HW4: Graph Neural Networks - Final Report

Objective

The task is to predict molecular properties using a Graph Neural Network. Molecules are represented as graphs with atoms as nodes and bonds as edges. The challenge lies in designing a performant GNN that generalizes well across diverse molecular structures.

Architecture & Enhancements

1. Model:

GIN (Graph Isomorphism Network)

- 3 stacked GINConv layers with ReLU activations
- BatchNorm after each layer
- Residual connection after second GIN layer
- Readout: concatenation of global **add**, **max**, and **mean** pooling
- Final MLP: 128-dim → GELU → dropout → regression output

2. Feature Engineering

- Degree of nodes (1D scalar) added to each node's features
- A virtual node with mean features connected to all other nodes
- Node features scaled with `StandardScaler` across train+test
- Edge index extended to include virtual edges (bi-directional)

3. Optimization & Regularization

- Adam optimizer

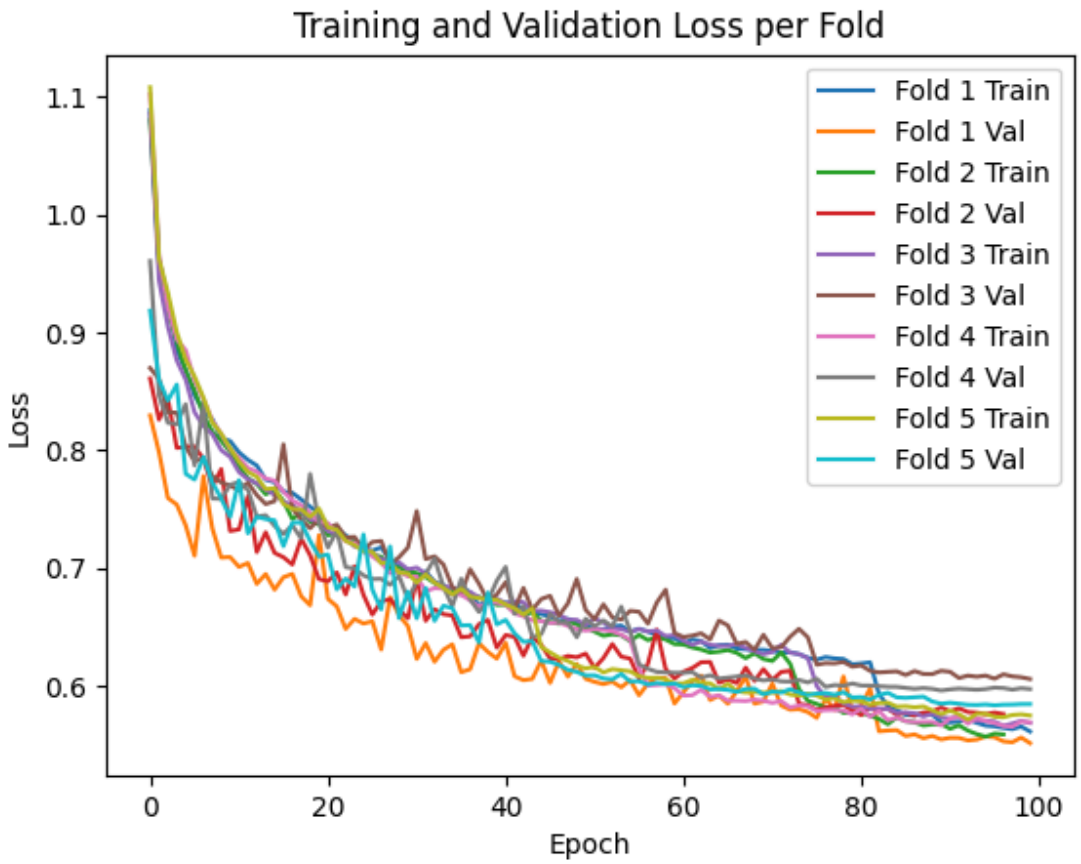
- Learning rate: `0.001133` (tuned via Optuna)
- Weight decay: `1.66e-5`
- Dropout: `0.45388`
- Early stopping with patience of 10 epochs
- Scheduler: `ReduceLROnPlateau` on validation MAE

4. Training Protocol

- 5-fold K-Fold cross-validation
- Train: Validation split = 80:20
- Batch size: 32

Results & Evaluation

Kaggle Score Achieved: MAE = 0.54260



Loss Curve Insights:

- Training and validation losses show a consistent downward trend.
- Minimal overfitting due to dropout and early stopping.
- Best performance typically reached by ~80th epoch.