Uncertainty Aware Anomaly Prediction with Siamese Twin Models

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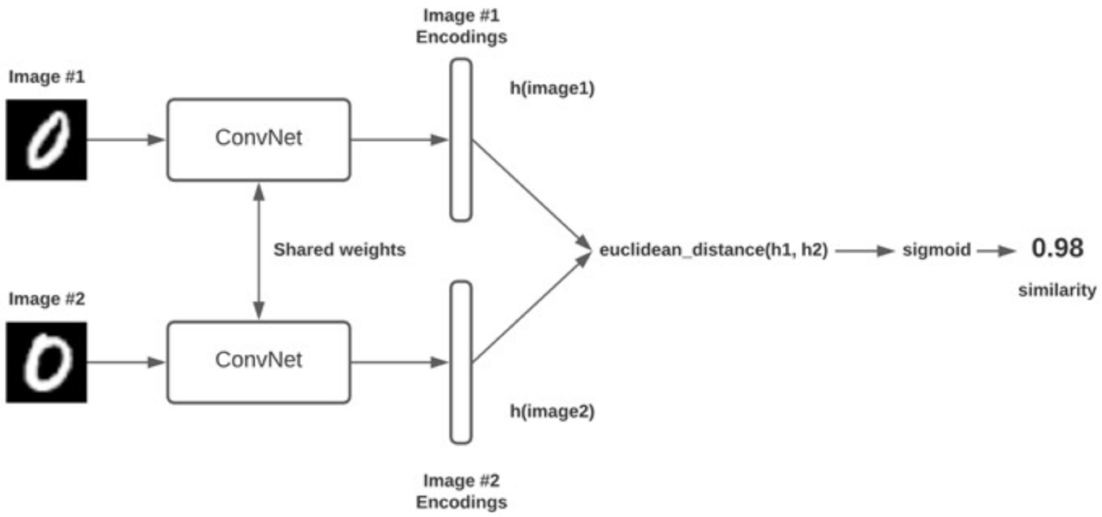
Outline

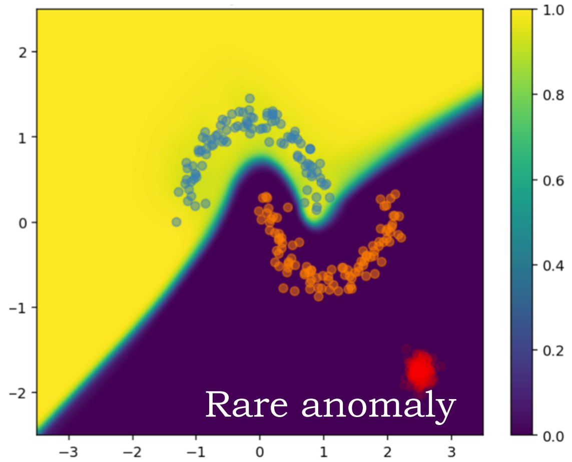
- Siamese Twin Models
- Siamese Twin for DQM
- Uncertainty Aware Siamese Models
- Errant Beam Prediction at Spallation Neutron Source Accelerator
  - Data Preparation
  - Model and Training
  - Results and Deployment in real time system
- Conclusion
- References

Siamese Twin Models

- Siamese Model consist of twin networks (shared weights and biases) that learn to transform inputs into a reduced representation (feature extraction)
- The reduced representation is compared with an appropriate distance function
- Further processing may require to provide final similarity score



