Unsupervised Cross-Domain Functional MRI Adaptation for Automated Major Depressive Disorder Identification – Supplementary Materials

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Besides the experimental results reported in the main text, in the following, we present the detailed process of parameter tunning for two competing methods and report the corresponding results with different parameter values. To validate the generalization ability of the proposed unsupervised cross-domain fMRI adaptation (UFA-Net) method, we directly apply a well-trained UFA-Net to five unseen sites from the REST-meta-MDD Consortium [1]. We also test our method on the public Autism Brain Imaging Data Exchange (ABIDE) initiative in differentiating autism spectrum disorder (ASD) patients from healthy controls (HCs). More details can be found in the following.

1. Parameter Tuning Process

For **BC-SVM-N-G**, the node-based features and graph-based topology features are concatenated and fed into an SVM model for MDD diagnosis. We try three different SVM kernels (*i.e.*, polynomial, Gaussian, and linear) for classification, and their prediction results are reported in Table SI. From Table SI, we can see that the AUC score in linear SVM is much higher than that in polynomial or Gaussian SVM. Even though Gaussian SVM has a higher ACC value than the other two models, its SEN and SPE scores are much imbalanced. Therefore, we finally choose the linear SVM as the competing method.

For **DANN**, the adjustable hyperparameters are (1) learning rate (LR) and (2) epoch for step decay (ESD), where ESD=30 denotes that LR drops every 30 epochs. LR and ESD are tuned within the range of {0.0001, 0.001, 0.01, 0.1} and {20, 30, 40, 50} respectively, and the corresponding classification results are shown in Table SII. From Table SII, we can see that DANN-0.01-50 generally achieves the superior performance, especially in terms of ACC, SEN, and PRE, which is finally chosen as the competing method.

Table SI: Results of the BC-SVM-N-G with different kernels in the task of MDD vs. HC classification. Best results are shown in bold.

Method	ACC (%)	AUC (%)	SEN (%)	SPE (%)	PRE (%)
BC-SVM-N-G (polynomial kernel)	49.32	46.79	51.35	47.30	49.35
BC-SVM-N-G (Gaussian kernel)	54.05	46.09	66.22	41.89	53.26
BC-SVM-N-G (linear kernel) (Ours)	52.03	55.50	52.70	51.35	52.00

2. Results on Unseen MDD Sites

To validate the generalization capability of the proposed UFA-Net, we directly apply the model trained with Site-20 (source domain) and Site-1 (target domain) on five unseen/held-out MDD sites from the REST-meta-MDD Consortium [1], without any model retraining or finetuning. That is, no test data/domain is used for model training. In this group of experiments, we only select sites with a number of subjects greater than 100 as unseen test domains. The classification results yielded by the proposed UFA-Net on these five MDD sites are shown in Fig. SI. From the figure, we can observe that the UFA-Net generally achieves satisfactory classification results. Although data acquisition parameters (*e.g.*, scanner type, receive coil, voxel size) of these sites are different from those of source and target domains¹ used in model training, our method

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DANN-LR-ESD	ACC (%)	AUC (%)	SEN (%)	SPE (%)	PRE (%)
DANN-0.0001-20	51.49±3.74	51.42±2.91	52.97±5.09	50.00±6.62	51.52±3.68
DANN-0.0001-30	51.49±3.74	51.42 ± 2.91	52.97±5.09	50.00±6.62	51.52 ± 3.68
DANN-0.0001-40	51.62±3.57	51.43±2.92	53.24±5.24	50.00±6.62	51.64±3.54
DANN-0.0001-50	51.62±3.57	51.42±2.89	53.24±5.24	50.00±6.62	51.64±3.54
DANN-0.001-20	51.22±3.24	51.35±2.83	53.24±5.51	49.19±5.96	51.18±3.19
DANN-0.001-30	51.35±3.36	51.37±2.71	52.97±5.69	49.73±6.36	51.34±3.33
DANN-0.001-40	51.22±3.24	51.42±2.69	52.43±5.23	50.00 ± 5.86	51.21±3.23
DANN-0.001-50	50.81±2.97	51.56±2.69	52.70±5.47	48.92±5.23	50.76±2.93
DANN-0.01-20	51.89 ± 2.85	51.86±2.62	53.24±3.88	50.54±4.15	51.86 ± 2.81
DANN-0.01-30	51.22±2.39	51.71±2.50	53.78±3.76	48.65±4.44	51.18 ± 2.28
DANN-0.01-40	51.49±2.75	51.87±2.46	53.78±3.35	49.19±4.57	51.47±2.65
DANN-0.01-50 (Ours)	52.43±2.32	51.86±2.61	54.32±2.62	50.54±3.88	52.39 ± 2.26
DANN-0.1-20	51.76±1.69	51.99±2.36	54.59 ± 5.03	48.92±7.71	51.85±1.79
DANN-0.1-30	51.76±3.76	52.39±1.95	54.32±8.43	49.19±10.66	51.97 ± 3.70
DANN-0.1-40	52.03±2.30	52.26±2.34	54.59 ± 6.97	49.46±6.54	51.95 ± 2.30
DANN-0.1-50	50.54±1.93	52.02±3.08	55.41±7.50	45.68±7.52	50.50±1.66

Table SII: Results of the DANN with different hyperparameters in the task of MDD vs. HC classification. LR: learning rate; ESD: epoch for step decay. Best results are shown in bold.

can still obtain good prediction results without any model finetuning, verifying the generalizability of the proposed UFA-Net.



Figure SI: Results of the proposed UFA-Net on five unseen/held-out MDD sites from the REST-meta-MDD Consortium [1] in the task of MDD vs. HC classification. Note that no test data/domain is used for model training.

3. Application on ABIDE Dataset

Besides the MDD dataset, we further apply the proposed UFA-Net on the ABIDE dataset² to identify autism spectrum disorder (ASD) patients from healthy controls (HCs). Two largest sites (*i.e.*, *NYU* and *UM*) are used in this group of experiments, while *NYU* (79 ASD and 105 HCs) and *UM* (68 ASD and 77 HCs) are used as the source domain and the target domain, respectively. The classification results of our UFA-Net and nine competing methods are reported in Fig. SII. It can be observed that our UFA-Net generally achieves superior performance compared with the competing methods.

In the current literature, we find that a recent study [2] achieves superior cross-domain classification results on the ABIDE dataset, with functional connectivity (FC) features based on Pearson's correlation coefficients used as input data. The possible reason why our method shows inferior performance could be that we directly leverage fMRI BOLD signals as model inputs, while BOLD signals may contain much noise [3, 4]. Even though our method can model spatial-temporal characteristics of fMRI data and provide interpretability to some extent, the noise will negatively affect effective fMRI representation learning. A possible solution to tackle this problem is to improve input data quality by reducing noisy information in raw BOLD signals via building FC matrices/networks (*e.g.*, using the Pearson's correlation technique as done in [2]). Accordingly, as future work, we will first segment fMRI BOLD signals using the sliding window technique, and then build an FC network for each time segment. The resulting sequential FC networks will be used as input data of the proposed UFA-Net, followed by spatial-temporal fMRI feature learning and cross-domain data adaptation.

²https://fcon_1000.projects.nitrc.org/indi/abide/



Figure SII: Results of ten methods in cross-domain ASD vs. HC classification on the ABIDE dataset, with NYU and UM used as the source domain and the target domain, respectively. ASD: autism spectrum disorder.

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