Google Summer of Code

ML 4 SCI

MidTerm Update: Quantum Contrastive Representation Learning

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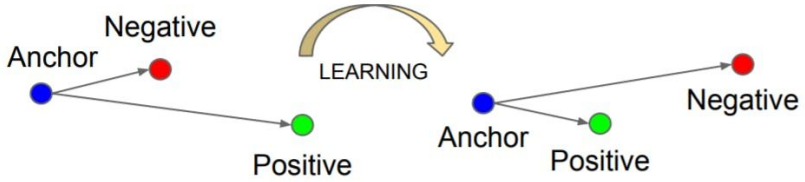
Project Overview



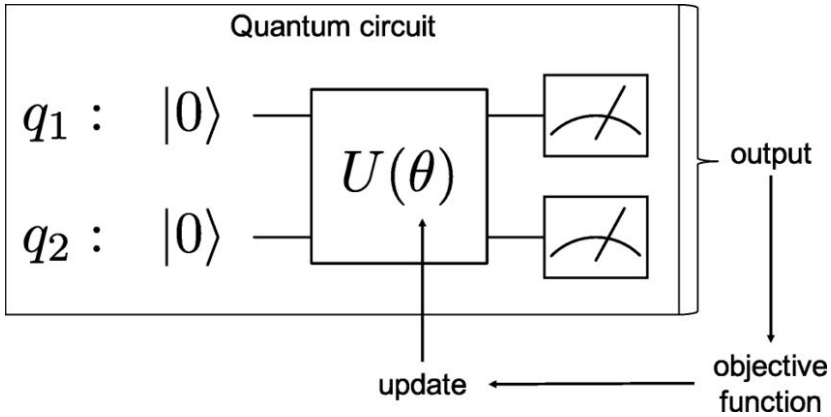
Contrastive Representation Learning: *Learn the latent space to predict a metric (distance) instead of a likelihood*

Objectives:

- Self-supervised Contrastive Learning
- Supervised Contrastive Learning

Methods:

- **Quantum Variational Circuits Encoder**
- Equivariant Network Encoder
- Data Augmentations



Datasets:

- MNIST
- HEP Data: Photon Electron Image, Quark Gluon Image, Quark Gluon Particle Cloud
- Molecule Data: QM7, QM9

Contrastive Losses

Temperature-Scaled CE Loss

$$\mathcal{L} = -\log \frac{\exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_j)/\tau)}{\sum_{k=1}^{2N} \mathbf{1}_{[k \neq i]} \exp(\text{sim}(\mathbf{z}_i, \mathbf{z}_k)/\tau)}$$

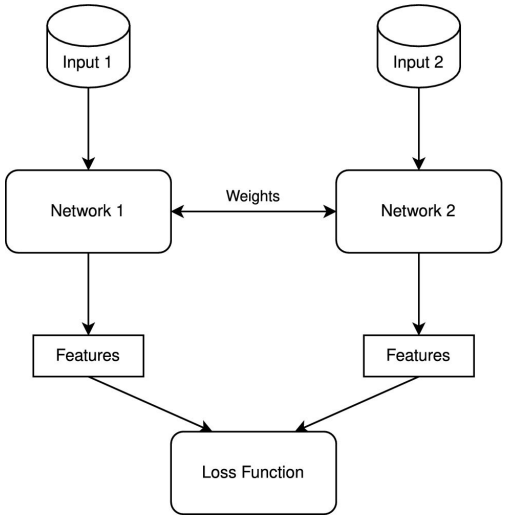
Pairwise Contrastive Loss

$$\mathcal{L} = \frac{1}{2N} \sum_{i=1}^{N} \left(y_i d^2 + (1 - y_i) \max(m - d, 0)^2 \right)$$

Fidelity Loss in QVC

For pure states *psi* and *phi*, the fidelity loss:

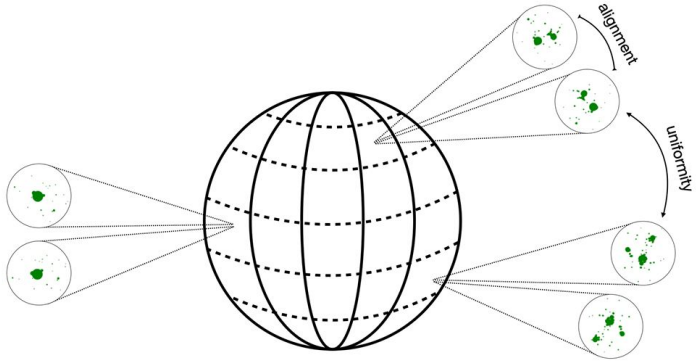
$$\mathcal{L}_{fidelity} = 1 - F(|\psi\rangle, |\phi\rangle)$$



