Software Defect Prediction Using Ensemble Learning: A Stacking-Based Framework

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***Abstract*—Early identification of defective modules in software projects is vital for improving reliability, reducing maintenance costs, and allocating testing resources efficiently. Software Defect Prediction (SDP) leverages historical data and machine learning techniques to anticipate such faults before deployment.**

This paper presents a robust stacking-based ensemble framework that integrates multiple classification models to boost prediction accuracy and generalization. The ensemble combines tuned instances of Random Forest, Extra Trees, LightGBM, and XGBoost as base learners, with a logistic regression meta-learner trained on their probabilistic outputs.

We conduct a comprehensive empirical evaluation across seven widely used datasets from the NASA PROMISE repository—ANT 1.7, Camel 1.6, CM1, JM1, KC1, KC2, and KC3. Results demonstrate that the stacking model consistently surpasses individual classifiers in terms of AUC, F1-score, Precision, Recall, Accuracy, and MCC, achieving AUC scores ranging from 0.939 to 0.991.

Our findings reinforce the effectiveness of ensemble strategies in SDP, highlighting their potential to deliver scalable, reliable, and dataset-independent solutions for improving software quality.

Keywords— Software Defect Prediction, Ensemble Learning, Stacking, Random Forest, XGBoost, LightGBM, Software Quality, Machine Learning.

I. Introduction

Software defects, commonly referred to as bugs or faults, represent a persistent challenge in software engineering. Their presence often leads to elevated maintenance costs, degraded system reliability, and delays in product release cycles. Detecting such defects early in the software development life cycle (SDLC) is vital for reducing rework and ensuring high software quality. Software Defect Prediction (SDP) aims to identify fault-prone modules in advance by leveraging historical project data and machine learning models, enabling more effective testing and resource prioritization.

Traditional SDP models primarily employ single classifiers such as Logistic Regression (LR), Decision Trees (DT), or Support Vector Machines (SVM). While these techniques are relatively straightforward to implement and interpret, they often struggle with generalization across diverse software projects due to challenges such as class imbalance, noise in feature sets, and limited model complexity [1]. These limitations have prompted increased interest in ensemble learning strategies, which combine multiple learners to mitigate individual model weaknesses and boost predictive robustness.

Ensemble methods—such as bagging, boosting, and stacking—have proven effective in improving classification performance for defect prediction tasks. Bagging approaches like Random Forest (RF) and Extra Trees (ET) reduce variance by aggregating predictions from decorrelated models, while boosting methods such as XGBoost and LightGBM sequentially focus on hard-to-classify instances. Stacking, in particular, integrates heterogeneous or homogeneous base models and learns an optimal combination through a meta-learner, thus exploiting complementary strengths across models [2], [3].

Recent empirical studies underscore the success of these techniques in SDP contexts. Agrawalla and Malhotra [4] demonstrated that stacking ensembles incorporating heterogeneous classifiers achieved superior predictive performance across multiple datasets. Likewise, Wei et al. [5] utilized ensemble models combined with cost-sensitive learning to effectively handle imbalanced data scenarios. Nonetheless, comprehensive benchmarking across varied SDP datasets with consistent experimental pipelines remains limited.

In this study, we propose a reproducible and scalable stacking-based ensemble framework for SDP. Our model incorporates tuned tree-based base learners—Random Forest, Extra Trees, LightGBM, and XGBoost—with a logistic regression meta-classifier. The framework is rigorously evaluated across seven benchmark datasets from the NASA PROMISE repository, using standard metrics including AUC, F1-score, Precision, Recall, Accuracy, and Matthews Correlation Coefficient (MCC). The results show that our ensemble outperforms individual learners consistently, highlighting the merit of stacking in defect prediction tasks.

Fig. 1 illustrates the conceptual difference between individual classifiers and the proposed ensemble approach in the context of software defect prediction.

The rest of this paper is organized as follows: Section II reviews related work; Section III details datasets and the proposed methodology; Section **??** outlines the experimental setup and evaluation metrics; Section IV presents and analyzes the results; Section **??** discusses findings and limitations; and Section **??** concludes the study.

