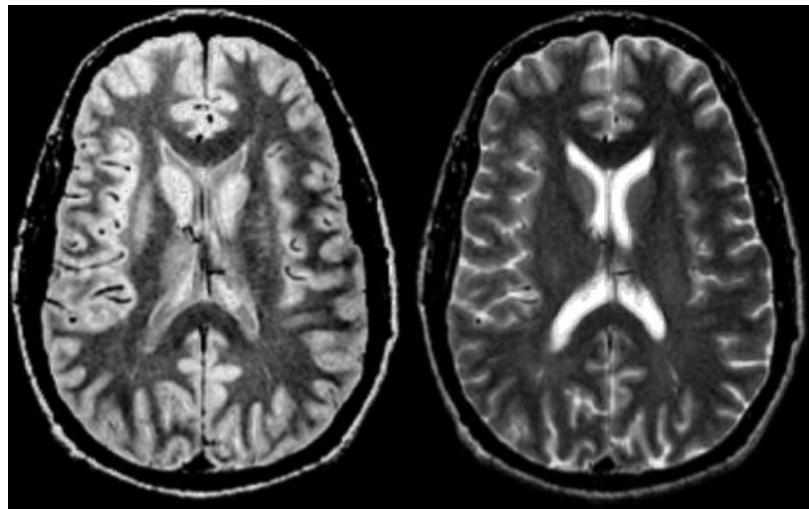


# GNN for Brain Network Analysis

Xuan Lin, Nilay Shah, Nima Zaghari, Daisy Zheng

# Motivation

- Identify relationships between brain regions and specific neurological disorders
- GNNs have been used to perform graph classification on brain networks composed from fMRI data
- Seek to validate agnosticity and robustness of framework and further increase its interpretability



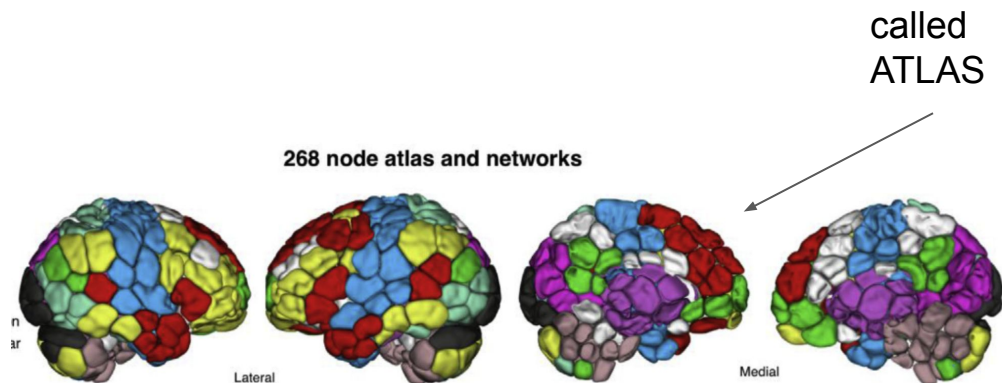
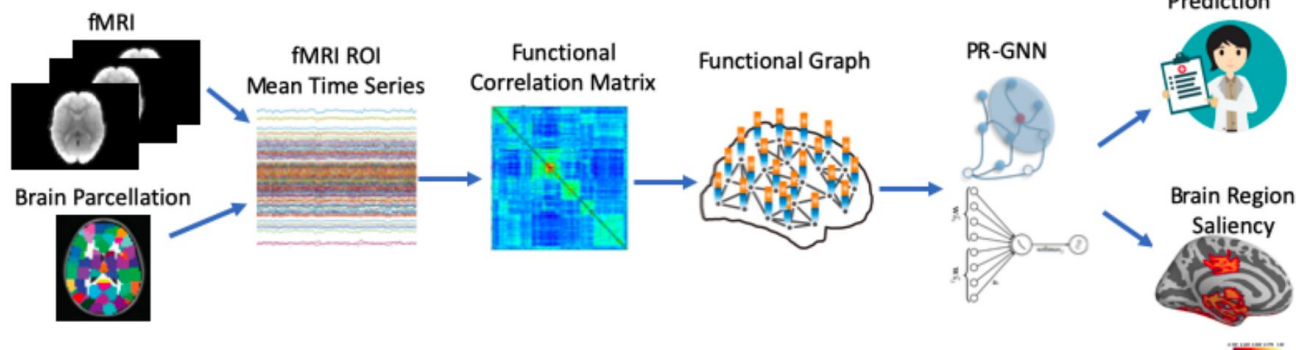
# Problem Definition

