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Interpretable Hybrid Machine Learning Models for Renewable-Powered Smart Grid Stability Prediction

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Abstract

Power grids today operate under unpredictable and rapidly changing conditions, making it essential to develop reliable predictive systems for stability management. This study explores two hybrid learning frameworks that combine deep feature transformation with ensemble classification to improve grid stability prediction. Specifically, an autoencoder (AE) and a TabTransformer (TT) are used for feature encoding, followed by Extreme Gradient Boosting (XGBoost) classifiers. Additionally, two conventional ensemble models (Random Forest and standalone LightGBM) are evaluated for comparison. Models are assessed using standard classification metrics and stratified cross-validation. The autoencoder-based hybrid model outperforms others by producing enriched feature representations, while the standard LightGBM delivers stable and interpretable results. Although the TabTransformer-based model offers architectural novelty, it exhibits less consistency. These findings highlight that optimal grid stability prediction depends not solely on model complexity but on synergy between feature processing and learning architecture, supporting the development of confidence-aware models for smart grid decision systems.

Index-words: *Grid stability prediction, Random Forest, Autoencoder-XGBoost, TabTransformer, Ensemble classifier, Light GBM.*

I. Introduction

Modern electric grids are changing rapidly with the growing share of renewable energy, varying load behavior, and decentralized generation. These changes add uncertainty and complexity, making conventional rule-based controls less effective for maintaining stability [1-3]. As a result, there is a clear shift toward data-driven systems that can use real-time information from generation, transmission, and distribution layers to predict and manage stability.

Machine learning (ML) has become a valuable tool for this task. Ensemble models such as Random Forest, Gradient Boosting, and LightGBM have shown strong results in fault diagnosis, load forecasting, and stability analysis, especially when data are large, noisy, or imbalanced [4-7]. Deep learning (DL) methods further extend these capabilities. Autoencoders, for example, can compress features while preserving key patterns [8-9], while attention-based methods like TabTransformer can capture relationships between variables in tabular data [10-11].

Still, major challenges remain. Many existing models have limited interpretability, struggle with class imbalance, or fail to provide reliable probability estimates. While some hybrid approaches combining deep features and ensemble classifiers have been explored, their use in grid stability is limited. Most past work has focused mainly on improving

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accuracy, without considering interpretability or prediction confidence, both of which are critical in real grid operations. Beyond power-grid studies, hybrid and ensemble machine learning frameworks have also been successfully applied in renewable-energy forecasting, microgrid voltage management, and sustainable energy systems, reinforcing the broader relevance of such hybrid approaches [12-15].

To highlight this gap, Table 1 compares recent studies. It shows that while earlier works improved accuracy through Deep Neural Networks (DNNs), boosting, or optimization, none addressed accuracy, interpretability, and calibration together.

Table 1: Summary of related works on grid stability prediction compared with this study

Year	Reference	Method / Model	Dataset	Key Contribution	Limitation
2024	Lahon et al. [4]	Deep Neural Network (DNN)	National power system data	Improved grid resilience with DNN-based stability analysis	Limited interpretability; no confidence assessment
2024	Raju et al. [7]	Bayesian-optimized LightGBM	Smart Grid Stability (Kaggle)	Boosted ensemble with Bayesian tuning	Focused only on optimization; no hybrid deep features
2025	Binbusayyis & Sha [11]	PSO-optimized XGBoost	Simulated grid data	Enhanced prediction using metaheuristic tuning	No interpretability or calibration of predictions
2023	Yao et al. [8]	LightGBM–XGBoost hybrid	Load forecasting dataset	Effective short-term load forecasting	Different domain (load), not grid stability
2024	Lakshmanarao et al. [18]	ML–DL fusion model	Grid stability dataset	Combined ML and DL for better prediction	Limited analysis of model interpretability
2024	Oyucu et al. [20]	RNN + LSTM hybrid	Smart grid signals	Sequence-based learning for stability estimation	High complexity; lacks calibration and feature analysis
2025	This Work	AE-XGBoost, TT-XGBoost	Smart Grid Stability (Kaggle)	Hybrid feature learning with ensemble boosting; interpretable outputs; confidence calibration	First to jointly address accuracy, interpretability, and calibration in smart grid stability.

This study builds on these gaps. We propose two hybrid architectures: one combining an autoencoder with XGBoost, and another combining TabTransformer with XGBoost [16]. Unlike earlier efforts, our work emphasizes three key points:

- Direct comparison of Autoencoder and TabTransformer hybrids with standard ensemble baselines.
- Feature importance analysis to provide operational insights for grid operators.
- Calibration assessment to ensure predictions are not only accurate but also reliable.

These models are benchmarked against conventional ensemble methods on a public dataset. The evaluation includes accuracy, F1-score, class balance, interpretability, and calibration [13-14]. The results contribute to building smarter and more reliable ML frameworks for future power grids [19].

II. Methodology

A. Dataset description

This study uses a publicly available dataset titled “Smart Grid Stability”, sourced from Kaggle. It contains 60,000 records, each representing a specific operational state of an electric power grid. The dataset includes 12 continuous input features, categorized into three layers of the power system:

- **Generation layer**: Four internal damping coefficients ($\tau 1$ to $\tau 4$)
- **Transmission layer**: Four power output readings ($p1$ to $p4$)
- **Distribution layer**: Four phase angle indicators ($g1$ to $g4$)

Two target outputs are provided:

- A **continuous stability index** (stab)
- A **categorical label** (stabf) indicating whether the grid state is "stable" or "unstable"

This study focuses on the binary classification task using the stabf label. All features are continuous, and the dataset contains no missing values. Before model training, input features were normalized using standard scaling. The diversity of grid conditions in the dataset provides a rich environment for evaluating the performance and robustness of predictive models [6], [20]. Figure 1 illustrates the mapping of generation ($\tau 1$ to $\tau 4$), transmission ($p1$ to $p4$), and distribution ($g1$ to $g4$) variables to their respective phases in the electric grid, leading to a binary grid stability output.

