Brain Graph Super-Resolution Challenge

DGL 2024 Kaggle Competition

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[Team: Edge Engineers]

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Introduction

Problem Statement

The challenge of predicting high-resolution brain connectivity graphs from low-resolution ones using generative Graph Neural Networks (GNNs).

Objectives

- Design a generative GNN model named EnGIN that accurately infers high-resolution brain graphs from low-resolution inputs.
- Ensure the model exhibits expressiveness, enabling it to capture the complex data of brain connectivity effectively.
- Achieve generalizability, allowing the model to accurately process unseen graphs.

Significant (Motivation)

- Inspired by the challenge of upgrading brain graph resolution while preserving intricate connectivity patterns—critical for advancing neuroscience research and clinical applications.
- Push the boundaries of GNN capabilities in brain connectivity analysis, leveraging a thorough literature review of existing methodologies.

Proposed Method: EnGIN Architecture

Solution Overview

Developed EnGIN, a cutting-edge generative GNN framework designed to upscale low-resolution brain graphs to high-resolution counterparts with unprecedented accuracy.

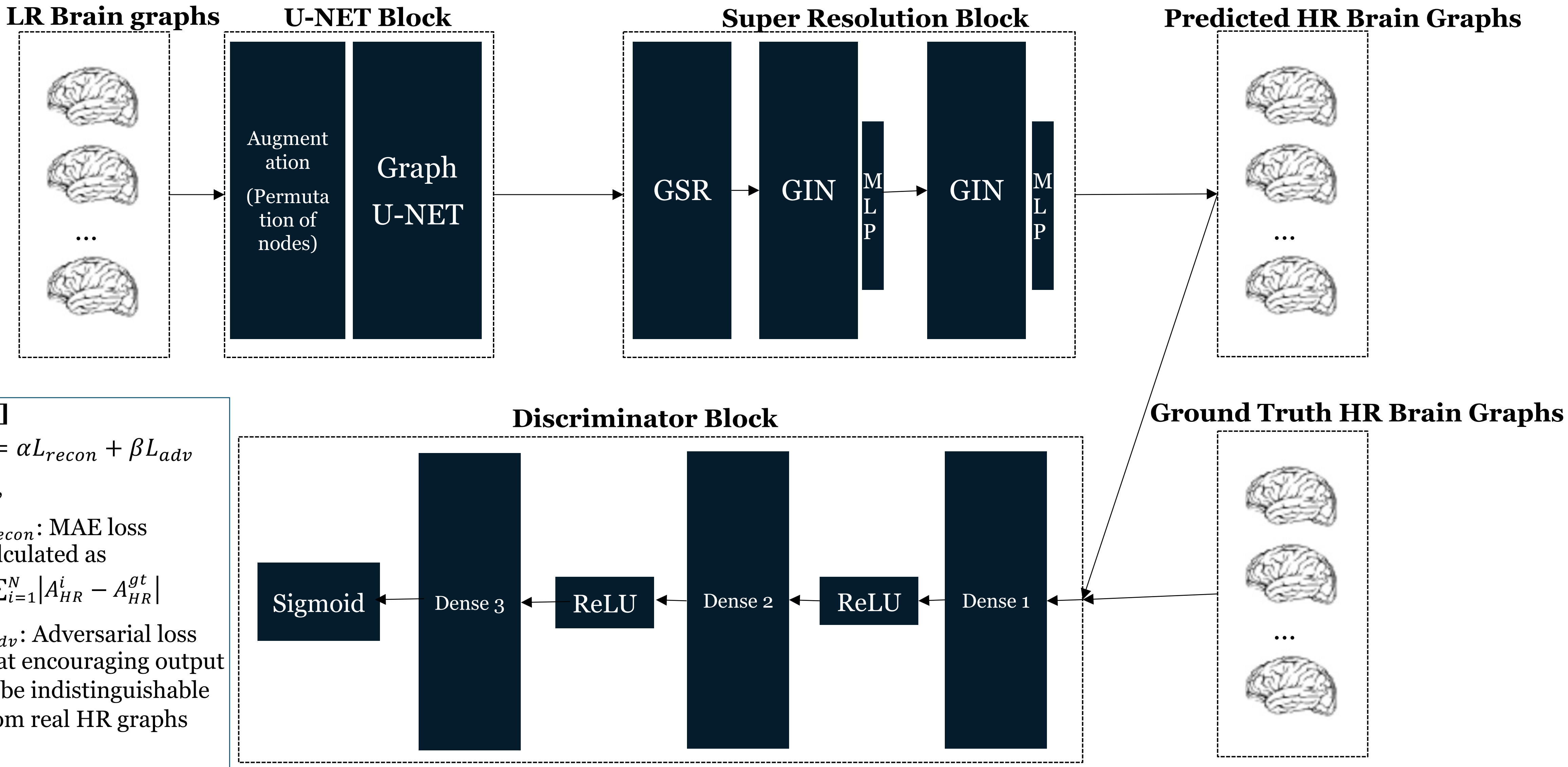
EnGIN Components