Input: brain fMRI data

Output: Predictions/Salient Regions

Pipeline:

fMRI  $\xrightarrow{\text{pre-process}}$  Graph  $\xrightarrow{\text{GNN}}$  Predictions



# Experimental Data

We utilized fMRI datasets from the following databases:

- ABIDE (Autism Brain Imaging Data Exchange)
  - fMRIs from neurotypical individuals and individuals with ASD
  - 539 individuals suffering from ASD and 573 control
- HCP (Human Connectome Project)
  - rfMRI, tfMRI, dMRI, and connectome data from healthy individuals
  - 1113 subjects 7 tasks - Gambling, Language, Motor, Relational, Social, Working Memory, Emotion



# Data Pre-processing

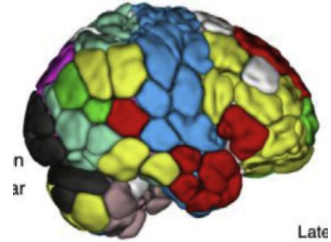
ABIDE(Autism Brain Imaging Data Exchange) - 116 ROIs

HCP(Human Connectome Project) - 268 ROIs, needs pre-process

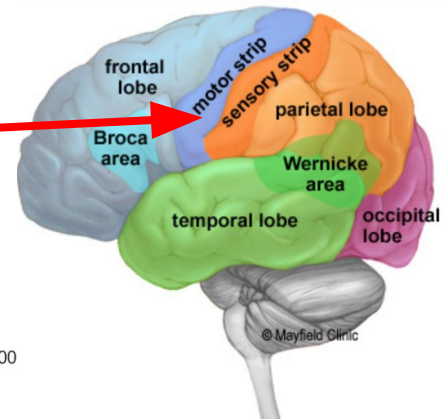
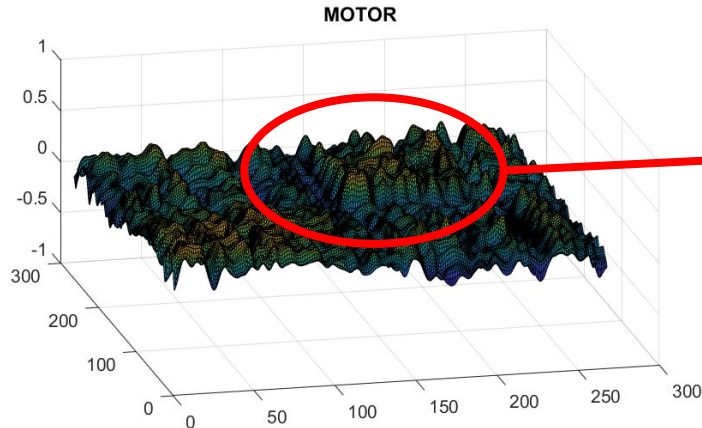
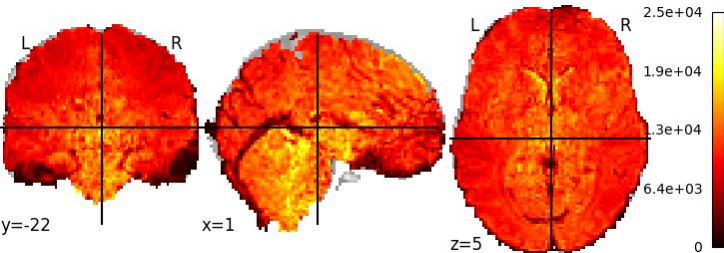
Average time series for each ROI  $\Rightarrow$  Correlation matrix