To prepare the data for training and evaluation, two slightly different splitting strategies were applied depending on the model. For the AE-XGBoost experiments, the dataset was divided into 80% training and 20% testing. For the TT-XGBoost experiments, a three-way split was used with 60% training, 20% validation, and 20% testing. In both cases, a stratified splitting strategy was used to maintain class balance across subsets, and the sets were kept fully independent with no overlap to ensure unbiased evaluation.

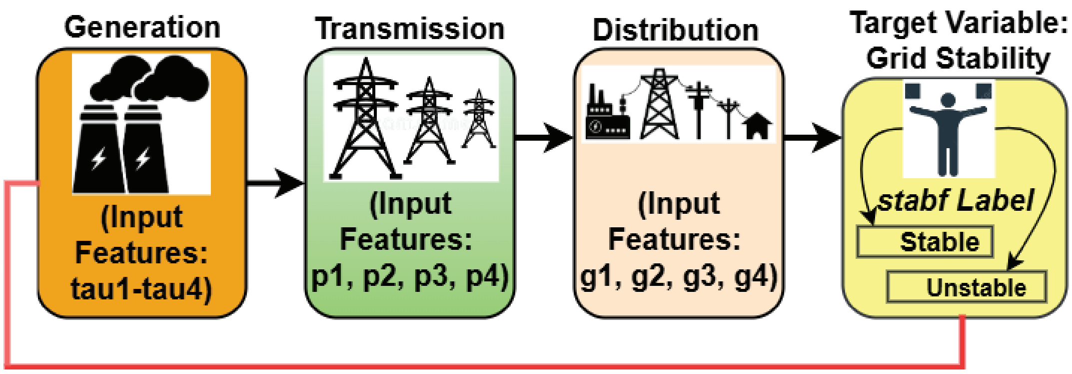

Figure 1: Feature groups in the dataset, showing generation, transmission, and distribution variables that determine grid stability.

B. TabTransformer with Extreme Gradient Boosting (TT-XGBoost)

This hybrid approach combines TabTransformer for feature transformation with XGBoost for Classification, aiming to capture feature interactions and improve prediction confidence in grid stability [22].

1. Feature transformation using TabTransformer

TabTransformer applies multi-head self-attention to model dependencies among features. In this work, it was adapted for continuous grid variables by embedding each of the 12 features into a 32-dimensional vector [23]. The model used four attention heads, two transformer layers, and a dropout rate of 0.2.

The embeddings are passed through the attention layers, where dependencies are captured as shown in Eq. (1).

$$Attention(Q, K, V) = \mathrm{Softmax}\left(\frac{\mathrm{Q_i K_i^T}}{\sqrt{\mathrm{d_k}}}\right)\mathrm{V} \tag{1}$$

Where Q, K, and V are the query, key, and value matrices, respectively. The enriched feature representation is then concatenated and projected as shown in Eq. (2).

$$\mathbf{Z} = \mathrm{Concat}\,(head_1, \cdots, head_h)W^0 \tag{2}$$

Here, the enriched matrix **Z** encodes contextual information among features, which is later passed to the XGBoost classifier.

2. Classification using XGBoost

XGBoost is a gradient-boosted ensemble of decision trees that improves performance through iterative learning and is widely known for its scalability and interpretability [23].

The objective function for each boosting round is given in Eq. (3).

$$\mathcal{L}^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) \quad (3)$$

Where:

- l is a differentiable loss function (e.g., logistic loss)
- f_t is the tree added at iteration t
- $\Omega(f_t)$ penalizes model complexity

Predictions are updated as shown in Eq. (4).

$$\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + \eta f_t(\mathbf{x}_i) \quad (4)$$

η is the learning rate used to control step size during optimization.

3. TT-XGBoost Workflow

The workflow has two phases:

- **Training:** Input features are embedded by TabTransformer to generate enriched vectors Z, which are used to train the XGBoost classifier.
- **Inference**: For a new sample x', its enriched form z' is passed to the trained XGBoost model for prediction.

For a new instance x', its enriched form z' is generated. The trained XGBoost model predicts the grid's stability class using z'.

This hybrid model effectively captures feature dependencies using attention while leveraging the predictive strength and interpretability of XGBoost [24]. The end-to-end training and inference flow of this hybrid model is illustrated in Figure 2.

