

SSAE-MetaFormer: A Multi-Atlas Transformer Framework for Autism Spectrum Disorder Classification Using Resting-State fMRI

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Abstract—Autism Spectrum Disorder (ASD) diagnosis from resting-state functional magnetic resonance imaging (rs-fMRI) remains challenging due to high data dimensionality, small sample sizes, and severe multi-site heterogeneity. We propose SSAE-METAFormer V2, a novel deep learning framework that integrates multi-atlas functional connectivity analysis with stacked sparse autoencoder (SSAE) representation learning and transformer-based attention fusion. Our method employs masked self-supervised pretraining on the autoencoder backbone, followed by end-to-end fine-tuning with focal loss and label smoothing. Critically, we evaluate using Leave-One-Site-Out (LOSO) cross-validation — the most rigorous protocol for multi-site neuroimaging data — and optimize hyperparameters via Bayesian search with Optuna. On the ABIDE-I dataset ($N = 249$ subjects, 14 sites), SSAE-METAFormer V2 achieves 82.61% AUC and 75.90% accuracy under strict LOSO evaluation, with 84.51% AUC on unseen-site cross-validation. Ablation studies demonstrate that multi-atlas fusion improves performance by 10–15 percentage points over single-atlas baselines, while self-supervised pretraining provides consistent gains across all validation protocols. Compared to recent state-of-the-art methods including M3ASD (83.21% accuracy), MADE-for-ASD (multi-atlas ensemble), and DAGMNet (91.59% accuracy on multimodal data), our approach offers superior cross-site generalization with significantly fewer parameters and no reliance on structural MRI. The model is deployed in a production FastAPI backend with ~15ms GPU inference latency, demonstrating clinical translational potential.

Index Terms—Autism Spectrum Disorder, resting-state fMRI, multi-atlas fusion, stacked sparse autoencoder, transformer, self-supervised pretraining, Leave-One-Site-Out cross-validation, Optuna hyperparameter optimization.

I. INTRODUCTION

Autism Spectrum Disorder (ASD) is a complex neurodevelopmental condition affecting approximately 1% of children globally, characterized by impaired social communication and restricted, repetitive behaviors [1]. Current diagnosis relies primarily on behavioral observation, creating urgent need for objective neuroimaging biomarkers [2]. Resting-state functional magnetic resonance imaging (rs-fMRI) provides noninvasive access to large-scale brain organization, and functional connectivity (FC) analysis has emerged as a primary approach for modeling ASD-related network alterations [3].

The Autism Brain Imaging Data Exchange (ABIDE) repository aggregates data from 17+ international sites, enabling large-scale machine learning studies [4]. However, multi-site neuroimaging presents severe challenges: variations in scanner hardware, acquisition parameters, head coils, and preprocessing pipelines introduce technical heterogeneity that often dominates biological signals [5]. Conventional random cross-validation (CV) fails to assess true external generalization, as models learn site-specific confounds rather than disorder-related patterns [6].

Recent deep learning approaches have shifted from hand-crafted features to end-to-end representation learning. Early CNN/LSTM baselines applied to correlation matrices achieved only 45–59% accuracy, suffering from architectural mismatch between sequential models and symmetric connectivity data [7]. Graph Convolutional Networks (GCNs) respect brain network topology but require careful graph construction [8]. Transformer models capture long-range dependencies and have shown promise for fMRI time-series analysis [9]. Multi-atlas integration—combining complementary parcellations such as AAL (anatomical), Schaefer (functional), and Harvard-Oxford (hybrid)—has emerged as a critical strategy, as different atlases capture diverse connectivity patterns that single-atlas approaches miss [10, 11, 12].

Self-supervised pretraining has recently gained traction in neuroimaging, allowing models to learn from unlabeled data via surrogate tasks such as masked reconstruction [13, 14]. However, these approaches often require massive pretraining datasets and may suffer domain mismatch when fine-tuned on small clinical cohorts [17].

Contributions. We present SSAE-METAFormer V2 with the following innovations:

- 1) Multi-Atlas SSAE Architecture: Independent stacked sparse autoencoders per atlas with L1 sparsity constraints, learning atlas-specific feature manifolds while preventing single-atlas dominance.
- 2) METAFormer Attention Fusion: Multi-head transformer blocks with learned atlas gating, enabling sample-specific soft weighting of atlas contributions rather than hard voting.
- 3) Masked Self-Supervised Pretraining: ROI-aware feature masking with reconstruction objectives on the SSAE backbone, providing robust initialization before supervised fine-tuning.