Alignment and Uniformity in Contrastive Representation Learning

Alignment Loss: $\mathcal{L}_{align} = \frac{1}{N} \sum_{i=1}^{N} \|f(x_i) - f(x_i^+)\|^2$

- Distance between the embeddings of positive pairs
- Ensures similar pairs are close in feature space

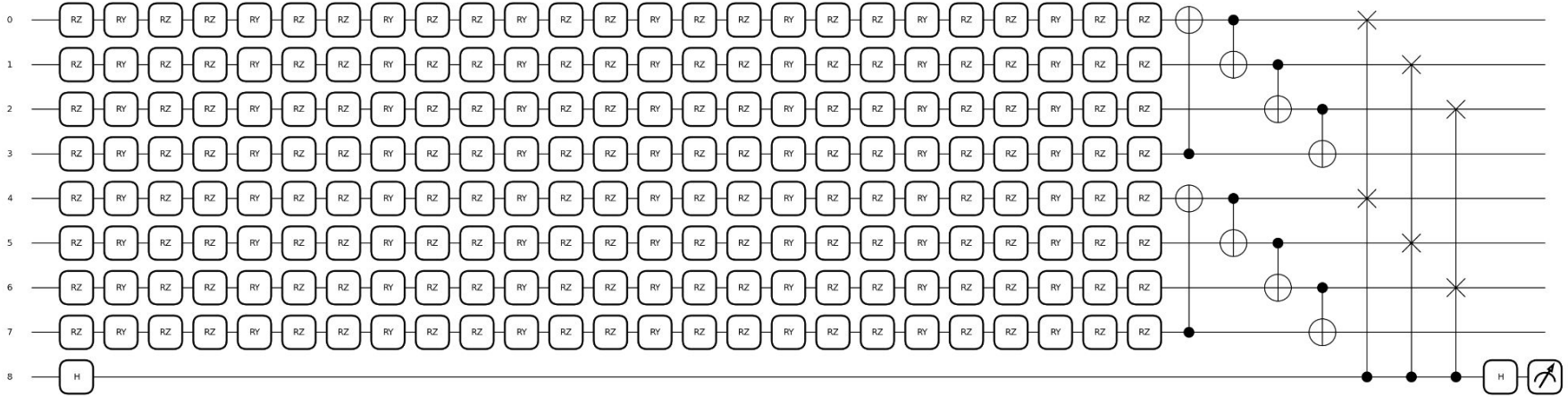


Uniformity Loss: $\mathcal{L}_{uniform} = \log \frac{1}{N^2} \sum_{i \neq j} \exp(-2\|f(x_i) - f(x_j)\|^2)$

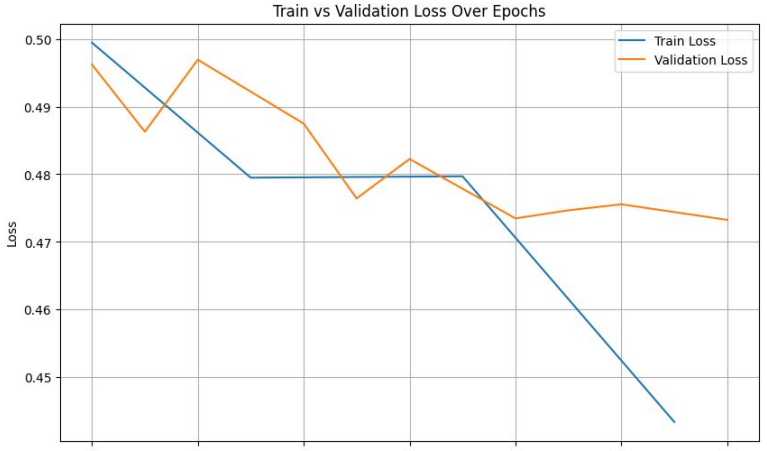
- Ensures that the feature embeddings are uniformly distributed over the feature space

