Machine Learning in Nuclear Physics

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This talk

Outline

1. Probably over-simplified introduction to Machine Learning
2. ML for Nuclear Physics
3. Interpretable Machine Learning

Caveats

4. I am not a data scientist
5. There are so many exciting developments that I cannot cover in 30 minutes

Artificial Intelligence and Machine Learning will be a core component of new discoveries in Nuclear Physics

AI-based technologies are *everywhere*

Self Driving Cars

.Tesla

SpaceX

Fraud Detection

Fraudulent purchases, insurance claims

Drug Discovery

AlphaFold

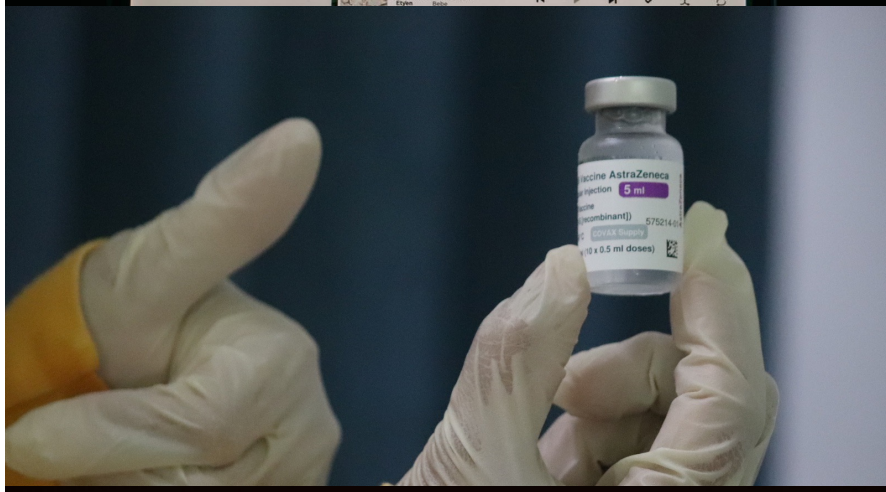
Pandemic response

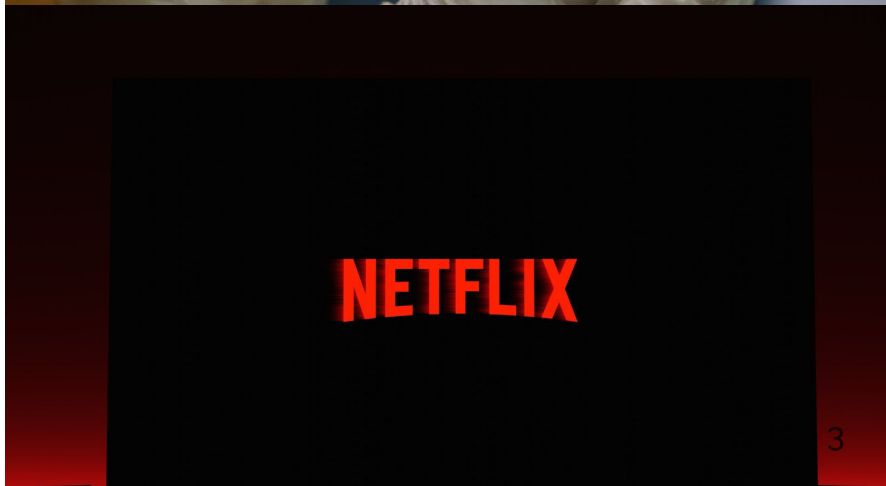
COVID-19

Recommendation Systems

Netflix

Amazon

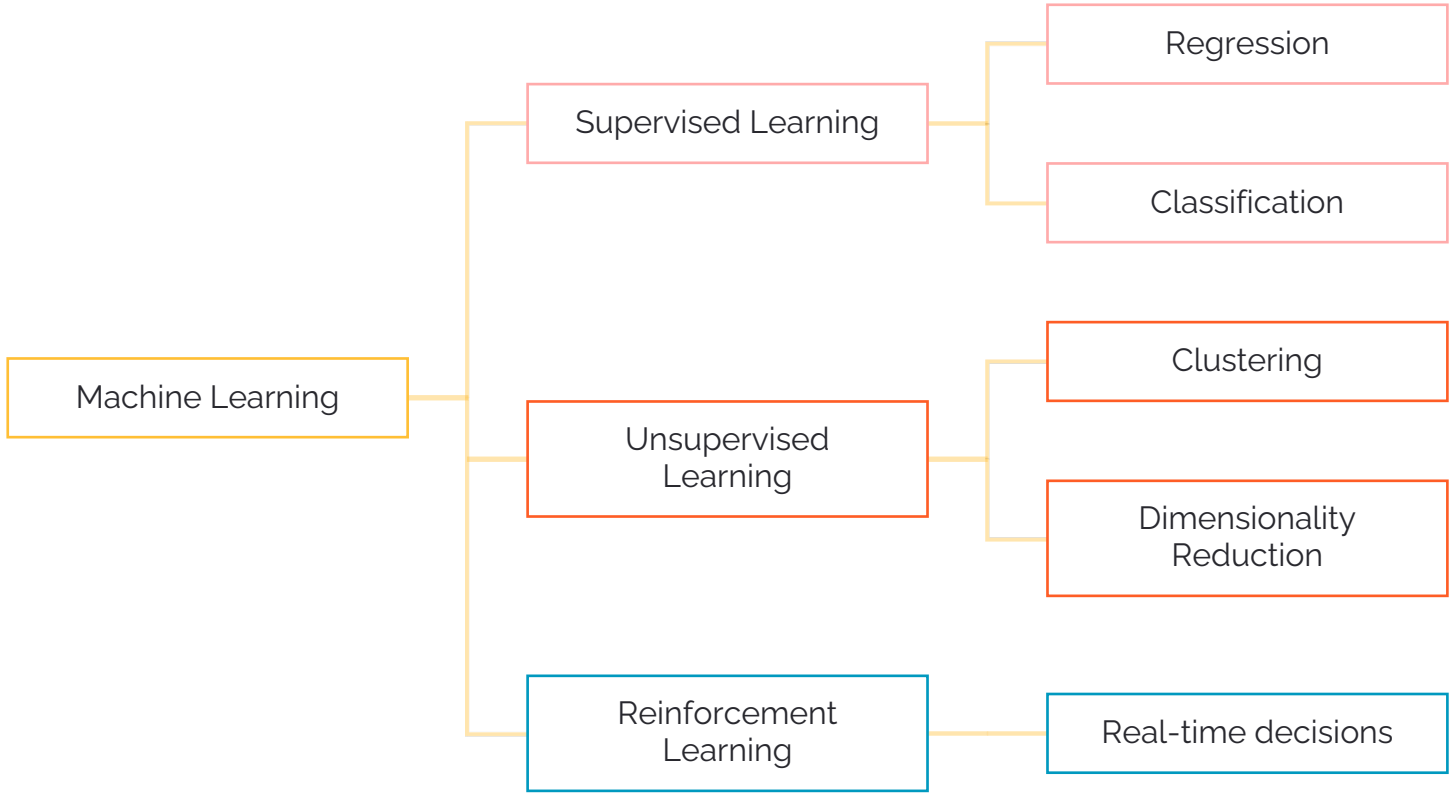




What is Machine Learning?

Machine Learning

Understanding and building methods that 'learn' a set of tasks



Supervised Machine Learning

Labeled training data

Let specific ML algorithm learn and deduce patterns in the datasets

Unsupervised Machine Learning

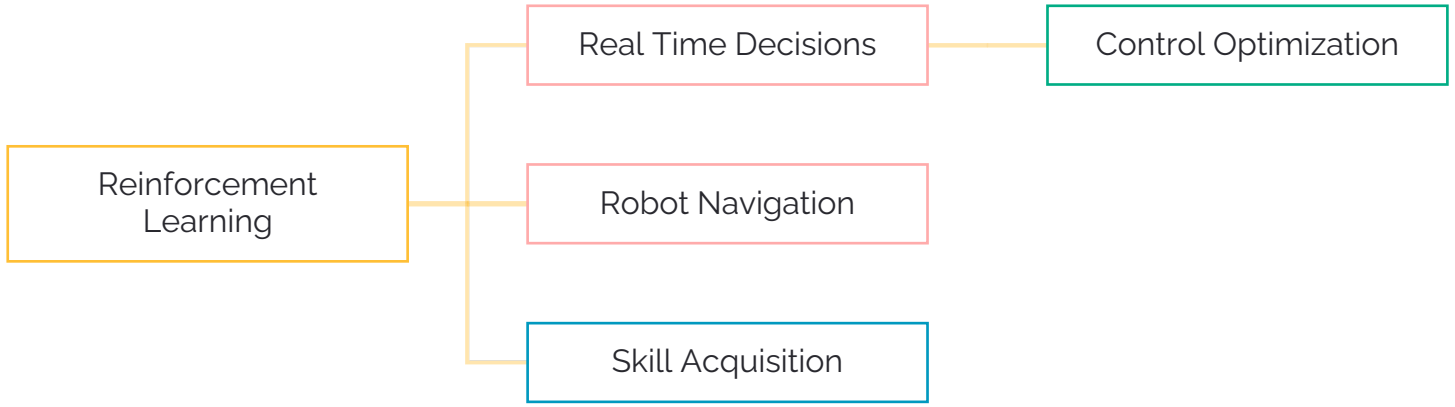
Unlabeled training data

Find patterns and relationships in datasets without any prior knowledge of the system