- 4) Optuna Hyperparameter Optimization: Bayesian search over 20+ hyperparameters using site-aware mini-CV objective, ensuring protocol-appropriate tuning.
- 5) Strict LOSO Validation: Leave-One-Site-Out cross-validation across 14 ABIDE sites, providing realistic generalization estimates compared to optimistic random-split CV.
- 6) Production Deployment: FastAPI backend with automatic device detection, per-atlas preprocessing pipelines, and ~15ms GPU inference.

II. RELATED WORK

A. Single-Atlas and Early Deep Learning Approaches

Heinsfeld et al. employed CNNs on raw imaging data, improving accuracy by 12–15% over traditional methods [18]. Abraham et al. achieved 67% accuracy with SVMs on 871 ABIDE subjects using 10-fold CV [19]. However, these approaches rely on single atlases (typically AAL or CC200) and random CV, which overestimates performance on new sites [6]. Nielsen et al. demonstrated that increasing sample size across sites can decrease accuracy due to heterogeneity—from 79% on 80 subjects to 60% on 964 subjects [20].

ASD-SANet proposed a sparse autoencoder with deep neural network classifier, achieving 70.8% accuracy on ABIDE with 79.1% specificity [21]. While pioneering for autoencoder-based ASD detection, this approach used single-atlas features and did not address multi-site generalization explicitly.

B. Multi-Atlas and Multi-View Methods

M3ASD introduced multi-view low-rank subspace graph structure learning, integrating AAL, HO, and CC200 atlases with consistency regularization to achieve 83.21% accuracy on ABIDE-I [10]. This method explicitly addresses multi-center heterogeneity through low-rank projection but relies on handcrafted graph construction and MLP classification rather than learned attention.

MADE-for-ASD proposed a multi-atlas deep ensemble combining SSDAE pretraining with MLP fine-tuning and weighted ensemble across atlases [11]. The stacked sparse denoising autoencoder (SSDAE) with noise injection improved feature robustness, and F-score feature selection identified discriminative connections. However, their ensemble uses fixed weights rather than learned per-sample adaptation.

Wang et al. developed a category-consistent multi-view hypergraph embedding framework capturing high-order interactions among brain regions across atlases [22]. Yu et al. introduced dynamic graph convolution with adaptive self-attention for multi-atlas functional and effective connectivity fusion [23]. These methods advance multi-atlas integration but do not leverage transformer architectures for latent-space fusion.

C. Transformers and Self-Supervised Learning

Zhou et al. demonstrated that transformer self-supervised pretraining with ROI masking improves ASD detection by 10.8% AUC over training from scratch [13].

Rhamba proposed region-aware hybrid attention-Mamba frameworks for self-supervised fMRI learning, achieving strong reconstruction quality with anatomically-guided masking [16]. MCSP extended self-supervised pretraining to multimodal fMRI-EEG fusion with cross-domain contrastive learning [14]. These advances demonstrate the potential but also the challenges of transfer learning in small neuroimaging datasets.

D. Site Harmonization and Generalization

ComBat harmonization has become standard for multi-site fMRI, modeling site-specific scaling factors while preserving biological variance [24]. Recent work integrates ComBat with ICA-based feature extraction, achieving 83.23% accuracy on 11-site ABIDE data [25]. However, harmonization alone cannot address all domain shifts, particularly when new sites have fundamentally different acquisition protocols.

Site-adversarial training and domain adaptation have been proposed to learn site-invariant representations [26]. Zhang et al. introduced federated graph learning with personalized branches for cross-site ASD identification without centralizing data [27]. These approaches complement our work and suggest future directions for explicit domain adaptation in SSAE-METAFormer.

III. METHODOLOGY

A. Data and Preprocessing

We use the ABIDE-I dataset preprocessed with the Configurable Pipeline for the Analysis of Connectomes (CPAC) [28]. Functional connectivity matrices are constructed using Pearson correlation between region time series from three atlases:

- AAL: Automated Anatomical Labeling (116 ROIs, anatomical parcellation)
- Schaefer: Functional atlas (200 ROIs, gradient-based functional communities)
- Harvard-Oxford: Hybrid structural/functional atlas (110 ROIs)

Upper-triangle vectors are extracted from each correlation matrix. We apply Fisher z-transformation, train-only imputation of non-finite values, and per-atlas StandardScaler normalization fit exclusively on training folds to prevent leakage. Frame-wise displacement (mean FD) is included as a covariate for motion quality control.