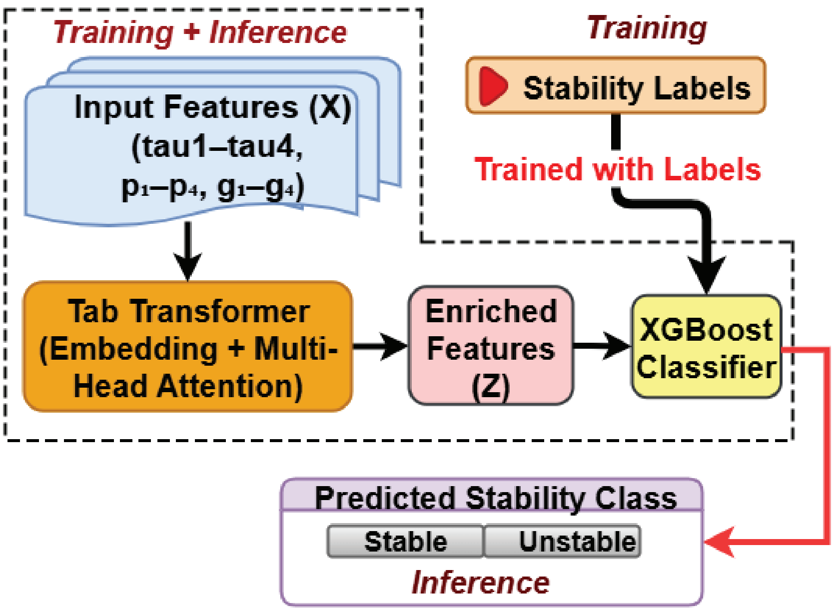

Figure 2: Architecture of the TT-XGBoost hybrid model, where TabTransformer extracts enriched feature representations that are classified by XGBoost during training and inference.

C. *Autoencoder with Extreme Gradient Boosting (AE-XGBoost)*

This hybrid model combines an Autoencoder for dimensionality reduction and XGBoost for Classification. The Autoencoder transforms high-dimensional inputs into compressed representations that preserve essential structure while removing redundancy [25].

1. Feature Extraction using Autoencoder

The Autoencoder compresses the 12 input features into a lower-dimensional latent space while minimizing reconstruction loss [26]. The encoder transforms each input x_i as shown in Eq. (5).

$$z_i = f_{enc}(x_i) = \sigma(W_{enc} x_i + b_{enc}) \quad (5)$$

And the decoder reconstructs it as represented in Eq. (6).

$$\hat{x}_i = f_{enc}(z_i) = \sigma'(W_{dec} z_i + b_{dec}) \quad (6)$$

The training objective is to minimize the reconstruction error, as given in Eq. (7).

$$\mathcal{L}_{AE} = \frac{1}{n}\sum_{i=1}^{n}\|x_i - \hat{x}_i\|^2 \quad (7)$$

In this study, the encoder used layers of size 64 → 32 → 16 with ReLU activations, and the decoder used layers 32 → 64 → 12 with a sigmoid output to preserve normalized ranges. Training was carried out for 50 epochs with a batch size of 256, using the Adam optimizer (learning rate = 0.001). The final 16-dimensional latent vector was passed to the XGBoost classifier.

2. Classification using XGBoost

The compressed latent vectors z_i produced by the Autoencoder are passed to the XGBoost classifier for training and prediction [27]. The classifier follows the same boosting objective and iterative update rule already described in Section 2.2.2, but here it operates on the compact representations rather than raw features.

3. AE-XGBoost workflow

The AE-XGBoost workflow has two phases:

- **Training**: The Autoencoder compresses the input features into compact latent vectors, which are then used to train the XGBoost classifier with stability labels.
- **Inference:** For a new input sample x', the encoder generates its compressed representation z', which the trained XGBoost model classifies as stable or unstable.

This setup reduces feature noise and emphasizes meaningful patterns, while preserving the predictive strength and interpretability of XGBoost [28-29]. The overall architecture is shown in Figure 3.

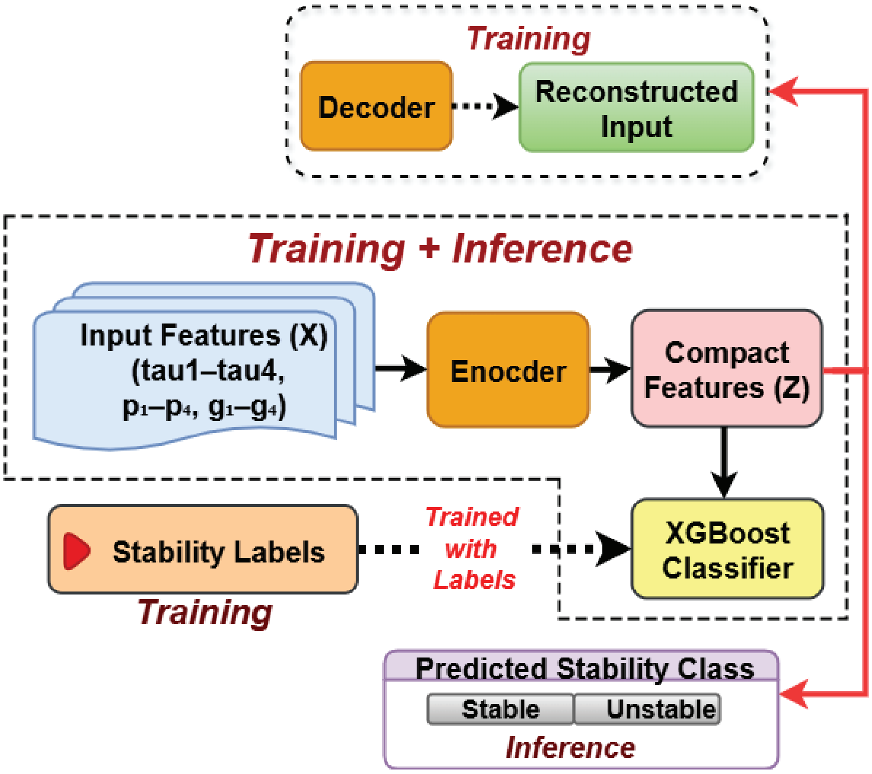

Figure 3: Architecture of the AE-XGBoost hybrid model, where the Autoencoder compresses input features into latent vectors that are used by XGBoost for final Classification.