Reinforcement Learning

Inspired by behavioral psychology

Actions are learned to maximize reward



Data Science Pipeline

- Real or synthetic
- Quality
- Dimensionality
- Format
- Size
- Time-to-acquire

- Data cleaning
- Restructuring
- Correlations
- Visualization

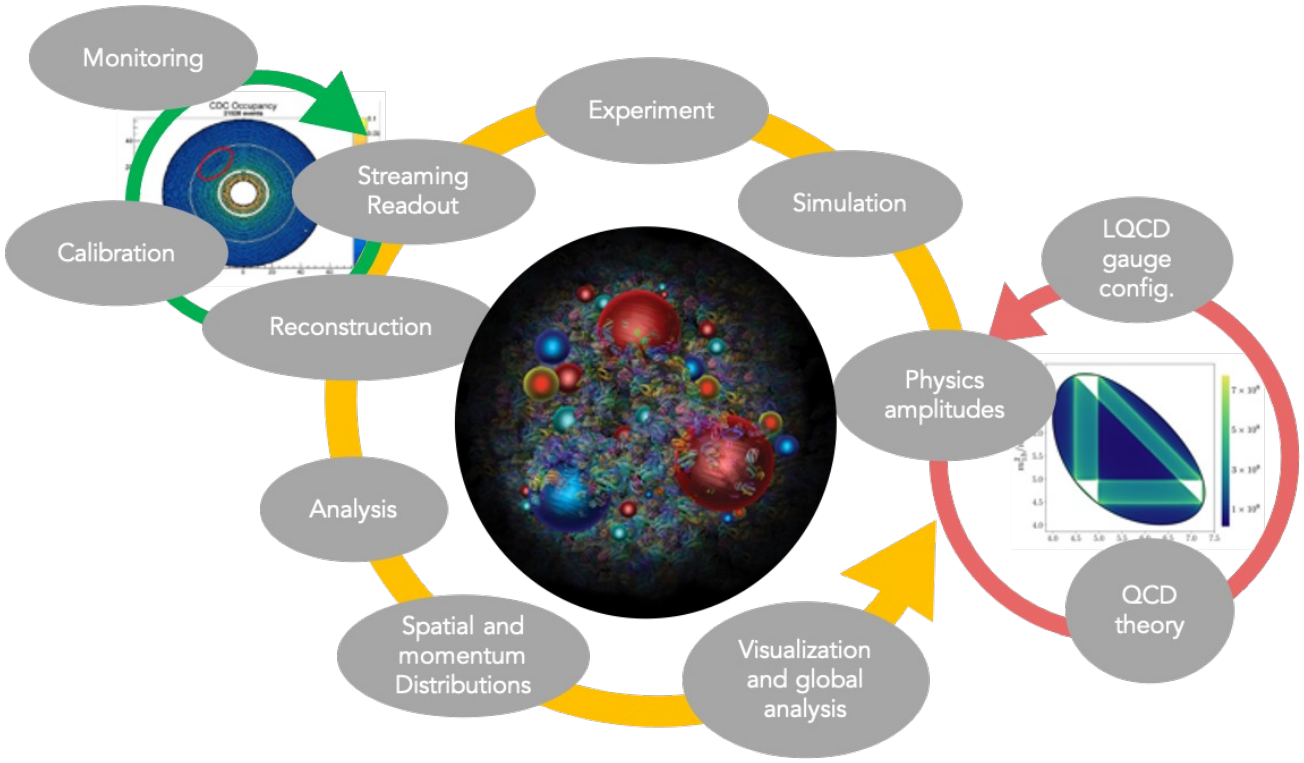
- Classification
- Regression
- Clustering
- Feature Extraction

- Cross validation
- Hyperparameter optimization

- Predictions
- Confidence level
- **Explainability**
- **Uncertainty Quantification**

Traditional Nuclear Physics workflow

AI and ML techniques are now actively being used in all aspects of Nuclear Physics



TYPICAL NP DISCOVERY PARADIGM, FROM A. BOEHNLEIN

Parallel Talks from Monday

- **AI/ML for Streaming Readout**
  Jin Huang
  Utilizing AI/ML on FPGAs and ASICs to use with streaming readout data acquisition
- **AI/ML for Nuclear Theory**
  Daniel Hackett
  Generative models for lattice quantum field theory
- **A(i)DAPT: AI for Data Analysis and Preservation**
  Marco Battaglieri
  AI-based algorithms to unfold detector effects and reveal interaction mechanisms at the vertex level
- **AI/ML for Experimental Physics**
  Diana McSpadden
  Motivations for ML use in Experimental Physics
- **AI-Assisted Detector Design**
  Cristiano Fanelli
  Utilizing AI to aid in detector design with applications
  to the Electron Ion Collider

ML for Experimental Nuclear Physics

Online Data Quality Monitoring: Hydra at Jefferson Lab

Traditional method:

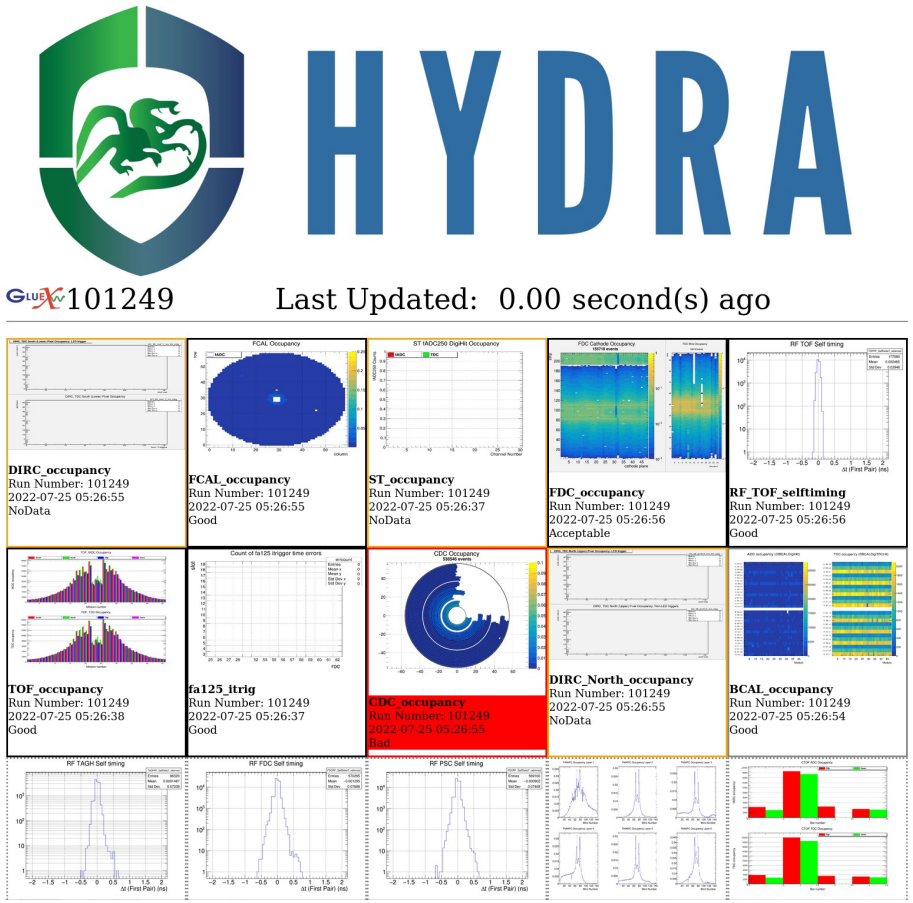
Shift takers monitor *hundreds* of histograms for all of the detector subsystems 24/7 during an experiment. Different shift takers look at the monitoring plots at different time intervals.

Hydra:

Re-train Google's InceptionV3 with labeled monitoring plots from previous experiments. Hydra evaluates all images and provides classification and confidence **every 30 seconds**. Can interface with alarm handler to audibly alert shift crew of problems.

Results:

Hydra discovers issues in monitoring plots faster and more reliably than humans.



ML for Nuclear Theory

Reducing cost of LQCD calculations

Computation of observables in LQCD is computationally expensive

Requires the inversion of a large matrix

ML methods are being developed to take cheaper inversions with low precision, and then recover the full precision propagator while saving computing resources

see Dan Hackett's talk on ML for Nuclear Theory

ML for Accelerator Physics

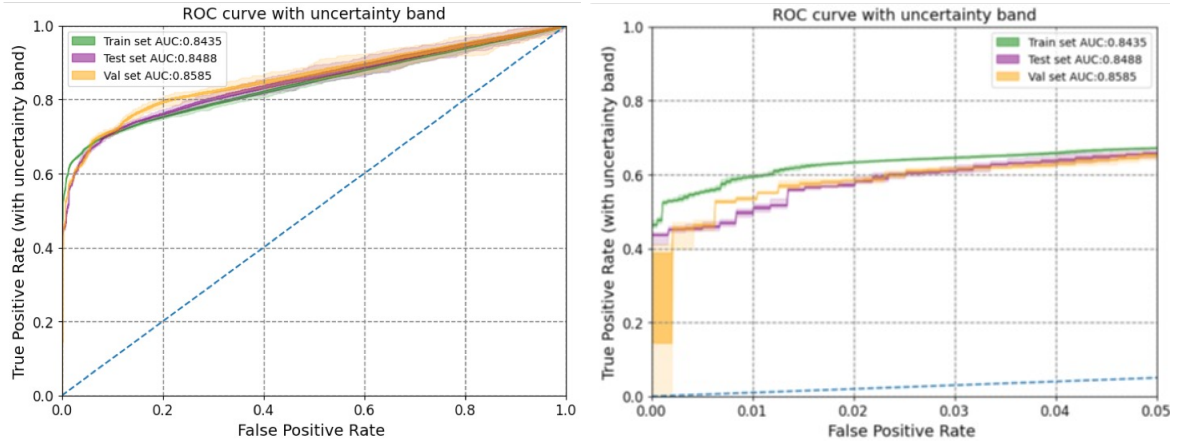
Detection of Errant Beam Pulses at ORNL

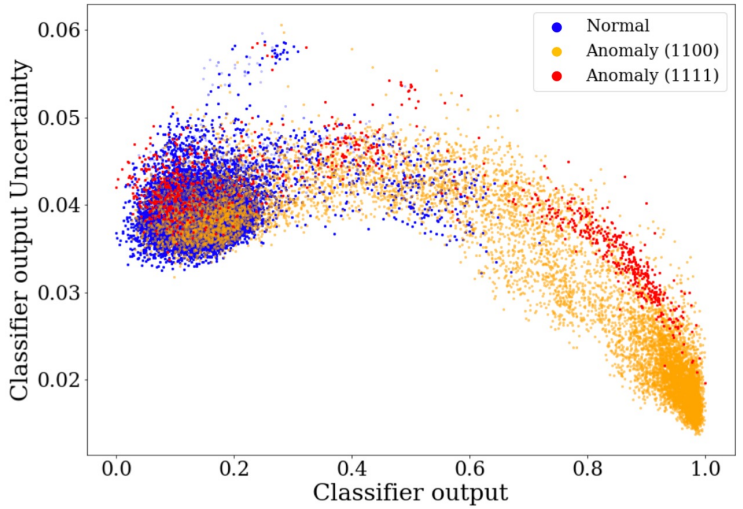
Predicting errant beam pulses ahead of time

Home of the Spallation Neutron Source

Uncertainty Aware Siamese Neural Network evaluates beam current traces and determines similarity to reference trace

Corrective action can be taken to reduce downtime or equipment damage caused by errant beam pulses





Interpretability + Uncertainty Quantification

Trustworthiness

> “The more you can understand how your ML system actually works, the more reason you might have to trust it”

Max Tegmark, MIT

Complexity vs Accuracy Trade Off

Interpretable or Accurate? Choose one!

