A Hybrid Approach for Binary Classification of Imbalanced Data

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ABSTRACT Binary classification with an imbalanced dataset is challenging. Models tend to consider all samples as belonging to the majority class. Although existing solutions such as sampling methods, cost-sensitive methods, and ensemble learning methods improve the poor accuracy of the minority class, these methods are limited by overfitting problems or cost parameters that are difficult to decide. We propose HADR, a hybrid approach with dimension reduction that consists of data block construction, dimentionality reduction, and ensemble learning with deep neural network classifiers. We evaluate the performance on eight imbalanced public datasets in terms of recall, G-mean, and AUC. The results show that our model outperforms state-of-the-art methods.

INDEX TERMS Imbalanced data, binary classification, sampling, cost-sensitive, ensemble learning

I. INTRODUCTION

Binary classification of imbalanced data is a highly active topic because it is a common scenario in the real world, for instance, credit card fraud detection, defect detection, and rare disease diagnosis. The main feature of imbalanced data is that most samples belong to a single class called the majority class and the rest of the samples belong to the other class, called the minority class. Typically, the minority class is more valuable than the majority class. However, it is challenging to train a classifier which accurately distinguishes the minority class. For example, consider a rare but fatal disease. Since it is fatal, it is more important to discover a confirmed case than to find a healthy case. However, as the probability of a person having the disease is very low, the trained classifier might tend to judge all cases as healthy cases if it is trained for high accuracy. Thus patients with the disease would tragically miss the opportunity to receive life-saving treatment. Hence, the challenge in training a classifier of imbalanced data is that the classifier easily ignores misclassification of the minority class.

The literature has shown that traditional machine learning methods often fail when applied to imbalanced data classification [18]. Studies on improving the performance of imbalanced data classification can be divided into three categories: sampling methods, cost-sensitive methods, and ensemble learning methods. The sampling method balances the number of instances between classes by generating new samples or deleting existing samples, using techniques called oversampling [6] and undersampling [4], respectively. Cost-sensitive methods improve the classifier by applying different cost functions for misclassified samples [7]. Ensemble learning is a general meta-method of machine learning, which seeks better prediction performance by combining predictions from multiple classifiers [15]. However, each method has limitations which must be accounted for. For sampling methods, undersampling may remove helpful information, and oversampling may yield overfitted classifiers [5]. For cost-sensitive methods, it is not trivial to decide the cost parameters for minority and majority classes. Also, the ensemble learning method may cause biased results due to the unstable samples, which means the number of positive predictions is close to the number of negative predictions.

Recently, a hybrid method called DDAE [19] has been proposed which integrates the advantages of the sampling, cost-sensitive, and ensemble learning methods. However, if the imbalance ratio is large and the amount of positive samples is small, the size of each data block constructed by the method’s data block construction (DBC) component is also small. The data space improvement (DSI) component then easily overfits on each data block. The following ensemble learning
(EL) component based on the adaptive weighted adjustment (AWA) component may fail if most of the unstable samples are positive.

In this paper, we propose a hybrid approach with dimension reduction (HADR) for binary imbalanced classification problems that addresses the problems of the above categories. HADR contains three components: (i) a data block construction (DBC) component responsible for dividing the input data into nearly balanced data blocks. (ii) A dimensionality reduction (DR) component which reduces the dimensionality of the features and improves the data space by using metric learning for kernel regression. DR not only encodes the features but also prunes redundant features. In this step, we seek to mitigate the overfitting problem of DDAE. (iii) An ensemble learning component which combines multiple classifiers via a voting mechanism. We apply multilayer perceptrons (MLPs) as classifiers because of their low bias. High variance can be reduced by the bagging ensemble method. We evaluate the performance on eight imbalanced public datasets in terms of the recall, G-mean, and AUC metrics. The results show that HADR outperforms state-of-the-art methods. In particular, in the Wine3vs5 dataset, the recall of HADR is 66.7% better than that of DDAE.

We summarize the rest of this paper as follows: we discuss related works in Section II, the proposed methodology in Section III, and the experiments in Section IV. We conclude in Section V.

