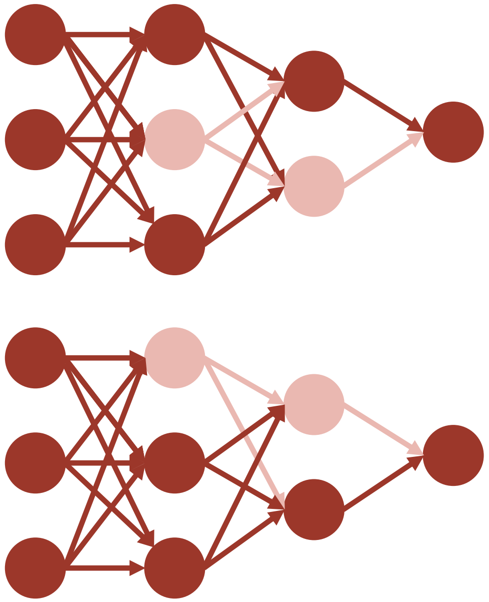




Uncertainty Types: Aleatoric vs Epistemic uncertainties

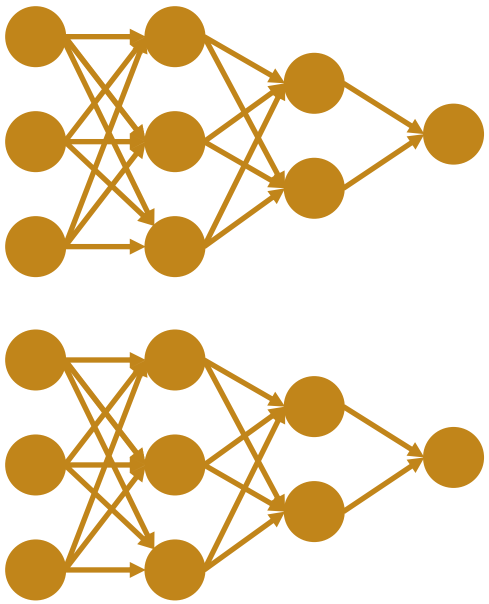
- Aleatoric → Data uncertainties
- Epistemic → Out of training distribution uncertainty (OOD)

Popular methods for UQ in DL



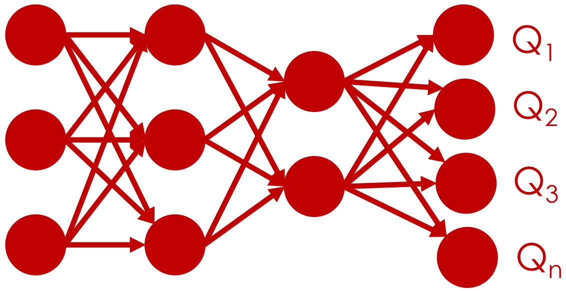
(a) MC Dropout

Use dropout during inference to create variability in the prediction which can be used to estimate the uncertainty. Requires offline calibration



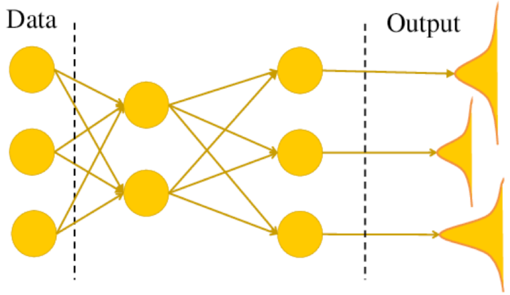
(b) Ensemble

Create multiple copies of the same model architecture trained with different parameters initialization. Requires calibration after training



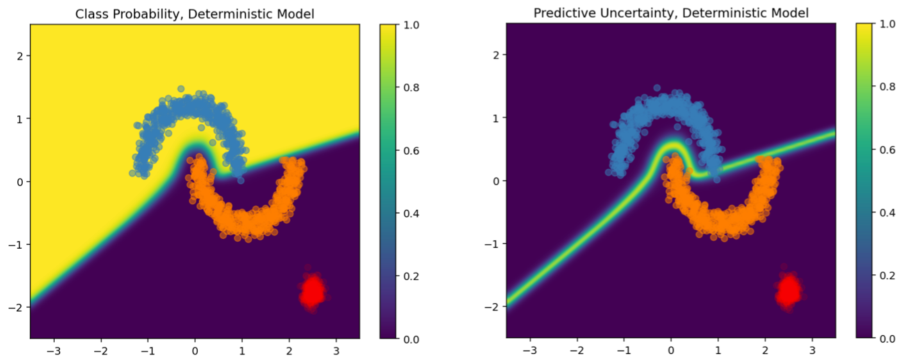
(c) Quantile Regression

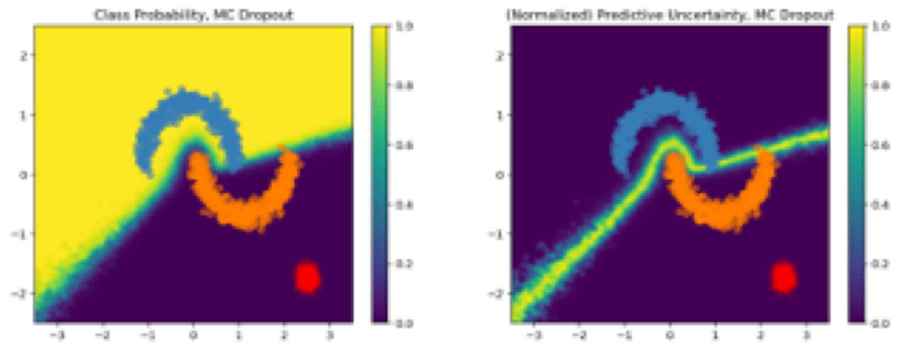
Model is trained to predict quantiles for the regression problem

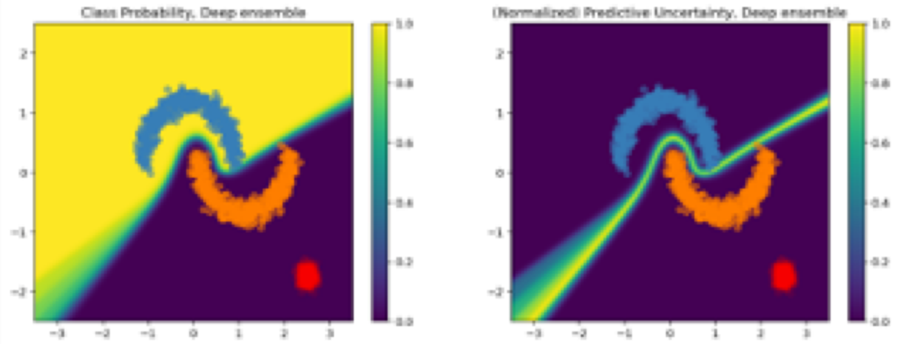


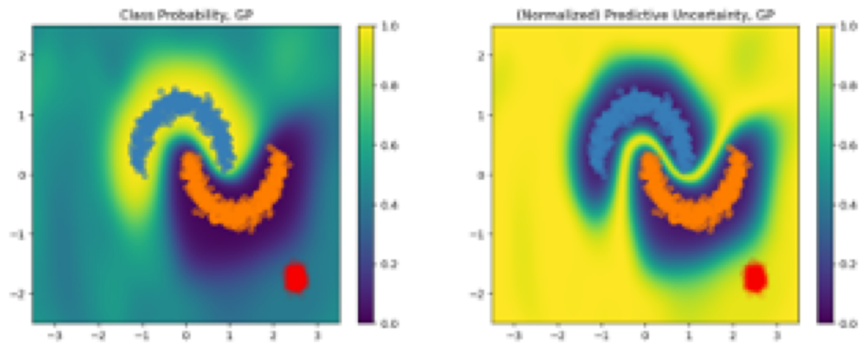
Popular methods for UQ in DL

- Unfortunately, majority UQ methods for DL do not account for OOD uncertainty
- This is critical in optimization or control problems
- For example, different methods yield vastly different uncertainty estimation
  - Deterministic (Prediction value)
  - MC Dropout
  - Deep Ensemble
  - Gaussian Processes (GP)





