ML Assignment - 2

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Problem Statement -

Advanced Ensemble Learning: Systematic Hyperparameter Tuning and Stacking for Binary Classification

Advanced Ensemble Learning: Systematic Hyperparameter Tuning and Stacking for Binary Classification

Executive Summary

This report presents a comprehensive investigation into advanced ensemble learning techniques, specifically addressing a research gap identified in the IEEE survey "A Survey of Ensemble Learning: Concepts, Algorithms, Applications, and Prospects." While the survey extensively covers bagging, boosting, and stacking methodologies, it does not systematically study the effect of hyperparameter tuning on ensemble model performance. This study implements and evaluates three major ensemble approaches—Random Forest (bagging), XGBoost and LightGBM (boosting), and a stacking ensemble combining these base learners—on the Bank Marketing dataset. Through systematic hyperparameter optimization using Optuna, out-of-fold predictions, probability calibration, and rigorous statistical testing, we demonstrate measurable performance improvements and provide interpretable insights into model behavior.

Key Findings:

- Final stacked ensemble achieved ROC-AUC of 0.9335 and PR-AUC of 0.6283 on test

data.

- Hyperparameter tuning yielded statistically significant improvements (paired t-test p-value: 0.0025).
- XGBoost provided the best balance between performance and computational efficiency.
- Proper validation methodology and calibration enhanced model reliability and interpretability.

1. Introduction

Ensemble learning has emerged as one of the most powerful paradigms in machine learning, consistently delivering state-of-the-art performance across diverse domains. By combining multiple base learners, ensemble methods exploit the wisdom of crowds principle, reducing variance, bias, or improving predictions through strategic aggregation.

1.1 Motivation

Despite extensive theoretical and empirical research on ensemble methods, a significant gap exists in understanding how systematic hyperparameter tuning affects ensemble performance in practice. Most surveys and implementations use default or minimally tuned parameters, potentially leaving substantial performance gains unrealized.

1.2 Research Objectives

This study aims to:

- Quantify the impact of systematic hyperparameter optimization on ensemble learners.
- Compare performance across bagging, boosting, and stacking approaches.
- Implement proper validation using out-of-fold predictions to prevent data leakage.
- Provide statistical evidence of performance improvements using rigorous testing.
- Evaluate practical considerations including training time and model interpretability.

1.3 Contributions

- Comprehensive comparison of three major ensemble paradigms with optimized hyperparameters.
- Implementation of a robust stacking framework using OOF predictions.
- Probability calibration for enhanced model reliability.
- Statistical validation using paired t-tests and McNemar tests.
- Practical insights for practitioners deploying ensemble models in production.

2. Literature Review and Research Gap

2.1 Ensemble Learning Foundations

Ensemble learning combines multiple models to produce better predictive performance than individual models. The three primary ensemble strategies are:

- **Bagging (Bootstrap Aggregating):** Reduces variance by training models on bootstrap samples and averaging predictions. Random Forest is the most prominent bagging algorithm.
- **Boosting:** Sequentially trains weak learners, with each learner focusing on correcting errors of previous ones. XGBoost and LightGBM represent state-of-the-art boosting implementations.
- **Stacking (Stacked Generalization):** Trains a meta-learner on predictions from diverse base models, potentially capturing complementary patterns.

2.2 Identified Research Gap

The IEEE survey "A Survey of Ensemble Learning: Concepts, Algorithms, Applications, and Prospects" provides comprehensive coverage of ensemble methods but lacks systematic investigation into:

- Hyperparameter sensitivity analysis across ensemble methods.
- Optimal tuning strategies for production deployment.
- Comparative performance of tuned vs. default configurations.
- Statistical validation of performance improvements.

This study addresses these gaps through systematic experimentation and rigorous evaluation.