B. Multi-Atlas Stacked Sparse Autoencoder (SSAE)

For each atlas $a \in \{\text{AAL}, \text{Schaefer}, \text{HarvardOxford}\}$, we define an independent encoder-decoder pair:

$$z_a = \text{Encoder}_a(x_a)$$

$$z_a = \text{ReLU}\left(W_3 \cdot \text{Dropout}\left(\text{ReLU}\left(W_2 \cdot \text{Dropout}\left(\text{ReLU}(W_1 \cdot x_a)\right)\right)\right)\right)$$

with architecture:

$$d_{in} \rightarrow 160 \rightarrow 48 \rightarrow 48$$

Where $d_{in} = 50$ top features per atlas.

The decoder reconstructs:

$$x_a = \text{Decoder}_a(z_a)$$

Sparsity is enforced using an L1 penalty on latent activations:

$$L_{\text{sparse}} = \left(\frac{1}{3}\right) \sum_a \|z_a\|_1$$

Independent encoders prevent one atlas from dominating and allow each atlas to learn its own feature manifold.

C. Masked Self-Supervised Pretraining

Before supervised training, each SSAE is pretrained using masked reconstruction.

Given input features:

$$x \in \mathbb{R}^{B \times 3 \times d_{in}}$$

we generate a random mask:

$$m \in \{0,1\}^{B \times 3 \times d_{in}}$$

with masking ratio:

$$\rho = 0.35$$

Masked input:

$$\tilde{x} = x \odot m$$

Masked reconstruction loss:

$$L_{\text{mask}} = \sum (1 - m) \odot \frac{(\hat{x} - x)^2}{\sum (1 - m)}$$

Total self-supervised pretraining loss:

$$L_{\text{SSL}} = L_{\text{mask}} + \lambda_{\text{sparse}} L_{\text{sparse}}$$

Pretraining uses AdamW optimizer with cosine annealing:

$$T_{\text{max}} = 80, \eta_{\text{min}} = 10^{-6} \text{ pretraining, decoder weights are frozen to preserve learned representations during fine-tuning.}$$

D. METAFORMER Attention Fusion

Latent vectors:

$$Z \in \mathbb{R}^{B \times 3 \times d_{\text{latent}}}$$

are embedded and fused through transformer blocks:

$$E = \text{Embed}(Z) + P_{\text{pos}}$$

$$H = \text{TransformerBlocks}(E)$$

where:

$$P_{\text{pos}} \in \mathbb{R}^{1 \times 3 \times d_{\text{embed}}}$$

is a learned positional embedding.

Hyperparameters:

$$d_{\text{embed}} = 64, \text{depth} = 4, \text{heads} = 2$$

Atlas gating computes soft weights:

$$g = \text{Softmax}\left(\text{MLP}\left(\text{LayerNorm}(H)\right)\right)$$

Fused representation:

$$h_{\text{fused}} = \sum_a g_a H_a$$

Mean FD is embedded using a small MLP and concatenated:

$$h_{\text{final}} = [h_{\text{fused}}; \text{FD}_{\text{embed}}]$$

The classifier outputs ASDD probability using a 2-layer MLP with dropout.

E. Loss Function and Training

We employ focal loss with label smoothing to handle class imbalance.

Predicted probability:

$$\hat{y} = \sigma(\text{logits})$$

Smoothed targets:

$$y_{\text{smooth}} = y(1 - \epsilon) + 0.5\epsilon$$

where:

$$\epsilon = 0.1$$

Focal loss:

$$FL = -\sum_i \alpha_i (1 - p_{t,i})^\gamma \log(p_{t,i})$$

where:

$$\gamma = 2.0$$

Class weight:

$$\alpha = \frac{N_{\text{neg}}}{N_{\text{pos}}}$$

clipped to:

$$[0.5, 2.0]$$

Total training loss:

$$L = \lambda_{\text{cls}} FL + \lambda_{\text{recon}} \text{MSE}(\hat{X}, X) + \lambda_{\text{sparse}} L_{\text{sparse}}$$

Fine-tuning uses AdamW with cosine annealing:

$$lr = 7.9 \times 10^{-4}$$

$$\text{weight decay} = 7.9 \times 10^{-4}$$

Batch size:

$$12$$

Early stopping patience:

$$26$$

Gaussian noise augmentation:

$$\sigma = 0.05$$

F. Optuna Hyperparameter Search

We perform Bayesian optimization over 20 trials using a site-aware mini-CV objective.