Can make simple models more accurate, and complex models more interpretable

	Interpretable	Accurate
Simple Model	✔	✖
Complex Model	✖	✔

What happens if we don't fully understand our model?

The Rise and Fall of Knight Capital — Buy High, Sell Low. Rinse and Repeat.

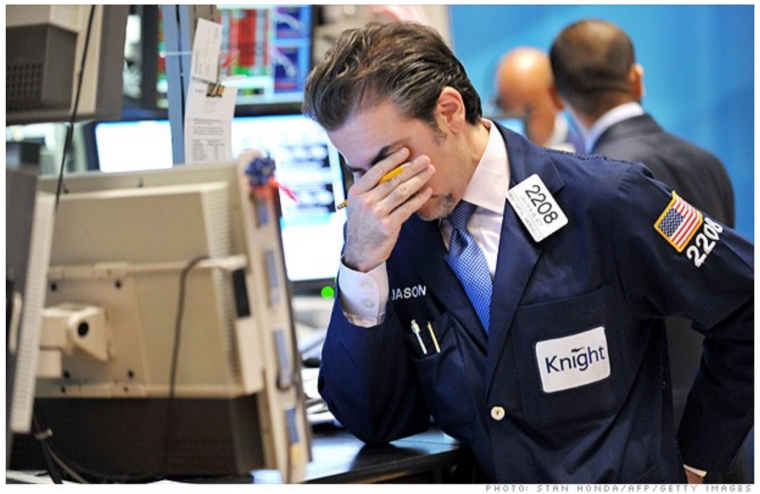
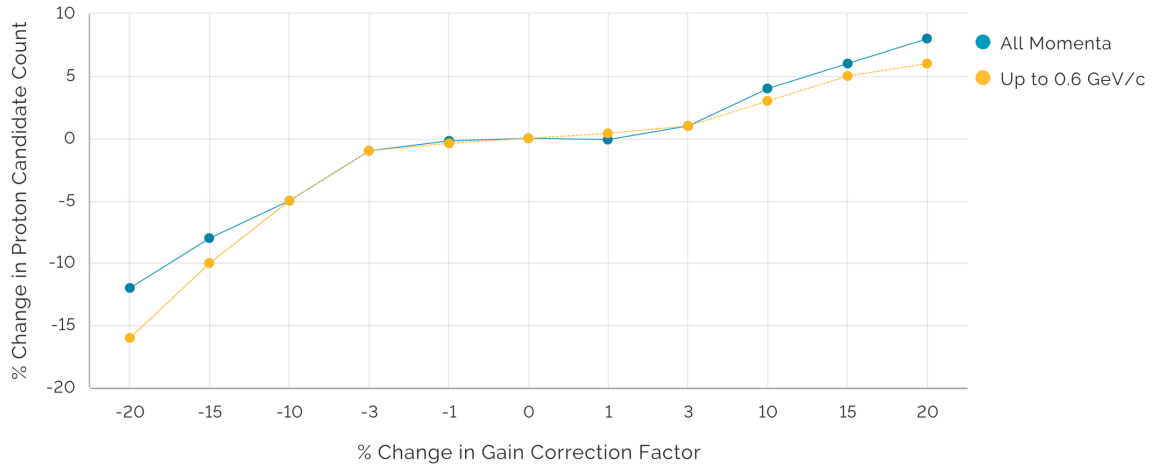


PHOTO: STAN HONDA/AFP/GETTY IMAGES

Knight Capital Trading

In 2012, software error lost ~$10M per minute for 44 minutes before it was noticed.



Incorrect Calibrations

The GlueX Central Drift Chamber is used for charged particle identification. Poorly calibrated detector would negatively affect all physics analyses.

Interpretability

Understand model predictions and stability

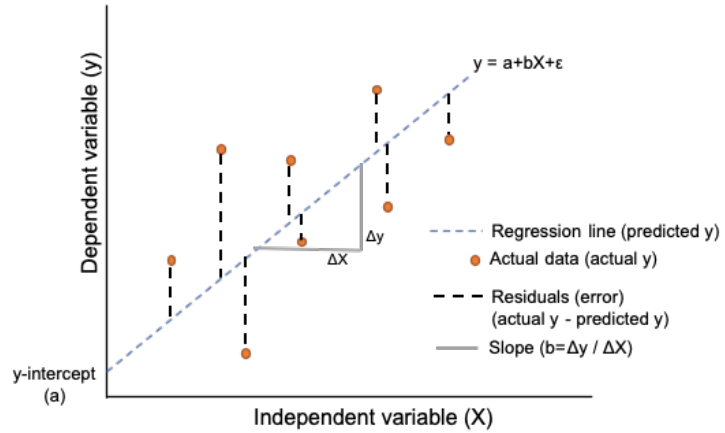
How does a model come up with its prediction?