- 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

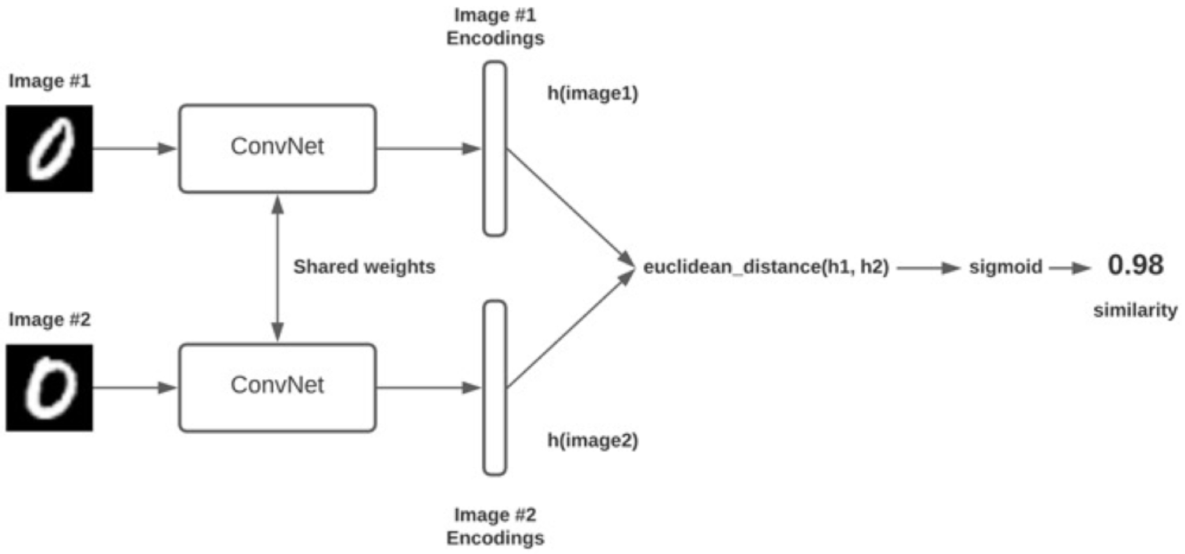


Siamese Twin Models for DQM

- Systems are designed to work -> A lot of normal operation data (good quality data)
- Profile of good quality data available
- In most cases, normal operation data is similar
- Siamese Models can be trained to produce similarity with normal operation data – Monitor new data
- References can be changed (or masked) on the fly upon change in the system – Adaptive

Reference

Inference

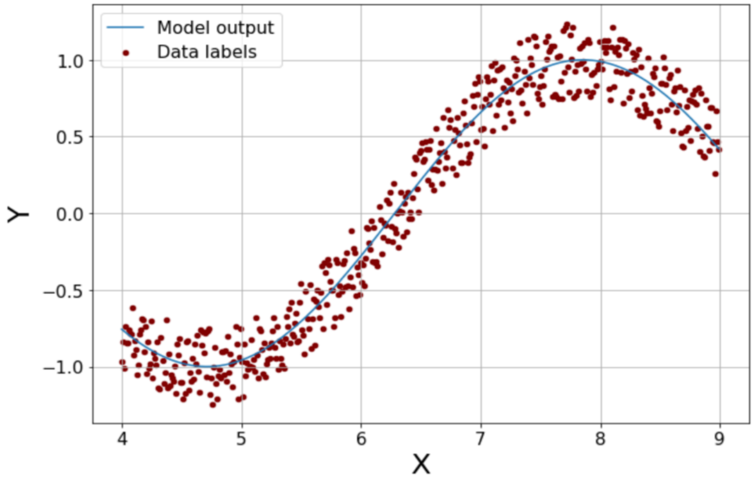


How about the uncertainties?

Uncertainty Quantification in Machine Learning

- ➢ Deterministic transformation functions

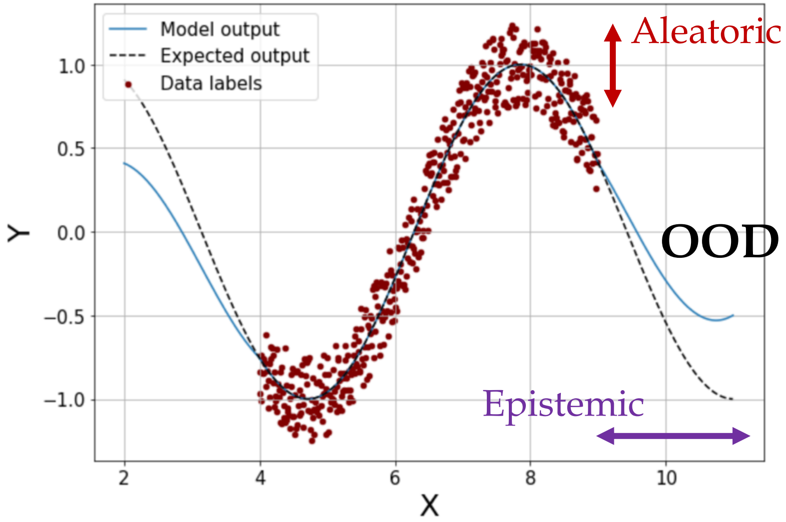
Input(s) → ML model → Output(s)