II. RELATED WORK
Our DR component uses metric learning to reduce the dimensionality of the dataset to find an effective data representation. Studies on data representation apply techniques such as metric learning [20], [21] or data space improvement [19]. Several techniques can be used to address data imbalance. Based on the different balancing techniques for data imbalance, we classify the most relevant studies into three types: sampling methods [1], [6], cost-sensitive methods [7]–[12], and ensemble learning methods [13]–[16]. Each method effectively alleviates the influence of imbalanced data. Multiple methods may also be combined for further improvements [17]–[19]. In recent years, due to the growth of deep learning, some components (sampling, cost-sensitive, ensemble, and data representation components) have been replaced with neural networks [22]–[24].

In the following subsections, we will review sampling, cost-sensitive, and ensemble methods. We will also discuss the state-of-the-art DDAE model [19].

A. SAMPLING METHODS
The purpose of a sampling method is to turn imbalanced data into balanced data either by generating new samples or deleting existing samples. Hence sampling methods fall into two categories: undersampling and oversampling.

1) Undersampling
The concept of undersampling is to remove majority samples to balance the data. Selection approaches include random undersampling and informed undersampling. Random undersampling techniques [3] involve randomly selecting examples from the majority class and removing them from the training data. The limitation with this technique is the removal of samples without accounting for their usefulness or importance while determining the decision boundary between the classes. That is, we lose valuable information with this technique. To account for this, Liu et al. [4] propose informed undersampling. They sample the majority data into several subsets and train a classifier for each subset. Then they combine the classifiers to produce the final prediction. This makes better use of the majority class than random undersampling.

2) Oversampling
Oversampling duplicates or generates sufficient minority samples to achieve a balanced state. Here we also have two main approaches: random oversampling and synthetic oversampling. In random oversampling, we randomly select and duplicate minority samples until the data is balanced. Then we train the classifier on the derived balanced data. Although this prevents the classifier from predicting all samples as the majority class, such random oversampling often results in data overfitting, as the prediction of the minority class relies on the information in the minority samples. The synthetic minority oversampling technique (SMOTE) [6] addresses this limitation by generating synthetic samples from minority classes. The idea of SMOTE is to apply the k-nearest neighbors algorithm, choose n samples, and then generate the synthetic sample between the sample in question and its neighbors. SMOTE prompted a number of related studies [1], [23]. Alam et al. [15] propose a new method for addressing multi-class imbalance which differs from other data balancing methods like sampling and underbagging. The basic idea is to partition data from multi-class imbalanced problems into several balanced problems. This is a unique recursion-based approach that partitions the imbalanced data into balanced data.

B. COST-SENSITIVE METHODS
Cost-sensitive methods help to improve the classifier by applying different costs to different misclassified samples [7]. First, we review the cost matrix in Table I. Following the notation in [12], let $C(i, j)$ be the cost when class $i$ is predicted and class $j$ is the ground truth. Thus $C(0, 0)$, $C(0, 1)$, $C(1, 0)$, and $C(1, 1)$ are true negative (TN), false negative (FN), false positive (FP), and true positive (TP), respectively. The optimal classifier can be trained by minimizing the cost function

$$L(x, i) = \sum_j P(j|x)C(i, j).$$

(1)
TABLE 1. Cost matrix

| Predicted negative | Actual negative | Predicted positive |
|--------------------|----------------|-------------------|
| \( C(0, 0) \)       | \( C(0, 1) \)   | \( C(1, 0) \)     |
| \( C(1, 0) \)       | \( C(0, 1) \)   | \( C(1, 1) \)     |

It is intuitive to set the costs in FN and FP to be greater than TN and TP. When optimizing \( \text{1} \), the classifier learns to focus on false predicted samples. However, it is still a challenge to define the cost matrix. One heuristic is to assign costs based on the inverse class distribution. For example, if we have an imbalance ratio of 100 : 1 between the majority and minority classes, we can set \( C(0, 0) = 0, C(0, 1) = 100, C(1, 0) = 1, \) and \( C(1, 1) = 0 \). This will force the classifier to focus on correctly predicting the minority class. However, this heuristic assumes the class distribution of the training data is equal to that of the test data. Another simple way is to use a machine-learning model that predicts the probability of each class, and combine this with a line search on a threshold, where samples are assigned to every clear class label, to ultimately minimize the cost of misclassification. The cost-sensitive method is a commonly-used method, despite the difficulty in obtaining precise misclassification cost parameters for minority and majority classes.

