A Comparative Evaluation of RandomForest and XGBoost within the ELDB Multi-Instance Learning Framework

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ABSTRACT

Multi-Instance Learning (MIL) addresses classification problems where labels are as- signed to bags of instances rather than indi- vidual instances. The Multi-Instance Ensem- ble Learning with Discriminative Bags (ELDB) algorithm is a notable mapping- based MIL approach that transforms bags into a new feature space before classification. The performance of ELDB depends signifi- cantly on the classifier employed on this mapped representation. This study investi- gates the integration and performance of modern ensemble classifiers, specifically RandomForest (RF) and XGBoost (XGB), within the ELDB framework, using their de- fault parameters. These were compared against the baseline classifiers originally con- sidered (k-Nearest Neighbors (kNN), Sup- port Vector Machines (SVM), and Decision Trees (J48)) using an implementation based on the work by Yang et al. (2022). Experi- ments were conducted using 10-fold cross-validation on standard MIL benchmark da- tasets including Musk1+, Fox+, and Tiger+, with F1-score as the primary evaluation met- ric. Results indicated that performance is highly dataset-dependent; while XGBoost showed strong performance on Fox+, kNN remained the top performer on Musk1+. Sig- nificant variability in performance across folds was also observed, particularly on the Tiger+ dataset. This study demonstrates the feasibility of integrating RF and XGBoost into ELDB and highlights that while these models are competitive, the optimal classifier choice is contingent on the dataset character- istics, warranting careful selection or further tuning within the ELDB framework.

Keywords: Multi-Instance Learning, En- semble Learning, ELDB, RandomForest, XGBoost, Machine Learning, Classification, Benchmark Datasets

INTRODUCTION

Machine learning often deals with scenarios where labels are available for each data point. However, in various real-world applications, such as drug activity prediction, image classifi- cation, and text categorization, labels are only assigned to groups (or "bags") of instances, while the labels of individual instances within the bags remain unknown. This paradigm is known as Multi-Instance Learning (MIL). Since its introduction, MIL has garnered signif- icant attention due to its ability to handle weakly labeled data.

Several approaches have been developed to tackle MIL problems. Instance-based methods attempt to identify key instances within bags to drive classification. Bag-based methods define distance metrics directly between bags. Another prominent strategy involves embedding or mapping methods, which transform each bag into a single feature vector in a new space, al- lowing standard supervised learning algorithms to be applied.

The Multi-Instance Ensemble Learning with Discriminative Bags (ELDB) algorithm, pro- posed by Yang et al., falls into the mapping- based category. ELDB employs a two-stage process: first, it selects a subset of "discrimina- tive" bags (dBagSet) based on spatial and label information, potentially refining this set using self-reinforcement; second, it maps all bags into a new feature space based on their distances to the bags in the selected dBagSet(s). Finally, an ensemble of classifiers trained on these mapped representations provides the final prediction. The effectiveness of the mapping relies

on thesubsequent classifier's ability to model the pat- terns in the transformed space.

The original ELDB study primarily evaluated its performance using relatively standard clas- sifiers like k-Nearest Neighbors (kNN), Sup- port Vector Machines (SVM), and Decision Trees (J48/C4.5). While effective, the advent of more powerful ensemble methods like Ran- domForest (RF) and XGBoost (XGB) raises the question of whether these modern techniques could further enhance ELDB's performance when applied to its generated feature space. These ensemble methods are often highly effec- tive on tabular data, potentially capable of cap- turing complex interactions within the mapped features derived from bag relationships.

Therefore, the objective of this paper is to inte- grate and empirically evaluate the performance of RandomForest and XGBoost, using their standard default hyperparameters, within the established ELDB framework. We compare their performance against the baseline classifi- ers (kNN, SVM, J48) on several standard MIL benchmark datasets to understand their suitabil- ity and potential benefits in this specific algo- rithmic context. This study provides insights into classifier selection for the ELDB algorithm and assesses the out-of-the-box effectiveness of modern ensemble methods on ELDB's mapped representations.

I. BACKGROUND AND RELATED WORK

A. Multi-Instance Learning (MIL)

In contrast to traditional supervised learning, MIL deals with data where a single label Y_i is assigned to a bag B_i = {x_i1, x_i2, ..., x_iN_i}, composed of N_i instances x_ij. The labels of individual instances x_ij are unknown during training. The standard MIL assumption, originating from drug activity prediction, posits that a bag is labeled positive if at least one in- stance within it is positive, and negative other- wise. The goal is typically to train a classifier that can predict the labels of unseen bags.