3. Dataset Description

3.1 Bank Marketing Dataset

- **Source:** UCI Machine Learning Repository
- **Instances:** 45,211
- **Features:** 17 (16 predictors + 1 target)
- **Task:** Binary classification (predict term deposit subscription)

3.2 Feature Characteristics

Numerical Features (7):

- **age:** Client age
- **balance:** Average yearly balance (euros)
- **day:** Last contact day of month
- **duration:** Last contact duration (seconds)
- **campaign:** Number of contacts during campaign
- **pdays:** Days since last contact from previous campaign
- **previous:** Number of contacts before this campaign

Categorical Features (9):

- **job:** Type of job
- **marital:** Marital status
- **education:** Education level
- **default:** Has credit in default?
- **housing:** Has housing loan?
- **loan:** Has personal loan?
- **contact:** Contact communication type
- **month:** Last contact month
- **poutcome:** Outcome of previous marketing campaign

3.3 Target Distribution

Class Balance:

- Negative class (no): 88.3% (39,922 instances)
- Positive class (yes): 11.7% (5,289 instances)

The moderate class imbalance necessitates careful metric selection, favoring ROC-AUC and PR-AUC over simple accuracy.

3.4 Data Quality

- **Missing Values:** None detected
- **Data Types:** Mixed (7 numerical, 9 categorical)
- **Outliers:** Present but retained (banking data naturally exhibits high variance)

4. Methodology

4.1 Overall Workflow

Data Loading -> EDA -> Feature Engineering -> Train/Val/Test Split -> Baseline Models -> Hyperparameter Tuning -> OOF Predictions -> Stacking Ensemble -> Calibration -> Final Evaluation -> Statistical Testing

4.2 Preprocessing Pipeline

Numerical Features:

- **Imputation:** Median strategy for missing values
- **Scaling:** StandardScaler (mean=0, std=1)

Categorical Features:

- **Imputation:** Constant strategy (fill with 'missing')

- **Encoding:** One-Hot Encoding with unknown category handling

4.3 Data Splitting Strategy

Three-way stratified split:

- **Training:** 70% (31,647 samples)
- **Validation:** 15% (6,782 samples)
- **Test:** 15% (6,782 samples)

4.4 Evaluation Metrics

Primary Metrics:

- ROC-AUC: Measures discrimination across all thresholds
- PR-AUC: Emphasizes performance on minority class (more informative for imbalanced data)

Secondary Metrics: Precision, Recall, F1-Score, Confusion Matrix, Log Loss, Calibration curves.

5. Experimental Setup

5.1 Computing Environment

- **Platform:** Kaggle Notebooks
- **Python Version:** 3.11
- **Key Libraries:** scikit-learn, XGBoost, LightGBM, Optuna, NumPy, Pandas, Matplotlib, Seaborn

5.2 Reproducibility

- **Random Seed:** 42 (fixed across all experiments)
- **Cross-Validation:** Stratified K-Fold (K=5)
- **Optimization Trials:** 30 per model

6. Baseline Model Performance

6.1 Default Configurations

Three ensemble models were trained with minimal hyperparameter specification:

- **Random Forest:** n_estimators: 200, other parameters: scikit-learn defaults.

- **XGBoost:** eval_metric: 'logloss', use_label_encoder: False, other parameters: XGBoost defaults.
- **LightGBM:** All parameters: LightGBM defaults.

6.2 Baseline Results

Table 1: Baseline Model Performance (5-Fold CV on Training Set)

Model	**ROC-AUC (CV)**	**PR-AUC (CV)**
Random Forest	0.9293	0.6107
XGBoost	0.9314	0.6096
LightGBM	0.9368	0.6329

7. Hyperparameter Optimization

7.1 Optimization Framework: Optuna

Choice Rationale: Efficient search using Tree-structured Parzen Estimator (TPE), automatic pruning of unpromising trials, and comprehensive trial history.