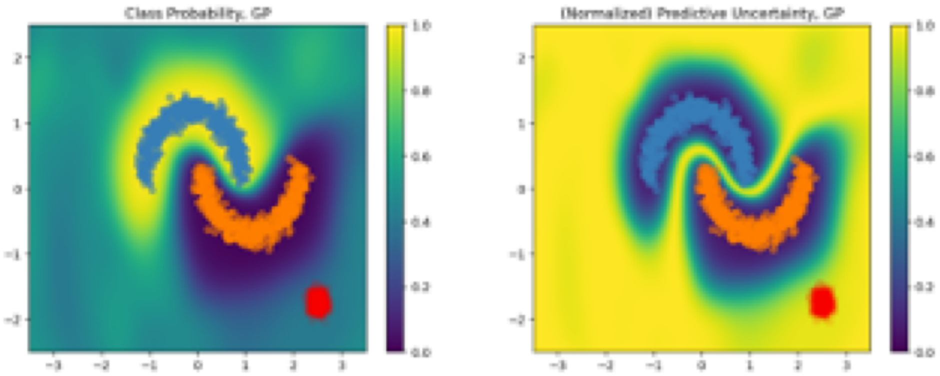


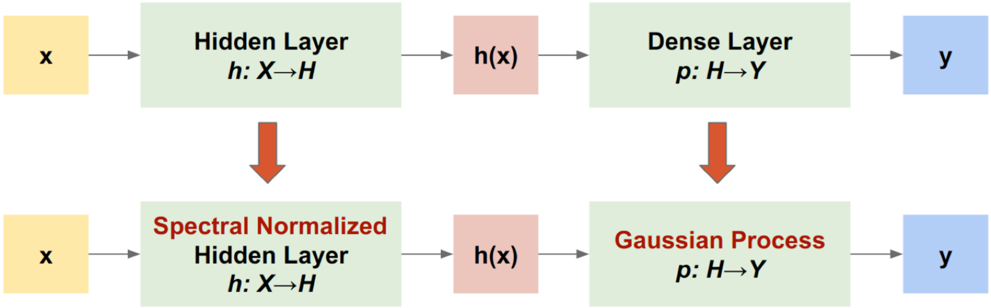


https://arxiv.org/abs/2006.10108

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 measure between different input samples
- This allows GP to intrinsically provide uncertainty estimates including OOD
- GP is limited in terms of Scaling and data reduction techniques are usually required for large data sets
- Recent study presented a way to introduce Gaussian Process approximation within a neural network
- This allows to use highly expressive deep networks and provide uncertainty estimation





Spectral Neural Gaussian Process*

https://arxiv.org/abs/2006.10108

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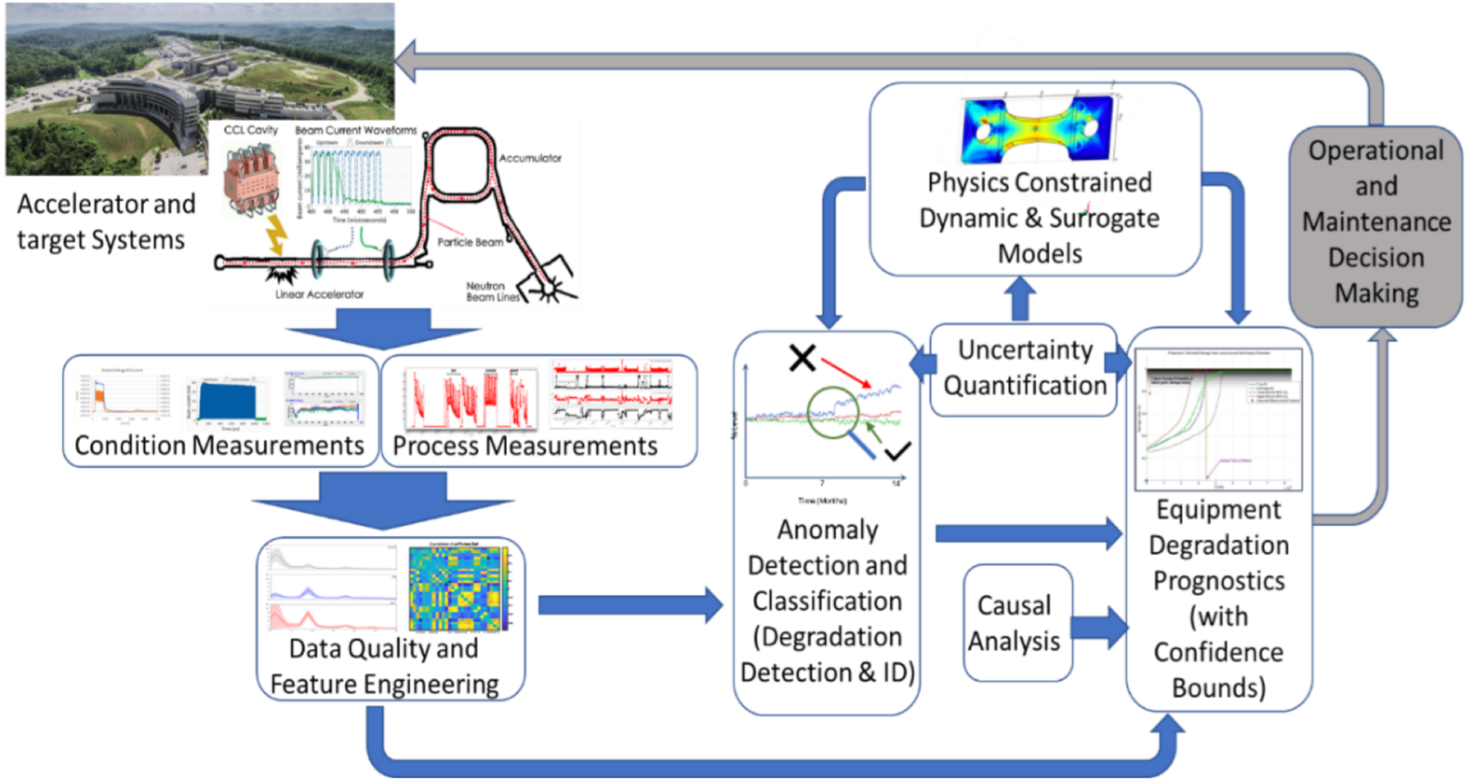
Errant Beam Prediction for SNS Accelerator

- Spallation Neutron Source (SNS) accelerator at ORNL delivers 1.4 MW of a 1 GeV pulsed beam at 60 Hz
- Ongoing work to **predict errant beam pulses** as well as equipment degradation and prognostics
- Continuous data collection is done by **Differential Current Monitor (DCM)**, Beam Position Monitor (BPM) etc.
- Errant beam prediction on one pulse before it occurs to potentially avoid it



Errant Beam Prediction for SNS Accelerator

- **Goal**: Predict an upcoming machine trip before it occurs to potentially allow the crew to change settings to avoid it
- **How:** We use pulses leading to a trip (tagged "Before") and identify features that indicate an upcoming failure
- **Data science pipeline used**:

Data Source → Data Preparation → ML Approach → Training Tools → Results

Data Source:
- Real or synthetic
- Quality
- Dimensionality
- Format
- Density
- Size

Data Preparation:
- Data cleaning
- Data restructuring
- Correlations
- Dynamics
- Visualization

ML Approach:
- Classification
- Regression
- Clustering
- Feature extraction

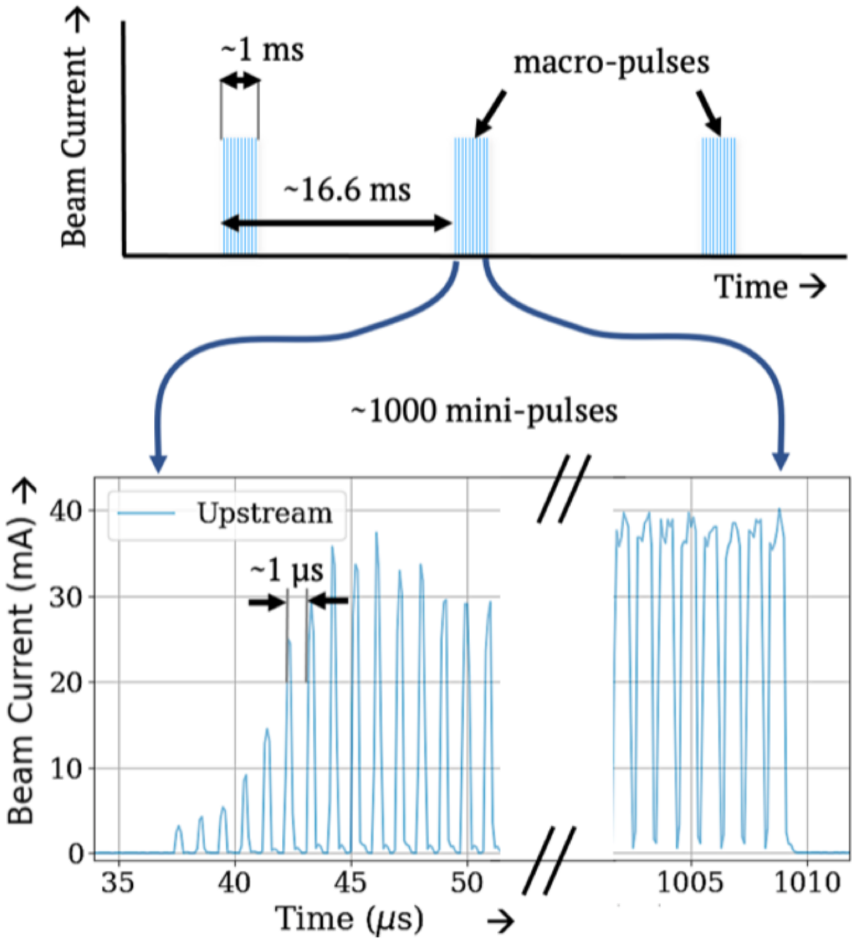
Training Tools:
- Cross-validation
- HPO

Results:
- Predictions
- Confidence Level
- Explainability

Data Collection and Preparation

How was the data collected and labeled?