C. ENSEMBLE METHODS

Ensemble learning combines the results from several classifiers to improve prediction performance \( \text{14} \). The bagging (bootstrap aggregating) algorithm \( \text{15} \) and the boosting algorithm are two main ensemble learning methods. One difference between the bagging algorithm and the boosting algorithm is that boosting aggregates the results using weights. Given the effectiveness of ensemble learning, many studies combine data partitioning with ensemble learning for imbalanced classification \( \text{15} \).

D. DDAE

DDAE \( \text{19} \) is a novel model based on k-nearest-neighbor classifiers for imbalanced data classification. DDAE contains four main components: (i) a data block construction (DBC) component responsible for dividing the input data into nearly balanced data blocks; (ii) a data space improvement (DSI) component which brings samples in the same class closer together and further separates samples from different classes; (iii) an adaptive weight adjustment (AWA) component which adjusts the ensemble learning weight for each classifier; and (iv) an ensemble learning (EL) component which combines multiple base classifiers via the use of weighted voting.

III. METHOD

A. MODEL DESCRIPTION

Figure 1 depicts the HADR architecture. There are three components in the training phase: (i) a data block construction (DBC) component, which divides the training set into nearly balanced data blocks; (ii) a dimensionality reduction (DR) component, which reduces the dimensionality of the data and improves the data space by using metric learning for kernel regression; and (iii) an ensemble learning (EL) component, which combines multiple classifiers via a voting mechanism. In the testing phase, we directly apply the trained DR component to the test set and then combine the predictions of the trained classifiers.

B. DATA BLOCK CONSTRUCTION (DBC) COMPONENT

To generate balanced data blocks, we divide the training data into multiple blocks by partitioning the data \( \text{15} \). We also modify the partitioning method \( \text{15} \) to make it more suitable for binary classification. Let \( S_{\text{min}} \) and \( S_{\text{maj}} \) be the set of minority and majority samples, respectively. Let \( N_{\text{min}} \) and \( N_{\text{maj}} \) be the number of samples in \( S_{\text{min}} \) and \( S_{\text{maj}} \), respectively. Let \( ir = N_{\text{maj}}/N_{\text{min}} \) be the imbalance ratio of the dataset. Algorithm 1 shows the data block construction process. In the algorithm, \( ir^* \) can be either \( \lceil ir \rceil \) or \( \lfloor ir \rfloor \).

**Algorithm 1 Data Block Construction**

**Input:** Dataset \( D \)

**Output:** A set \( B \) of \( ir^* \) data blocks

1. Obtain \( S_{\text{min}}, S_{\text{maj}}, N_{\text{min}}, \) and \( N_{\text{maj}} \) based on \( D \);
2. Divide \( S_{\text{maj}} \) into \( ir^* \) chunks \( \{C_1, C_2, \ldots, C_{ir^*}\} \);
3. for \( i = 1 \) to \( ir^* \) do
   4. \( B_i = C_i \cup S_{\text{min}} \);
5. end for
6. return \( B = \{B_1, B_2, \ldots, B_{ir^*}\} \)

Figure 2 illustrates Algorithm 1. First, we obtain \( S_{\text{maj}}, S_{\text{min}}, N_{\text{maj}}, \) and \( N_{\text{min}} \) according to their classes. Then we obtain the imbalance ratio \( ir = N_{\text{maj}}/N_{\text{min}} \) and split \( S_{\text{maj}} \) into \( ir \) chunks \( \{C_1, C_2, \ldots, C_{ir}\} \). Since we seek to maintain the balance in each data block \( B_i, i = 1, \ldots, ir \), we combine every \( C_i \) with the minority data \( S_{\text{min}} \) and form \( ir \) nearly balanced data blocks \( \{B_1, B_2, \ldots, B_{ir}\} \).