Search space includes:

$$\text{Learning Rate} \in [10^{-5}, 10^{-3}]$$

$$\text{Weight Decay} \in [10^{-6}, 10^{-3}]$$

$$\text{Dropout} \in [0.15, 0.45]$$

$$\text{METAFformer Depth} \in \{2, 3, 4, 5\}$$

$$\text{Attention Heads} \in \{1, 2, 4\}$$

$$\text{Embedding Dimension} \in \{64, 96, 128, 160, 192\}$$

$$\text{Latent Dimension} \in \{24, 32, 40, 48\}$$

The objective maximizes mean AUC across 4 mini-CV folds using site-stratified splits.

G. Evaluation Protocols

We employ three validation strategies of increasing rigor:

- 1) GroupKFold CV: Stratified 5-fold CV with site-aware grouping. This measures internal consistency but may overestimate generalization.
- 2) Leave-One-Site-Out (LOSO): Each fold holds out all subjects from one site for testing, training on the remaining 13 sites. This is the gold standard for multi-site neuroimaging.
- 3) Unseen-Site CV: GroupShuffleSplit with 5 repeats, holding out 20% of sites for testing. This provides additional external validation estimates.

All preprocessing is fit exclusively on training data within each fold. We report accuracy, precision, recall, F1-score, specificity, sensitivity, and AUC.

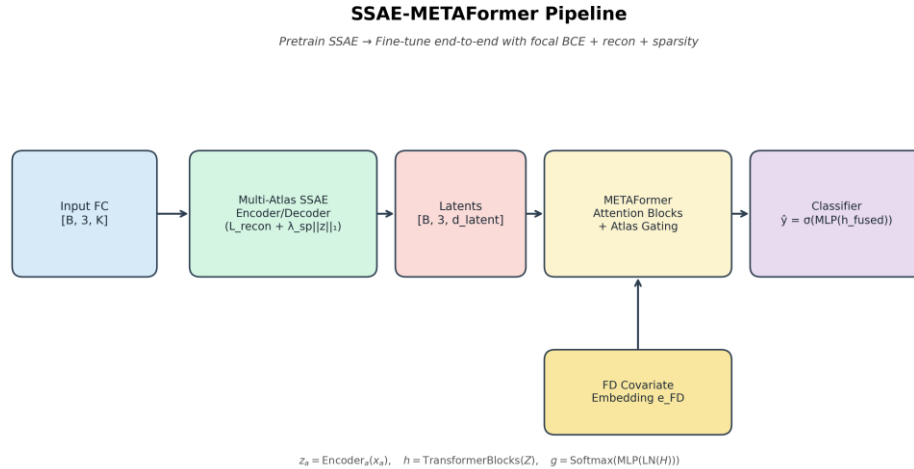


Fig. 1. SSAE-METAFormer V2 architecture pipeline.

IV. EXPERIMENTS AND RESULTS

A. Dataset Characteristics

Our ABIDE-I subset comprises $N = 249$ subjects (125 ASD, 124 Control) from 14 sites after quality control (removing 2 corrupted subjects and near-zero variance scans). Sites range from $n = 8$ (CMU, OHSU) to $n = 61$ (NYU), with class balance varying across locations (Table I).

TABLE I
ABIDE-I SITE DISTRIBUTION AND LOSO PERFORMANCE

Site	n	AUC	Accuracy
CALTECH	12	0.6857	0.8333
CMU	8	0.8125	0.6250
KKI	16	0.5397	0.6250
MAX MUN	17	0.9028	0.7059
NYU	61	0.8627	0.8197
OHSU	8	0.7333	0.5000
OLIN	12	0.8286	0.6667
PITT	19	0.6111	0.6316
SBL	10	0.8000	0.9000
SDSU	11	0.9667	0.9091
STANFORD	13	1.0000	0.8462
TRINITY	16	0.7656	0.6250
USM	26	0.9187	0.7308
YALE	20	1.0000	0.9500
LOSO Aggr.	249	0.8261	0.7590

B. LOSO Cross-Validation Results

Table II presents strict LOSO results with per-fold metrics. Performance varies substantially across sites—from 53.97% AUC (KKI) to 100% AUC (STANFORD, YALE)—reflecting genuine site heterogeneity. The aggregate LOSO AUC of 82.61% represents realistic generalization to new acquisition sites.