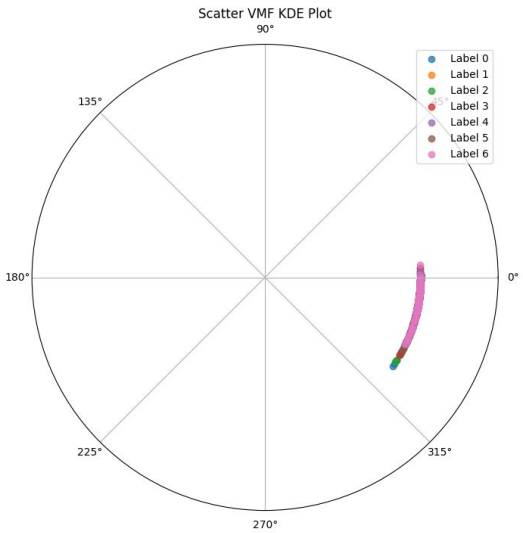
T. Wang and P. Isola, “Understanding Contrastive Representation Learning through Alignment and Uniformity on the Hypersphere.” arXiv, Aug. 15, 2022. doi: 10.48550/arXiv.2005.10242.

Quantum Reuploading CNN Contrastive Model

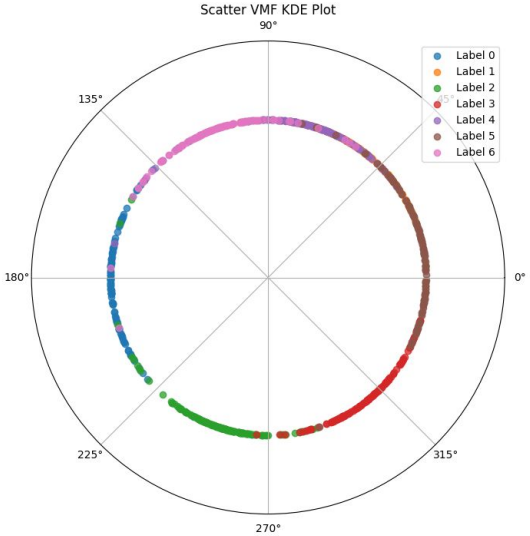



```
IMG_DIM = 10

DRCs = 1
EPOCHS = 10

KERNEL_SIZE = 5
STRIDE = 5

DATA_QBITS = 4 # int(((INPUT_DATA_SIZE - KERNEL_S
LATENT_QBITS = 3
AUX_QBITS = 1
```