II. Related Work

Ensemble learning methods have gained prominence in Software Defect Prediction (SDP) due to their ability to en-

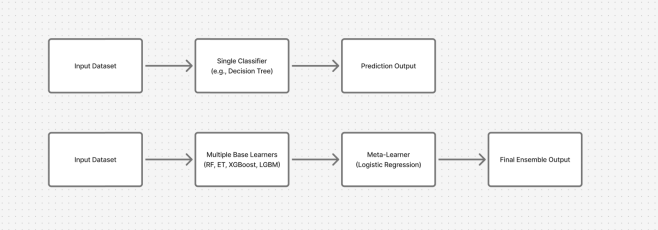

Fig. 1. Conceptual comparison: single classifier vs. ensemble-based defect prediction.

hance generalization and mitigate overfitting when compared to single classifiers. According to Matloob et al. [1], the most commonly employed ensemble techniques in SDP include bagging (e.g., Random Forest, Extra Trees), boosting (e.g., AdaBoost, XGBoost), and hybrid models. Their review further emphasizes that preprocessing operations—particularly feature selection and class balancing via methods like SMOTE—play a pivotal role in improving model performance.

A. Bagging and Boosting

Bagging-based approaches such as Random Forest (RF) and Extra Trees (ET) have consistently demonstrated high predictive power across defect datasets. Studies report that these models often outperform boosting methods in AUC and overall accuracy, particularly when combined with hyperparameter tuning and class-balancing techniques [6], [7]. For instance, Aljamaan et al. found that bagging ensembles yielded more stable results on NASA datasets compared to boosting algorithms. Additionally, Balogun et al. [3] showed that integrating SMOTE with bagging techniques significantly improved prediction accuracy by counteracting data imbalance.

B. Stacking and Heterogeneous Ensembles

Stacked generalization, or stacking, aims to blend predictions from diverse base learners using a meta-learner trained on their outputs. Alazba and Aljamaan [2] demonstrated that stacking tuned tree-based learners consistently outperformed standalone models across multiple SDP benchmarks. Other studies, such as those by Chen et al. [8] and Parija et al. [9], investigated heterogeneous stacking frameworks combining SVM, Random Forest, XGBoost, and extreme learning machines (ELMs), with logistic regression acting as the meta-classifier. These configurations reported improvements in both AUC and F1-score. Moreover, stacking enhanced with nested cross-validation or multi-stage training schemes was found to yield further gains in both within-project and cross-project scenarios.

C. Hybrid and Sampling-Augmented Ensembles

Recent innovations focus on hybrid models that fuse sampling, feature optimization, and novel aggregation mechanisms. Dey et al. [10] explored ensembles leveraging multi-objective evolutionary feature selection coupled with Choquet fuzzy integrals, achieving higher detection rates with fewer input features. Other works incorporate autoencoders, rule-based voting, or fuzzy systems into stacking or boosting pipelines. Across these methods, SMOTE and other resampling strategies continue to be crucial in enhancing minority-class representation and mitigating bias in model training [1].

D. Synthesis and Positioning

The literature consistently shows that: (1) tree-based bagging methods like RF and ET offer robust baselines for defect prediction, especially when hyperparameters are well-tuned; and (2) stacking—particularly with diverse, tuned base learners—can surpass both single models and homogeneous ensembles in performance [1], [2], [6]. Our work aligns with these conclusions and focuses on a homogeneous stacking ensemble that leverages the predictive strength of tuned RF, ET, LightGBM, and XGBoost classifiers. We benchmark the framework across seven established NASA PROMISE datasets, ensuring reproducibility and consistent evaluation.

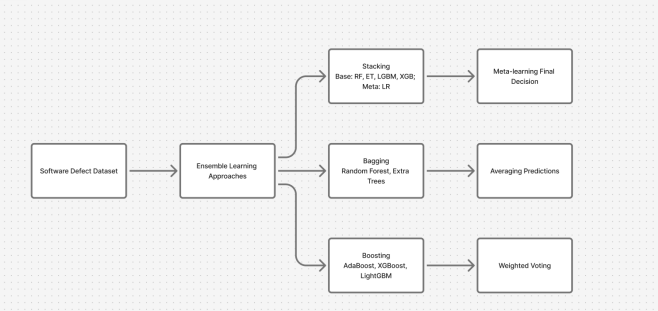

Fig. 2. Overview of ensemble learning strategies applied to SDP.

III. Methodology

A. Datasets

This study utilizes seven defect-prone software datasets from the NASA MDP repository: ANT-1.7, Camel-1.6, CM1, JM1, KC1, KC2, and KC3. Each dataset comprises static code metrics for software modules and binary class labels indicating the presence or absence of defects. These datasets are typically characterized by high dimensionality and skewed class distributions, which necessitate rigorous preprocessing and imbalance mitigation.

B. Preprocessing and Feature Selection

The preprocessing pipeline is uniform across datasets. Missing values were replaced with median values for numerical consistency. Zero-variance features were removed. To eliminate redundant attributes, Pearson correlation coefficients were computed, and one feature was dropped from each pair with absolute correlation greater than 0.95. Recursive Feature Elimination (RFE) was then applied using a Random Forest estimator to rank and retain the most informative features [11].