D. Hyperparameter tuning

Hyperparameters were tuned through a combination of small grid search and manual adjustment. For XGBoost, we tested the number of trees (100, 300, 500), maximum depth (4, 6, 8), learning rate (0.01, 0.05, 0.1), and subsample ratios (0.7, 0.8, 1.0). The best setup used 300 trees, depth 6, learning rate 0.1, and subsample 0.8. For the Autoencoder, latent sizes (8, 16, 32), epochs (30, 50, 70), and batch sizes (256, 512) were explored. The final choice was 16 latent dimensions, 50 epochs, batch size 256,

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with Adam optimizer at learning rate 0.001. For the TabTransformer, we experimented with embedding dimensions (16, 32, 64), attention heads (2, 4, 8), and dropout rates (0.1, 0.2). The selected model used 32 dimensions, four heads, and a dropout of 0.2.

III. Results & discussion

We evaluated the proposed hybrid models against common machine learning techniques for grid stability prediction. Standard metrics such as validation accuracy, test accuracy, precision, recall, and F1-score (Table 2) were used, along with additional checks like statistical testing and calibration analysis, discussed later in this section.

Table 2: Performance metrics of baseline and hybrid models for grid stability prediction

Model	Validation Accuracy	Test Accuracy	Precision		Recall		F1-Score	
			Class 0	Class 1	Class 0	Class 1	Class 0	Class 1
Random Forest	0.945	0.939	0.940	0.930	0.960	0.900	0.950	0.910
LightGBM	0.957	0.958	0.960	0.950	0.970	0.930	0.970	0.940
TT-XGBoost	0.892	0.894	0.910	0.870	0.930	0.840	0.920	0.850
AE-XGBoost	0.977	0.977	0.980	0.970	0.980	0.970	0.980	0.970

AE-XGBoost achieved the best performance, with 97.7% accuracy and an F1-score of 0.98 for both classes, showing a strong balance between precision and recall. In contrast, TT-XGBoost reached only 89.4% accuracy and performed poorly on Class 1, indicating difficulty in identifying unstable grid states.

Table 3 shows composite metrics (MCC, balanced accuracy, ROC AUC). AE-XGBoost again leads across all three, confirming its reliability in distinguishing stable from unstable states. LightGBM also performs strongly, while TT-XGBoost falls behind, especially in MCC and balanced accuracy.

Table 3: Composite evaluation metrics of baseline and hybrid models

Metric	Random Forest	LightGBM	TT-XGBoost	AE-XGBoost
MCC	0.867	0.910	0.771	0.951
Balanced Accuracy	0.930	0.953	0.883	0.976
ROC AUC Score	0.989	0.994	0.965	0.998

Table 4 adds two more metrics, Cohen's Kappa, which accounts for chance agreement, and Log-loss, which reflects the quality of probability estimates. AE-XGBoost and LightGBM have the lowest log-loss values, showing better calibration. TT-XGBoost again performs the weakest.

Table 4: Additional evaluation metrics of baseline and hybrid models

Model	Cohen's Kappa	Log-loss
Random Forest	0.882	0.194
LightGBM	0.912	0.133
AE-XGBoost	0.862	0.154
TT-XGBoost	0.764	0.236

To make sure that the observed improvements were not just due to random variation, we carried out a statistical validation. A McNemar's test was used to compare AE-XGBoost with LightGBM, the strongest baseline model, on the same test set. The test gave a chi-square statistic of 99.0 with a p-value of 3.7×10^{-95}. Since this value is far below the 0.05 threshold, the result confirms that the performance difference is statistically significant. This gives us additional confidence that the superiority of AE-XGBoost is genuine and not simply a chance effect.

AE-XGBoost shows the cleanest separation, with the fewest errors. LightGBM and Random Forest are also reliable, while TT-XGBoost shows more confusion in unstable states, as shown in Figure 4.