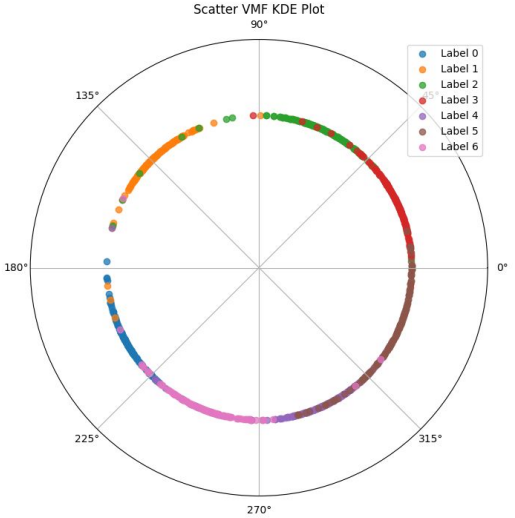




Untrained

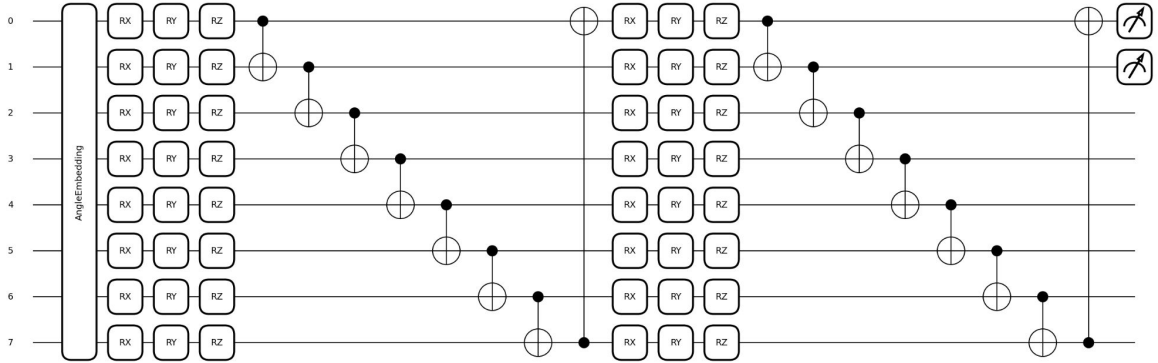


Quantum Head

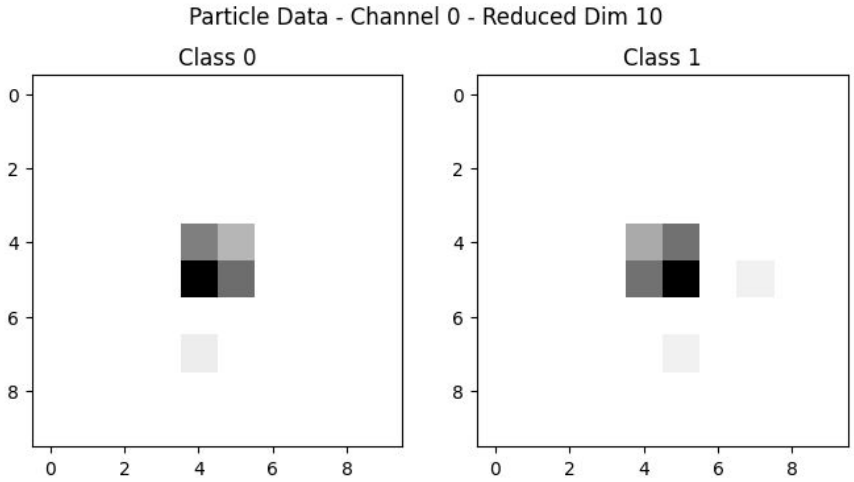


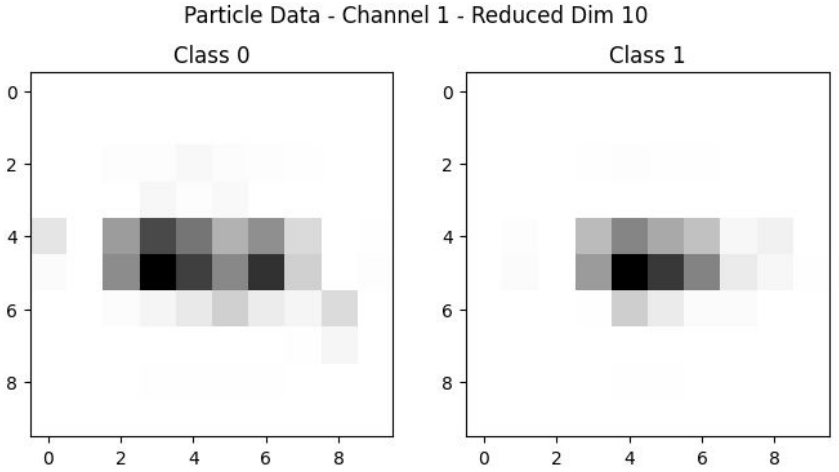