B. The ELDB Algorithm

The ELDB algorithm aims to improve upon standard mapping-based MIL methods by cre- ating more discriminative bag representations and using an ensemble approach. Its key com- ponents are:

1. *Discriminative Bag Set (dBagSet) Se- lection:* ELDB first analyzes the spatial and label distribution of a subset of the training data (Td) to identify bags that are effective at distinguishing between classes. This involves constructing a graph Laplacian-based matrix (L) and calculating a discriminative score (p_k) for bags based on their mapping rela- tive to Td (using a bag-to-bag distance metric like Average Hausdorff) and the L matrix. An initial dBagSet is formed by selecting bags with high scores.

2. *Self-Reinforcement:* An optional step where bags from another subset of the training data (Ts) are evaluated. If a bag from Ts demonstrates higher discrimi- native potential than the current worstbag in the dBagSet, it can either be added to the set (mode 'a') or replace the worst bag (mode 'r'). This iteratively re- fines the dBagSet, potentially creating multiple versions.

3. *Mapping Function:* For a given dBagSet state, each bag in the dataset (training and test) is mapped to a new feature vector. Each dimension of this vector typically represents the distance from the bag to one of the bags in the current dBagSet.

4. *Ensemble Construction:* ELDB trains a standard single-instance classifier (like kNN) on the mapped data correspond- ing to *each* generated dBagSet state (the initial one and any updated ver- sions). The performance of the classi- fier on a validation portion (like Ts) is used to assign a weight to the predic- tions made by that classifier using that specific dBagSet mapping. The final prediction for a test bag is derived by combining the weighted predictions from all ensemble members.

C. Classifiers Overview

The performance of ELDB relies heavily on the classifier used in the final stage on the mapped data. This study compares:

1. *k-Nearest Neighbors (kNN):* A non- parametric instance-based learner that classifies a point based on the majority label of its k nearest neighbors in the feature space. Simple and often effec- tive if proximity is meaningful.
2. *Support Vector Machine (SVM):* A powerful classifier that finds an opti- mal hyperplane to separate classes in a high-dimensional space, often using kernel functions.
3. *Decision Tree (J48/C4.5):* A tree-based model that recursively partitions the feature space based on simple rules learned from the data. Prone to overfit- ting individually but forms the basis of ensembles.
4. *RandomForest (RF):* An ensemble method that builds multiple decision trees on bootstrapped subsets of data and features, averaging their predic- tions. It reduces variance and often im- proves accuracy over single trees.
5. *XGBoost (XGB):* An efficient and highly regularized implementation of Gradient Boosting Machines. It builds trees sequentially, with each tree cor- recting the errors of the previous ones. Often achieves state-of-the-art perfor- mance on tabular data due to its han- dling of regularization and optimiza- tion.

RF and XGBoost are particularly relevant as they can potentially model complex, non-linear relationships and feature interactions that might exist in the mapped feature space generated by ELDB's distance-based transformation.

II. METHODOLOGY

A. Framework Implementation

This study utilized the core ELDB algorithm structure as presented by Yang et al.. The imple- mentation involved adapting and extending ex- isting Python code modules responsible for data handling (MIL), distance calculation (Dis- tance), classification (ClassifyTool), and the main ELDB workflow (ELDB), including fixes identified during development for robustness.

B. Classifier Integration

The primary modification involved extending the classification module (ClassifyTool.py) to support sklearn.ensemble.RandomForestClas- sifier and xgboost.XGBClassifier alongside the original kNN, SVM, and DecisionTree classifi- ers. For this study, these newly integrated clas- sifiers were used with their **default hyperpa- rameters** as defined in scikit-learn and XGBoost For example, RandomForestClassi- fier used n_estimators=100, and XGBoost used its standard defaults with eval_metric='logloss'. No hyperparameter tuning was performed in the experiments reported here.

C. Datasets

The experiments were conducted on standard MIL benchmark datasets obtained from The da- tasets used include:

- **Musk1+:** A drug activity prediction dataset.
- **Fox+:** An image classification dataset (identifying foxes).
- **Tiger+:** An image classification da- taset (identifying tigers).
- **Musk2+:** A drug activity prediction da- taset (2)

A summary of dataset characteristics is pro- vided in Table 1.

Table 1: Benchmark Dataset Characteristics

Dataset	Bags(N)	Total Instances(n)	Features(d)
Musk1+	92	476	166
Fox+	200	1320	230
Tiger+	200	1220	230

D. Experimental Setup

- **Evaluation Protocol:** A 10-fold Cross- Validation (CV) strategy was employed for all experiments. The data was ran- domly shuffled, then split into 10 folds. For each fold, 9 folds were used for training (further split into Td/Ts within ELDB) and 1 fold for testing.
- **Performance Metric:** The primary metric reported is the average **F1- score** across the 10 test folds. Standard deviation is also reported to indicate re- sult variability. (Mention if binary, macro, or weighted F1 was used if rel- evant).
- **ELDB Parameters:** Unless otherwise specified, the standard ELDB parame- ters were used: alpha (Td/Ts split ratio)
= 0.75, psi (dBagSet selection ratio) = 0.9, psi_max (max dBagSet size) = 200, mode_action = 'a' (addi- tion), type_b2b (distance metric) ='ave' (Average Hausdorff).
- **Environment:** Experiments were con- ducted using Python [Latest version] with libraries including scikit-learn, XGBoost NumPy and SciPy

RESULTS

The performance of kNN, SVM, J48 (Decision Tree), RandomForest (RF), and XGBoost clas- sifiers, all using default parameters within the ELDB framework ('a' mode), was evaluated us- ing 10-fold cross-validation on the benchmark datasets. The average F1-score and standard de- viation across the folds are presented in Table 2.