- DCM creates a series of pulses ("macro-pulses") with each macro-pulse composed of ~1k mini-pulses
  - An errant-beam data file is composed of 25 "good" macro-pulses followed by the errant beam pulse
  - A "normal" data file has no errant beam pulse
- We used the macro-pulse before the errant beam pulse (and labeled it as anomaly) and macro-pulses from the normal file (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
- Samples were divided into 3 orthogonal dataset:
  - Train (64%)/Test(20%)/Validation(16%)



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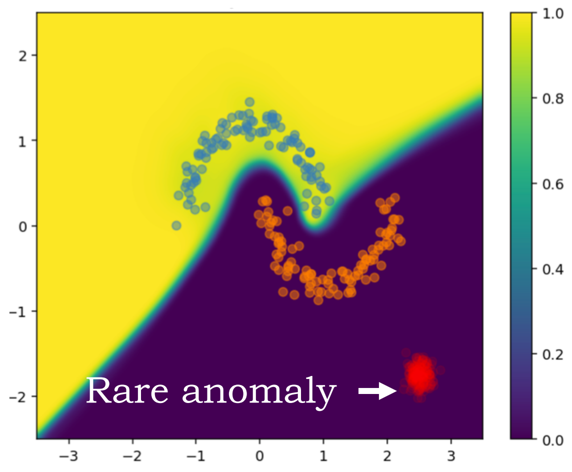
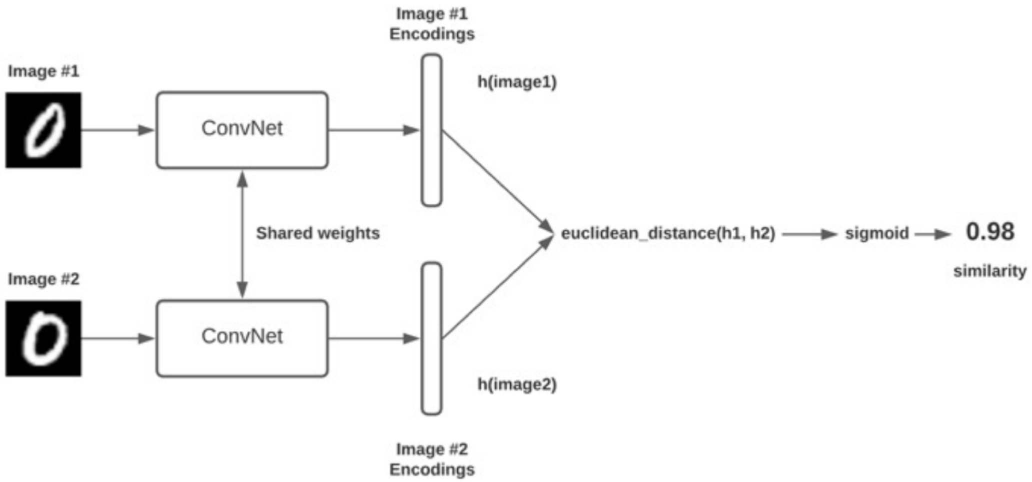
Siamese Neural Network (SNN) Model

Traditional classification models vs Siamese model

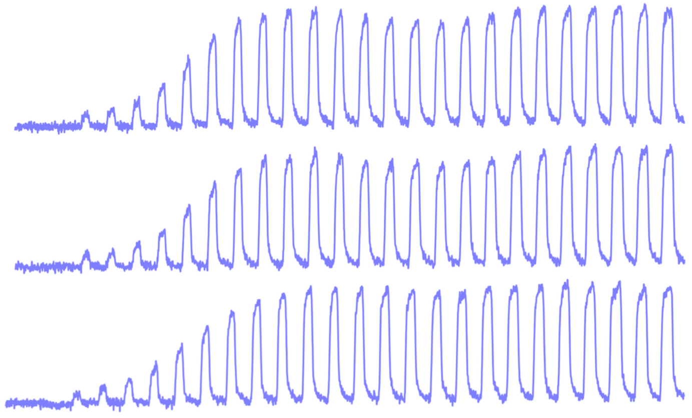


- Traditional DL classification models fails to identify unseen anomalies (OOD)
- Similarity based models can correctly classify unseen anomalies. Ex Siamese model
- Siamese model does not explicitly model the classification but focuses on the similarities
- It learns twin embedding models to transform inputs into a latent space
- Distance measures are applied at latent space to compute the similarity

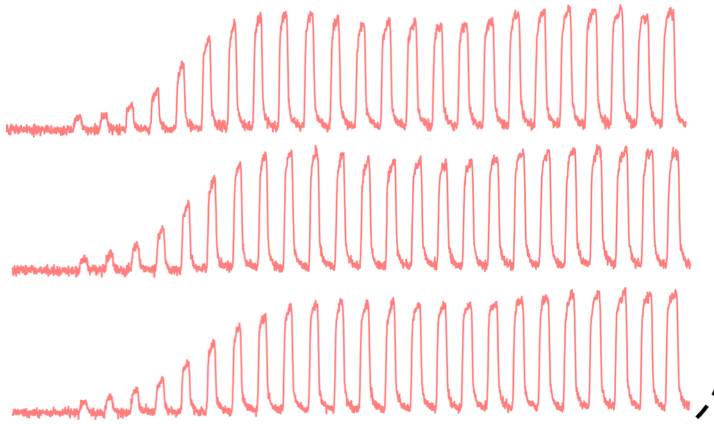


Data Preparation for SNN Model Training

Reference Normal Pulses

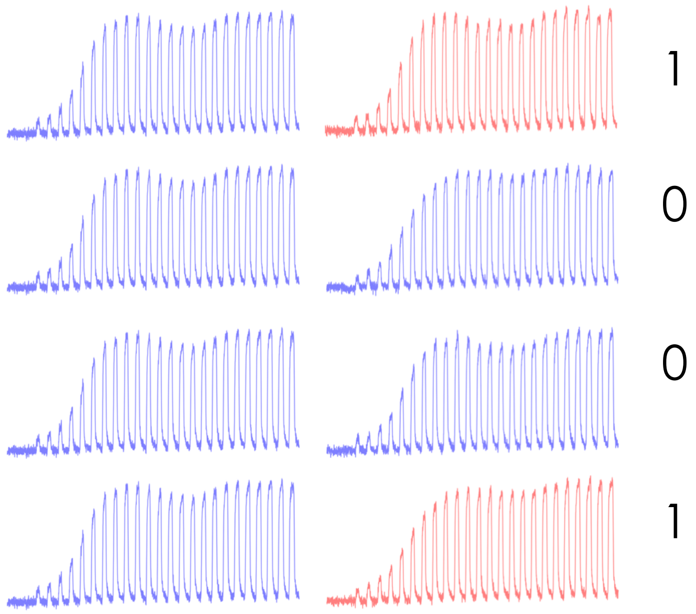


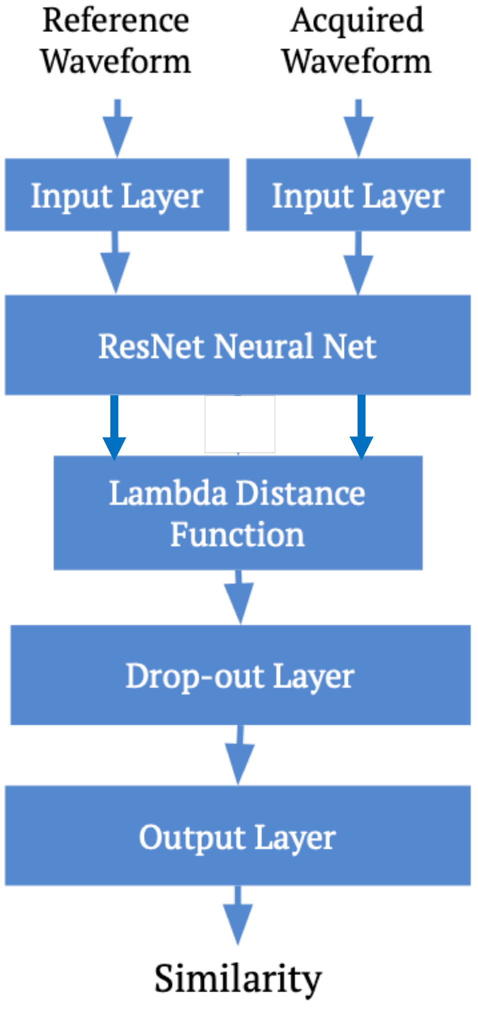
Pulses before Anomalies



Data for the SNN Model

Different Combinations of Normal to Normal (labeled 0) and Normal to "Before" pulses (labeled 1)