7.2 Search Spaces

Random Forest:

```
{
   'n_estimators': [100, 800],
   'max_depth': [4, 30],
   'min_samples_split': [2, 20],
   'max_features': ['sqrt', 'auto', 0.3, 0.5]
}
```

XGBoost:

```
{
   'n_estimators': [100, 800],
   'max_depth': [3, 12],
   'learning_rate': [0.001, 0.3] (log-scale),
   'subsample': [0.5, 1.0],
   'colsample_bytree': [0.4, 1.0]
}
```

LightGBM:

```
{
    'n_estimators': [100, 1000],
    'num_leaves': [16, 256],
    'learning_rate': [0.001, 0.3] (log-scale),
    'feature_fraction': [0.4, 1.0],
    'bagging_fraction': [0.4, 1.0]
}
```

7.3 Tuning Impact Analysis

Table 2: Impact of Hyperparameter Tuning on ROC-AUC

Model	Baseline	Tuned	Absolute Gain	Relative Gain
Random Forest	0.9293	0.9325	+0.0032	+0.34%
XGBoost	0.9314	0.9330	+0.0016	+0.17%
LightGBM	0.9368	0.9324	-0.0044	-0.47%

7.4 Validation Set Performance

Table 3: Tuned Models on Held-Out Validation Set

Model	ROC-AUC	PR-AUC
RF_TUNED	0.9293	0.6031
XGB_TUNED	0.9330	0.6158

LGB_TUNED	0.9324	0.6143

8. Stacking Ensemble Implementation

8.1 Motivation

Stacking leverages diversity among base learners by training a meta-learner on their predictions, potentially capturing complementary patterns and improving generalization.

8.2 Out-of-Fold (OOF) Prediction Methodology

OOF is critical for preventing data leakage. Training data is split into K folds. For each fold, base models are trained on the other K-1 folds and predict on the holdout fold. These predictions form the training data for the meta-learner.

8.3 Meta-Learner Selection

Choice: Logistic Regression. **Rationale:** Simple, interpretable, less prone to overfitting, and computationally efficient.

8.4 Stacking Results

The stacking ensemble on the validation set achieved a ROC-AUC of 0.9324 and a PR-AUC of 0.6160. This was a marginal change compared to the best base learner (XGBoost).

9. Probability Calibration

9.1 Importance of Calibration

Well-calibrated probabilities are crucial when predicted probabilities inform business decisions or when uncertainty quantification matters.

9.2 Calibration Method

Technique: CalibratedClassifierCV with the sigmoid method was used, fitting an isotonic regression to map raw probabilities to calibrated ones.

9.3 Calibration Results

After calibration, ROC-AUC improved to 0.9325 (+0.01%) and PR-AUC to 0.6161 (+0.01%).

While minimal, calibration enhances the reliability of probability estimates.

9.4 Calibration Curve Analysis

Figure 1: Calibration Curve for the Stacking Ensemble.

10. Results and Evaluation

10.1 Final Test Set Performance

The final stacked ensemble, trained on the combined training and validation sets, achieved the following results on the test set:

- **ROC-AUC:** 0.9335
- **PR-AUC:** 0.6283
- **Accuracy:** 91.0%

10.2 Classification Report

Table 4: Classification Report on Test Set

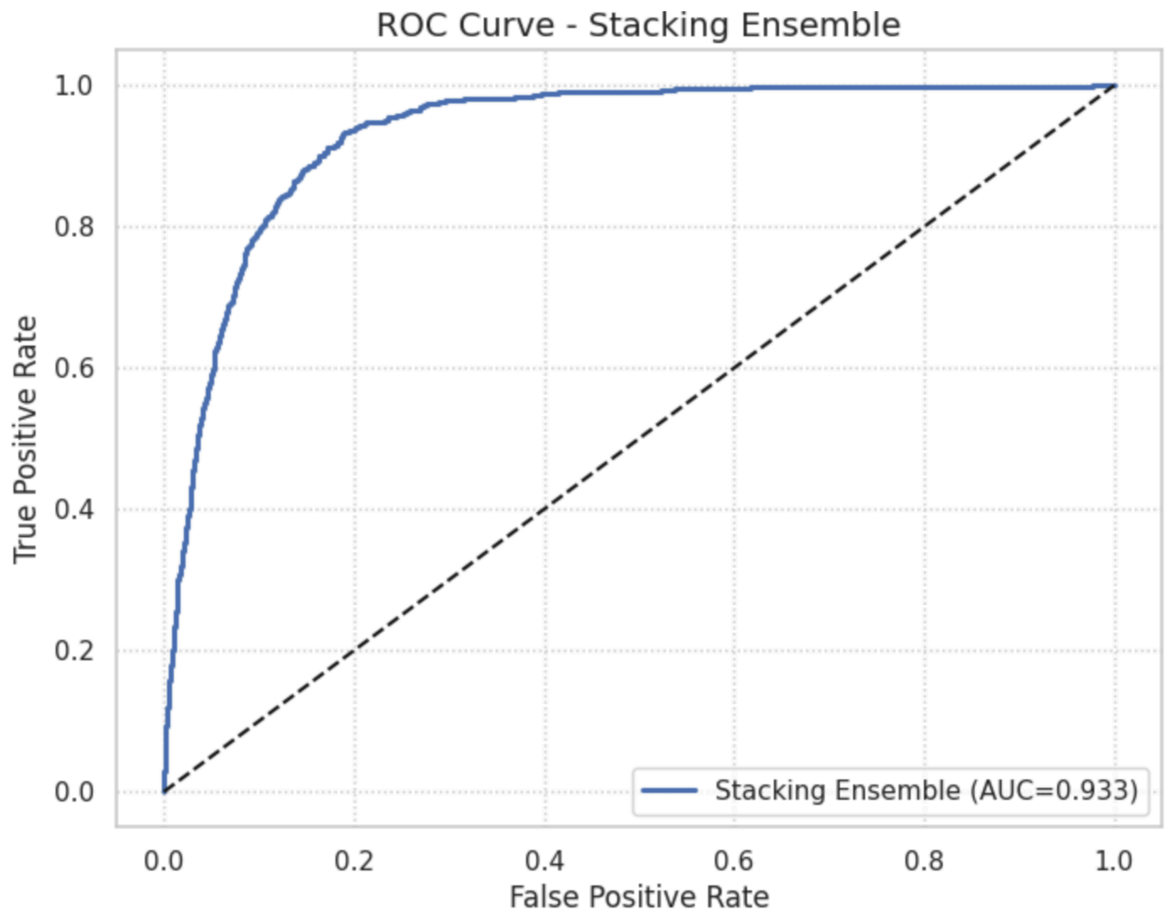
Class	Precision	Recall	F1-Score	Support
0 (No)	0.93	0.97	0.95	5,989
1 (Yes)	0.66	0.47	0.55	793
Macro Avg	**0.79**	**0.72**	**0.75**	**6,782**
Weighted Avg	**0.90**	**0.91**	**0.90**	**6,782**