- **Graph U-NET Block:** The block facilitates the transition from node-centric models to graph-oriented processing for initial feature embedding.
- **Graph Super-Resolution Block:** Incorporates a GSR layer followed by GIN layers to upscale and refine the feature embeddings of the high-resolution output.
- **Discriminator Block:** Evaluates the fidelity of generated graphs against actual high-resolution graphs, guiding the GSR block towards producing more accurate predictions.
- **Ensemble Block:** Implements ensemble learning by averaging predictions from models trained with varied parameters to enhance accuracy and generalizability.

Engineering Logic

- **Graph U-NET Block:** Enables robust initial feature embedding for effective super-resolution.
- **GSR and GIN Layers:** Utilized for their ability to upscale input while preserving graph topology through advanced aggregation methods.
- **Discriminator Block:** Applies adversarial learning to align generated graphs with real high-resolution matrices.
- **Ensemble Approach:** Leverages multiple models to enhance prediction accuracy and generalizability.

Proposed Method: Main Figure I



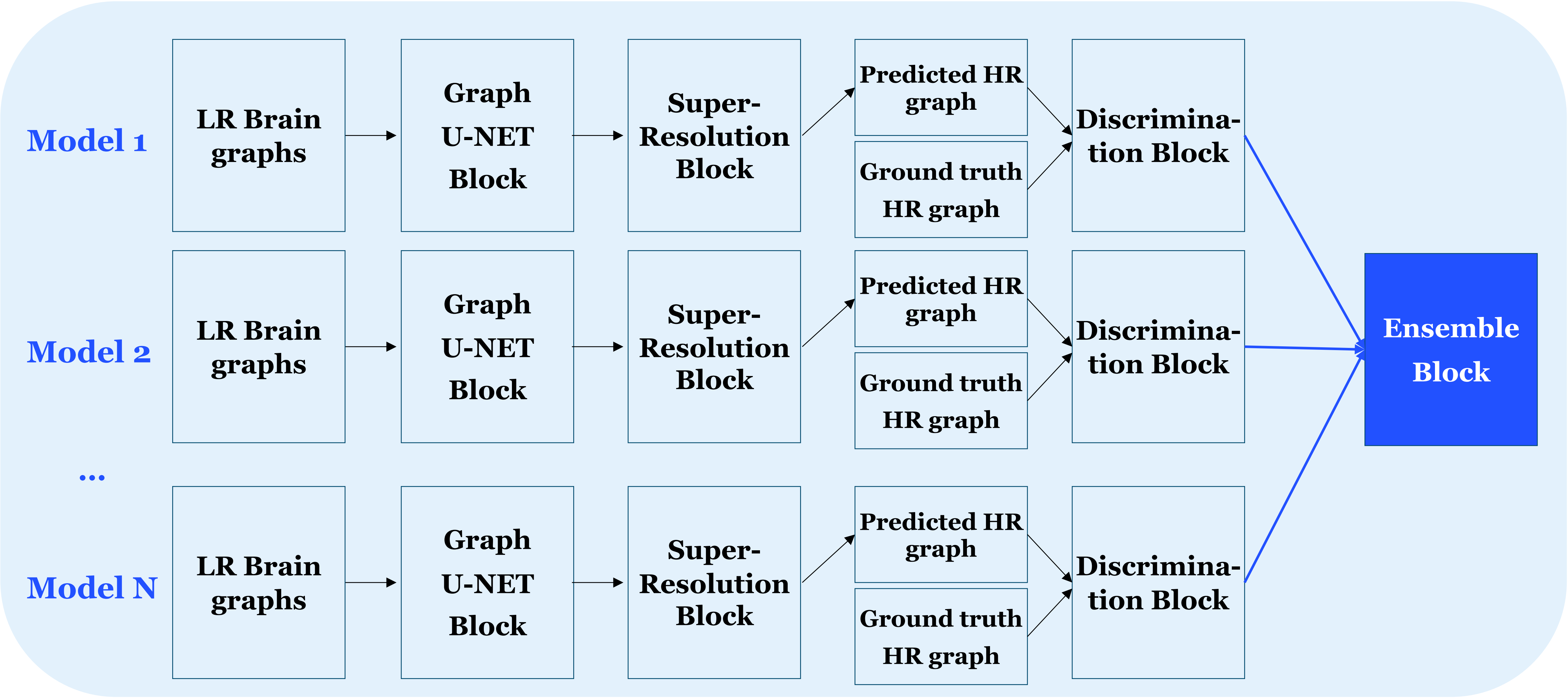
[Loss]

$$L = \alpha L_{recon} + \beta L_{adv}$$

where,

- L_{recon}: MAE loss calculated as $\frac{1}{N}\sum_{i=1}^{N}\left|A_{HR}^{i} - A_{HR}^{gt}\right|$
- L_{adv}: Adversarial loss that encouraging output to be indistinguishable from real HR graphs