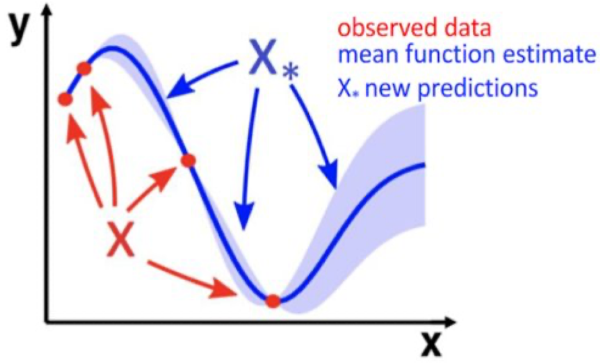
- ➢ Decision making based on predictions from ML models
  - ➢ Uncertainty Quantification is required to make an informed decision

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



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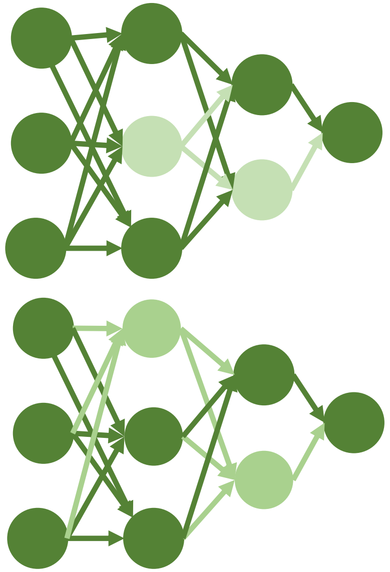
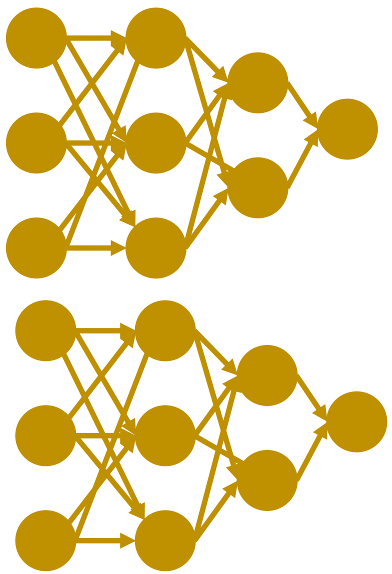
Large data sets with higher dimensions and GP

- **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?