C. DIMENSIONALITY REDUCTION (DR) COMPONENT

In machine learning or deep learning, dimensionality reduction is an important step which extracts useful features and decreases the effect of noise. Principal component analy-
sis (PCA) [26] is a well-known dimensionality reduction technique. However, one limitation is that the projection is entirely unsupervised; thus side information is sometimes ignored. Hence, we apply metric learning kernel regression (MLKR), another dimensionality reduction technique which can be viewed as a supervised PCA.

We will demonstrate how PCA reduces the dimensionality of the data. Assume that $x_i \in \mathbb{R}^m$ is a sample with $m$ features.

1) PCA

First, we calculate the covariance matrix as

$$C = \sum_i x_i x_i^\top \in \mathbb{R}^{m \times m},$$

(2)

after which we compute eigenvalues $\lambda_j$ of $C$ in descending order and the corresponding eigenvectors $v_j$ using

$$Cv_j = \lambda_j v_j,$$

(3)

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$ and $j = 1, 2, \ldots, m$. Then we project the sample $x_i$ onto the lower dimensional space and derive $\hat{x}_i$ as

$$\hat{x}_i = [v_1^\top x_i, v_2^\top x_i, \ldots, v_l^\top x_i]^\top,$$

(4)

where $l \leq m$.

Due to the above-mentioned limitation with standard PCA, we apply MLKR instead. We demonstrate it as follows.

2) MLKR

In the proposed method, we apply MLKR [25] as the tool for dimensionality reduction for each data block. MLKR learns a distance function $d(\cdot, \cdot)$ by minimizing the loss function

$$\mathcal{L} = \sum_i (y_i - \hat{y}_i)^2,$$

(5)

where

$$\hat{y}_i = \frac{\sum_{j \neq i} y_j k_{ij}}{\sum_{j \neq i} k_{ij}},$$

(6)

and

$$k_{ij} = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{d(x_i, x_j)^2}{2\sigma^2}}.$$  

(7)

In [5], $\hat{y}_i$ represents the approximated $y_i$ and is calculated as the weighted average of the nearby $y_j$ in [6]. The kernel function $k_{ij}$ is usually defined as a Gaussian kernel in [7]. The distance function $d(x_i, x_j)$ measures the “distance” between two samples $x_i$ and $x_j$. The distance function is defined as

$$d(x_i, x_j) = (x_i - x_j)^\top M(x_i - x_j),$$

(8)

where the matrix $M$ represents a Mahalanobis matrix, which is symmetric positive semi-definite. That is, for any vector $v$, $M$ satisfies $v^\top M v \geq 0$. The distance function $d$ can be interpreted as a generalized Euclidean metric. It is indeed an Euclidean metric if $M$ is an identity matrix. The authors of [25] expect the matrix $M$ to help $d$ to measure the distance more appropriately. However, it is difficult to maintain the positive semi-definite property in the training procedure. They solve this problem by defining $M = A^\top A$ which transforms the learning target from the constrained $M$ to the unconstrained $A$. Thus we rewrite [6] as

$$d(x_i, x_j) = \|A(x_i - x_j)\|^2.$$  

(9)

After optimization of [5], the learned $A$ projects the data $x_i$ onto the embedding space [10], yielding improved regression performance:

$$x_i \rightarrow Ax_i.$$  

(10)

3) Supervised PCA

In [25], the authors showed that MLKR also can be interpreted as a supervised PCA. Assume that the covariance matrix $C$ of the input $x_i$ is an identity matrix (this can be accomplished by whitening $x_i$). Thus the covariance matrix of $Ax_i$ is $C^A = AA^\top$. Suppose $\gamma_j$ and $w_j$ are the eigenvalue and the corresponding eigenvector of $C^A$, where $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_m$. According to the PCA algorithm, we can derive the reduced feature space by multiplying $x_i$ by the selected number of eigenvectors as

$$\hat{x}_i = [w_1^\top Ax_i, w_2^\top Ax_i, \ldots, w_l^\top Ax_i]^\top \in \mathbb{R}^l,$$

(11)

which yields

$$C^A w_j = AA^\top w_j = \gamma_j w_j.$$  

(12)