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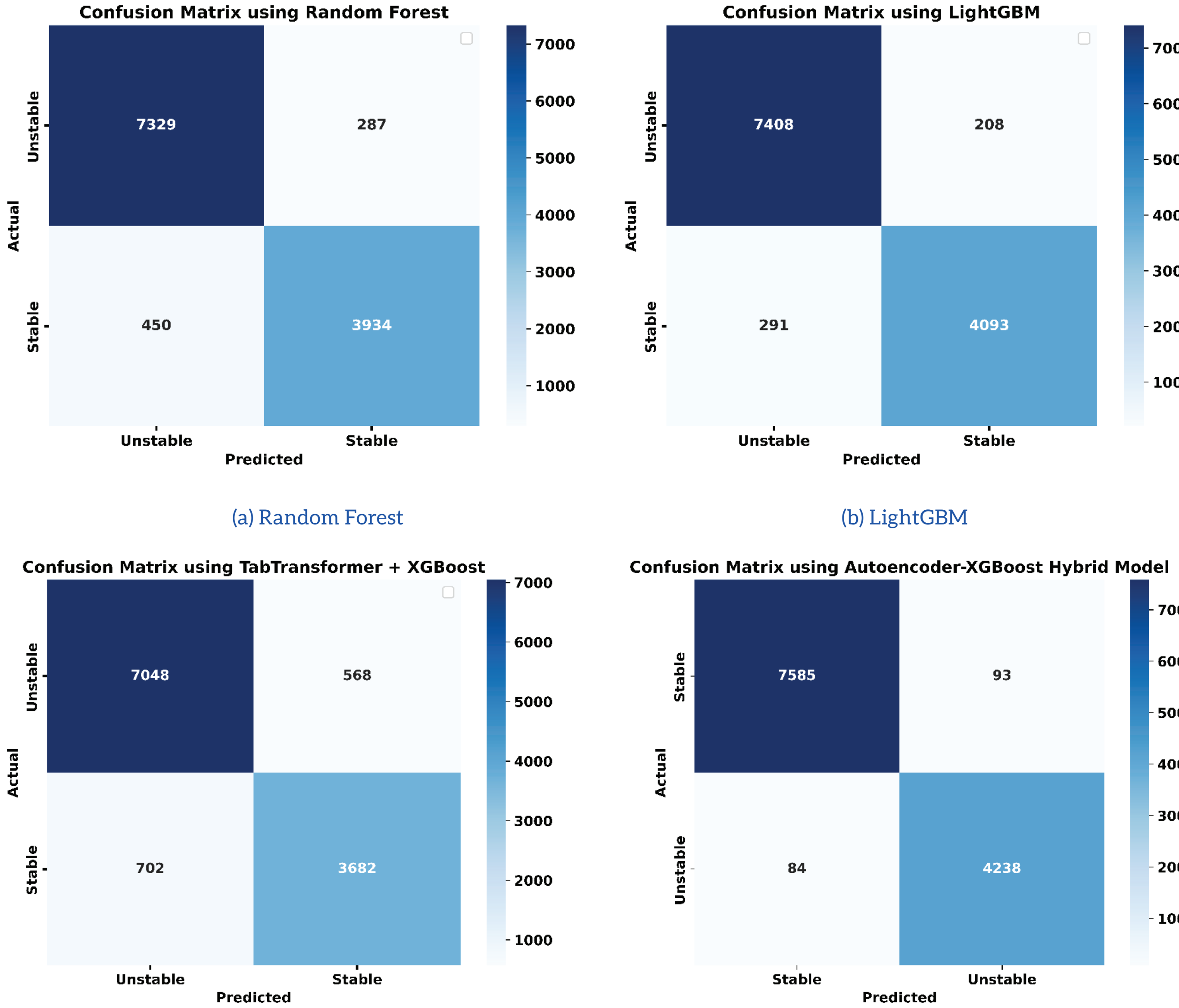

(a) Random Forest

(b) LightGBM

(c) TT-XGBoost

(d) AE-XGBoost

Figure 4: Confusion matrices of Random Forest, LightGBM, TT-XGBoost, and AE-XGBoost models.

Figure 5 shows the ROC curves of all models. AE-XGBoost is nearly perfect with an AUC close to 1.0. LightGBM also performs strongly, while Random Forest lags slightly in detecting unstable states. TT-XGBoost dips noticeably, confirming its weaker class separation.

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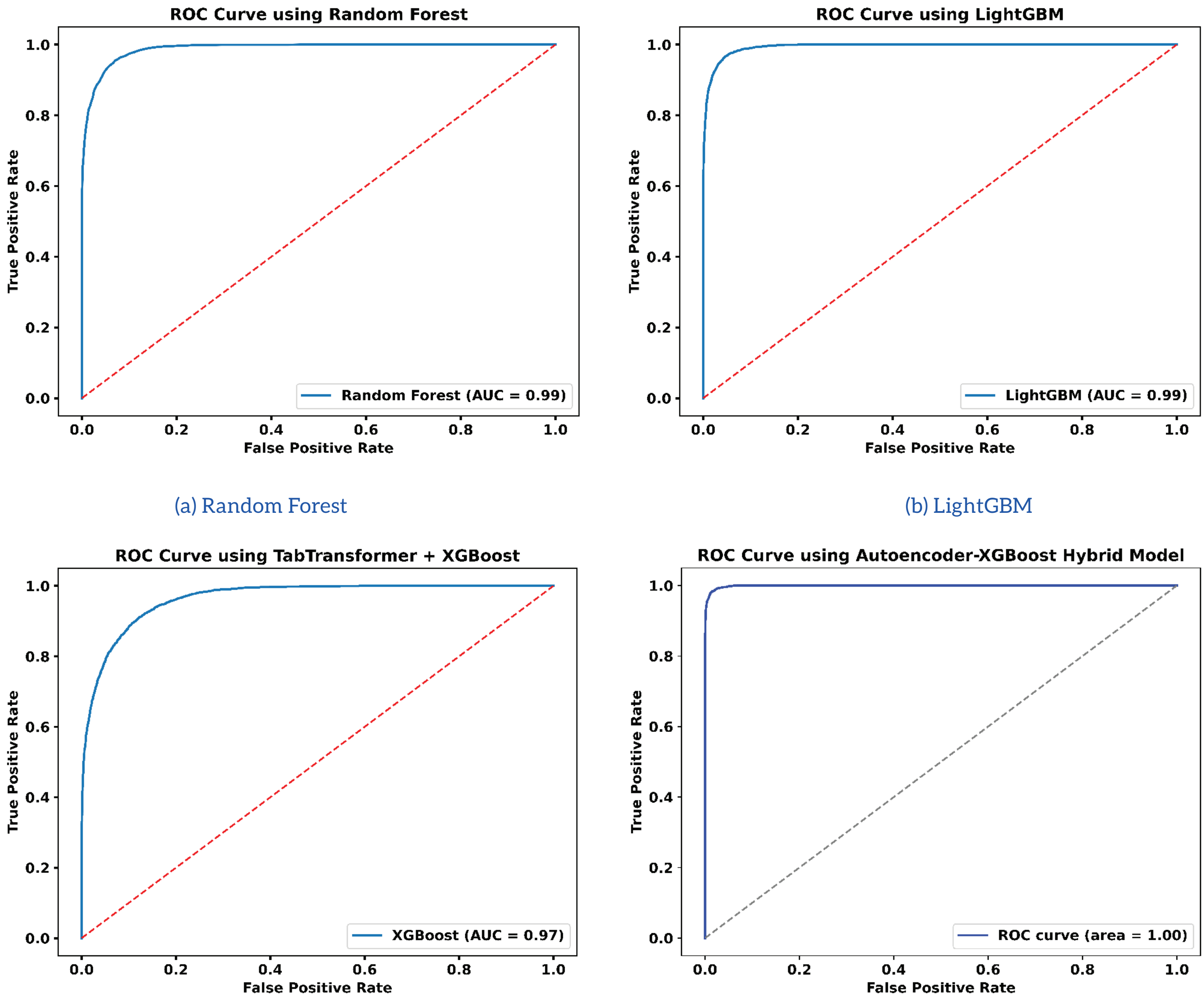