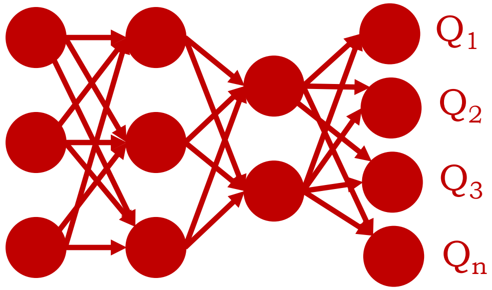
UQ in Deep Learning



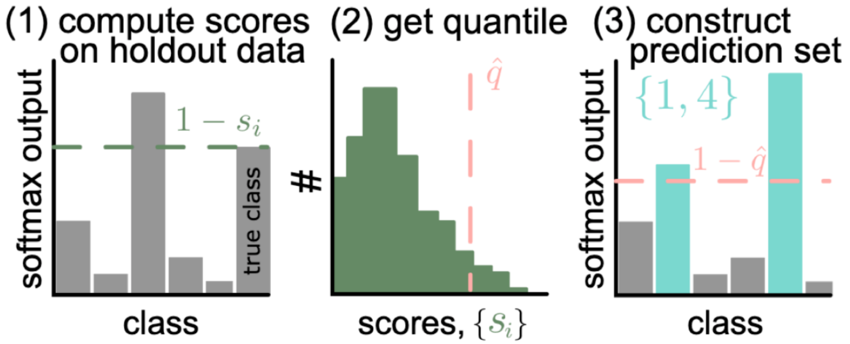
(a) MC Dropout



(b) Ensemble



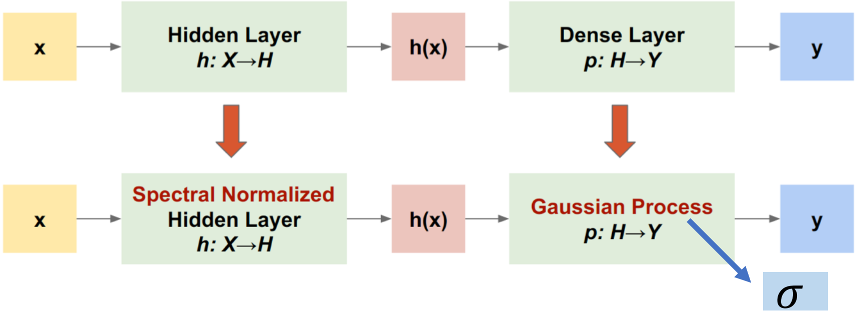
(c) Quantile Regression



https://arxiv.org/abs/2107.07511

(d) Conformal Predictions

GP takes into account distance between input samples explicitly



Spectral Neural Gaussian Process

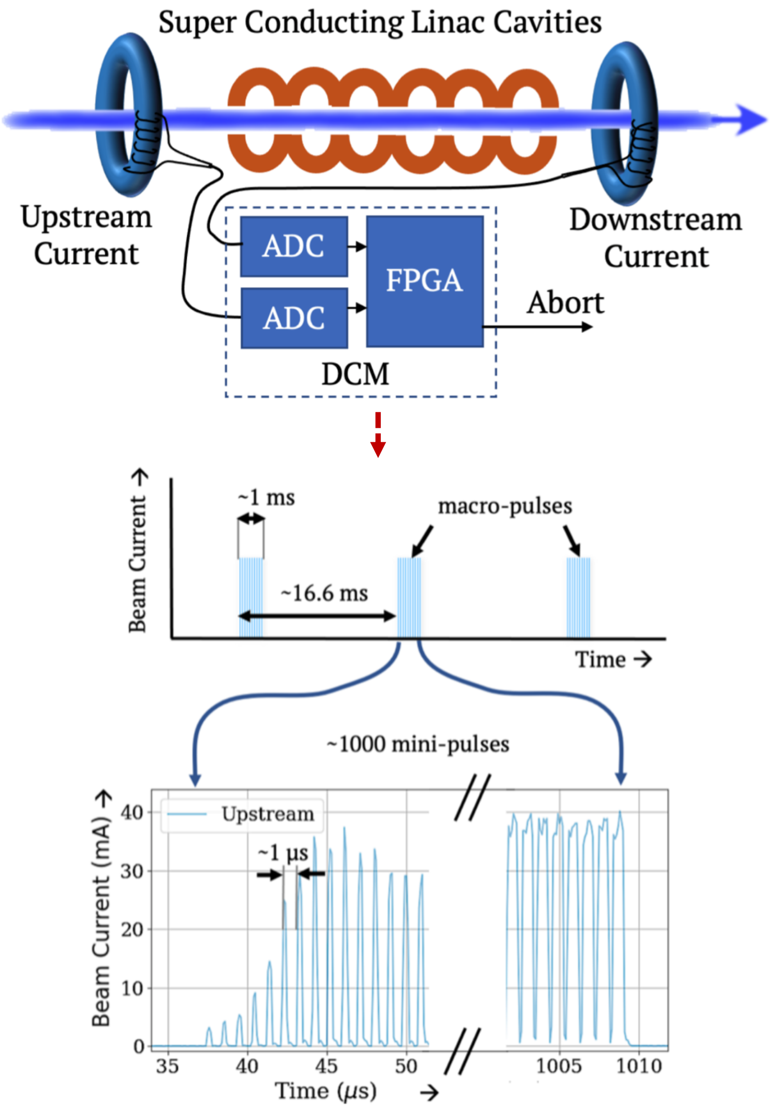
- Distance preservation via Spectral Norm on each hidden layer
  - Reduced expressivity, harder to learn
- Distance preservation via bi-lipschitz