Node attributes: correlation coefficients relative to other nodes

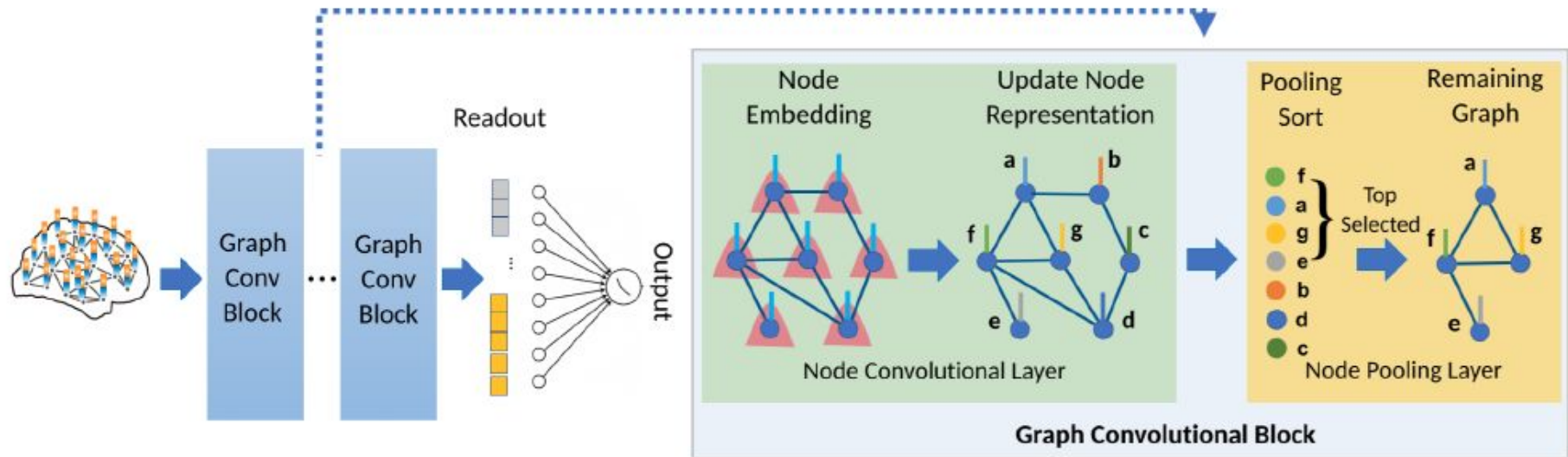
Edges: top 10% positive



268 node ATLAS



# Network Architecture



# Solution

- Proposed GNN structure may not be robust among atlases
- Generates different results with different atlases
- We use different preprocessing techniques of the data to validate and improve the robustness of the model, which is important for ensuring consistency of results