Even the simplest ML model architectures can be 'black boxes'

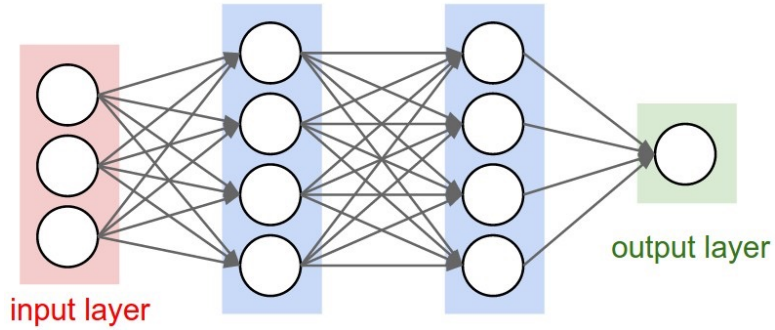
Benefits to nuclear physicists and data scientists

Nuclear physicists are more likely to implement a model they trust

From a data scientist's perspective, explanations can help better understand problem, the data, and when and why a model might fail



LINEAR REGRESSION

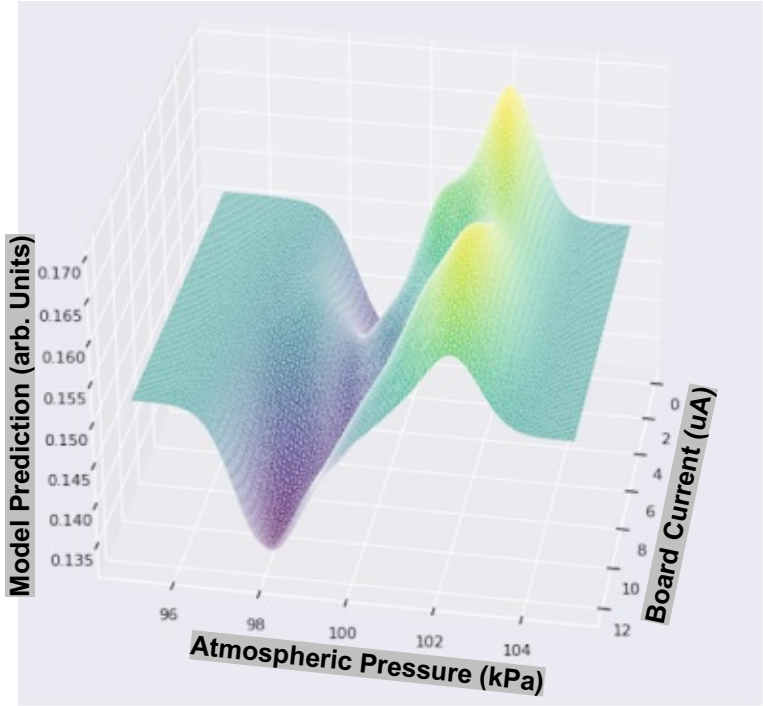


SIMPLE NEURAL NETWORK

Trustworthiness

- Implementing ML based systems for physics applications will **require** interpretability
- Much easier to adopt ML techniques if we understand model behavior

  Imagine trying to convince a detector expert to implement a ML system to control a detector during an experiment without validating its behavior in all circumstances (even if its rare!)