Multiplying by $A^\top$ then yields

$$A^\top AA^\top w_j = \gamma_j A^\top w_j,$$

(13)

$$A^\top A (A^\top w_j) = \gamma_j (A^\top w_j),$$

(14)

$$M(A^\top w_j) = \gamma_j (A^\top w_j).$$

(15)

Let $u_j$ be the eigenvector of $M$. From [15], we have $u_j = A^\top w_j$. Thus, we rewrite [11] to derive

$$x_i = [u_1^\top x_i, u_2^\top x_i, \ldots, u_l^\top x_i]^\top \in \mathbb{R}^l.$$  

(16)

Equations [15] and [16] show that since $M$ is actually the covariance matrix of $x_i$, we can directly apply the PCA
algorithm. Moreover, M is learned in such a way that it can be interpreted as a supervised form of PCA given input data \( x_i \). That is, it does not waste label information in the input data.

In the proposed method, DR is an important step since the DBC component may create multiple small data blocks if the positive samples are rare, in which case the classifiers are likely to overfit the data blocks. Moreover, the DSI component in DDAE may fail due to such outliers. DR by MLKR addresses this problem not only by reducing the dimensionality by pruning redundant features, but also by selecting important features via feature space encoding.

D. ENSEMBLE LEARNING

Ensemble learning, the last component of the proposed model architecture, combines the classifiers to achieve better results. In the previous component, we obtain blocks of features whose dimensionality is reduced. Then we utilize those features as inputs for classifiers. Each classifier is an independent multilayer perceptron (MLP) with the following design. The MLP contains two hidden layers (including the input layer) and a sigmoid function. Each hidden layer contains 10 nodes. Figure 3 shows the structure of the MLP classifier.

The additional settings are described as follows. We use 1000 epochs with a batch size of 10 and binary cross-entropy as the loss function. After training all the MLP classifiers, we apply the majority voting mechanism.

In deep learning, MLPs are usually applied as classifiers. They are easy to use while being sufficiently complicated to approach the actual classifier. MLP exhibits low bias but high variance. We use bagging ensemble methods like majority voting to average the variance and derive low-bias, low-variance results.

IV. EXPERIMENTS

In this section we will introduce the experimental setup and evaluate the proposed model on eight imbalanced public datasets. We will show that HADR outperforms state-of-the-art models.

A. EVALUATION METRICS

For an imbalanced classification model, we typically do not measure performance using accuracy. As an example, consider a dataset that contains one cancerous patient and 99 non-cancerous patients. The model achieves 99% accuracy if all patients receive negative predictions. However, we have a greater interest in correctly predicting positive cases. In this case, the sensitivity (recall) equals zero, so the model is essentially useless even if it has extremely high accuracy. In our experiments, we apply recall, G-mean [27], and ROC-AUC which consider samples from both majority and minority classes. To calculate these three metrics, we must first derive the true positives (TP), false negatives (FN), false positives (FP), and true negatives (TN) from the ground truths and predictions.

1) \( \text{Recall} = \frac{TP}{TP + FN} \), which also called the true positive rate (TPR) or sensitivity in the medical domain. The denominator represents the number of all positive samples and the numerator represents the number of positive samples that are correctly predicted. Recall focuses on the minority class.

2) \( G\text{-mean} = \sqrt{\text{Recall} \times \text{TNR}} \), where \( \text{TNR} = \frac{TN}{TN + FP} \) denotes the true negative rate. We have mentioned that recall is also called TPR. Thus G-mean is actually the product of TPR and TNR, which implies that this metric focuses on measuring the balance between majority class accuracy and minority class accuracy. In the previous example, if the model predicts all samples as negative, then the model has a high TNR but a low TPR, which translates to a low G-mean.

3) AUC, which refers to the area under the ROC curve. This is a number between zero and one. A higher AUC implies better performance. For the ROC curve, the x-axis represents the false positive rate (FPR) while the y-axis represents the TPR. To calculate AUC, we retrieve the predicted score from the model. This is usually a probability, but it need not be. Given this score, the final class prediction is based on a given threshold. Using different thresholds, we derive different TPR-FPR pairs which we then use to plot the ROC curve. The best performance occurs with a 0% FPR and a 100% TPR, which means AUC equals one. Thus a larger AUC means we have a higher probability to get a high TPR and a low FPR simultaneously. As described above, AUC simultaneously considers the performance of the majority class and the minority class. Hence, it is an appropriate metric to measure the classification of imbalanced data.