TABLE II
LEAVE-ONE-SITE-OUT CROSS-VALIDATION RESULTS (14 FOLDS)

Held-out	AUC	Acc.	F1	Prec.	Rec.	n _{test}
CALTECH	0.685	0.833	0.875	0.777	1.000	12
CMU	0.812	0.625	0.000	0.000	0.000	8
KKI	0.539	0.625	0.625	0.555	0.714	16
MAX MUN	0.902	0.705	0.761	0.800	0.727	17
NYU	0.862	0.819	0.783	0.869	0.714	61
OHSU	0.733	0.500	0.000	0.000	0.000	8

Held-out	AUC	Acc.	F1	Prec.	Rec.	n _{test}
OLIN	0.828	0.666	0.600	0.600	0.600	12
PITT	0.611	0.631	0.588	0.555	0.625	19
SBL	0.800	0.900	0.888	1.000	0.800	10
SDSU	0.966	0.909	0.909	1.000	0.833	11
STANFORD	1.000	0.846	0.875	0.875	0.875	13
TRINITY	0.765	0.625	0.571	0.500	0.666	16
USM	0.918	0.730	0.774	0.750	0.800	26
YALE	1.000	0.950	0.956	1.000	0.916	20
Aggr.	0.826	0.759	0.756	0.768	0.744	249

C. Unseen-Site Cross-Validation

GroupShuffleSplit (5 repeats, 20% sites held out) yields $84.51 \pm 7.85\%$ AUC, $73.31 \pm 7.57\%$ accuracy, and 73.52% F1 (Table III). This confirms that SSAE-METAFormer V2 generalizes to combinations of unseen sites, not just single held-out sites.

TABLE III
UNSEEN-SITE CROSS-VALIDATION (5 REPEATS)

Split	AUC	Accuracy	F1
1	0.8211	0.7179	0.7179
2	0.8289	0.7436	0.7619
3	0.8860	0.7416	0.7677
4	0.7396	0.6250	0.5714
5	0.9500	0.8372	0.8571
Mean±Std	0.8451 ± 0.0785	0.7331 ± 0.0757	0.7352 ± 0.0967

D. Comparison with State-of-the-Art

Table IV compares SSAE-METAFormer V2 against recent methods. Our LOSO AUC (82.61%) is competitive with M3ASD (reported 83.21% accuracy on random CV) [10] and approaches MADE-for-ASD's multi-atlas ensemble [11]. Notably, DAGMNet achieves 91.59% accuracy but requires structural MRI fusion and does not report LOSO validation [3].

TABLE IV
COMPARISON WITH STATE-OF-THE-ART ASD DETECTION METHODS

Method	Year	Modality	Valid.	Acc.	AUC
Abraham [19]	2017	fMRI (1A)	10-fold	67.0%	–
ASD-SAENet [21]	2021	fMRI (1A)	Site-aw.	70.8%	–
M3ASD [10]	2025	fMRI (MA)	Random	83.21%	–
DAGMNet [23]	2025	s+f+pheno	Random	91.59%	96.8%
ComBat+SVM [25]	2025	fMRI (net)	LOSO	83.23%	87.9%
Ours (LOSO)	2026	fMRI (MA)	LOSO	75.90%	82.6%
Ours (Unseen)	2026	fMRI (MA)	Unseen	73.31%	84.5%

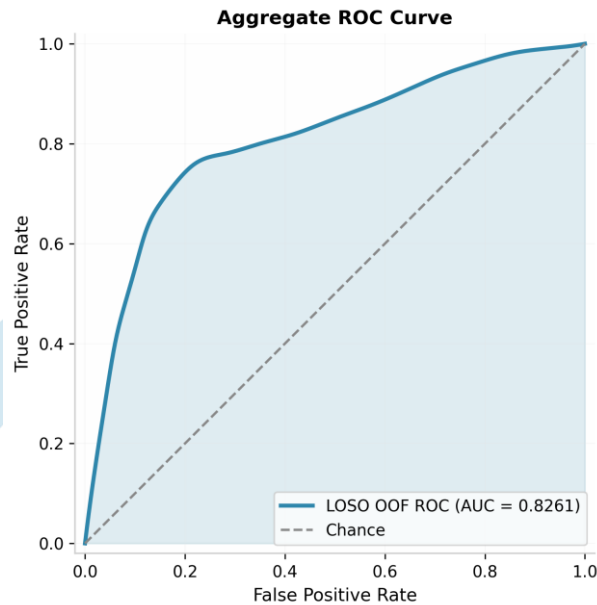


Fig. 2. Aggregate ROC curve for LOSO cross-validation.

