

# Codes and Data Availability

## Data Availability

The data is collected in-house and due to proprietary reasons, the data cannot be released.

## Codes

The following is a short description of all the codes that are used and uploaded with the submission.

Our codes contain 6 different folders. Here, we describe each of these folders along with some description about the files within each folder.

### Preprocessing

The codes within this folder have been used to generate the data which is used in repeated 10-fold cross validation and during pretraining.

**create\_train\_test\_gcn\_joint\_mode.m:** This matlab code is used to generate the training and validation data which is used during pretraining.

**create\_multiple\_runs.m:** This matlab code is used to generate the training, validation, and test split of out imaging genetics data which are used for repeated 10-fold cross validations.

**cv\_partition.m:** This code is used to generate train and validation indices.

**generate\_training\_nback.m:** Here we generate the contrast maps of our training Nback data which are used as imaging inputs to our model.

**generate\_training\_sdmr.m:** Here we generate the contrast maps of our training SDMT data which are used as imaging inputs to our model.

**generate\_testing\_nback.m:** This generates the contrast maps of out testing Nback data.

**generate\_testing\_sdmr.m:** This generates the contrast maps of out testing SDMT data.

## Pretraining

The codes within this folder are used to pretrain the genetic branch and the classifier of GUIDE.

**wrapper.py:** This python code is used to train the genetic branch and the classifier of our model. We save the performance for each epoch which are later used.

**find\_checkpoints.m:** Here we track the validation performance to find the early stopping point.

**model\_random.py:** The model architecture of the genetic branch and classifier of GUIDE.

**net\_train.py, net\_test.py:** These scripts used to train and test our model.

## Cross Validation

The codes within this folder are used to cross validate GUIDE. The performance obtained here is shown in Table. 1.

**wrapper\_img.py:** We warm start our model and train it on the imaging-genetics data in repeated 10-fold validation setting. This script trains the model, saves the intermediate results, plot them, and also store the model parameters as checkpoints.

**model\_joint.py:** Full model architecture of GUIDE.

**net\_train\_joint.py:** The script to train the model using backpropagation.

## Compare Random Graphs

The codes within this folder are used to train HG-ACN, and HG-DCN with random graphs.

**wrapper.py:** This python script is used to train the genetic branch using random graph embedding. We save the performance for each epoch which are later used.

**find\_checkpoint.m:** Here we track the validation performance to find the early stopping point.

**run\_checkpoint\_on\_img\_gen\_data.py:** Using the checkpoint model we evaluate the performance over the 208 test data as described in Section. 3.6 of manuscript.

**run\_checkpoint\_on\_training\_img\_gen\_data.py:** Using the checkpoint model we evaluate the performance over the training data.

**net\_train.py, net\_test.py:** These scripts used to train and test our model.

**model\_random.py:** The model architecture of the genetic branch.

### Bayes vs kshap

**Guide\_importance -> guide\_topk\_importance.py:** This python script is used to identify top-K imaging features using Bayes importance. They are then used to mask the test data of each fold. The script saves the testing performance which is later compared with K-SHAP.

**Shap\_importance -> shap\_importance.py:** This python script is used to identify top-K imaging features using K-SHAP. This script stores the testing performance and the K-SHAP values of each feature which are later used for comparison, as described in Section. 3.6 of manuscript.

**evaluate\_performance.m:** This script identifies the early stopping epoch for each fold based on lowest validation loss.

**importance\_compare.m:** It compares and plots the testing performance as shown in Figure. 2 of manuscript.

**guide\_bayes\_cross\_cosine:** Plots the pairwise cosine similarity across fold for Bayes feature selection scheme.

**shap\_cross\_cosine:** Plots the pairwise cosine similarity across fold for K-SHAP feature selection scheme.

### Identifying Pathways

This set of codes are used to identify paths that exist between each root node and leaf node and are associated with the disorder.

**wrapper.py:** This python script train GUIDE over multiple random subsets of the data as explained in Section. 3.6 of the manuscript.

**find\_checkpoint.m:** Here we track the validation performance to find the early stopping point.

**extract\_iterations.py:** This python script uses the checkpoint models of GUIDE to store interaction scores between each pair node.

**find\_all\_path.py:** It finds and stores all possible paths that exist between each root node and each leaf node.

**remaining\_paths\_to\_run.py:** It prepares the paths that will then fed to logistic regression model to identify potential discriminative pathways.

**lrt\_logistic\_regression\_multiple\_pretrain.py:** This takes in the patient specific interaction scores as input and runs logistic regression followed by likelihood ratio test. The p-values of the statistical test are stores for further evaluation.

**pathway\_importance.m:** This script identifies statistically significant pathways.

**embed\_pathway\_and\_display.py:** Embeds the pathway information using t-SNE and display 10 different categories of pathways.

### Auxilliary Codes

**convert\_to\_cpu.py:** Sends a tensor to CPU.

**convert\_to\_gpu.py:** Sends a tensor to GPU.

**convert\_to\_gpu\_and\_tensor.py:** Converts an array to tensor and sends to GPU.

**convert\_to\_gpu\_scalar.py:** Converts a scalar to tensor and sends to GPU.