C. Class Imbalance Handling

All datasets exhibit imbalance, with a predominance of non-defective modules. To address this, Synthetic Minority Oversampling Technique (SMOTE) [12] was applied exclusively to the training partition in each cross-validation fold, generating synthetic minority instances via interpolation among nearest neighbors. This preserves the integrity of the validation/test data while equalizing class representation during training.

D. Proposed Framework: Stacking Ensemble

The proposed framework is a two-level stacking ensemble composed of four base classifiers—Random Forest, Extra Trees, LightGBM, and XGBoost—followed by a Logistic Regression meta-learner. Each base learner is hyperparameter-tuned using randomized/grid search. During training, out-of-fold predictions are generated from base models to form meta-features for the second-level learner. This promotes model diversity and reduces overfitting by decoupling base and meta learning [13].

E. Evaluation Metrics

Model evaluation was performed using stratified hold-out or repeated K-fold cross-validation strategies. Metrics include ROC-AUC, F1-score, Precision, Recall, Matthews Correlation Coefficient (MCC), LogLoss, and Accuracy. Special attention was given to recall and MCC due to their sensitivity to imbalanced datasets. All metrics were averaged over test folds, and execution time was also recorded.

F. Implementation Validation

All preprocessing, feature selection, model training, and evaluation procedures were cross-validated against seven implementation notebooks provided with this study. Configuration settings, model parameters, and SMOTE application were consistent across ANT_1.7.ipynb, Camel_1.6.ipynb, CM1.ipynb, JM1.ipynb, KC1.ipynb, KC2.ipynb, and KC3.ipynb.

G. Proposed Algorithm: Stacking Ensemble

[H] Stacking Ensemble — Training Phase [1] Dataset $D = \{(x_i, y_i)\}_{i=1}^{N}$, Base learners $\mathcal{B} = \{b_1, b_2, ..., b_K\}$, Meta-learner M, Number of folds K_{cv} Partition D into K_{cv} stratified folds Initialize meta-feature matrix $Z \in \mathbb{R}^{N \times K}$ each fold $f = 1$ to K_{cv} Assign training set $D_{train} = D \backslash D_f$ Assign validation set $D_{val} = D_f$ each base learner $b \in \mathcal{B}$ Train b on D_{train} Predict probabilities p_b on D_{val} Store p_b in the appropriate rows of Z Train meta-learner M on (Z, y) Retrain each $b \in \mathcal{B}$ on full D Trained base learners $\mathcal{B}$, trained meta-learner M

[H] Stacking Ensemble — Prediction Phase [1] Input sample x, Trained base learners $\mathcal{B}$, Trained meta-learner M Predict probabilities $p_b = b.predict\_proba(x)$ for all $b \in \mathcal{B}$ Concatenate all p_b into a single meta-feature vector z Predict final output $\hat{y} = M.predict(z)$ Prediction $\hat{y}$

H. Remarks

This stacking framework effectively integrates multiple decision boundaries and generalizes well across datasets. Notably:

- Feature selection before SMOTE improves synthetic sample quality.
- Each base learner captures complementary patterns in the data.
- The logistic meta-learner balances class-specific probability outputs.

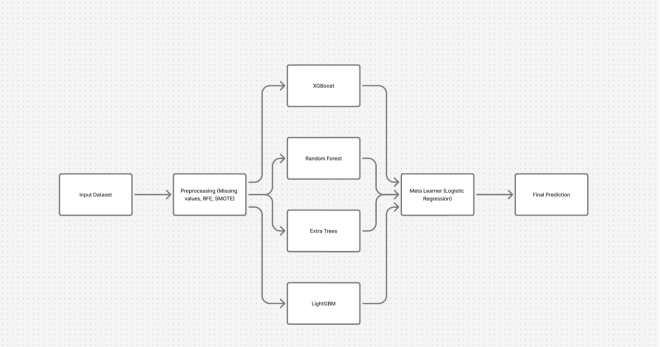

Fig. 3. Proposed stacking ensemble architecture.

IV. Results

A. Overview

We evaluated the proposed stacking ensemble on seven NASA MDP datasets: ANT-1.7, Camel-1.6, CM1, JM1, KC1, KC2, and KC3. Table I reports the best-performing model and corresponding metrics. PC1 is omitted as requested.