Classical Head

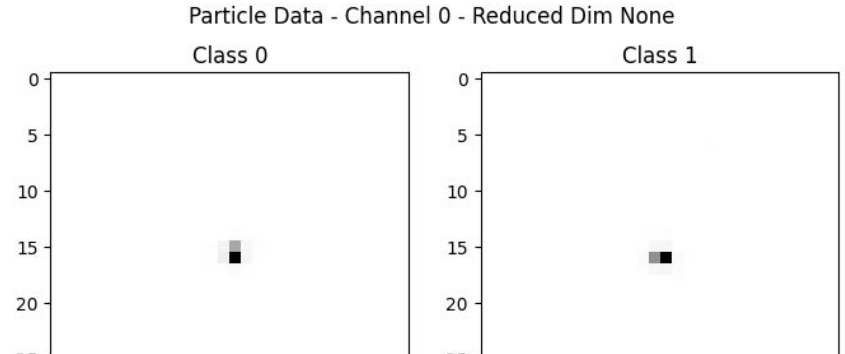
Classical and Quantum-Hybrid Models

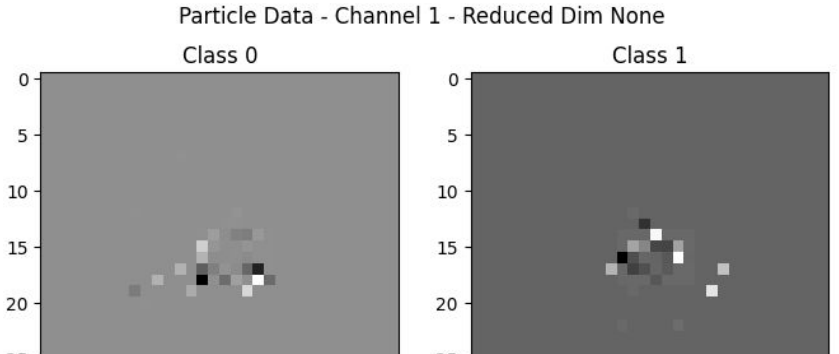


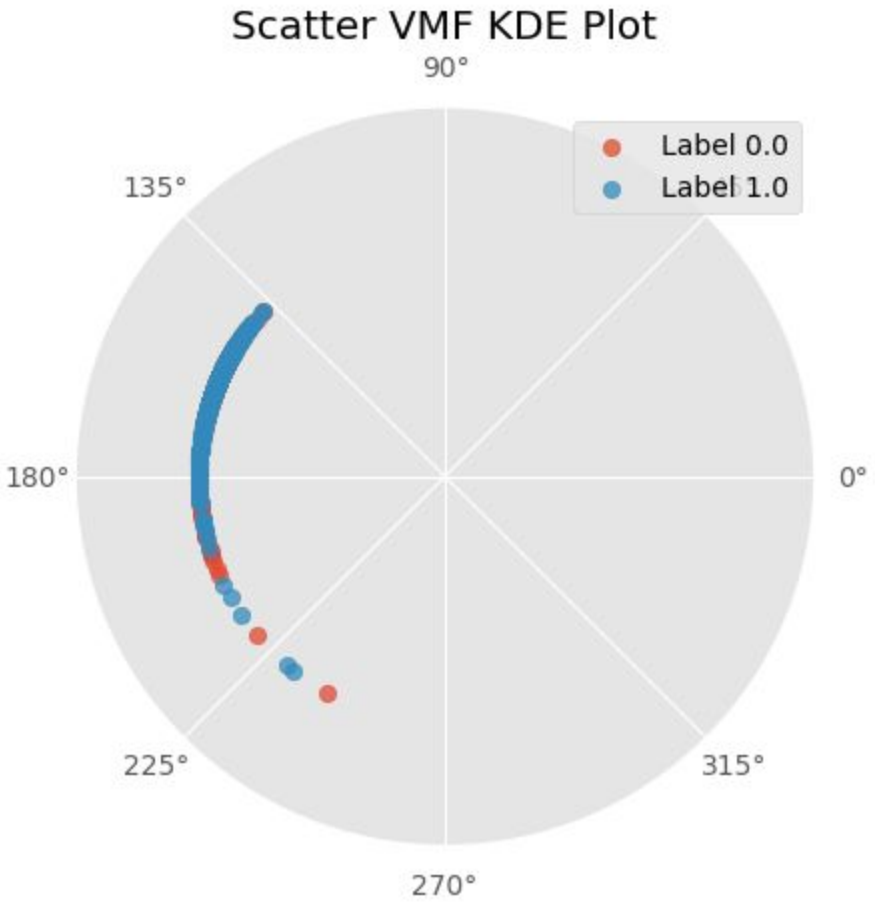
Photon - Electron Dataset