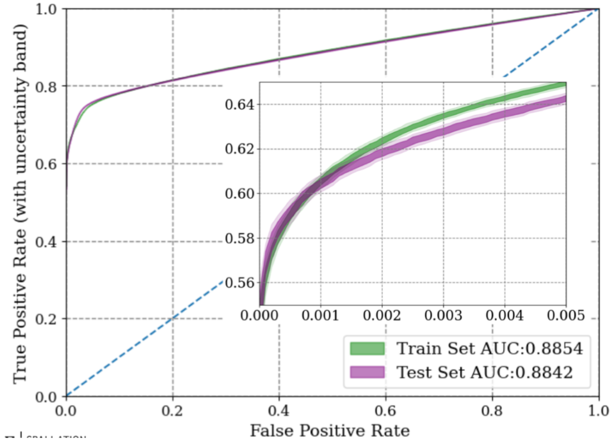


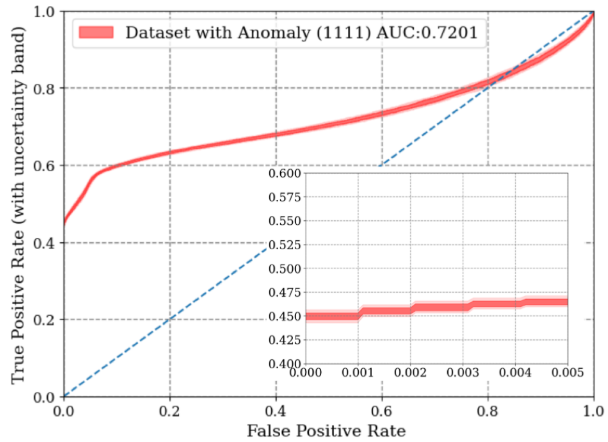


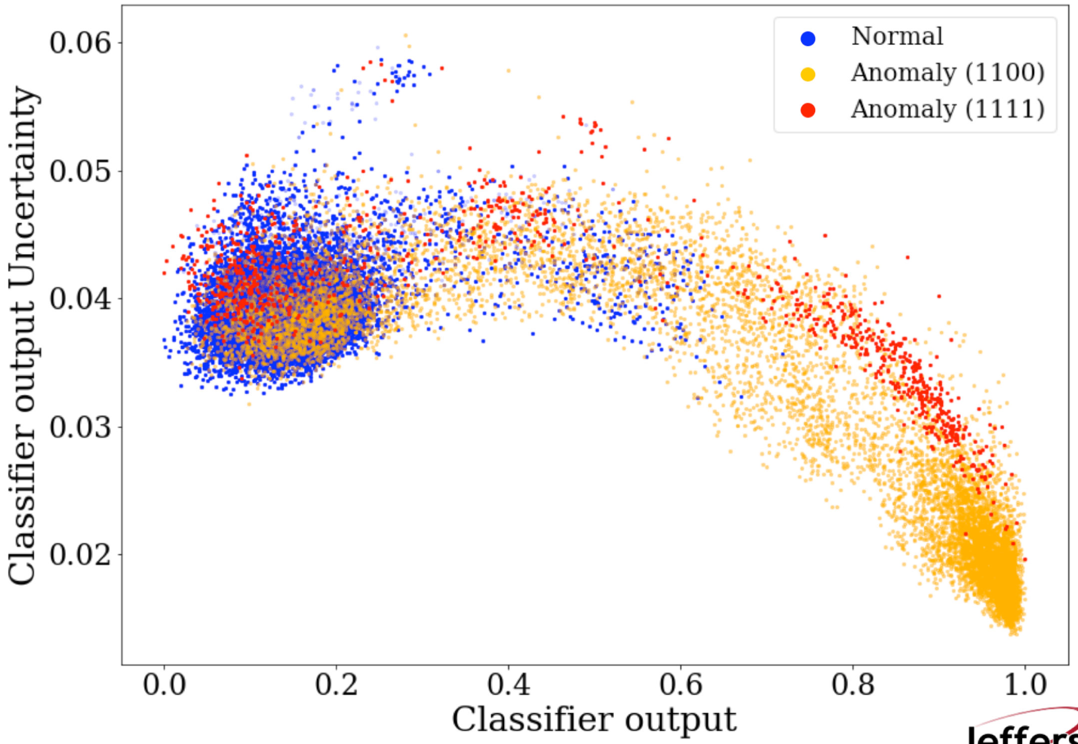
Uncertainty aware Siamese model

- We enhanced our Siamese model by adding GP layer providing an uncertainty estimate
- Results from similarity model showed a ~4x improvement in performance over previously published results, it is also much better than a vanilla Auto-encoder
- The ROC curves shows true fault detection rate above 60% while keeping the false alarms below 0.5% (not optimized)
- We introduced an out-of-domain anomaly, labelled 1111 (red), the UQ-based model performed similar in classifying the anomalies and indicated high uncertainty (as expected)

After a fault is predicted, is it possible to associate with a particular equipment failure?

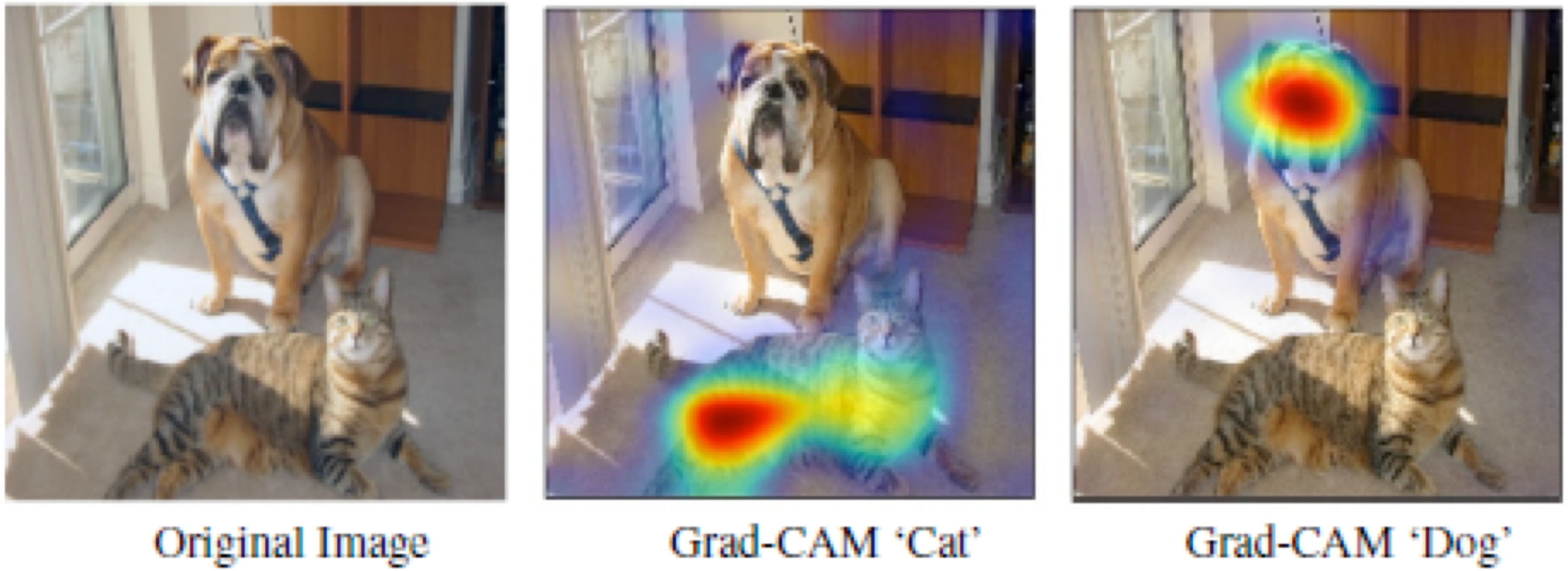






Gradient Class Activation Mapping (GradCAM)

