Optimization in Machine Learning for Neutrino Classification

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What Are Neutrinos?—fundamental particles (leptons) with neutral charge

that have puzzlingly small masses and interact only with the Weak Force

- Three flavors (mass states)
- Paired with charged partner

  ν_e with electrons

  ν_μ with muons

  ν_τ with tau particles

Where do they come from?

- Collisions following Big Bang
- Proton-proton fusion in stars
- Cosmic rays
- Beta decay

What makes them so weird?

- Change flavors
  - Superposition of mass states $\nu_{1,2,3}$
  - Probability oscillation obeys Schrödinger Equation
- Leptons => don't interact with Strong Force
- Neutral charge => don't interact with EM Force
- Mysterious and sneaky
  - "Normal" hierarchy of masses assumed but not required

Oscillation frequency—function of mass, distance traveled, and energy: $\sin^2(\varphi)(\Delta m)^2 \frac{L}{E}$

- In detectors, $\cos(\varphi)$ = zenith angle from entry point
- **Mixing angles** give amplitude of periodic flavor oscillation
- **Mixing matrices**: rows = flavors, columns = mass eigenstates

Lepton Mixing (PMNS) Matrix—unitary matrix with mixing angles and complex phases

- Components $U_{\alpha i}$ with α = flavor, i = eigenstate

$$\begin{bmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{bmatrix} = \begin{bmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu 1} & U_{\mu 2} & U_{\mu 3} \\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3} \end{bmatrix} \begin{bmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{bmatrix}$$

  - Parameterized by mixing angles:

    θ_{13} = probability (small) that ν_μ turns into ν_e

    θ_{12} = probability that ν_e turns into ν_μ or ν_τ

    θ_{23} = probability (close to 45°, nearly max.) that ν_μ turns into ν_τ

Charge-Pairity (CP) Violation—contradiction of conservation laws, charge conjugation, and pairity

- Complex phase angles invert spacial dimension
  - Change in charge sign
- Occurences in quarks too small to detect alone
- Explanations offered by Standard Model have yet to be proven

DUNE: Deep Underground Neutrino Detector — detectors at Fermilab and in South Dakota; anticipated 2026

- Graphite and Liquid Argon
  - Charged Lepton emitted or neutral current
    - Number of neutrinos and antineutrinos
  - Localize atmospheric oscillations
- Prototype detector ProtoDUNE at CERN
  - Testing AI programs
- Cherenkov radiation detected by light reflectors
  - Treat alternating orientations as pixelated images
- Seeking answers
  - Matter vs. antimatter
  - Sourced from core-collapse supernovae—black hole formation
  - Matter stability and grand unification

Problems:

- ν_τ hard to detect, looks like other particles
- ν_τ hits take up a lot of image space
  - 500 pixels x 500 pixels for just 4.5 mm
- Need extreme detail, lots of data
- 500 x 500 dataset doesn't entirely fit ν_τ
  - Smarter algorithms
- Data processed as images at various angles
  - Need flat selection efficiency over all angles

There are no standard methods to do this!

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Sparse Network— how the Aurisano Machine Learning Group is curating an algorithm

- Sparse tensors: only contain pixels with hits in them
  - Reduced amount of data and computational cost
- Train the network to have rotation invariance
- What could make a machine correctly identify ν_τ in the atmosphere?

Classes of particles: muons, pions, kaons, michel electrons, particle shower, diffuse scattering, and highly ionized particles (HIP)

Hyperparameters: learning rate (LR), weight decay (WD), gamma, step size, network depth