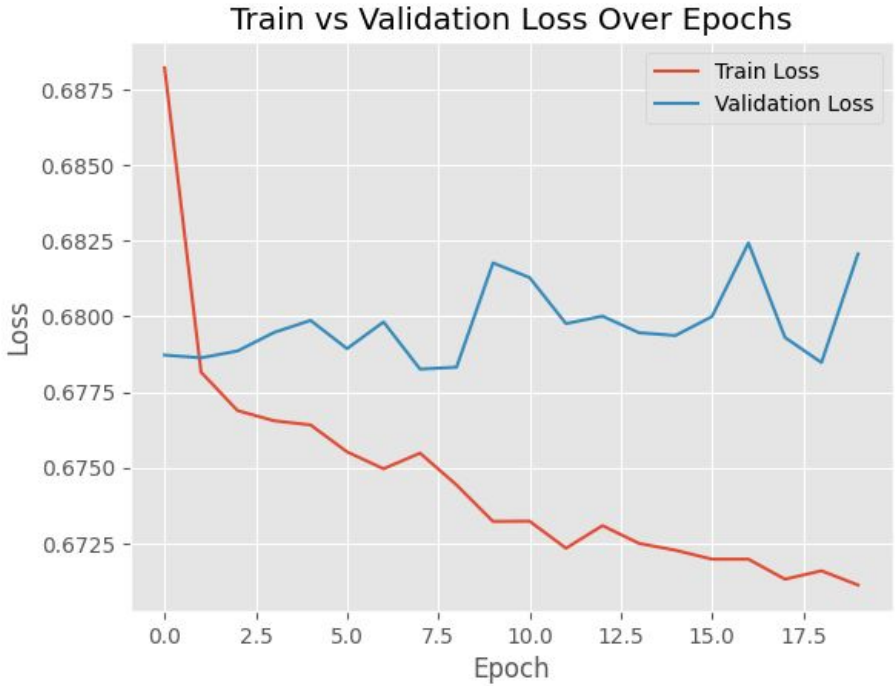




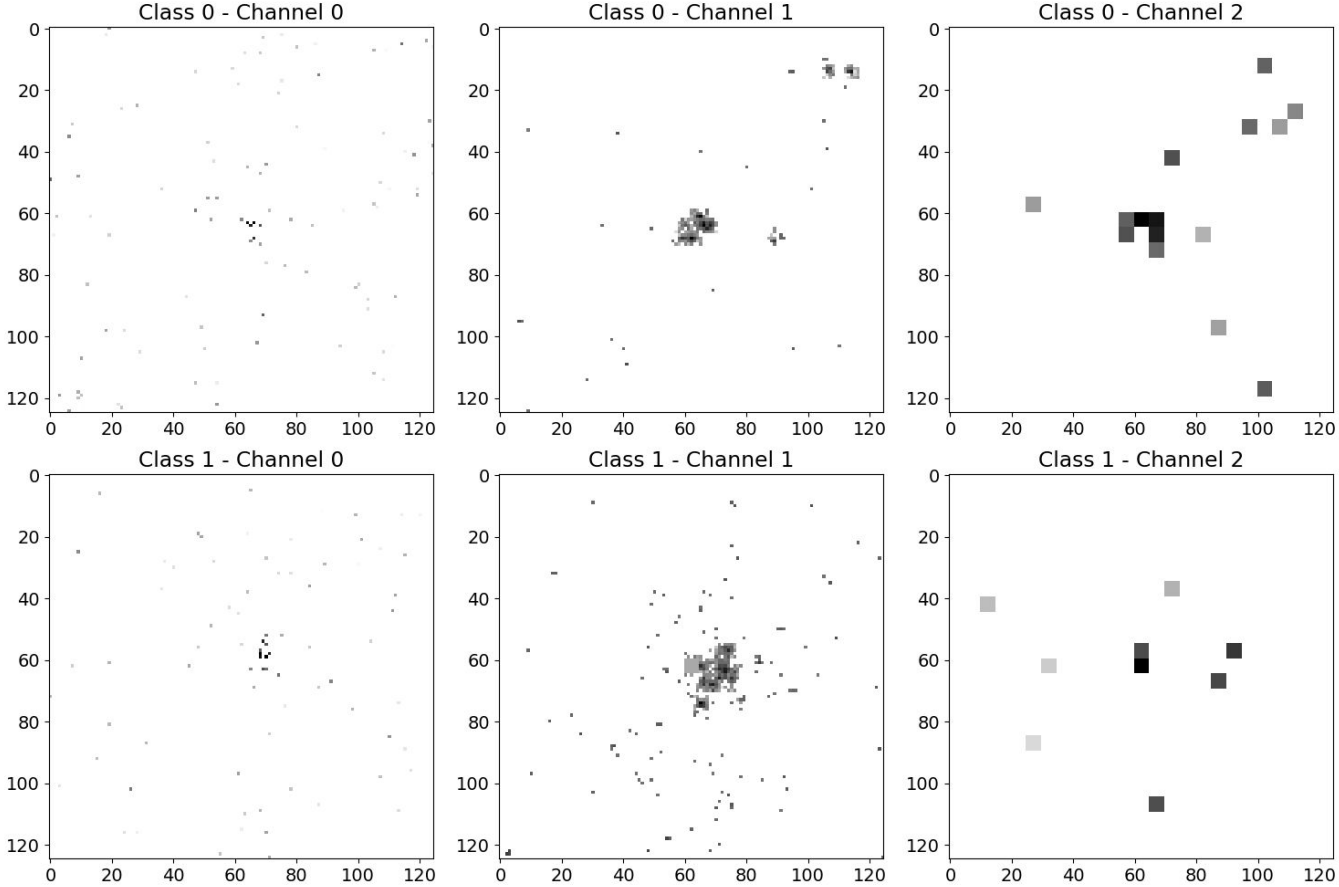




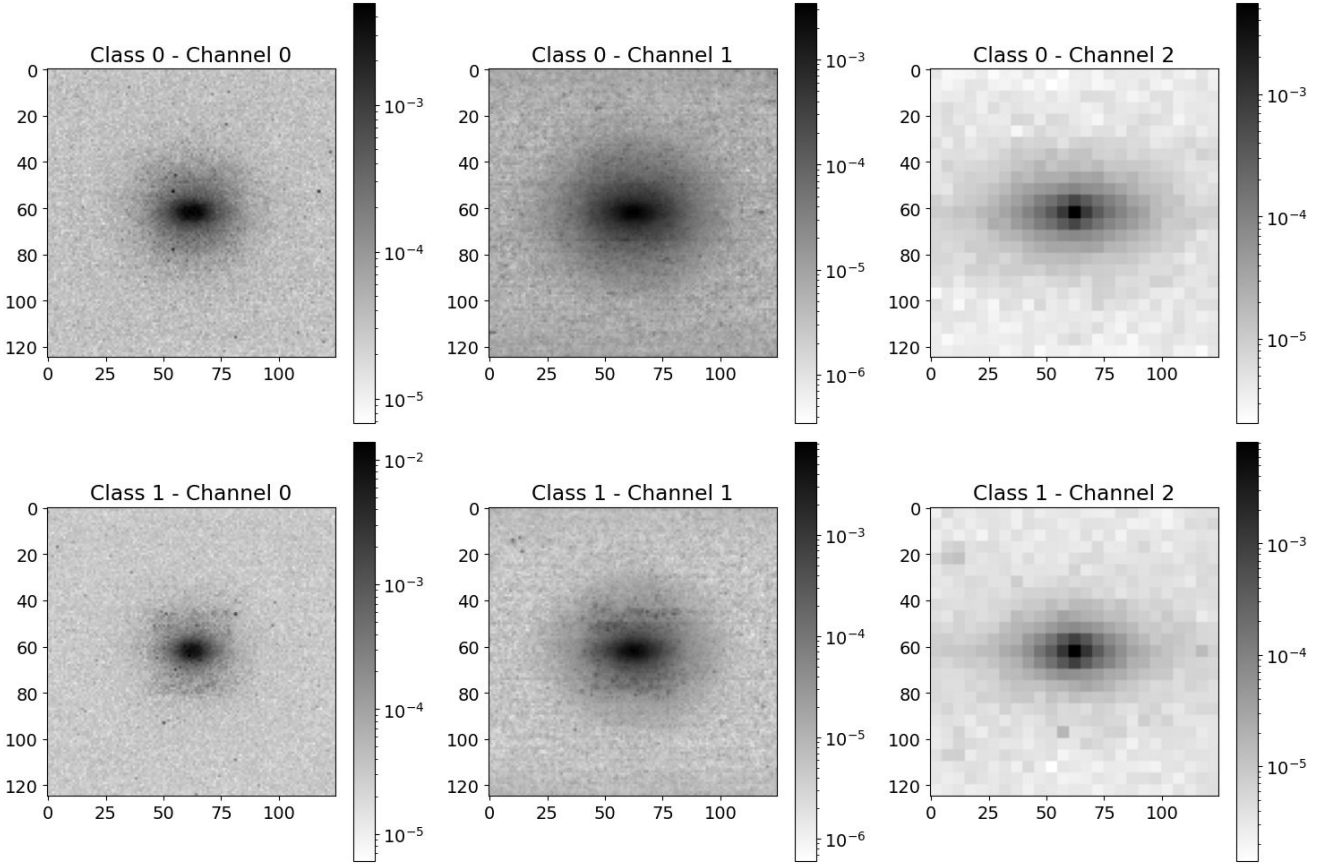

Scatter VMF KDE Plot
90°
135°
180°
0°
225°
315°
270°
Label 0.0
Label 1.0


Train vs Validation Loss Over Epochs
Train Loss
Validation Loss
Loss
0.6875
0.6850
0.6825
0.6800
0.6775
0.6750
0.6725
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Epoch