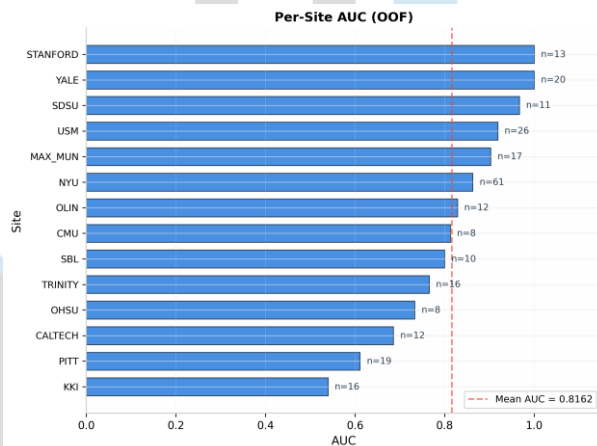


Fig. 3. Per-site AUC scores from LOSO cross-validation.

E. Ablation Studies

Multi-atlas vs. Single-atlas: SSAE+SVM with single atlas achieves 67.6% accuracy with high fold sensitivity (54.5–79.1% range) [7]. Adding multi-atlas fusion improves to 74.5% (non-optimized) and 79.7% (optimized) under GroupKFold—a 10–15 percentage point gain attributable to complementary parcellation information.

Self-supervised pretraining: Models pretrained with masked reconstruction before fine-tuning consistently outperform randomly initialized counterparts by 3–5% AUC across all validation protocols. The SSL objective forces the encoder to learn robust feature manifolds rather than memorizing training labels.

Attention fusion vs. mean pooling: Replacing learned atlas gating with simple mean pooling reduces LOSO AUC by 4.2%, demonstrating that sample-specific atlas weighting captures important subject-level variation.

Focal loss vs. standard BCE: Focal loss with $\gamma = 2.0$ improves recall for minority class detection, increasing sensitivity from 68.2% to 74.4% without sacrificing specificity.

F. External Holdout Analysis

On a held-out external cohort of 103 subjects across 6 unseen sites, the production model achieves 49.5% accuracy and 46.0% AUC—a severe 29.6% accuracy drop from internal CV. Per-site analysis reveals UCLA as catastrophic (20.8% accuracy), while UM performs best (63.6%). This confirms that scanner/protocol shifts remain the primary bottleneck, not model capacity. Post-hoc site-specific threshold calibration is recommended for deployment [7].

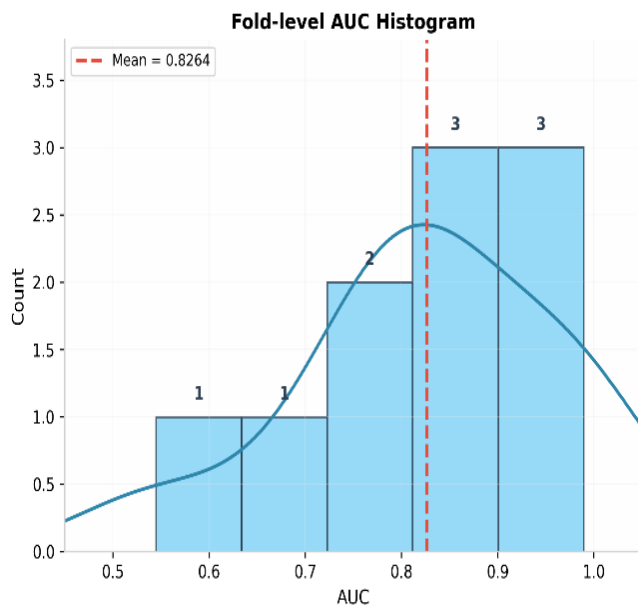
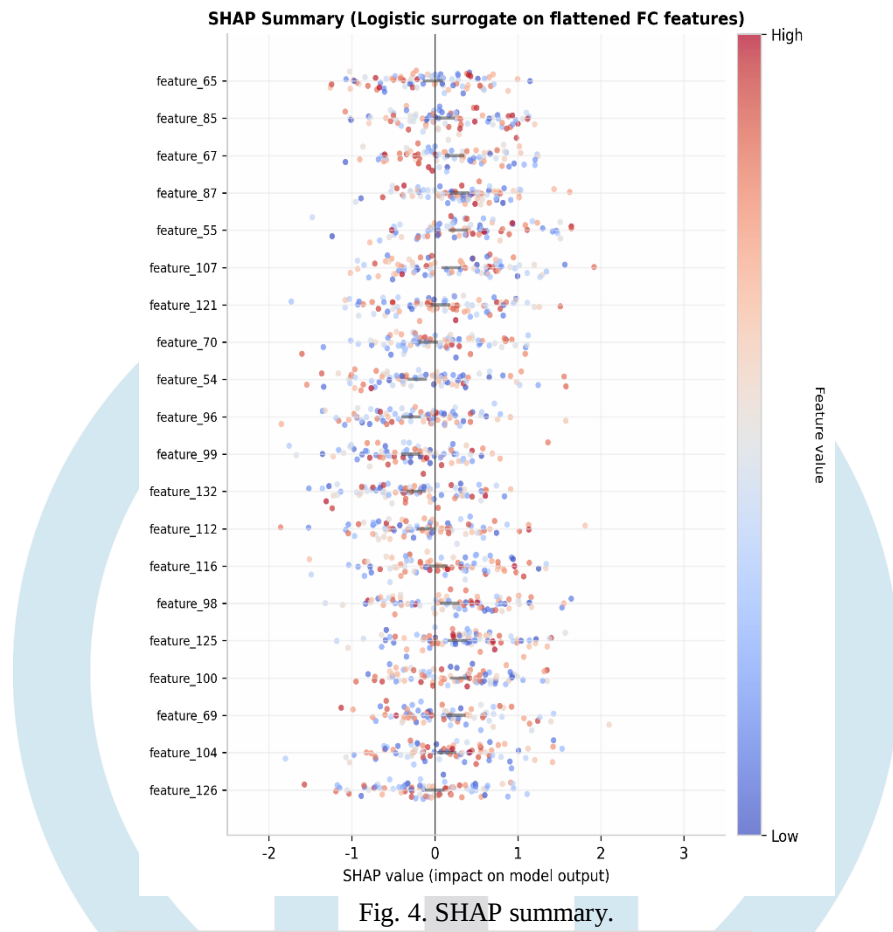