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

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



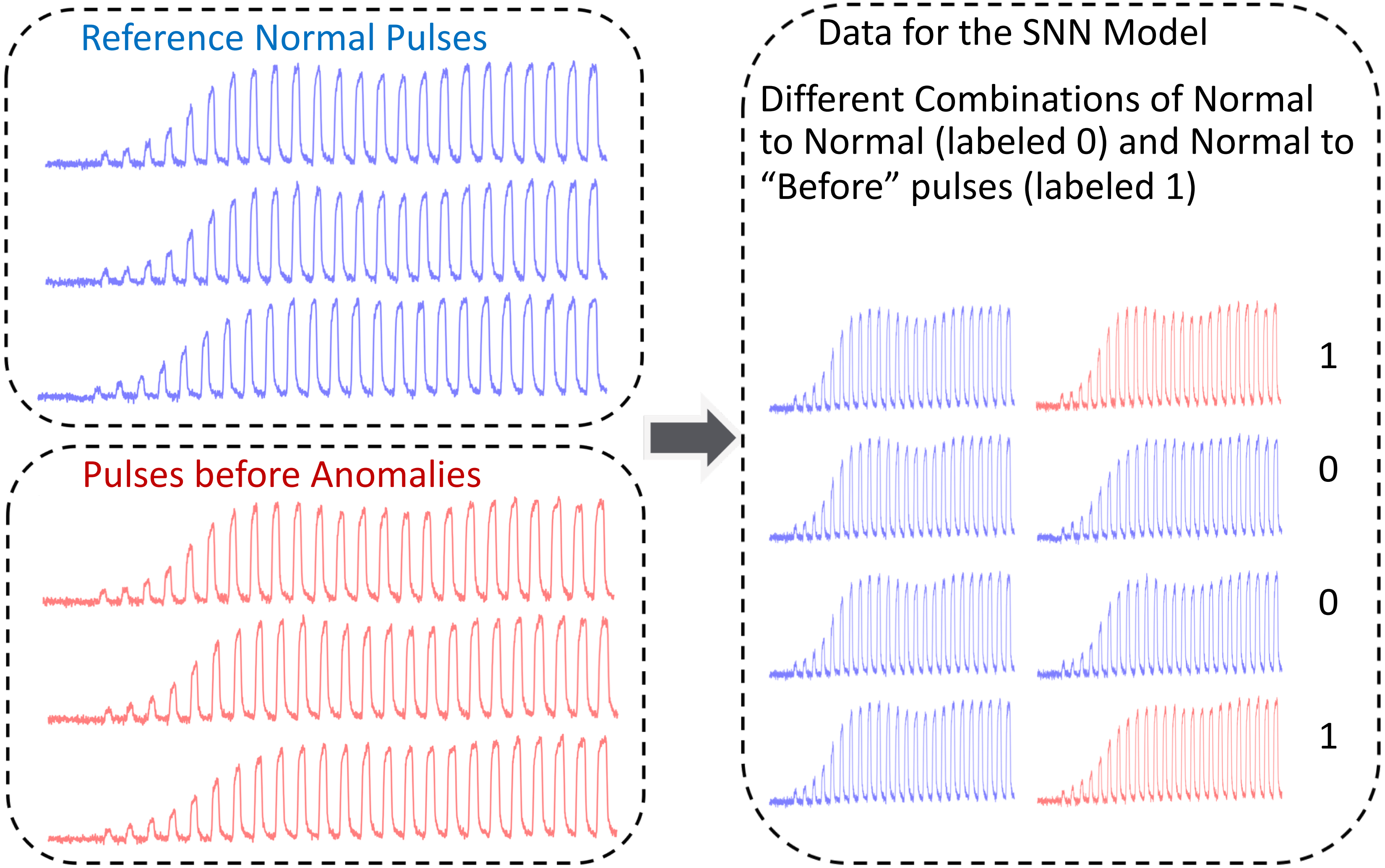
Goal: To predict errant beam pulses (with uncertainty quantification) before they occur to avoid potential damage to the equipment(s) and reduce the downtime