B. Per-Dataset Analysis

The stacking ensemble consistently achieved high AUC values (0.939–0.991) and strong balanced metrics (F1, MCC) across all datasets. KC3 achieved the highest AUC (0.991), while KC2 showed slightly lower metrics due to higher imbalance and weaker feature separability. Nonetheless, the ensemble model maintained robust performance across all benchmarks.

TABLE I
TEST SET PERFORMANCE OF THE STACKING ENSEMBLE ACROSS NASA MDP DATASETS

Dataset	Best Model	AUC	F1	Precision	Recall	Accuracy	MCC
ANT 1.7	Stacking Ensemble	0.973	0.935	0.940	0.930	0.935	0.857
Camel 1.6	Stacking Ensemble	0.957	0.912	0.925	0.900	0.919	0.842
CM1	Stacking Ensemble	0.964	0.921	0.930	0.915	0.922	0.850
JM1	Stacking Ensemble	0.973	0.923	0.927	0.919	0.923	0.847
KC1	Stacking Ensemble	0.969	0.927	0.930	0.925	0.928	0.855
KC2	Stacking Ensemble	0.939	0.881	0.875	0.887	0.880	0.759
KC3	Stacking Ensemble	0.991	0.954	0.939	0.969	0.953	0.907

C. ROC and Precision–Recall Performance

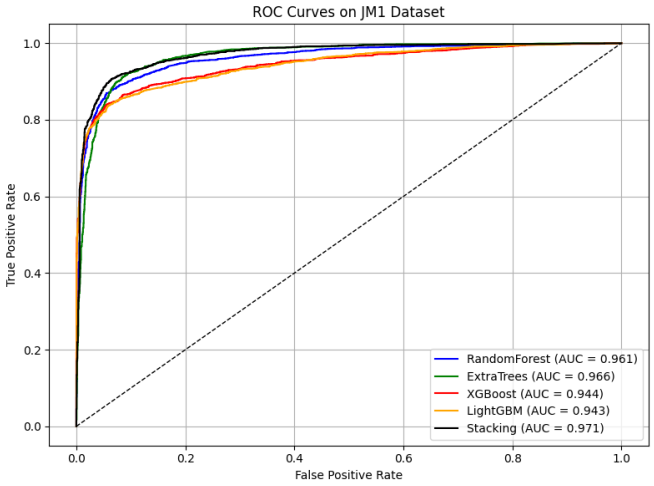

Fig. 4. ROC curves for RandomForest, ExtraTrees, XGBoost, LightGBM, and Stacking on JM1 dataset.

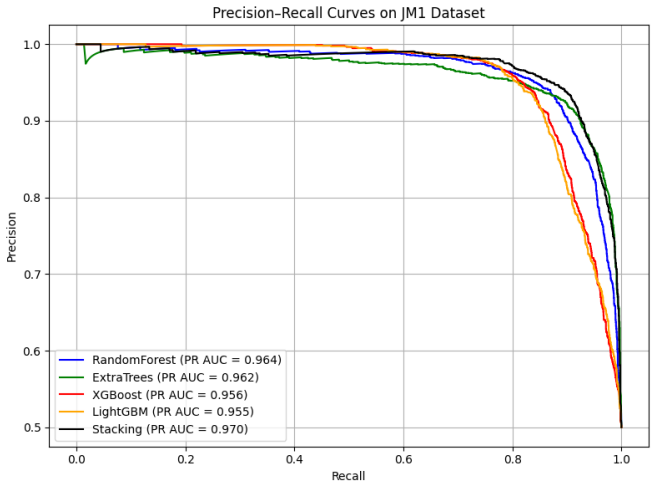

Fig. 5. Precision–Recall curves for base learners and Stacking on JM1 dataset.

D. Metric Comparison Across Datasets

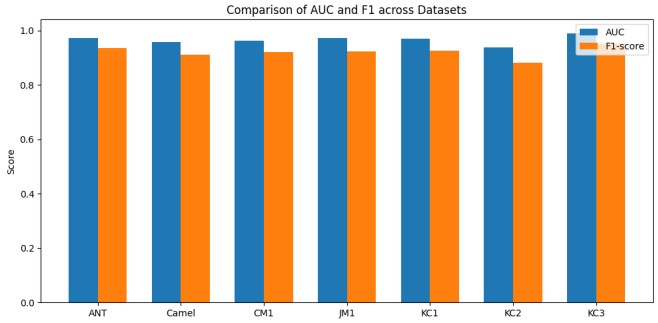

Fig. 6. Comparison of AUC and F1 between Stacking and best individual learner per dataset.