Optimization: loss function, activation function, automated optimizers

Optimization Algorithms: AdamW vs. Ranger

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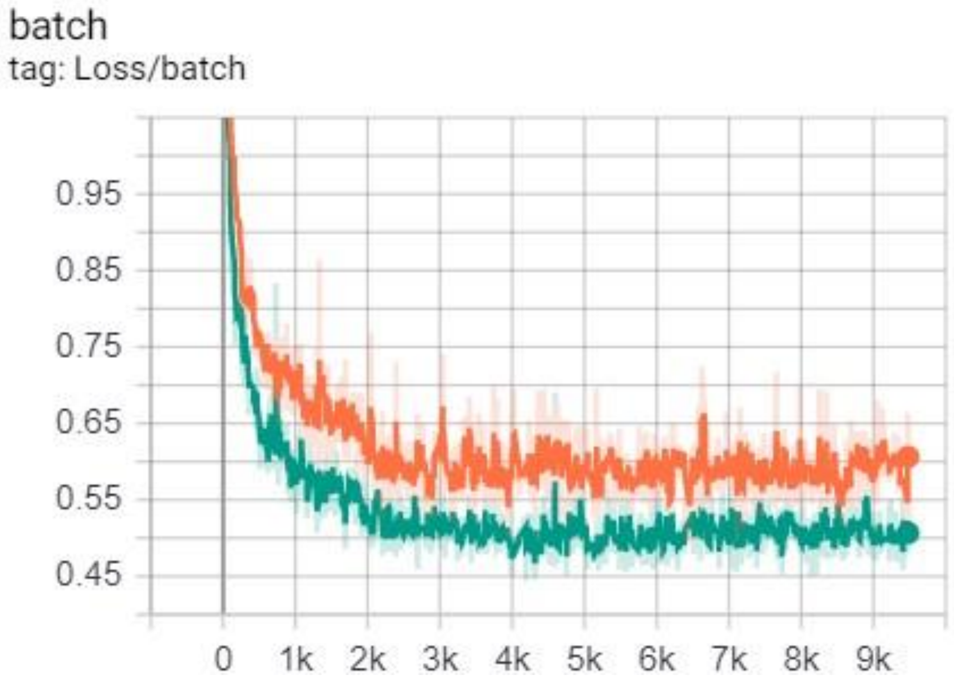
AdamW—adaptive moment estimation

- Adaptive Gradient Algorithm + Root Mean Square Propogation
- Memory usage minimized
- Efficient when properly tuned
- History of successful super convergence

Ranger—RAdam (Rectified Adam) + LookAhead

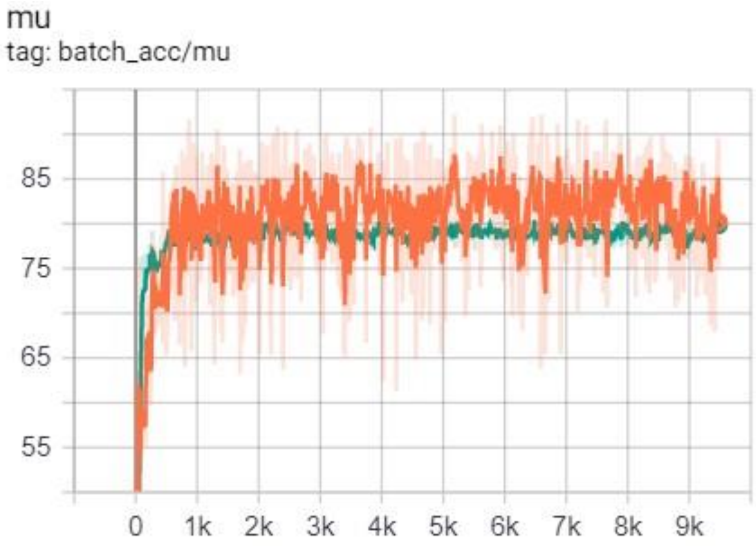
- Incorporates gradient centralization
  - Restricted loss function
- Quickly converges efficiency of multiple tasks
- Computationally efficient
- Compatible with Mish activation function

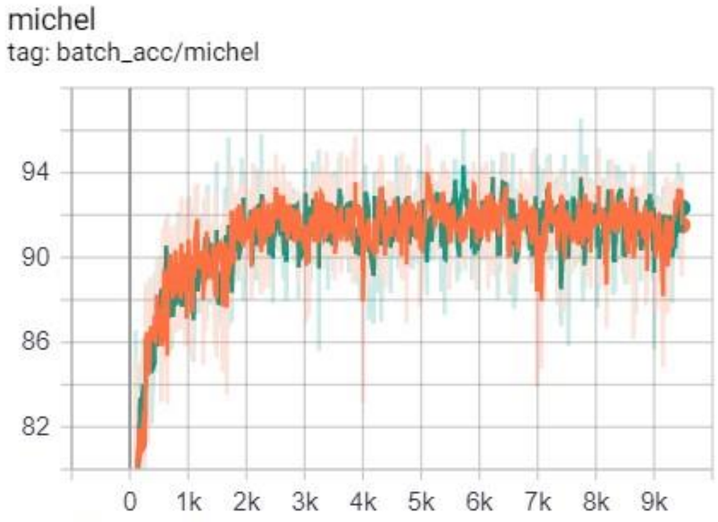
Default Values:
Weight Decay = 0.01, **Gamma** = 0.1