(a) Random Forest (b) LightGBM

(c) TT-XGBoost (d) AE-XGBoost

Figure 5: ROC curves of Random Forest, LightGBM, TT-XGBoost, and AE-XGBoost models.

Figure 6 presents the Precision–Recall curves. AE-XGBoost and LightGBM stay near the top-right corner, showing strong balance. Random Forest is slightly lower, while TT-XGBoost drops at higher recall, consistent with its weaker F1-scores.

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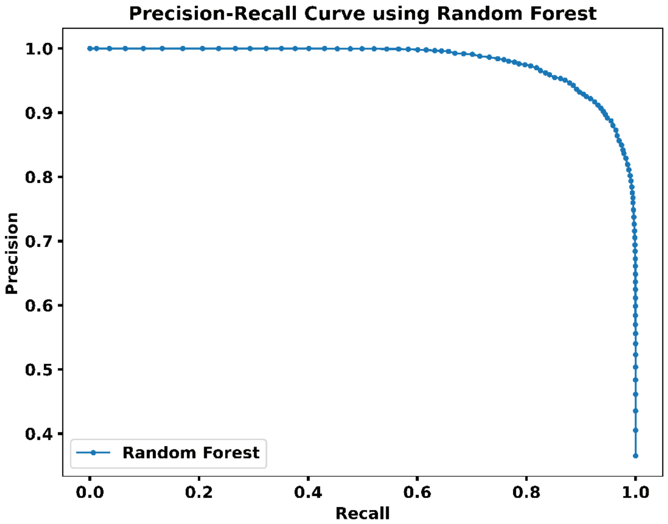
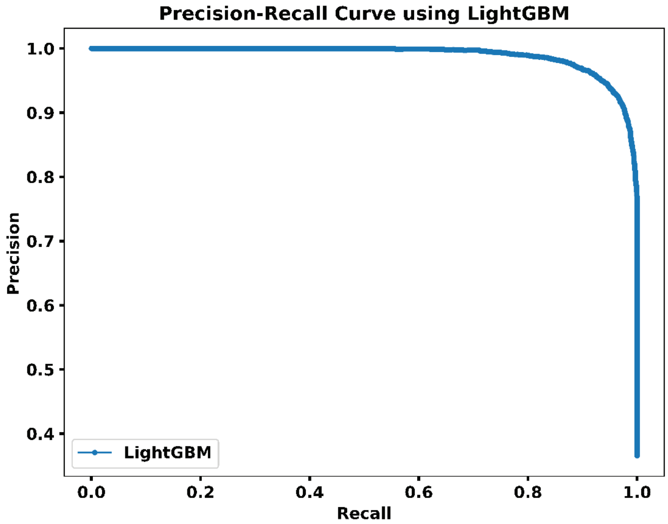
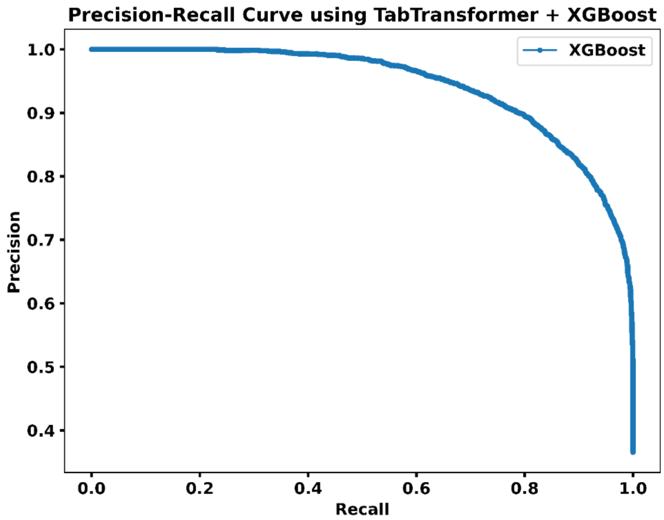