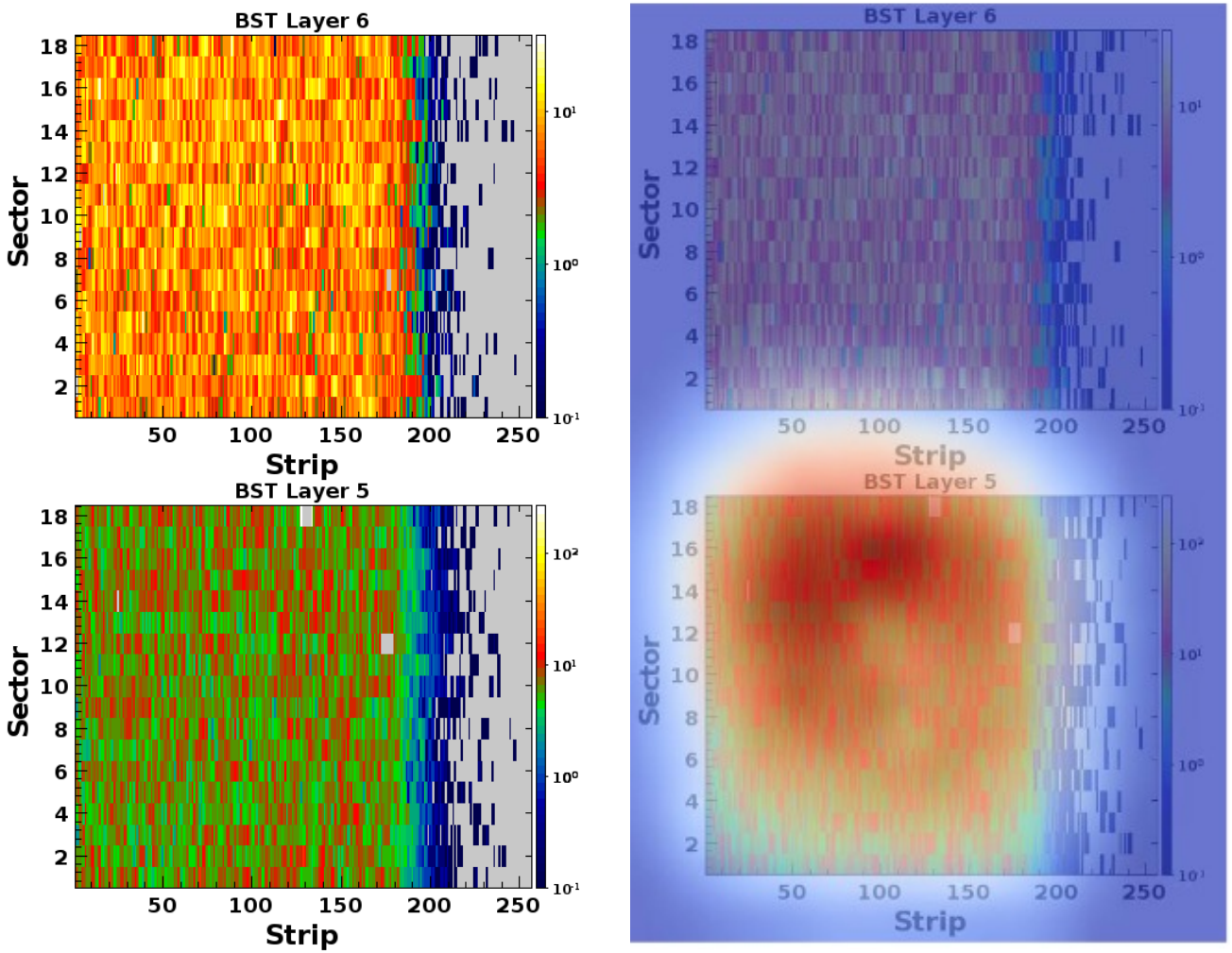
MODEL PREDICTIONS REGRESSING TO MEAN FOR OUT OF DOMAIN INFERENCES

Interpretability

GradCAM with Hydra

Gradient Class Activation Map

What region of the image is important to the model when making the classification?



LEFT: MONITORING PLOT FROM BARREL SILICON VERTEX TRACKER IN CLAS12. **RIGHT**: HEAT MAP INDICATING REGION OF IMPORTANCE FOR CLASSIFICATION.