Dataset	**kNN (k=3)**	**SVM**	**J48**	**RF (Default)**	**XGB (De- fault)**
Musk1+	**[90.56±1.28]**	[86.59±1.38]	[77.18±4.51]	[88.94±1.21]	[85.68±1.83]
Fox+	[62.46±1.86]	[26.32±1.62]	[59.21±2.40]	[61.4±2.2]	**[62.96±2.2]**
Tiger+	[70.15±2.11]	[67.76±1.13]	[67.67±3.00]	[72.06±1.44]	**[72.42±1.28]**

Table 2: Average F1-Score (%) ± Standard Deviation across 10 CV Folds

As shown in Table 2, the performance varied significantly across datasets. On the **Musk1+** dataset, the kNN classifier achieved the highest average F1-score ([approx. 90.56%]), outperforming both the traditional SVM/J48 and the newly integrated RF and XGBoost models using their default parame- ters.

For the **Fox+** dataset, the results were different. [XGBoost or RF - specify which based on your results] yielded the best average F1-score ([ap- prox. 60%]), slightly better than [second best model]. All classifiers showed moderate stand- ard deviations on this dataset.

On the **Tiger+** dataset, considerable variability was observed across folds for most classifiers, as indicated by high standard deviations (often
>10%). In the runs conducted, [XGBoost or other model] achieved the highest recorded av- erage F1-score across multiple runs ([approx. 75%], although individual runs varied signifi- cantly, sometimes yielding much lower scores like 50%). This suggests high sensitivity to the specific train/test splits generated during cross- validation for this dataset within the ELDB framework.

III. DISCUSSION AND CONCLUSION

This study aimed to evaluate the integration and performance of default RandomForest and XGBoost classifiers within the existing ELDBmulti-instance learning framework, comparing them to baseline methods (kNN, SVM, J48) on benchmark datasets.

The results clearly demonstrate that while inte- grating RF and XGBoost is straightforward, their out-of-the-box performance relative to simpler models like kNN is highly **dataset-de- pendent**. On Musk1+, kNN remained the top performer, suggesting that for this dataset, the feature space generated by ELDB's mapping might be effectively captured by instance prox- imity, which kNN excels at. The more complex ensemble models did not offer an advantage with their default settings.

Conversely, on the Fox+ and Tiger+ datasets, XGBoost (or RF, depending on your results) showed competitive or superior performance compared to kNN and the other baselines. This suggests that on these datasets, the mapped fea- ture space might contain more complex interac- tions or patterns that the tree ensemble methods are better equipped to model, even without spe- cific tuning.

A key observation across multiple datasets, par- ticularly Tiger+, was the **high variability** in performance across different folds of the cross- validation, indicated by large standard devia- tions. This suggests that the performance of the ELDB algorithm, combined with any of these classifiers, can be quite sensitive to the specific random partitioning of data into training and testing sets. This highlights the importance of using cross-validation but also indicates that single run results should be interpreted with caution. The mechanism for saving the best his-

torical result proved useful in capturing peak

performance across runs but also underscored this run-to-run variance.

Limitations of this study include the use of de- fault hyperparameters for RF and XGBoost. While providing a baseline, this does not repre- sent their optimal potential. Extensive hyperpa- rameter tuning, although computationally ex- pensive (as observed in preliminary tuning at- tempts), would be necessary for a definitive comparison of the classifiers' peak capabilities within ELDB. Furthermore, the evaluation was conducted on a limited number of datasets, and performance could differ on other MIL prob- lems. Lastly, statistical significance tests were not performed to rigorously confirm the ob- served performance differences.

In **conclusion**, this work successfully inte- grated RandomForest and XGBoost into the ELDB framework. The empirical results show that these modern classifiers are viable options, performing competitively and sometimes ex- ceeding baseline models on specific MIL benchmarks, even with default parameters. However, no single classifier was

universally superior, emphasizing the dataset-dependent nature of classifier performance on ELDB's generated feature representations. The observed variability also underscores the sensitivity of the approach to data splits. Future work should focus on extensive hyperparameter tuning for RF and XGBoost, evaluation across a broader range of datasets, and statistical testing to pro- vide more robust conclusions about classifier choice for the ELDB algorithm.

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