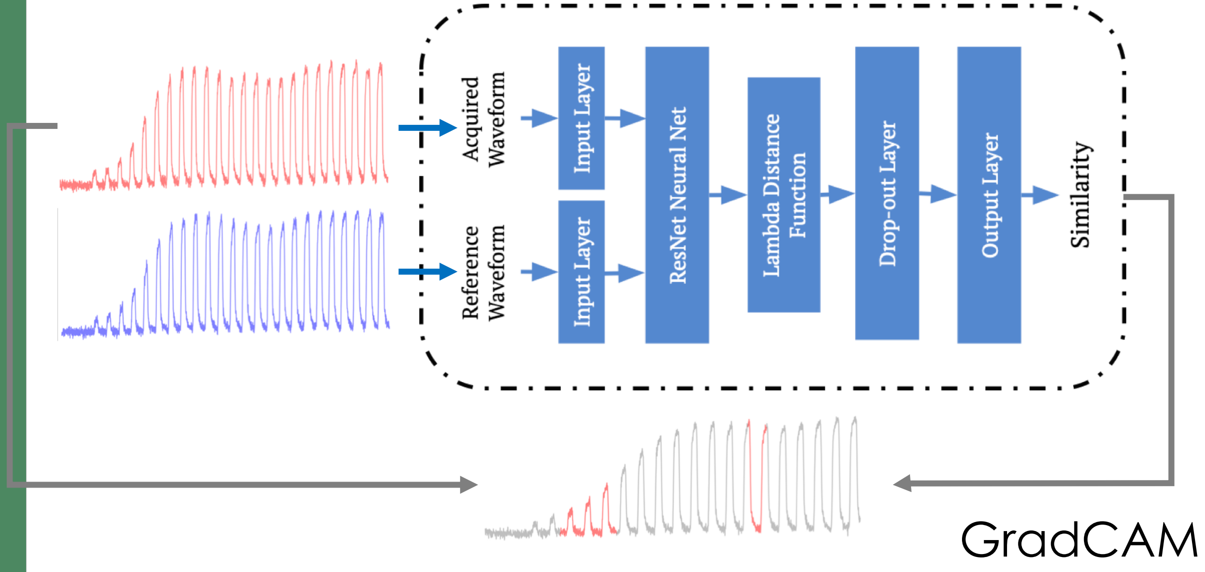
- GradCAM provides mapping between the the model output to the features in the input that the model thinks are the most relevant
- Extracts the most active features in the last convolutional layer and maps them back to the input



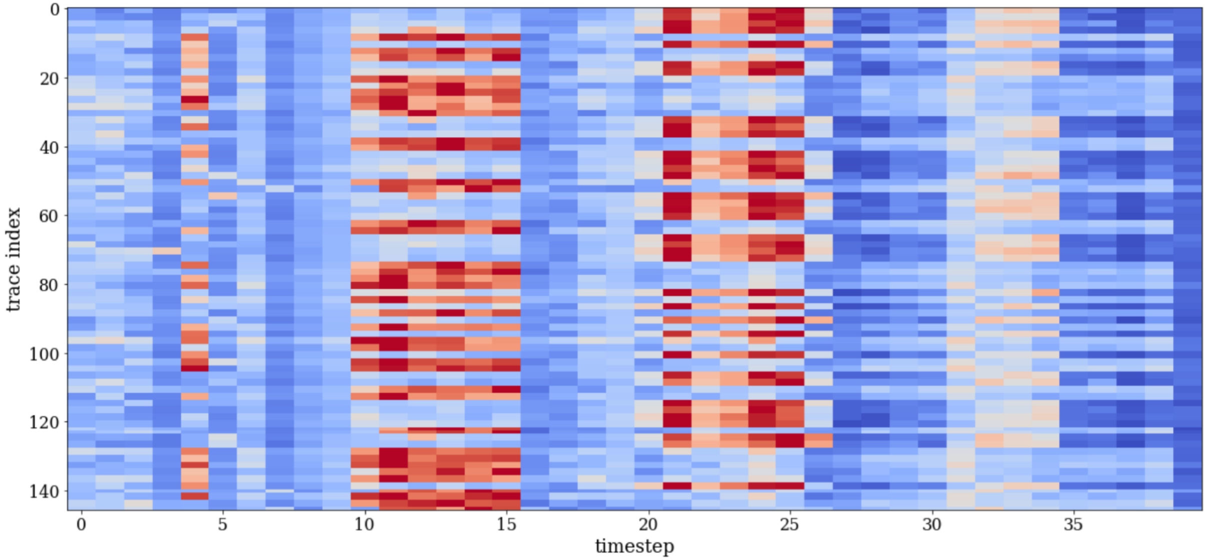
https://arxiv.org/abs/1610.02391

Equipment Fault Classification using GradCAM

- Applied GradCAM on SNN model trained to predict Errant Beam Pulses
- It identified sections of the waveform most relevant for a particular decision from the model

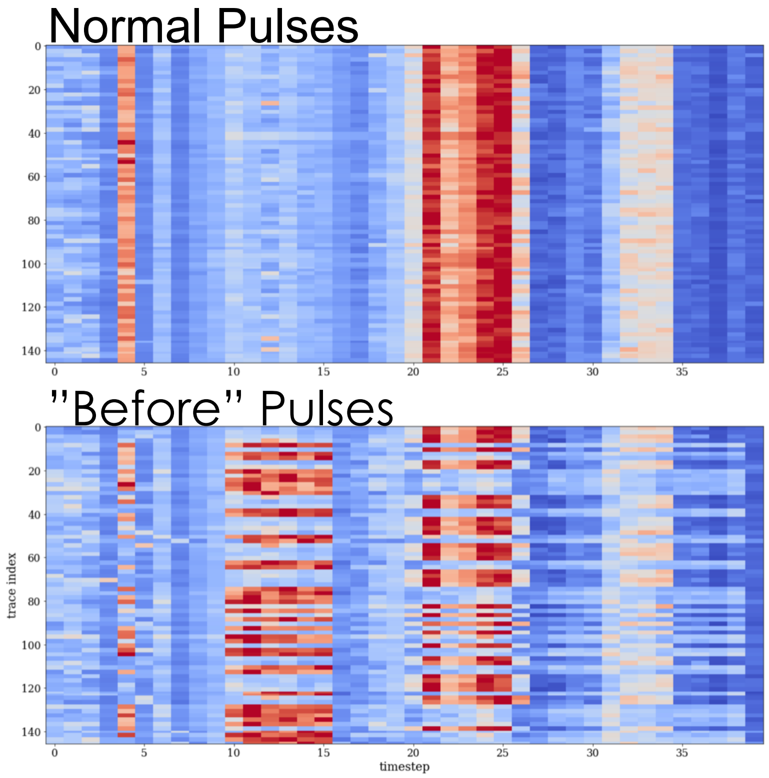


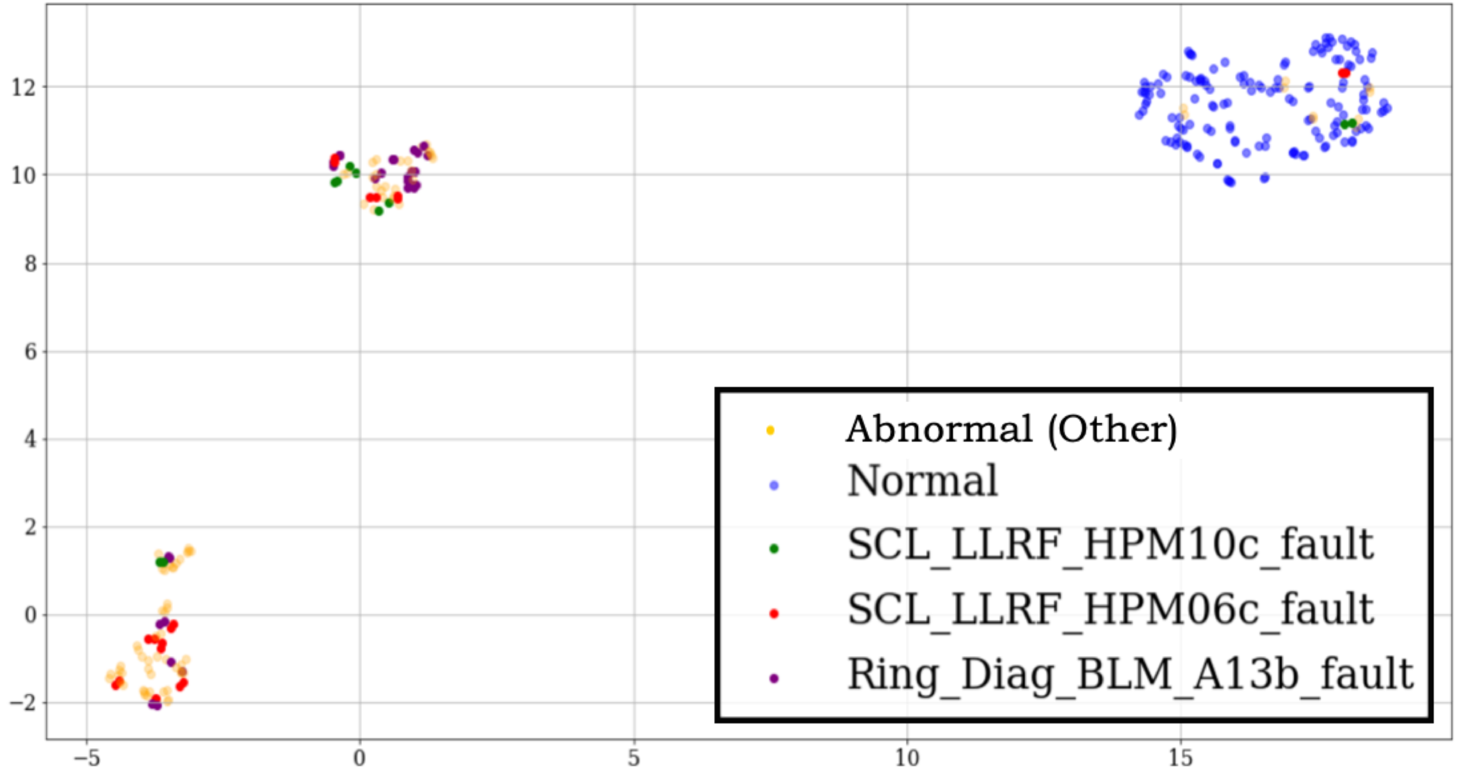
Stacked Relevance Vectors (“Before” Pulses)