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

Data Preparation

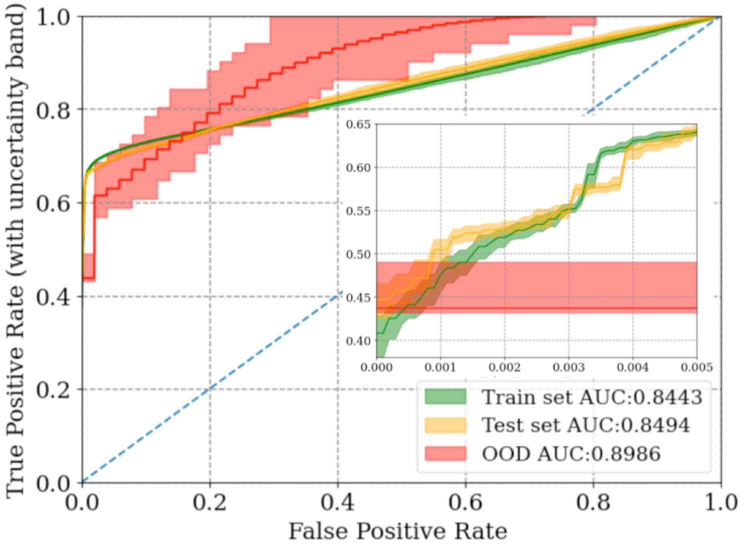
- Pair data from normal operation to other data (both normal and anomaly)
- The data before anomalies are used for training to be able to predict future anomalies
- A training data generator (keras) is used to generate combination of normal-normal and normal-anomaly pairs
- Labels are marked according to the pairs

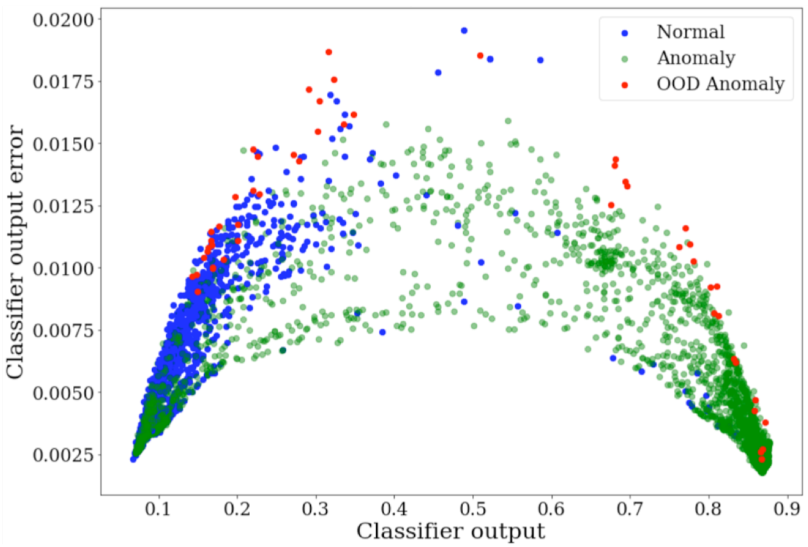


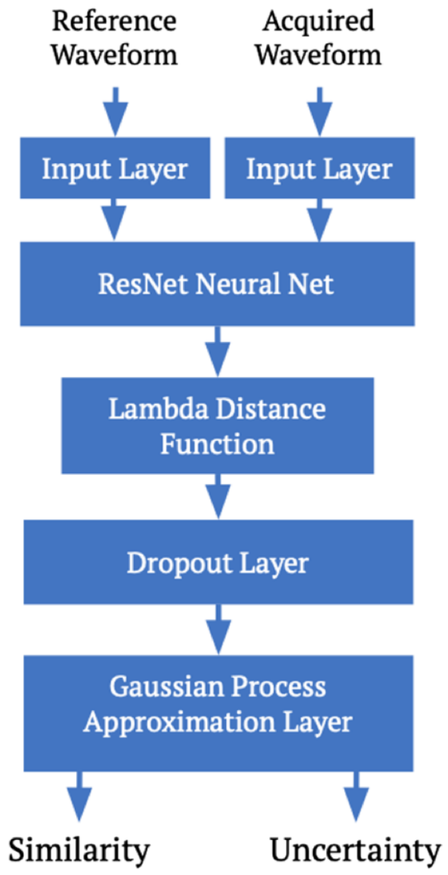
Uncertainty Aware Siamese Model and Results