Proposed Method: Main Figure II



Proposed Method (Main Equation)

$$A_{\mathrm{HR}}^{(i)} = \mathrm{Sigmoid}(\mathrm{Dense}_3(\mathrm{ReLU}(\mathrm{Dense}_2(\mathrm{ReLU}(\mathrm{Dense}_1(\mathrm{GIN}(\mathrm{GIN}(\mathrm{GSR}(\text{Graph U-NET}(LR))))))))))$$

$$\bar{A}_{\mathrm{HR}} = \frac{1}{N}\sum_{i=1}^{N} A_{\mathrm{HR}}^{(i)}$$

1. Graph U-NET block:

- *Input*: LR adjacency matric $A_{LR} \epsilon R^{N_{LR}*N_{LR}}$, where $N_{LR}$is the number of nodes in the LR graph.
- *Output*: Feature-embedded LR matrix $F_{LR} \epsilon R^{N_{LR}*D}$, where D is the feature dimension.

2. GSR block:

- *GSR layer:*
  - Upscales F_{LR} to a preliminary HR feature matrix using learned transformation weights.
  - *Equation*: $\mathrm{F}_{\mathrm{HR}}^{\mathrm{prelim}} = \mathrm{GSR}(\mathrm{F}_{\mathrm{LR}})$, where $\mathrm{F}_{\mathrm{HR}}^{\mathrm{prelim}} \epsilon R^{N_{HR}*D}$ and N_{HR} is the number of nodes in HR graph
- *GIN Layers:*
  - Refines F_{HR}^{prelim} to produce F_{HR}, the final HR feature matrix
  - *Equation*: $F_{HR} = GIN(F_{HR}^{prelim})$, applying GIN transformation iteratively.

3. Discriminator Block:

- *Input*: F_{HR} and the ground truth HR adjacency matrix A_{HR}^{true}.
- *Function*: Assesses the similarity between the generated graph and the real HR graph, providing feedback for model training.
- *Output*: Discriminator score indicating the performance of F_{HR}.

4. Ensemble Approach

- Ensemble prediction: Averages HR predictions from multiple models to obtain final HR graph.
- *Equation*: $\bar{\boldsymbol{A}}_{\boldsymbol{HR}} = \frac{1}{M}\sum_{i=1}^{M} A_{HR}^{i}$, where M is the number of models in the ensemble, and A_{HR}^{i} is the HR adjacency matrix predicted by the (i)-th model.

Data Augmentation

Data Augmentation/Processing Steps:

- **Edge Modifications:** Implemented *add_random_edges* and *drop_random_edges* to introduce and remove connections, enhancing data diversity.
- **Feature Shuffling:** Used *shuffle_node_features* to randomize feature order, promoting model robustness against feature position bias.

Feature Initialization

AGSR-NET and Advanced Techniques:

- **Weight Variable Glorot:** Initializes weights within a specific range by following the Glorot uniform distribution principle. This aims to maintain activation variances and back-propagated gradients at a stable level across layers.
- **Centrality-Based Initialization:** Explored node centrality metrics to assign initial feature values, hypothesizing that nodes with higher centrality might play pivotal roles in graph structure.

Results: Model Training

Hyper-parameters and Training

•**Learning Rate:** Started with **0.0001**, decreased by **10%** every 50 epochs based on validation loss plateau. (StepLR)

•**Epoch**: Over **200 epochs per fold** with **retraining** on the entire dataset to optimizer accuracy

•**Dropout Rate:** Evaluated rates from 0.1 to 0.5 in 0.1 increments, selecting **0.3** to prevent overfitting without overly dampening feature learning.

•**One-sided Label Smoothing:** Replaced the 1.0 (target) classifier with slightly **smoother rates**, selecting 0.9 to reduce certainty in-turn producing a much more robust, model.

Training time and Resource Usage

- Total training completed in approximately **50 minutes** across all folds, demonstrating EnGIN's efficiency.
- RAM usage was efficiently managed, averaging between **150-200MB** per epoch, underscoring the model's scalability.