# Hyperparameter Tuning through Bayesian Optimization

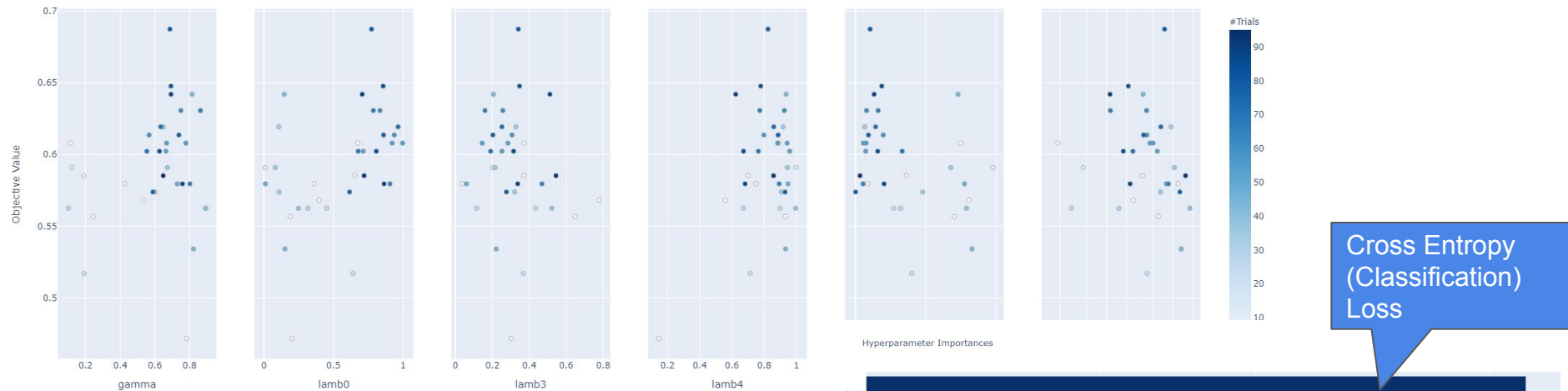
- Employed Optuna, a hyperparameter optimization framework
- Uses the Tree-structured Parzen Estimator) algorithm
- Key Hyperparameters considered:
  - Learning Rate: controls amount that weights are updated during back-propagation
  - Gamma: multiplicative factor for learning rate decay
  - Lambda 0 - hyperparameter controlling weight of negative log likelihood loss
  - Lambda 1 - hyperparameter controlling weight of distance loss
  - Lambda 2 - hyperparameter controlling weight of consistence loss

$$L_{total} = L_{ce} + \lambda_1 \sum_{l=1}^L L_{Dist}^{(l)} + \lambda_2 \sum_c^C L_{GLC}^c$$



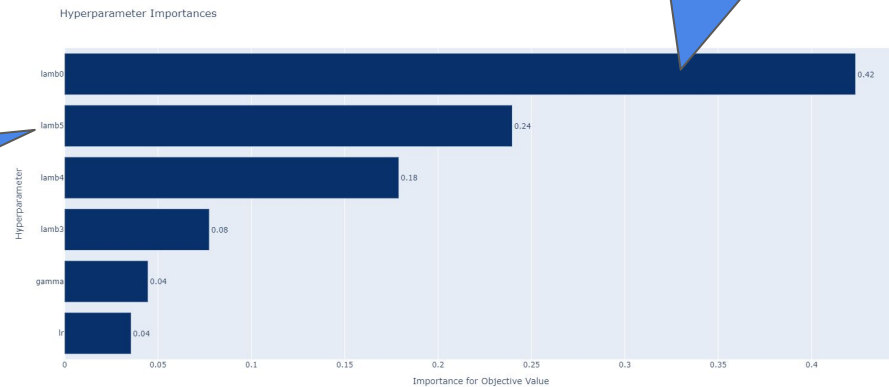
# Hyperparameter Tuning Results

Slice Plot



Cross Entropy  
(Classification)  
Loss

Consistence  
Regularization



# Evaluation

| Dataset | Classification Accuracy |
|---------|-------------------------|
| HCP     | 39%                     |
| ABIDE   | 63%                     |

|          | Predict HC | Predict ASD |
|----------|------------|-------------|
| True HC  | 20         | 15          |
| True ASD | 8          | 35          |



# Discussion and Conclusions

## Future direction

- Increase interpretability of results (add GNN-Explainer)

## Summary

- Graph classification of brain fMRI scans
  - ASD (binary classification)
  - Tasks (multiclass classification)
- Extended the model to handle multiclass classification
- Evaluated model robustness over new datasets, brain atlases, and preprocessing flows
- Attached hyperparameter search framework to the validation process

# References

Cameron Craddock, Yassine Benhajali, Carlton Chu, Francois Chouinard, Alan Evans, András Jakab, Budhachandra Singh Khundrakpam, John David Lewis, Qingyang Li, Michael Milham, Chaogan Yan, Pierre Bellec (2013). The Neuro Bureau Preprocessing Initiative: open sharing of preprocessed neuroimaging data and derivatives. *In Neuroinformatics 2013, Stockholm, Sweden.*

*<https://www.humanconnectome.org/study/hcp-young-adult/document/extensively-processed-fmri-data-documentation>*