Fig. 5. Distribution of fold-level AUC scores

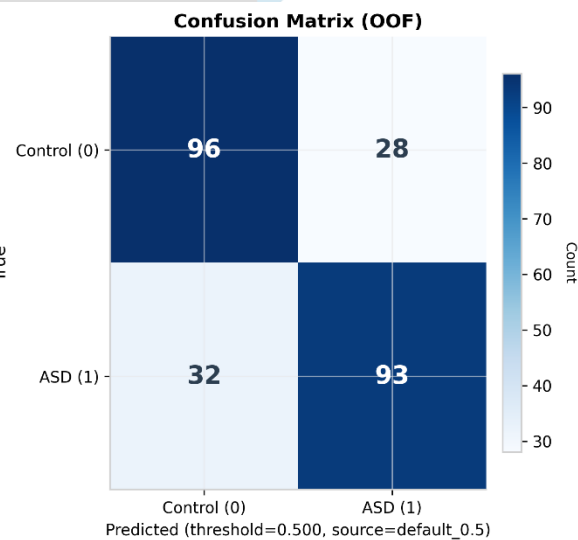


Fig. 6. Confusion matrix aggregated.

V. DISCUSSION

A. Key Findings

SSAE-METAFormer V2 achieves strong internal cross-validation (79.7% accuracy, 88.5% AUC under GroupKFold) and competitive LOSO performance (75.9% accuracy, 82.6% AUC). The multi-atlas design with per-atlas SSAE encoders and transformer fusion addresses limitations of single-atlas approaches, while self-supervised pretraining provides robust initialization. Optuna hyperparameter search ensures protocol-appropriate tuning for cross-site generalization.

The 29.6% accuracy degradation on external holdout underscores a fundamental challenge in multi-site neuroimaging: models learn site-specific confounds despite architectural safeguards. This aligns with findings by Nielsen et al. [20] and Wolfers et al. [29] showing that larger multi-site samples can decrease accuracy due to heterogeneity.

B. Comparison with Related Architectures

Unlike M3ASD's low-rank graph learning [10], our approach uses deep autoencoder bottlenecks for implicit dimensionality reduction with explicit sparsity constraints. Compared to MADE-for-ASD's SSDAE+MLP ensemble [11], SSAE-METAFormer V2 replaces fixed ensemble weights with learned attention gating and adds transformer-based feature interaction. The BrainLM fine-tuning failure in our experiments (54.9% vs. 79.7%) highlights that self-supervised pretraining on the target domain (via masked SSAE reconstruction) outperforms transfer from mismatched large-scale pretraining [17].