- 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%

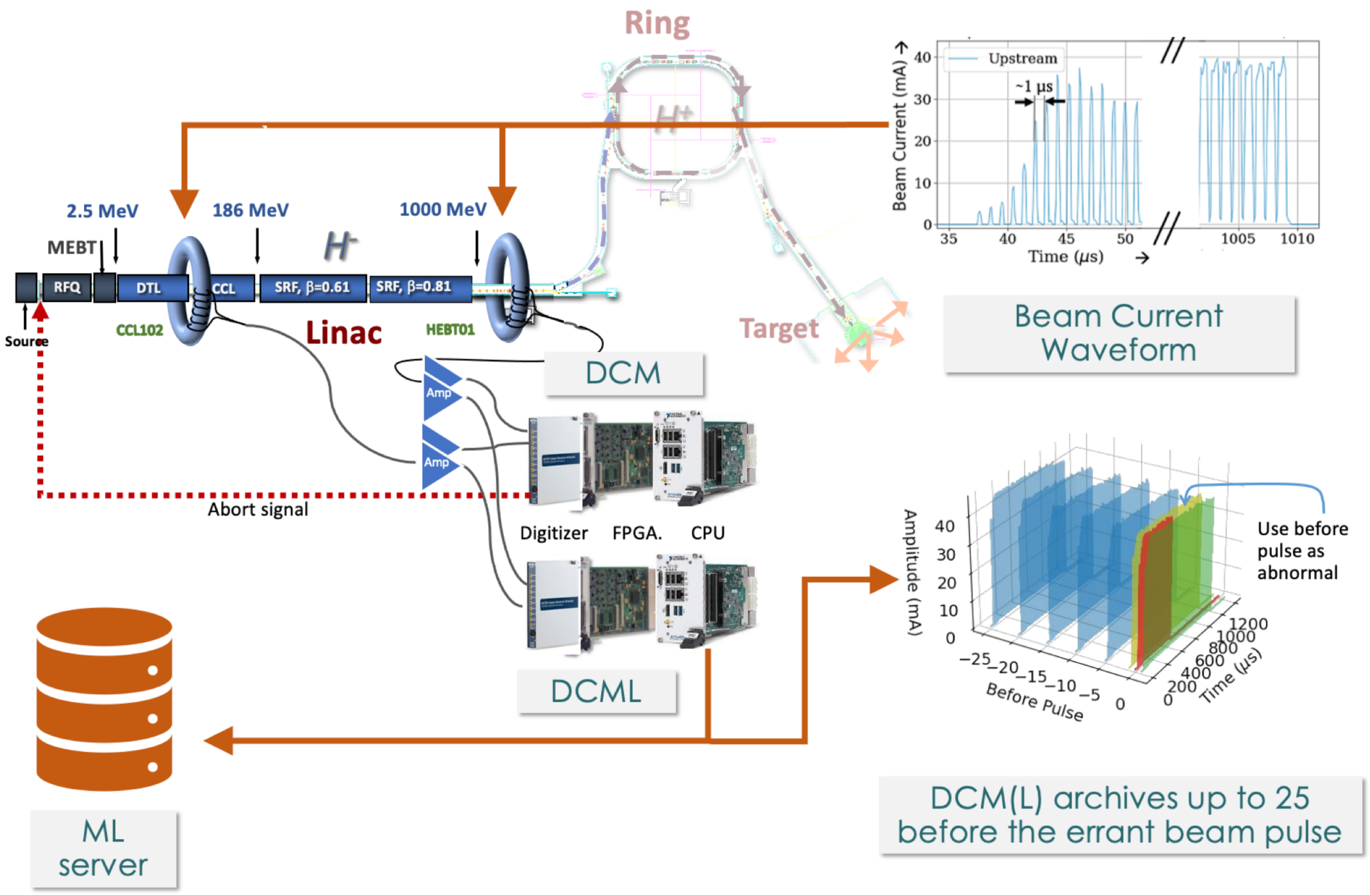






Online System

- ➢ 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 (JLab)
- ➢ DCML feeds data for machine learning training and inference while the original DCM still protects the machine