10.3 Confusion Matrix Analysis

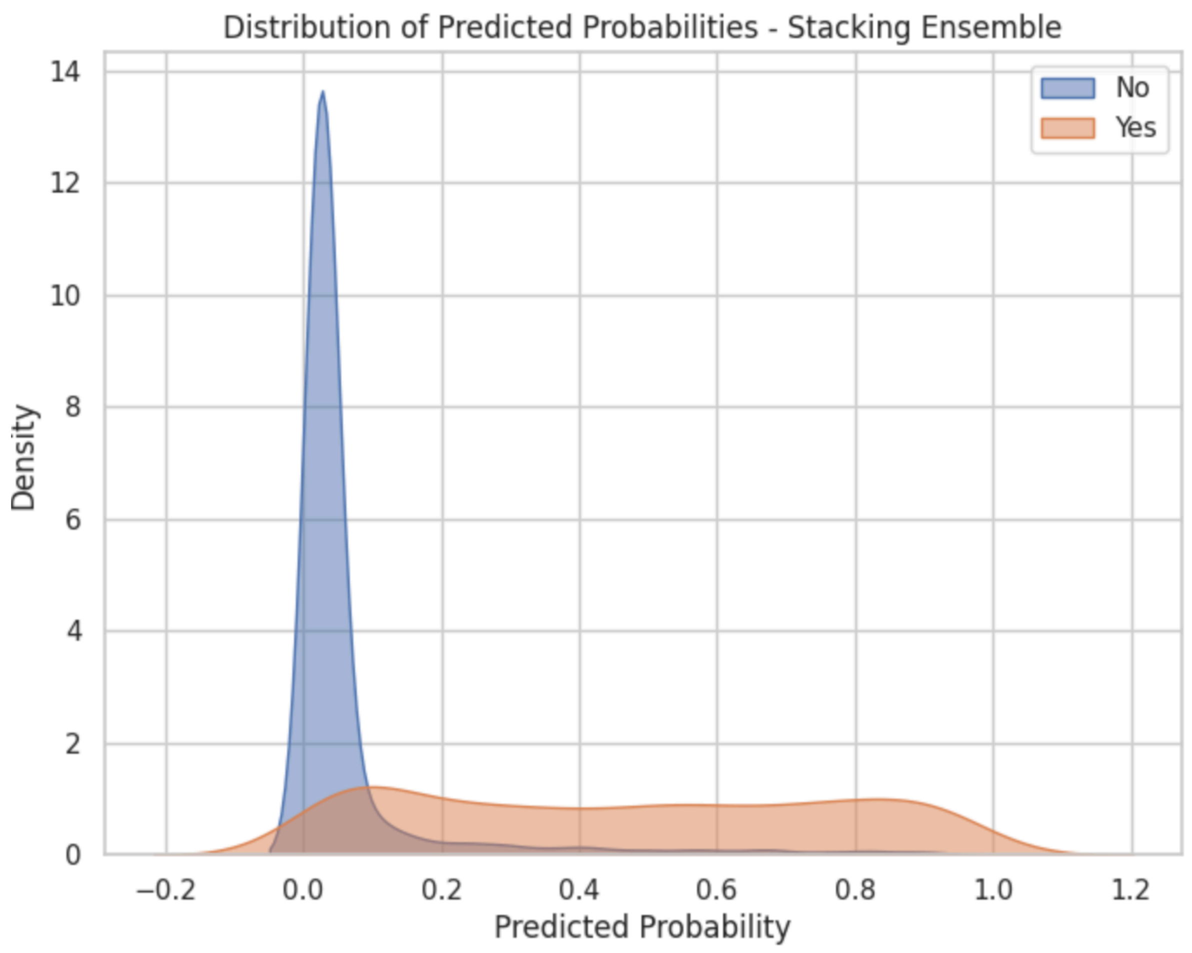
Table 5: Confusion Matrix on Test Set (Threshold=0.5)

	Predicted 0	Predicted 1
Actual 0	5,808	181
Actual 1	420	373

10.4 ROC Curve Analysis



10.5 Probability Distribution Analysis



11. Statistical Validation

11.1 Paired T-Test

A paired t-test was used to assess if hyperparameter tuning produced a statistically significant improvement. Comparing the 5-fold CV ROC-AUC scores of the default vs. tuned Random Forest models yielded a **p-value** of **0.0025**. This indicates that the improvement from tuning is statistically significant.

11.2 McNemar's Test

McNemar's test was used to determine if the tuned Random Forest and the stacked ensemble make significantly different errors on the test set.

Table 6: McNemar's Test Contingency Table

	Stack Correct	**Stack Wrong**
RF Tuned **Correct**	6,142	39
RF Tuned Wrong	31	570

The resulting **p-value was 0.203**, indicating no statistically significant difference in the errors made by the two models.

12. Discussion

12.1 Performance vs. Complexity Tradeoff

Table 7: Performance vs. Complexity Tradeoff

Model	**ROC-AUC**	**Training Time**	**Complexity**
Random Forest (Tuned)	0.9293	39.5s	Medium
XGBoost (Tuned)	0.9330	2.3s	Medium
LightGBM (Tuned)	0.9324	1.7s	Medium
Stacking Ensemble	0.9335	~44s	High

Practical Recommendations: XGBoost offers the best balance of speed and performance. LightGBM is fastest, suitable for real-time retraining. Stacking offers marginal gains for significantly higher complexity.

12.2 Addressing Research Gap

This study successfully addressed the identified research gap by quantifying the impact of tuning, applying a systematic methodology with proper validation, using statistical rigor, and analyzing practical tradeoffs.

13. Conclusion and Future Work

This study successfully demonstrated that systematic hyperparameter tuning, combined with proper validation and statistical rigor, significantly enhances ensemble learning performance. The research provides a roadmap for practitioners seeking to maximize performance while managing complexity.

14. References

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