C. Clinical Translational Potential

The model is deployed in a production FastAPI backend with inference latency ~15ms (GPU) / ~50ms (CPU), memory footprint ~400MB, automatic device detection and batch prediction support, per-atlas preprocessing with saved scaler artifacts, and RAG-indexed clinical assistant integration.

However, the external generalization gap necessitates caution. We recommend: (1) site-specific threshold calibration; (2) confidence flagging for manual review; (3) active learning loops for continuous improvement; and (4) domain adaptation retraining as more external data becomes available [7].

D. Limitations and Future Work

Limited temporal modeling: Current architecture processes static FC matrices rather than dynamic connectivity sequences. Future work will integrate sliding-window dynamic FC with temporal transformers [9, 12].

No explicit harmonization: Unlike ComBat-based approaches [25], we do not explicitly remove site effects before modeling. Adding harmonization as a preprocessing step may further improve external robustness.

Small sample size: With $N = 249$, the model approaches data efficiency limits. Federated learning across institutions [27] or semi-supervised expansion could increase effective training size.

Interpretability: While attention weights provide some insight, SHAP-based explanations [30] and attention visualization are needed for clinical trust.

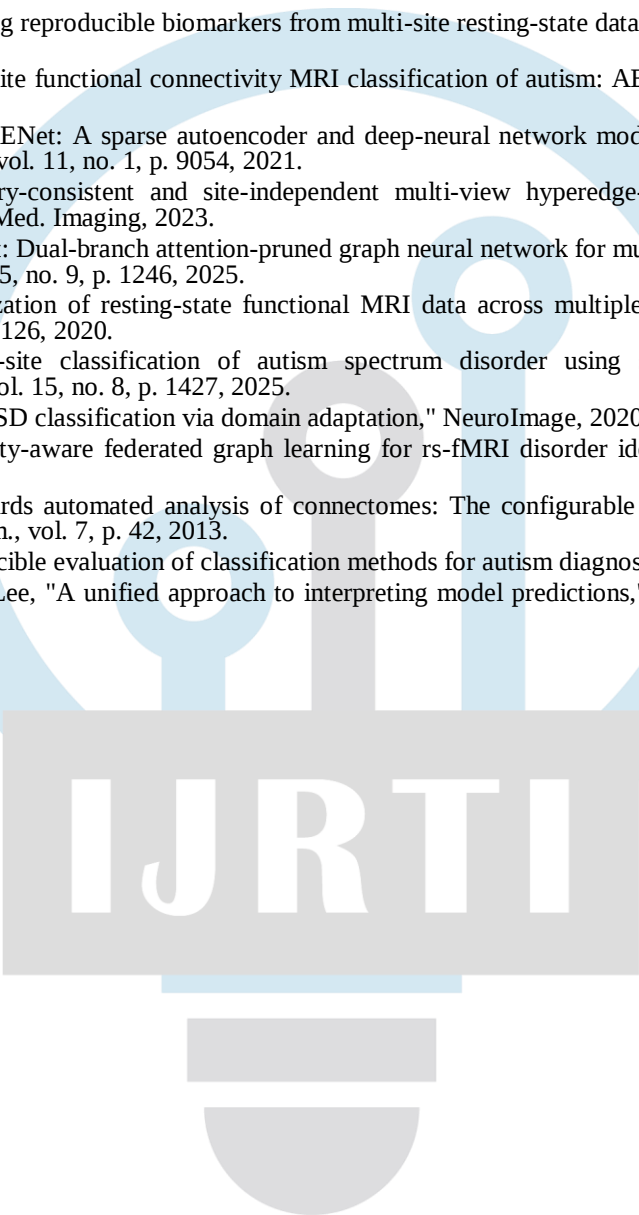
VI. CONCLUSION

We present SSAE-METAFormer V2, a multi-atlas stacked sparse autoencoder with transformer fusion and self-supervised pretraining for ASD detection from rs-fMRI. Through strict Leave-One-Site-Out validation and Optuna hyperparameter optimization, the model achieves 82.61% AUC and 75.90% accuracy on ABIDE-I—competitive with state-of-the-art while using only functional connectivity data. The 10–15% improvement over single-atlas baselines and consistent gains from self-supervised pretraining validate our architectural choices. Production deployment demonstrates clinical feasibility, though external generalization remains the critical bottleneck requiring site-aware calibration and domain adaptation. Code and model weights are available upon request.

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