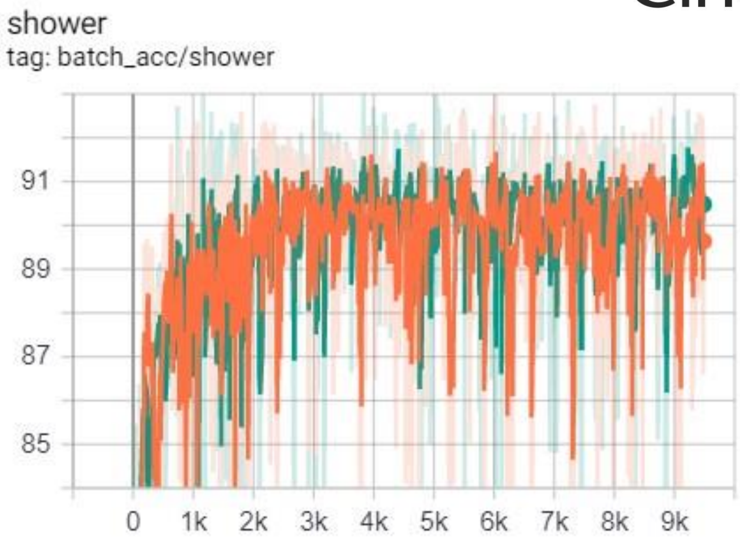


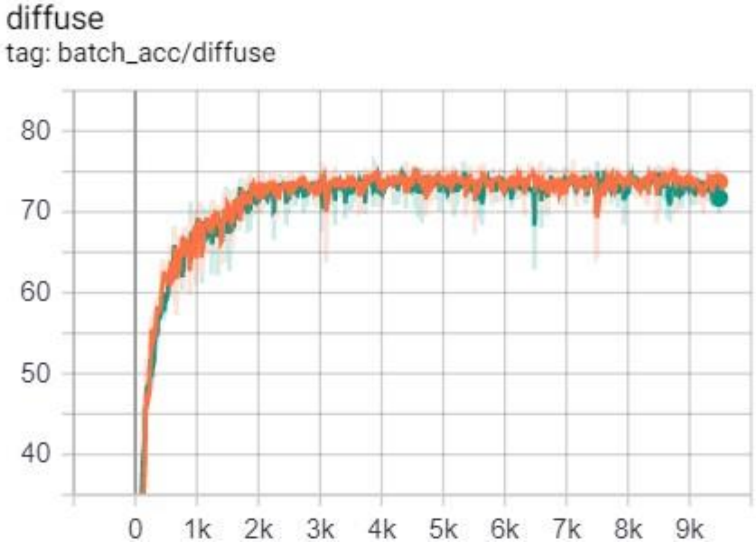
AdamW: End Accuracy = 79.48
Ranger: End Accuracy = 79.13

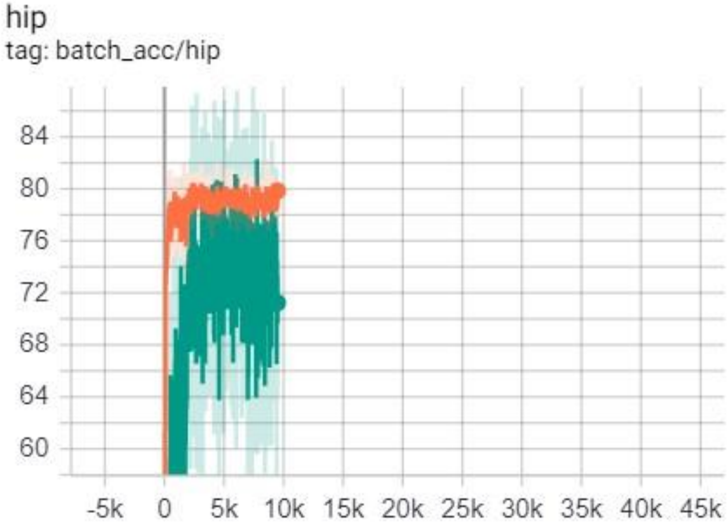
AdamW: End Loss = 0.4824
Ranger: End Loss = 0.6179