Equipment Fault Classification using GradCAM

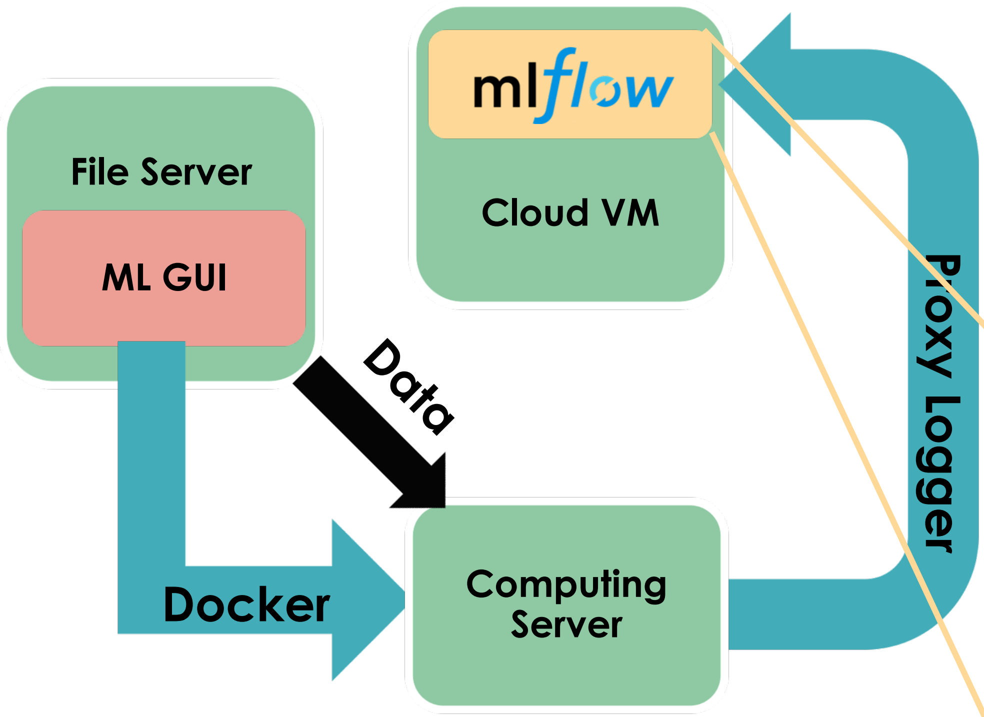
- The salient feature vectors are reduced to 2-dimensional space using UMAP*
- Studying how the cluster location from anomalies relate to specific equipment failures





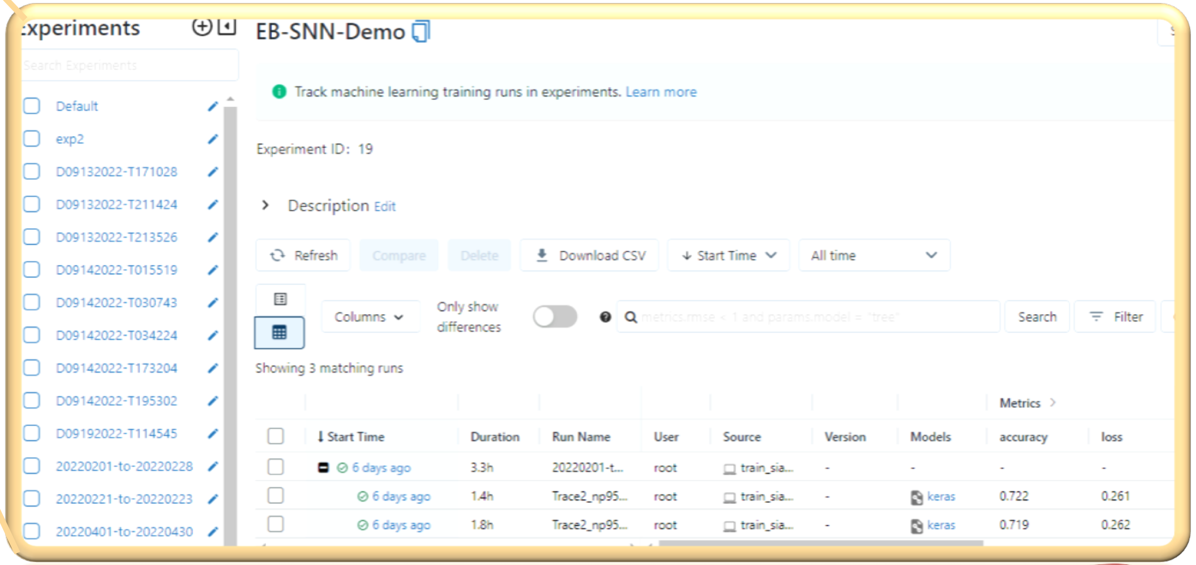
* https://arxiv.org/abs/1802.03426

Sustainable ML for SNS with MLflow



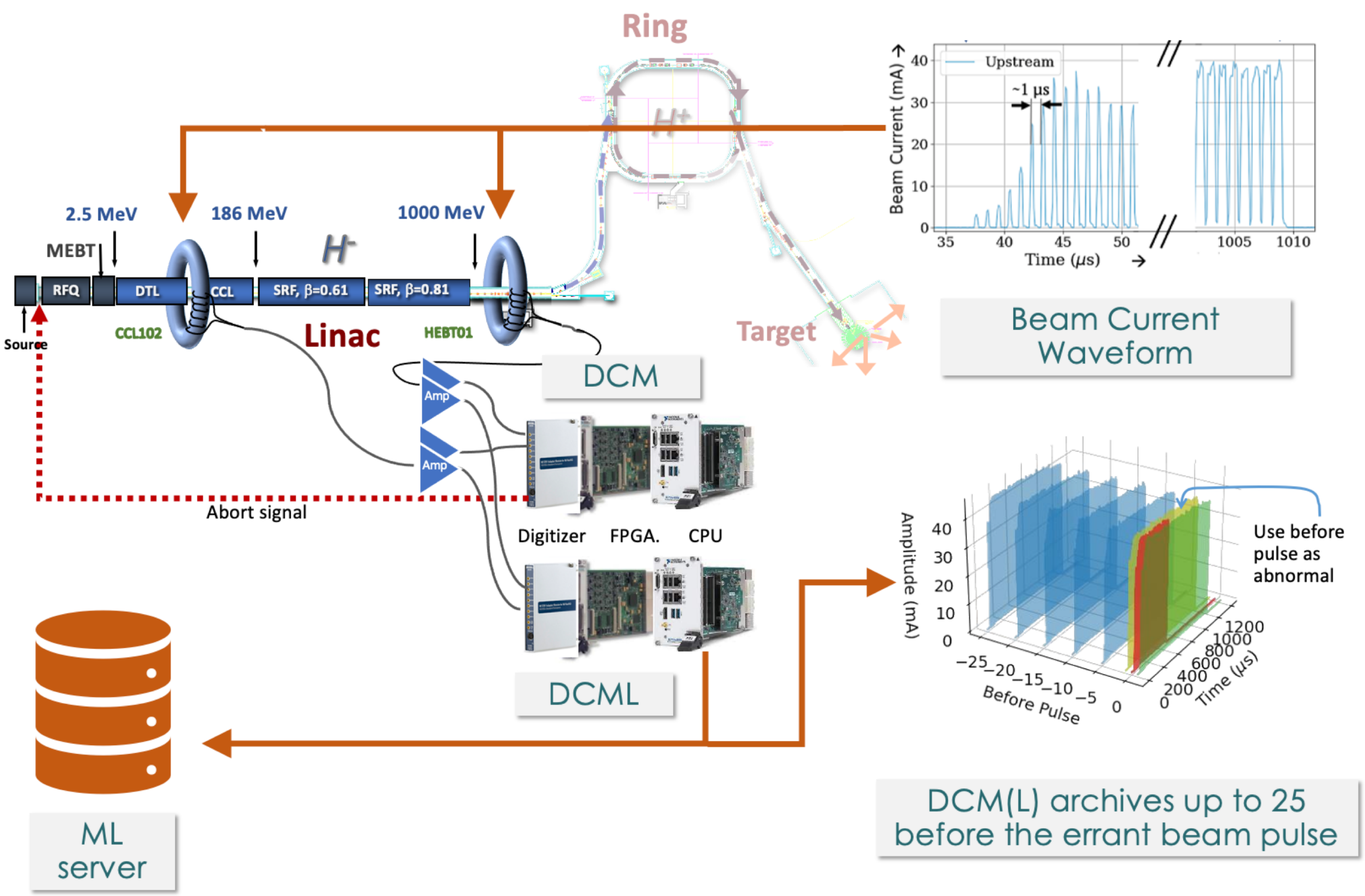
- Streamlined data processing
- Easy model generation and training for non-ML experts with an application
- Dockerized parallel training on GPUs (efficient training)
- MLflow hosted on Cloud VM for organized and multi-user model tracking
- Scalable with more models, use cases, projects