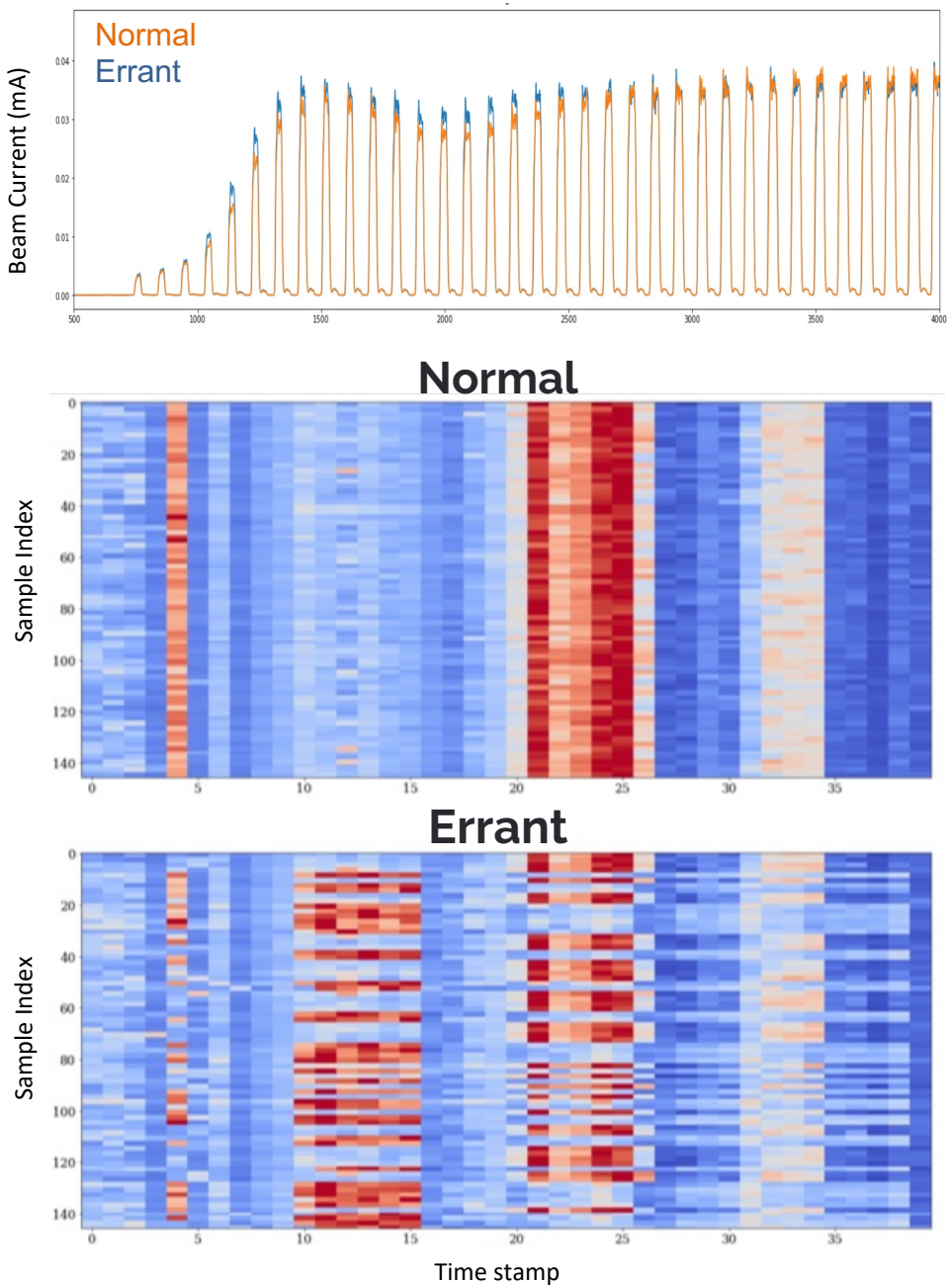
Interpretability

GradCAM + Siamese Neural Network

Can we distinguish heat maps produced from normal and errant beam pulses?

Can we associate heat maps from specific fault types to specific equipment failures?

Red indicates region of high importance, blue indicates region of low importance.



Interpretability

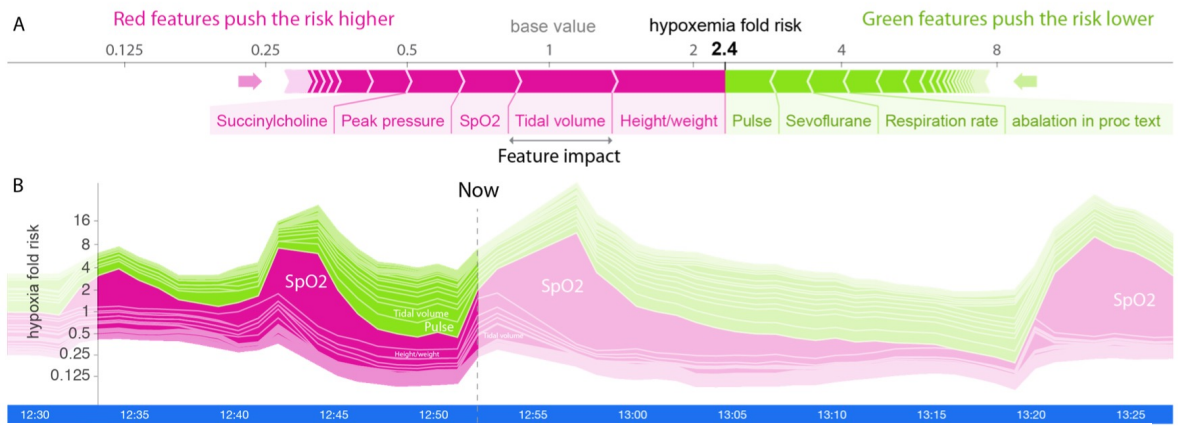
Shapley Values

Lloyd Shapley, Nobel Prize in Economics 2012

How does an individual input feature contribute to a prediction?

Based on 'fairness' properties from Game Theory

Model agnostic, but can be slow to evaluate



A) EXPLAINED RISK OF HYPOXEMIA IN THE NEXT 5 MINUTES DURING A SURGICAL PROCEDURE. B) EXPLAINED RISK EVOLVING OVER TIME.

Uncertainty Quantification

- Active area of research in AI

  Complicated by noisy data, limited data, hyperparameters, overparametrization, sampling errors, etc

- Critical for control related decisions

  Especially when it comes to maintaining safe operating conditions of an accelerator

  see Diana McSpadden's talk for UQ implementation at ORNL and FermiLab

- Need for designing human-interpretable explanations and developing comprehensive evaluation metrics

Take home messages

1. DOE has recognized the importance and benefits of implementing AI/ML techniques in Nuclear Physics
2. Numerous exciting applications and avenues to explore in experiment, theory, and accelerator fields
3. We have a unique opportunity to collaborate with data scientists to implement ML systems from the start at new facilities like the EIC and FRIB

References

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4. Uncertainty aware anomaly detection to predict errant beam pulses in the sns accelerator
   https://arxiv.org/pdf/2110.12006.pdf
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6. Uncertainty Quantification in Scientific Machine Learning: Methods, Metrics, and Comparisons
   https://arxiv.org/pdf/2201.07766.pdf

Community Identified Needs for AI Research in NP

AI for Nuclear Physics Workshop, Jefferson Lab

- ## Workforce development

  Retain talented students in AI-related fields, have community of researchers knowledgeable in AI technologies, strong collaborations between NP researchers and experts in AI/ML/Data Science

- ## Uncertainty Quantification

  Evaluation and comparison of uncertainty predictions using different modalities is required for widespread use in NP

- ## Comprehensive Data Management

  Establish standards for processing data, application of theoretical assumptions, and treatment of systematic uncertainties

- ## Adequate Computing Resources

  AI techniques are computationally intensive, will require access to GPU computing and disk storage at appropriate scales

EPSCI at Jefferson Lab

Experimental Physics Software and Computing Infrastructure

David Lawrence
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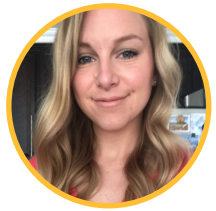
Nathan Brei

Thomas Britton

Michael Goodrich

Vardan Gyurjyan



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