B. EXPERIMENTAL SETUP

All experimental results were based on the eight imbalanced datasets. These include P1c1, P1c3, P1c4, and Mw1 from OpenML [28], all open datasets for the detection of software defects. The other datasets are from the KEEL repository [29], where Wine3vs5 is used for wine quality.
prediction, and the abalone datasets are used to predict the age of abalone. Table 2 shows the total number of samples, the number of features in each sample, and the imbalance ratio (majority/minority) of the eight datasets. We randomly split each dataset into two parts for all experiments: a training set (70%) and a testing set (30%). In the ensemble learning component for each MLP block, we further randomly split the training set into two parts: 80% for MLP training and 20% for validation. Due to the lack of open-source code, we compared the proposed method (HADR) with other methods following [19]. In addition to the comparison with the DDAE model, we also tested on other state-of-the-art models:

| Dataset          | Samples | Features | Imbalance ratio |
|------------------|---------|----------|-----------------|
| PC1              | 1109    | 21       | 13.4            |
| PC3              | 1563    | 37       | 8.8             |
| PC4              | 1458    | 37       | 7.2             |
| Mw1              | 403     | 37       | 12.0            |
| Wine3vs5         | 691     | 11       | 68.1            |
| abalone9vs18     | 731     | 8        | 16.4            |
| abalone19        | 4174    | 8        | 129.4           |
| abalone20        | 1916    | 8        | 72.7            |

- IML [21], which combines iterative metric learning for the construction of a stable data space and the k-nearest neighbors algorithm as a classifier.
- RP [15], which combines data partitioning for blocks generation and ensemble learning, with majority voting rules.
- CAdaMEC [9], a methodology that calibrates cost-sensitive learning methods and AdaMEC [30], which uses a decision tree as a classifier.
- MWMOTE [1], a synthetic oversampling method that weights minority class samples based on the Euclidean distance to the nearest majority sample. It uses the k-nearest neighbors algorithm as a classifier.

C. COMPARISON

Tables 3, 4, and 5 compare the AUC, Recall, and G-mean between the state-of-the-art methods and the proposed method (HADR). In general, HADR outperforms the state-of-the-art methods on all datasets. HADR is outperformed by DDAE on only two parts, one of which is the PC1 recall. Since the G-mean performance of the proposed method (HADR) is better than DDAE, this phenomenon implies that HADR tends to strike a better balance between majority and minority class, rather than identifying as many minority class samples as possible. The other case is the abalone20 G-mean. As the AUC in the proposed method is better, this is explained by the fact that the majority voting mechanism takes 0.5 as the positive/negative threshold. Thus it may be that the proposed method (HADR) would yield a better G-mean if a more appropriate threshold were chosen. Note that HADR outperforms DDAE significantly in terms of recall for Wine3vs5 and Mw1. As shown in Table 2, the Wine3vs5 imbalance ratio implies there are 69 data blocks and about 20 samples in each data block, but the number of features is 11. In this dataset, the 69 classifiers would easily overfit. A similar situation occurs in Mw1. Evidently, DDAE performs more poorly in this kind of situation. However, HADR achieves strong recall in both datasets, likely because both DR and EL of the MLPs alleviate the tendency to overfit.

D. ABLATION STUDY

To evaluate the effectiveness of the three HADR components—data block construction (DBC), dimensionality reduction (DR), and ensemble learning (EL)—we performed an ablation study of the model on two public datasets: PC1 and Wine3vs5.
We propose a hybrid approach with dimension reduction (HADR) for binary imbalanced dataset classification. This model contains components for data block construction (DBC), dimensionality reduction (DR), and ensemble learning (EL). The model outperforms state-of-the-art models on several imbalanced datasets, which demonstrates that HADR is competitive against existing model structures for imbalanced classification.

Currently, HADR is limited to binary imbalanced classification and is restricted to non-image data. We will consider multi-class classification on imbalanced data, image data, or medical problems as future work.

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