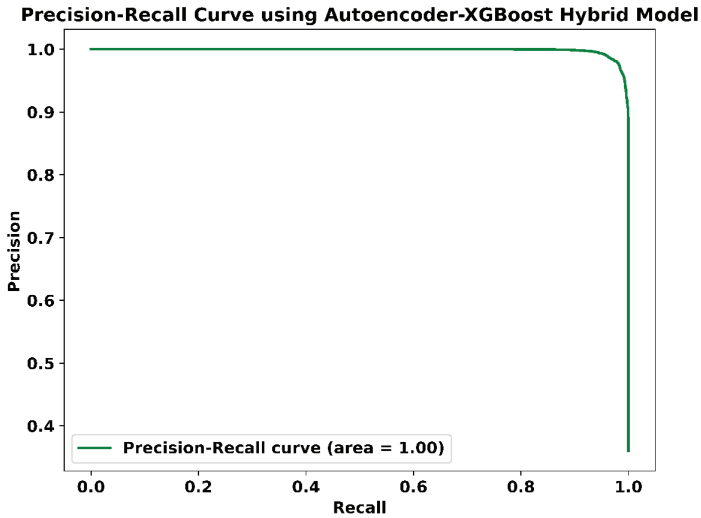
(a) Random Forest



(b) LightGBM



(c) TT-XGBoost



(d) AE-XGBoost

Figure 6: Precision–Recall curves of Random Forest, LightGBM, TT-XGBoost, and AE-XGBoost models.

Figure 7 shows the calibration curves with Expected Calibration Error (ECE) values. AE-XGBoost is closer to the diagonal and achieves a slightly lower ECE (0.036 vs. 0.037), giving more reliable probability estimates than LightGBM.

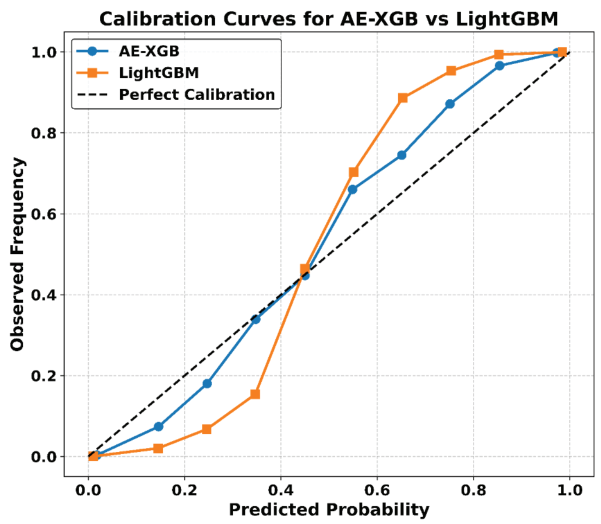


Figure 7: Calibration curves of AE-XGBoost and LightGBM models with reliability comparison.

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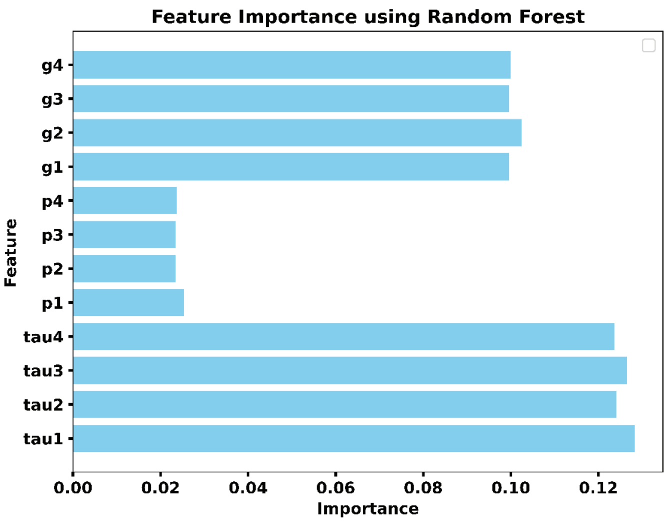
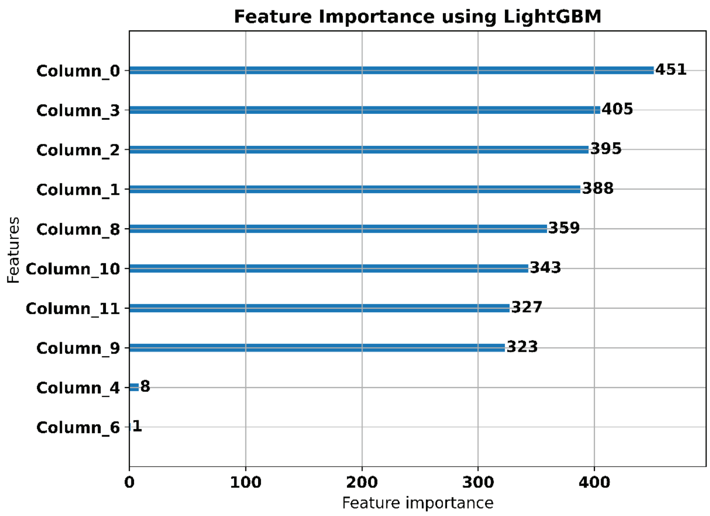
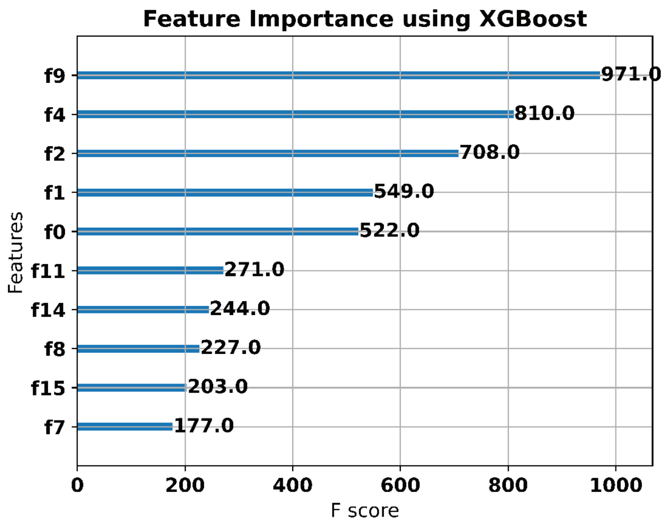
Figure 8 shows the feature importance rankings. AE-XGBoost and LightGBM both highlight phase angles and power outputs as key variables, while TT-XGBoost distributes focus more evenly, and Random Forest is less consistent.