MLflow's browser-based interface



Online system

- Upcoming pulse type decision (good or bad) must be made between pulses (≈15 milliseconds)
- Random Forest on LabVIEW FPGA
  - Developed by ORNL collaborators
- Siamese twin on LabVIEW RT DCML and Unix ML Server
- DCML feeds data for machine learning training and inference while the original DCM still protects the machine



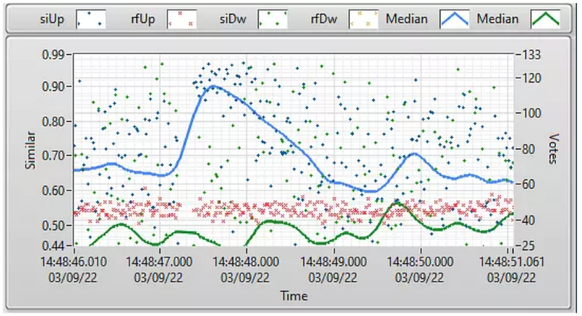
Online results

DCML:

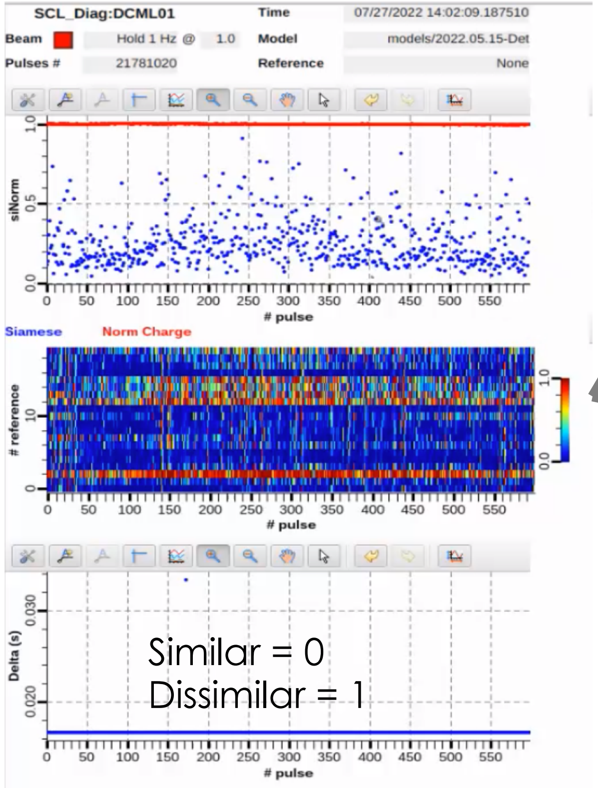
- Can run up to 4 deterministic SNN inferences

ML Server:

- Can run 20 deterministic inferences per pulse at 60 Hz to compare incoming waveform with multiple references (can be normal or abnormal)
- Create average similarity to improve results
- Presents results over EPICS

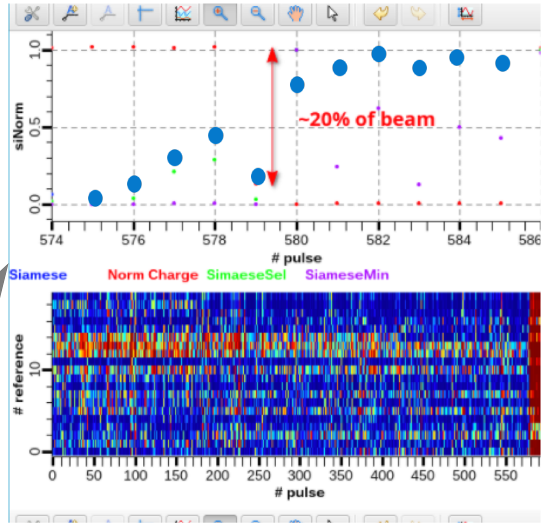


DCML live results (Siamese/RF upstream/downstream)

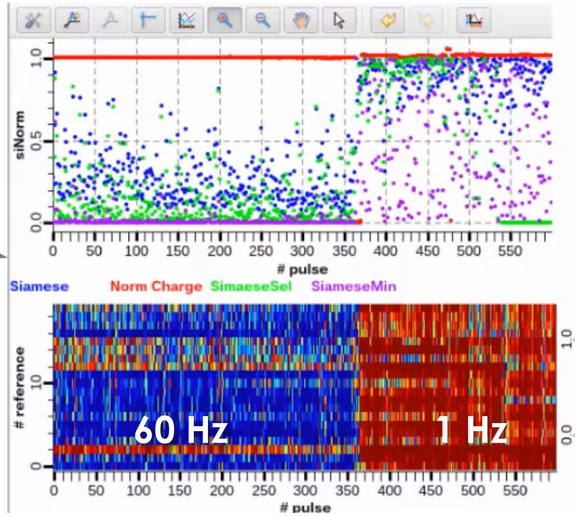


ML Server Results Control Room Screen

examples



Chopper partial failure is seen as abnormal beam



1 Hz beam (instead of 60 Hz) is seen as abnormal

Path Forward

- Currently deployed deterministic SNN model will be replaced by Uncertainty Aware SNN
- Continue the study on equipment fault classification via GradCAM and SNN model
- Because SNN focuses on similarity, it is sensitive to changes in the beam configuration
- Ongoing work to add beam configuration to the SNN model as conditional inputs

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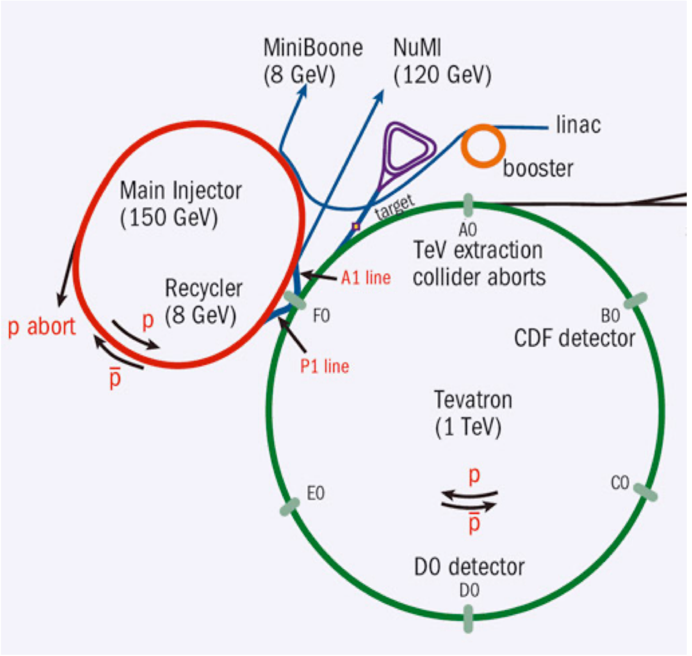
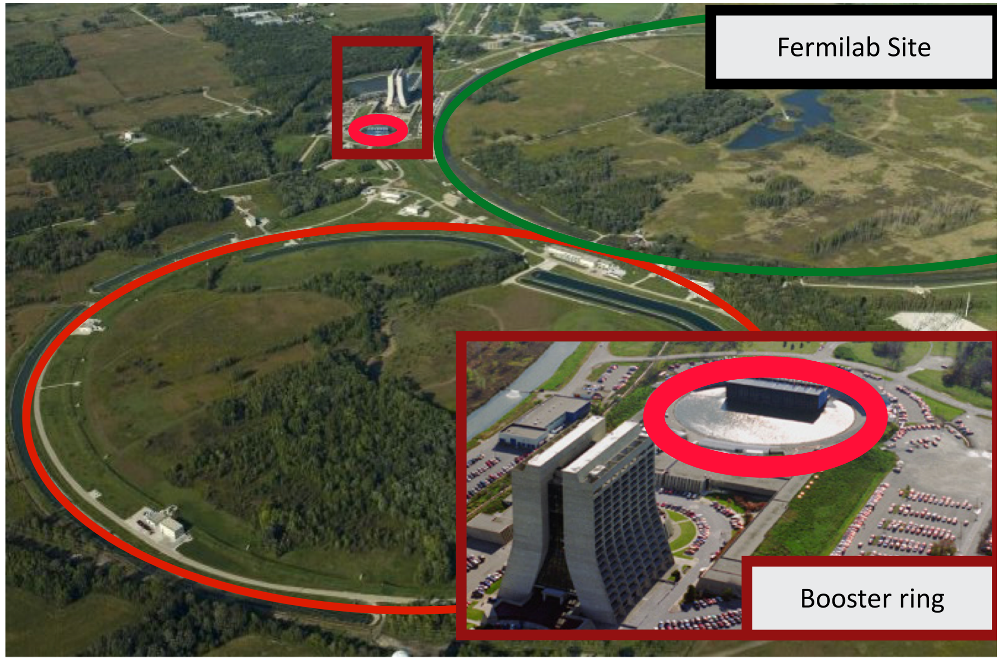
Uncertainty Aware Booster Surrogate