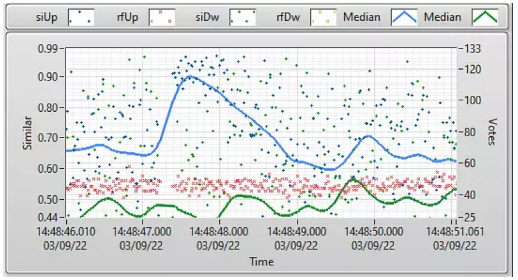
Online Results

DCML:

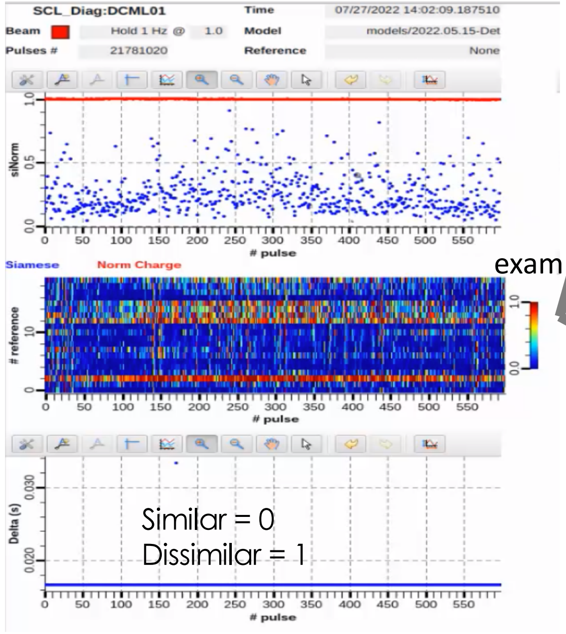
- Can run up to 4 deterministic SNN inferences

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

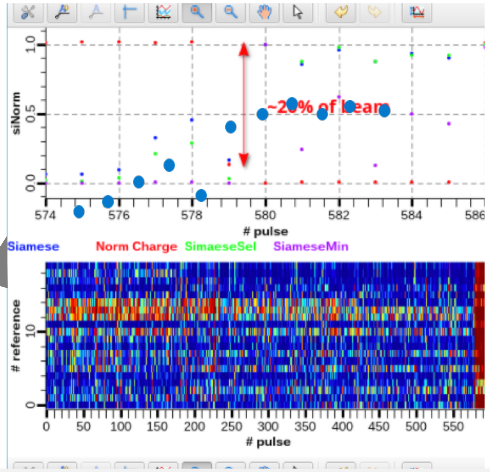


DCML live results (Siamese/RF upstream/downstream

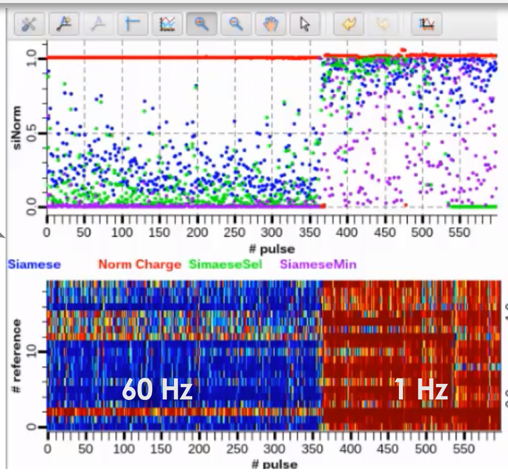


ML Server Results Control Room Screen

examples



Chopper partial failure is seen as abnormal beam



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

Conclusion

- Siamese Twin Models are used to learn the similarity between inputs
- Robust Adaptive Data Quality Monitoring can be achieved using Siamese Twin models
- DL models (including Siamese Twin) can be made OOD uncertainty aware by adding GP approximation
- Distance between input samples need to be preserved through hidden layers
- Presented uncertainty aware anomaly prediction is used for SNS accelerator
- The Model is able to identify unseen anomalies and provide confidence level
- Trained Models are deployed in real time system for fast anomaly prediction

Collaborators: Malachi Schram (JLab), Willem Blokland (ORNL), Yigit Yucesan (ORNL), Alexander Zukov (ORNL), Pradeep Ramuhali (ORNL), Frank Liu (ORNL), Charles Peters (ORNL), David Brown (ORNL), Cary Long (ORNL)

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