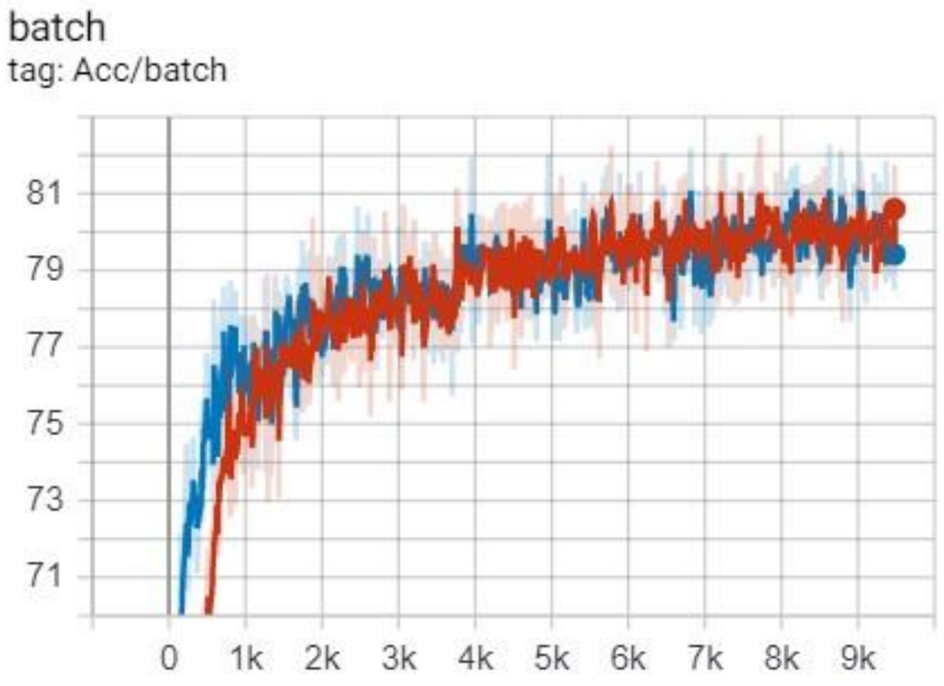


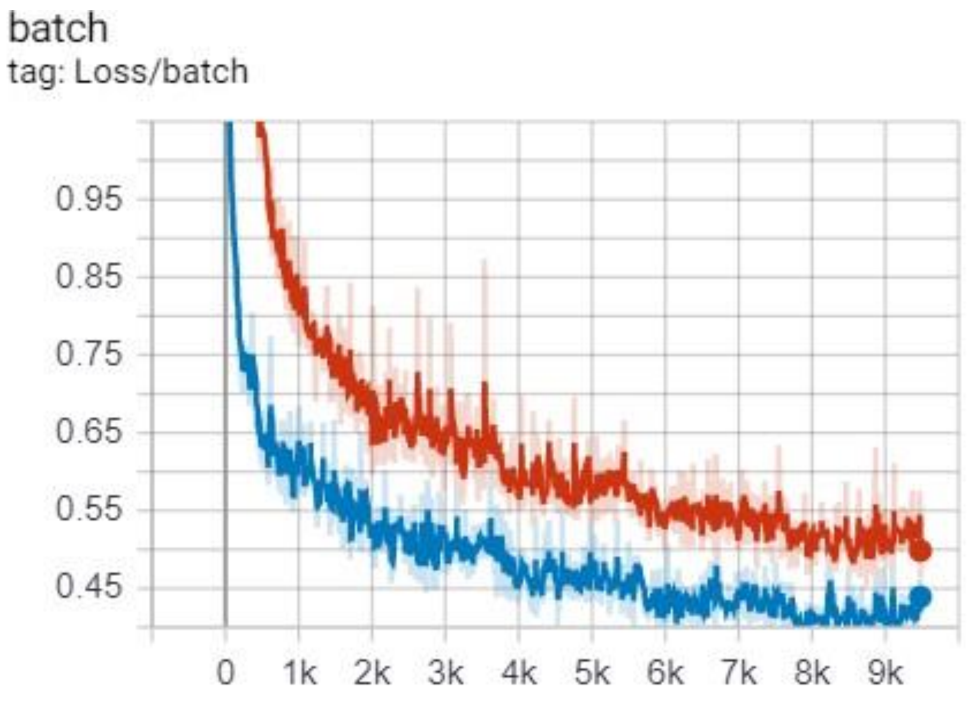


Conclusion: Ranger improved muon accuracy and HIP stability, but overall didn't outperform AdamW; no strong evidence that switching is worth it.

Chosen Values:

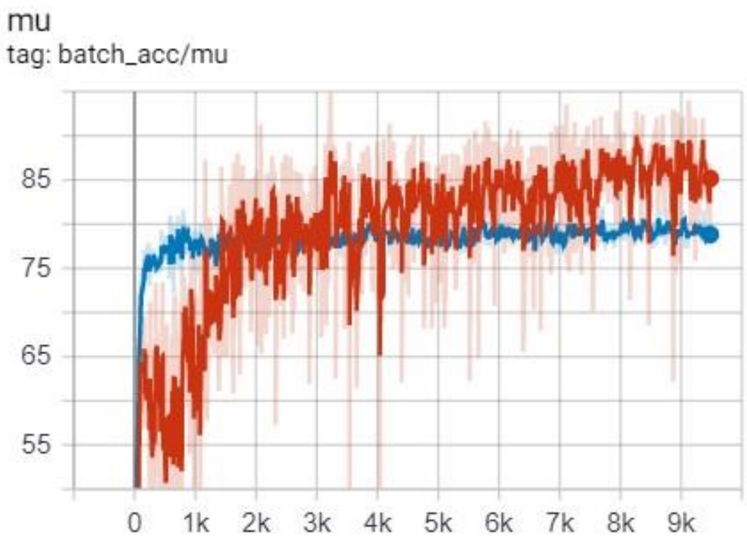
Weight Decay = 0.02, **Gamma** = 0.75

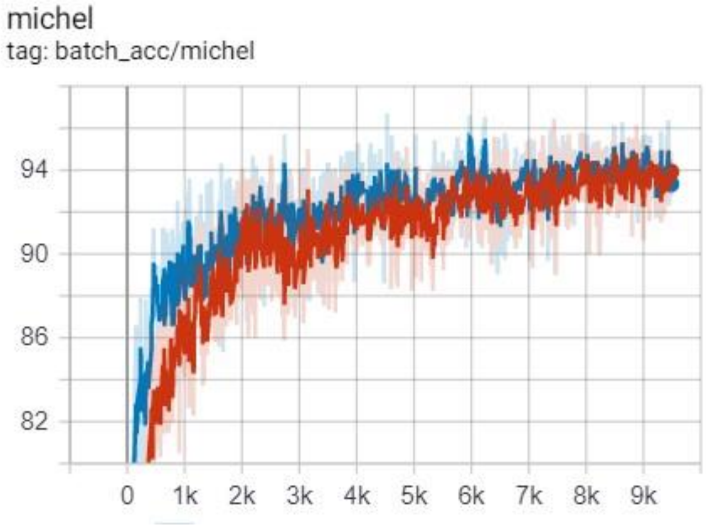


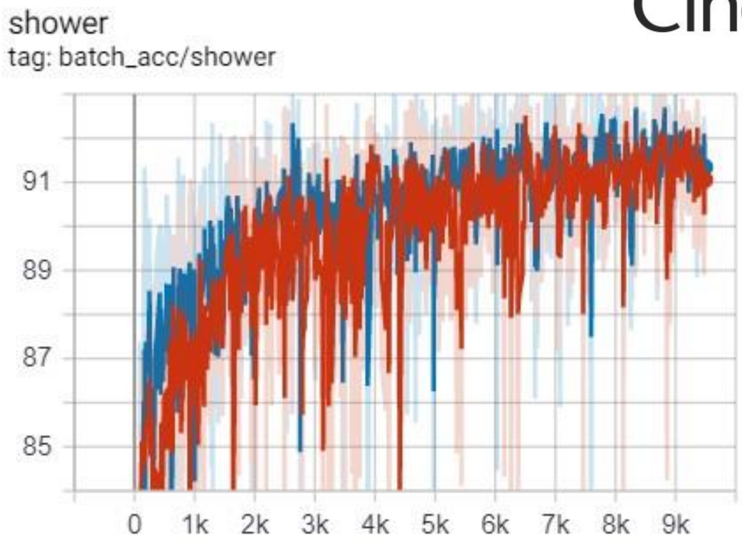


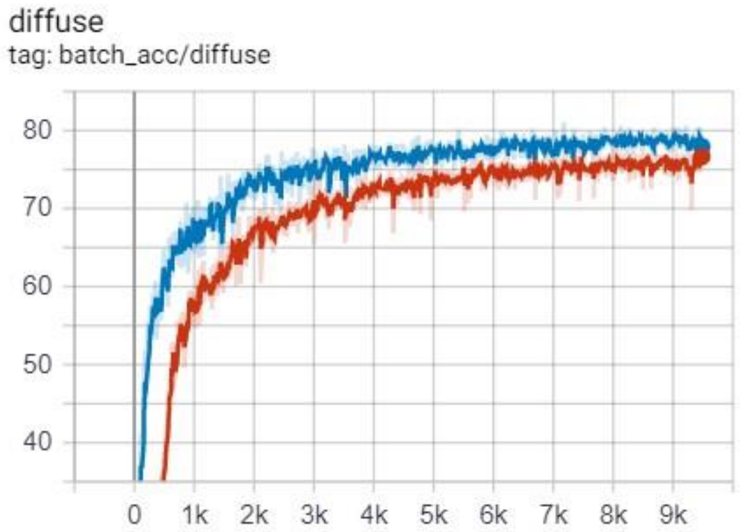
AdamW: End Accuracy = 78.48
Ranger: End Accuracy = 81.75

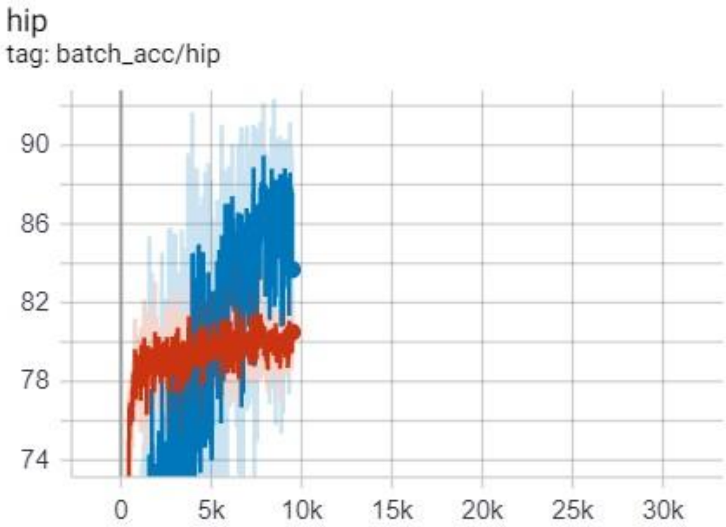
AdamW: End Loss = 0.4421
Ranger: End Loss = 0.4636











Conclusion: **Ranger** improved muon and diffuse accuracy, but overall didn't outperform **AdamW**; no strong evidence that switching is worth it.

Implementing SHERPA: "a Python Hyperparameter Optimization"

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Optimizing Parameters:

- Learning Rate

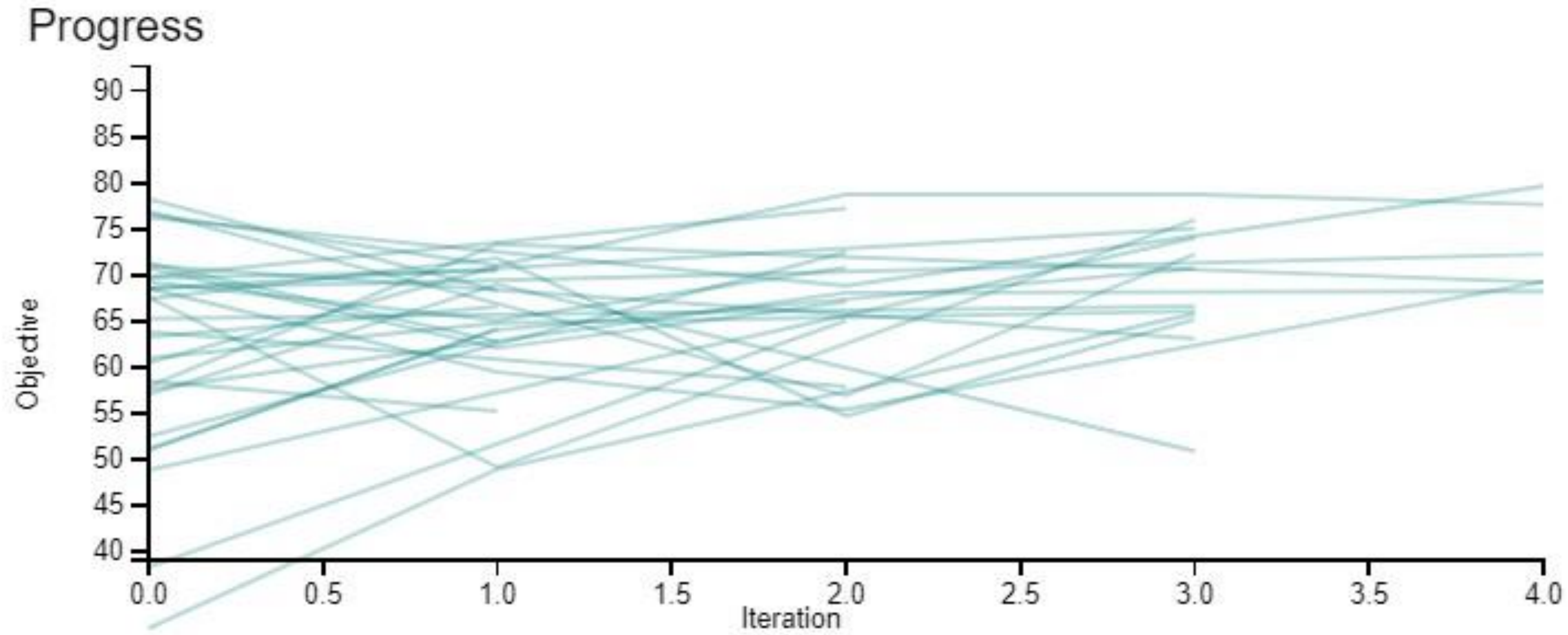
  Range = [0.0001, 0.1]

- Weight Decay

  Range = [0.01, 0.1]

- Network Depth

  Range = [2, 6]



Goals:

- Identify relationships: parameter values and objective score
- Narrow down ideal ranges for each parameter
- Test behavior with different algorithms

Parameters: LR, WD

Highest Accuracy: 70.8

- LR = 0.09907

Lowest Accuracy: 26.551

- LR = 0.08083

Algorithms—choosing and optimizing parameter values

Currently using: **GPyOpt Bayesian Optimization**

- Wrapper based on GPy
    - Gaussian modeling
- Good for many iterations

Loss Function: Currently using Categorical Cross Entropy, could consider customizing in the future.

Algorithms to consider in the future:

- **Asynchronous Successive Halving**—good for many hyperparametrs; stops early to reduce computational cost
- **Local Search**—analyzes small changes to the model; good when running fewer trials than GPyOpt

Moving Forward...

- Test the network on atmospheric datasets
- Push and identify limits of network parameters
- Verify previous results: AdamW vs Ranger

Moving Forward...

Unifying Workflow:

- Centralizing code for future use
- Implementing SHERPA
- Have been working with ProtoDUNE and NOvA data separately
- Translate from PyTorch dense tensors to MinkowskiEngine sparse convolution
    - Most activation functions are dense, so modify code to take only the sparse tensor's feature tensor, treat as dense

Preparing to test activation functions:

- LeakyReLU
    - Backpropogation
    - Downward slope for negative inputs
- SELU
    - ReLU for positive input, scaled exponential for negative input
    - Output: mean = 0, RMS = 1
- Swish
    - Bounded below, not above
    - Smooth

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Thank you!

Are there any questions?