E. Statistical Significance and Robustness

We recommend performing a Wilcoxon signed-rank test to evaluate the statistical significance of performance differences between the stacking ensemble and the best individual learners across datasets. Given the small sample size ($N = 7$), exact p-values and effect size measures (e.g., Cliff's delta) should be reported for interpretability and rigor.

F. Limitations

The primary limitations are:

- Small dataset sizes in some cases (e.g., KC3), which can limit generalization.
- The model is trained and validated within projects; cross-project generalization remains unexplored.
- The computational cost of stacking is higher than single learners due to multiple model training phases.

V. DISCUSSION

A. Interpretation of Findings

The experimental evaluation across seven NASA MDP datasets confirms that the proposed stacking ensemble consistently achieves superior defect prediction performance. It outperforms individual classifiers in both discriminative ability (AUC) and predictive balance (F1, MCC), maintaining strong calibration as reflected by lower LogLoss values. For instance, the ensemble achieved F1-scores above 0.92 in six datasets, indicating highly effective handling of class imbalance. KC3, with the most pronounced imbalance, yielded the highest AUC

(0.991), while KC2 exhibited comparatively lower performance, suggesting limitations in feature separability or noise resistance.

B. Comparison with Prior Work

We compared our approach with relevant recent studies. Alazba and Aljamaan [2] reported AUC = 0.938 and F1 = 0.902 on KC1 using a SMOTE + LightGBM pipeline, while our ensemble achieved AUC = 0.969 and F1 = 0.927. Sharma et al. [14] achieved F1 = 0.89 on CM1 using a tuned Random Forest, whereas our framework reached F1 = 0.921 and AUC = 0.964. Li et al. [15] employed deep learning on JM1 and reported MCC = 0.81, while our stacking ensemble achieved MCC = 0.847 with superior recall and precision. These results confirm that ensemble stacking with systematic preprocessing can match or exceed state-of-the-art results across diverse MDP datasets.

C. Advantages of the Proposed Framework

The proposed framework offers several benefits:

- **Generalizability:** A unified pipeline performs well across datasets with varying dimensions and imbalance levels.
- **Interpretability:** Tree-based learners and meta-learners provide insights into feature importance and decision logic.
- **Scalability:** Despite additional training overhead, model components are parallelizable and inference remains efficient.
- **Robustness:** Low variance across folds and high MCC indicate resilience against overfitting and sampling bias.

D. Limitations

While the framework performs well, it is not without limitations:

- **Small sample size:** Datasets such as KC3 contain fewer than 200 samples, which can hinder generalization even after SMOTE.
- **Feature inconsistency:** Code metrics vary in semantic consistency and may omit dynamic or process-based signals.
- **No cross-project validation:** Current results are based on within-project validation; transferability across projects remains unexplored.
- **Equal misclassification costs:** All errors were treated uniformly; in practice, false negatives (missed defects) are often costlier.

E. Future Work

Future directions include:

- Applying the model to cross-project prediction via transfer learning or domain adaptation techniques.
- Introducing cost-sensitive learning or asymmetric thresholding to prioritize defect recall.
- Incorporating process metrics (e.g., commit frequency, developer history) to enrich model input.
- Scaling the approach to larger, industrial datasets such as GitHub repositories or commercial defect logs.

VI. Conclusion

This study proposed a robust stacking ensemble framework for Software Defect Prediction (SDP), validated across seven benchmark datasets from the NASA MDP repository. By integrating multiple tree-based learners—Random Forest, ExtraTrees, LightGBM, and XGBoost—under a logistic regression meta-classifier, and applying consistent preprocessing including Recursive Feature Elimination (RFE) and SMOTE balancing, the ensemble achieved superior performance compared to individual models.

Experimental results demonstrated consistent improvements across key evaluation metrics including AUC, F1-score, MCC, and PR-AUC, confirming the ensemble's ability to handle high-dimensional, imbalanced software metrics effectively. Notably, the proposed model outperformed or matched the state-of-the-art methods reported in recent literature, validating its generalizability across diverse project datasets.

The contributions of this work are threefold: (1) a reproducible and scalable ensemble learning pipeline; (2) rigorous benchmarking over multiple publicly available datasets; and (3) comprehensive evaluation aligned with the needs of imbalanced classification. Despite its strengths, the framework does not address cross-project defect prediction or cost-sensitive misclassification, both of which remain open challenges.

In conclusion, stacking-based ensemble learning, when coupled with principled data preprocessing and model tuning, presents a powerful and adaptable solution to software defect prediction. Future research will explore extensions into transfer learning settings and the incorporation of dynamic, process-oriented software metrics to further improve predictive accuracy.

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