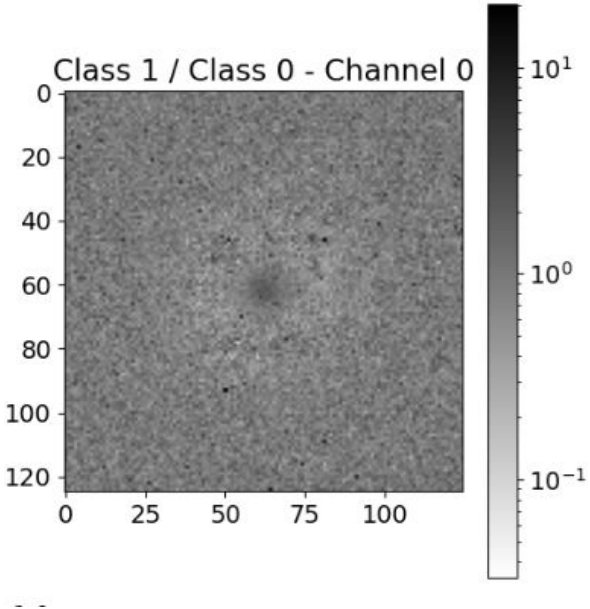
Quark Gluon Images Dataset

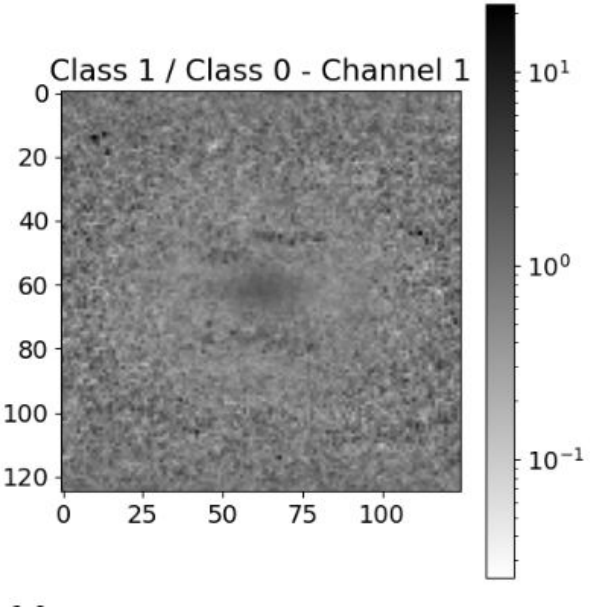


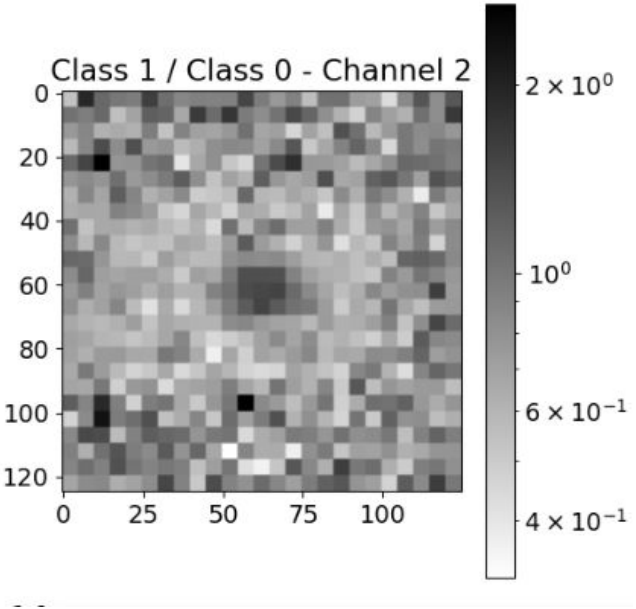
Quark Gluon Images Dataset



Quark Gluon Images Dataset







Self-Supervised Learning with Graph

- Rotation
- Momentum Perturbation
- Random (or Momentum Priority) Subsampling
- Noise Addition