Results: Evaluation and Discussion

Evaluation Measures and Results:

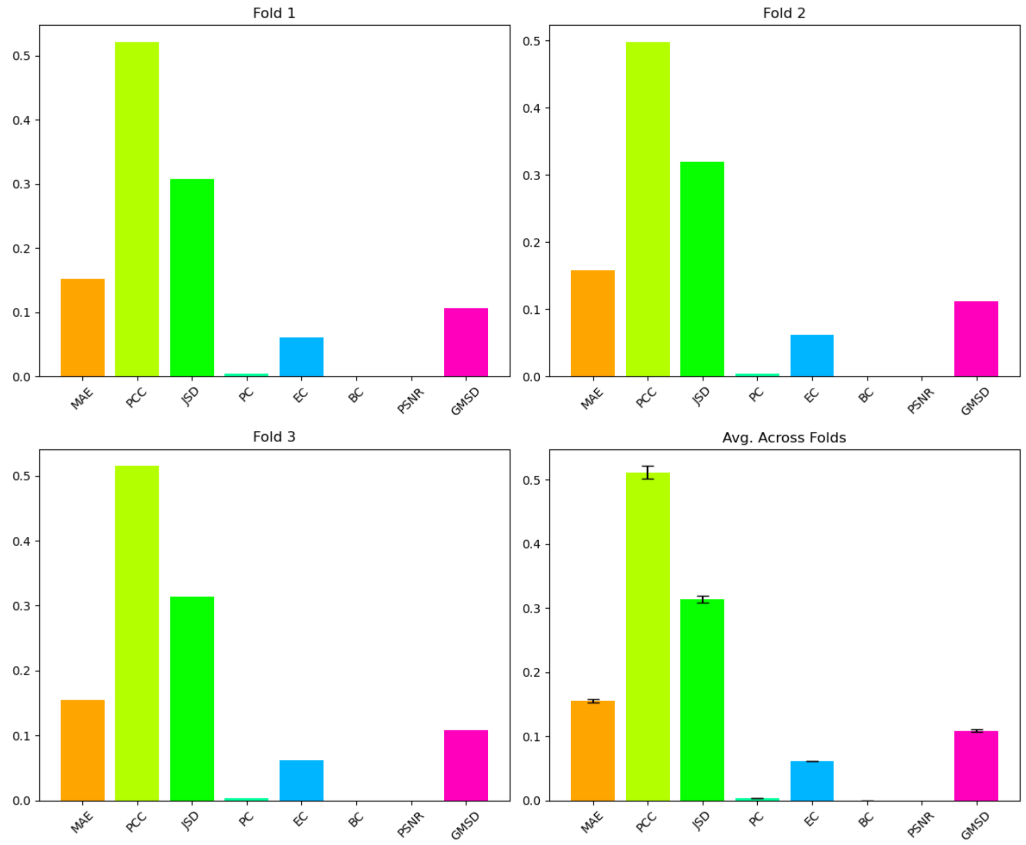
• **Cross-validation Metrics:** Demonstrated consistent performance across folds with Mean Absolute Error (MAE) around 0.155, Pearson Correlation Coefficient (PCC) approximating 0.51, and Jensen-Shannon Divergence (JSD) near 0.31, highlighting EnGIN's balanced approach to precision and correlation in graph predictions.

• **Performance Metrics:** Showed negligible Path Count (PC) and Betweenness Centrality (BC), and a Graph Matching Similarity Distance (GMSD) between 0.106 and 0.111, indicating a nuanced understanding of graph topology.

Training Insights:

• **Error Reduction and Loss Minimization:** Observed a consistent decrease in error rates from 12.7% to approximately 1.05%, alongside loss minimization from an initial 1.018 to a stable range around 13.08 over 200 epochs, evidencing effective model learning and convergence.

• **Training Dynamics:** Highlighted a notable transition from early error fluctuations to stable loss reductions and error minimization, indicative of the model's adaptive learning capability over successive epochs.



Discussion, Conclusion & Future Work

Challenges and Methodology Effectiveness

Challenges Overcome:

Addressed issues with model convergence and the intricacies of embedding features effectively, underscoring the resilience and adaptability of our approach

Methodology Insights:

The model's proficiency in generating accurate high-resolution brain graphs was affirmed, with ongoing efforts to amplify its generalizability and operational efficiency.

Conclusions and Future Directions

Project Achievements:

EnGIN has markedly advanced the field of brain graph super-resolution, showcasing the potential of generative GNN in complex domain.

Looking Ahead:

Future endeavours will focus on:

1. **GNN Variant Exploration**: Delving into more sophisticated GNN architectures to further refine prediction accuracy.
2. **Ensemble Method Enhancements**: Innovating ensemble strategies to elevate model robustness and accuracy
3. **Broader Applications**: Extending EnGIN's methodology to additional tasks across diverse fields.