Aim:
Reduce beam losses in the FNAL Booster by developing a Machine Learning (ML) model that provides an optimal set of actions for GMPS regulator

FNAL Accelerator Complex:



Courtesy: Christian Herwig



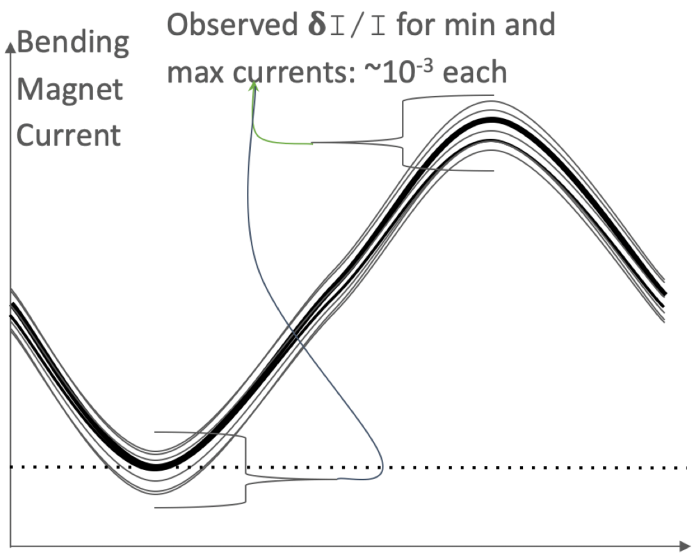
The Booster receives the 400 MeV (kinetic energy) beam from the Linac

It is then accelerated to 8GeV with the help of booster cavities and Combined-function bending and focusing electromagnets known as gradient magnets.

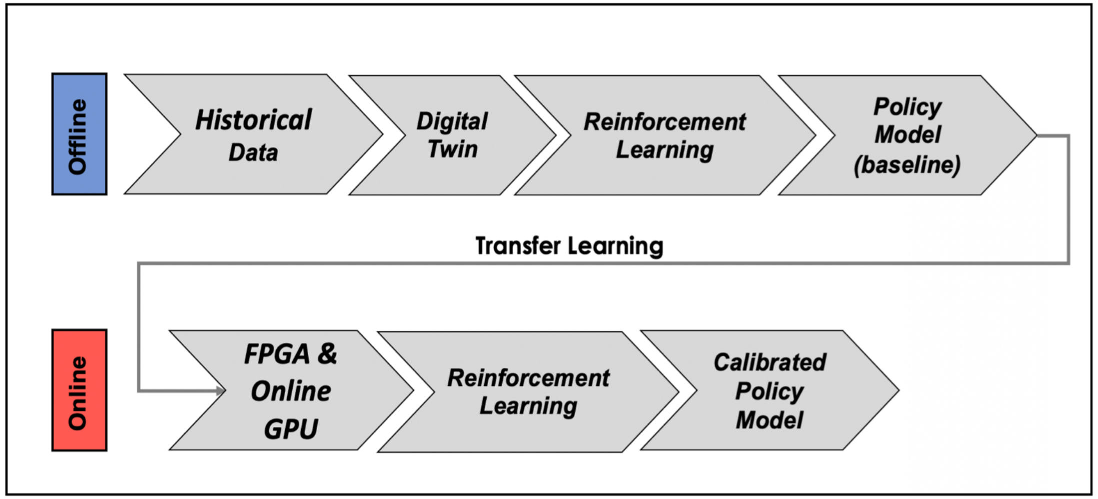
These magnets are powered by the gradient magnet power supply (GMPS)

Reinforcement Learning for Booster Control

- Other high-current, high-power electrical loads near GMPS varies in time
- Causing unwanted fluctuations of the actual GMPS electrical current and thus fluctuations of the magnetic field in the Booster gradient magnets
- This spread in B-field degrades the beam quality
- A GMPS regulator is required to calculate and apply small compensating offsets in the GMPS driving signal



- Use of RL to improve the existing PID based regulator
- Policy model is focused on controlling the regulator to reduce the error
- **This invokes a need of Surrogate model to build the RL environment**

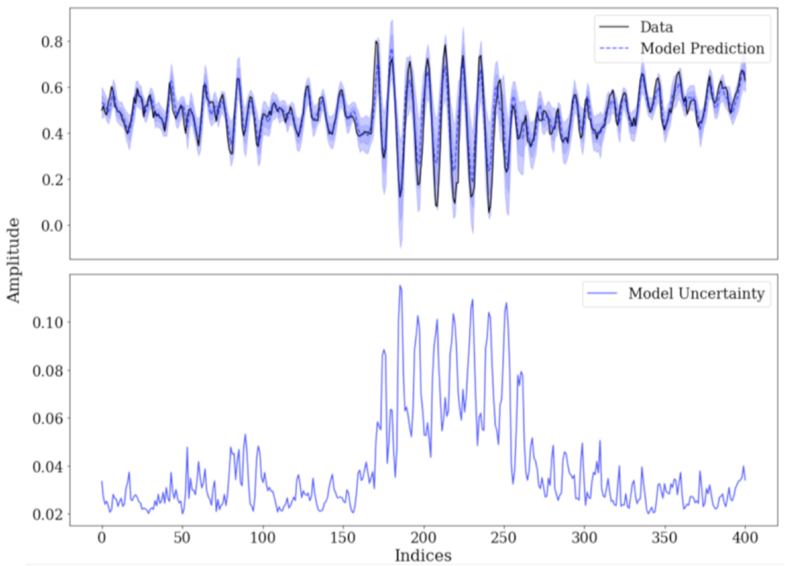


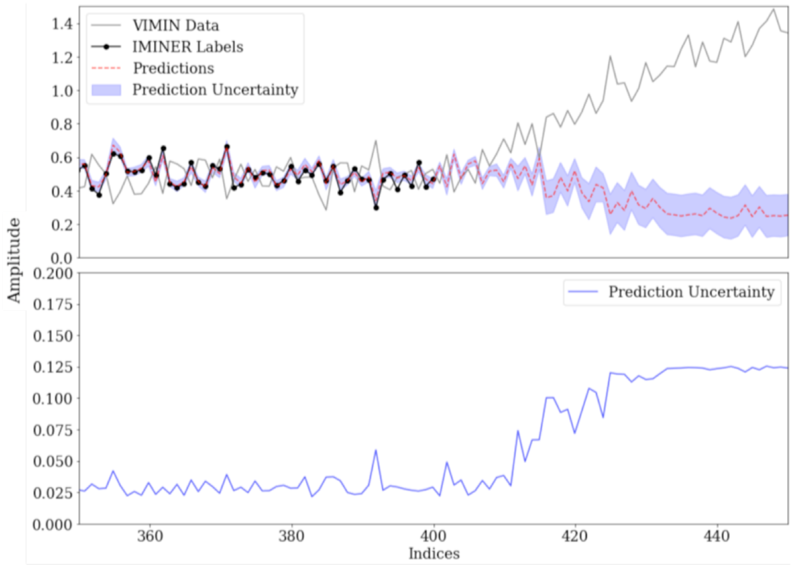
Uncertainty Aware DL Regression Model

Why uncertainty quantification is important in Digital Model?

- Uncertainty Quantification can help determine how well a region of a phase space is modeled by the surrogate

- Gaussian Process Approximation (DGPA) method to quantify the regression uncertainties for a DL model
- Unlike most other methods, DGPA does not require multiple inferences and does not require offline calibrations making it easy to deploy in online settings





Arxiv: https://arxiv.org/abs/2209.07458

Poster: NeurIPS Physical Science Workshop 2022

Paper: Under review at PRAB

Thank You!

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Developing Robust Digital Twins and Reinforcement Learning for Accelerator Control Systems at the Fermilab Booster
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