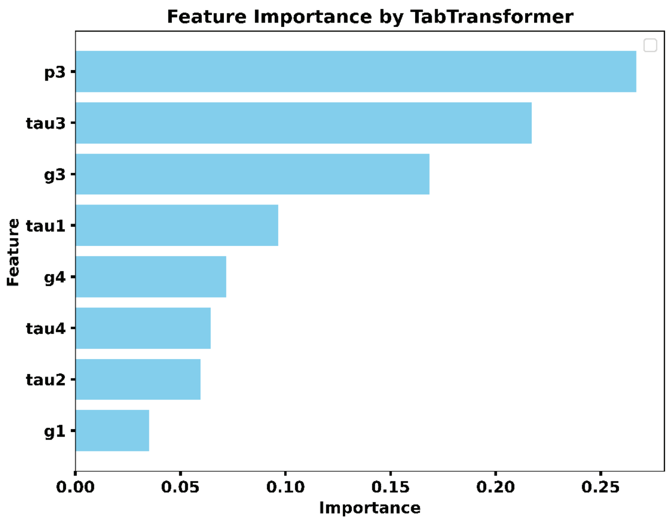
(a) Random Forest



(b) LightGBM



(c) XGBoost



(d) TabTransformer

Figure 8: Feature importance plots of Random Forest, LightGBM, XGBoost (from AE-XGBoost), and TabTransformer (from TT-XGBoost) models.

These results also have practical value. Both AE-XGBoost (through its XGBoost part) and LightGBM point to phase angles and power outputs as the most important variables. Random Forest highlights some of the same features but less consistently, while TT-XGBoost spreads its focus too widely, which likely affects its accuracy. For operators, this means keeping a close eye on phase angles ($g1$ to $g4$) can help spot early signs of instability, and watching power outputs ($p1$ to $p4$) can guide timely actions like load balancing or generator rescheduling.

Table 5: Ablation study results comparing baseline, individual components, and hybrid models.

Model	Accuracy	F1-Score	Balanced Accuracy	MCC	ROC AUC
XGBoost	0.961	0.946	0.955	0.916	0.995
AE	0.819	0.740	0.795	0.602	0.899
TT	0.978	0.970	0.978	0.953	0.998
AE-XGBoost	0.977	0.980	0.976	0.951	0.998
TT-XGBoost	0.894	0.850	0.883	0.771	0.965

Note: Results for AE-XGBoost, TT-XGBoost, and XGBoost are consistent with those reported in Tables 2 and 3, and are repeated here for completeness.

Table 5 compares the baseline, individual components, and hybrid models. XGBoost alone already performed strongly (96.1% accuracy, ROC AUC 0.995). Autoencoder alone reduced performance (81.9% accuracy), showing that compression by itself is insufficient. TabTransformer alone performed best among individual models (97.8% accuracy, ROC AUC 0.998), confirming the strength of attention-based feature learning. Among the hybrids, AE-XGBoost improved over plain XGBoost, while TT-XGBoost did not show consistent gains. These results show that combining the Autoencoder with XGBoost gives the strongest performance, supporting the proposed hybrid design.

IV. Conclusion

This study evaluated hybrid machine learning models for predicting grid stability, focusing on both accuracy and the reliability of predictions. Among the tested approaches, the Autoencoder combined with XGBoost (AE-XGBoost) consistently outperformed others, achieving high validation and test accuracy, excellent ROC separation, and balanced class-wise metrics. Its performance highlights its potential for real-world deployment in smart grid systems where stability decisions are critical. LightGBM also demonstrated strong results and useful feature insights, while TabTransformer with XGBoost (TT-XGBoost), despite its architectural depth, showed less consistent performance. These findings confirm that effectiveness depends more on alignment with data characteristics and careful evaluation than on complexity alone. This broader insight is also reflected in renewable-energy applications, where hybrid and interpretable learning frameworks have shown similar promise in enhancing forecasting accuracy and improving operational stability of sustainable grids.

At the same time, this study has certain limitations. The experiments were conducted on a single benchmark dataset and focused only on binary stability classification. Future work will test scalability to larger and more complex grids, explore extensions to multi-class and multi-label Classification, and investigate real-time integration of these models for adaptive grid management. These directions will further validate the robustness and practical utility of the proposed framework.

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