

Cluster-based Diversity Over-sampling: A Density and Diversity Oriented Synthetic Over-sampling for Imbalanced Data

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Abstract: In many real-life classification tasks, the issue of imbalanced data is commonly observed. The workings of mainstream machine learning algorithms typically assume the classes amongst underlying datasets are relatively well-balanced. The failure of this assumption can lead to a biased representation of the models' performance. This has encouraged the incorporation of re-sampling techniques to generate more balanced datasets. However, mainstream re-sampling methods fail to account for the distribution of minority data and the diversity within generated instances. Therefore, in this paper, we propose a data-generation algorithm, Cluster-based Diversity Over-sampling (CDO), to consider minority instance distribution during the process of data generation. Diversity optimisation is utilised to promote diversity within the generated data. We have conducted extensive experiments on synthetic and real-world datasets to evaluate the performance of CDO in comparison with SMOTE-based and diversity-based methods (DADO, DIWO, BL-SMOTE, DB-SMOTE, and MAHAKIL). The experiments show the superiority of CDO.

1 INTRODUCTION

Imbalanced data refers to a scenario whereby there is a large proportion of instances which are labelled as "Negative" (majority class) to the number of instances labelled as "Positive" (minority class). Performance of subsequent learning classifiers may be negatively impacted without further treatment of imbalanced labels. Specifically, the processing of minority instances would most likely be regarded as an outlier or anomaly within the dataset (Ali et al., 2013). The objective for most of the mainstream classification algorithms is either to minimise misclassification error or to maximise predictive accuracy. However, it is often overlooked that these classification algorithms are constructed on the basis that the distribution of instances within each class is relatively balanced. As such, when classifiers are built on imbalanced datasets, the accuracy of these algorithms is often biased or have an overwhelming tendency to predict the majority class, resulting in high False Negative Rates (FNR) (Sasaki, 2007; Thabtah et al., 2020).

In the current literature, there are 3 main concepts used to treat and address imbalanced data, which are cost-sensitive learning, ensemble-based method, and re-sampling techniques. The purpose of "re-sampling techniques" is to create, either randomly or synthetically, a more balanced representation of the underlying dataset used for learning. One form of re-sampling techniques is Over-sampling, where in its most basic form, involves random sampling. There are also synthetic ways used to over-sample data based on many years of research. Synthetic instances generated are not exact replicas of the original instances. They broaden the decision region compared to random over-sampling. As a result, synthetic methods minimise the likelihood of overfitting, and reduce False Negative Rate and stabilise the performance of classifiers (Japkowicz & Stephen, 2002). However, for most of the synthetic methods, the generated instances lies along a linear path between minority data points, and the creation of synthetic minority data points takes place in the "feature level" and not on the "data level" (Chawla et al., 2002). It implies the decision region of minority

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class does not consider a holistic view of the entire minority data space (Bennin et al., 2017).

In this paper, we designed an algorithm to address the above issue. The proposed algorithm generates diversified synthetic instances within the minority class while considering the distribution of the minority data space. It is done via optimising both similarity to minority instances and diversity in synthetic instances. The optimisation process is conducted based on genetic algorithm. Our proposed method guarantees proximity of the generated synthetic instances to the actual instances in the minority class. In addition to preserving the advantage of over-sampling, the proposed algorithm enables the optimal spread of generated instances in the data space and help to broaden the decision region as a result of diversity optimisation.

2 RELATED WORK

SMOTE is a well-known synthetic over-sampling technique in the literature (Chawla et al., 2002). The process of generating synthetic minority class instances is via a random selection of specified k -nearest neighbours of a minority sample, and applying a multiplier derived from a uniform random distribution $(0,1)$. This creates a “synthetic” instance which will be located between the 2 minority points. SMOTE has improved the performance of classifiers trained on imbalance dataset through the process of expanding decision regions housing nearby minority instances as compared to basic random over-sampling which enhanced and narrowed decision regions with contrasting effects (Chawla et al., 2002)

Recent studies have flagged a limitation of traditional over-sampling methods (i.e. SMOTE) to its casual tendency to generate synthetic instances which extends into the input region of the majority class instances, thereby negatively impacting the performance of the subsequent learning classifier built (Bennin et al., 2017; Sharma et al., 2018). These studies have identified the dual importance of maintaining the integrity of the minority sample region, in addition to enhancing the diversity of minority class data. Subsequent studies has aimed to address the above challenge.

ECO-ensemble is an Cluster-based synthetic oversampling ensemble method (Lim et al., 2016). Its idea originates on identifying suitable oversampling cluster regions with Evolutionary Algorithm (EA) to derive at the optimised ensemble. The SMOTE-Simple Genetic Algorithm (SMOTE-SGA) method is proposed to enhance the diversity within the

generated dataset (Tallo & Musdholifah, 2018). The algorithm determines instances to be generated and the number of synthetic instances created from the selected instance (sampling rate) to overcome the overgeneralization problem in SMOTE.

MAHAKIL is created with the purpose of generating more diverse synthetic instances (Bennin et al., 2017). It works by pairing minority instances with previously generated synthetic instances to generate instances inspired by the Chromosomal Theory of Inheritance. It utilised the core concept of Mahalanobis Distance as the measure for diversity, in conjunction with inheritance and genetic algorithm. The fundamental idea is to create synthetic minority instances which are unique using 2 relatively distant parent instances which are different to their parents (i.e. existing minority class). In 2018, SWIM (Sampling With the Majority) was proposed (Sharma et al., 2018). Synthetic minority instances are generated based on the distribution of majority class instances which are effective against extremely imbalanced data. In 2021, a diversity-based sampling method with a drop-in functionality was proposed to evaluate diversity. It is achieved via a greedy algorithm that is used to identify and discard subsets that share the most similarity (Yang et al., 2021).

Most recently, Diversity-based Average Distance Over-sampling (DADO) and Diversity-based Instance-Wise Over-sampling (DIWO) are proposed to promote diversity (Khorshidi & Aickelin, 2021). The objective of the 2 techniques is to generate well-diverse synthetic instances close to minority class instances. DADO aims to ensure diversity in the region among minority class instances. Whereas in the case of DIWO, the contrasting approach is taken to ensure synthetic instances are clustered as closely to the actual minority class instances. DADO performs better when minority instances are compact, and immediate surrounding area is located within minority space. DIWO performs better when minority instances are widely distributed, and the surrounding area does not sit within the minority space.

In this paper, we propose a new synthetic sampling method, namely Cluster-based diversity oversampling (CDO). Our proposed method combines the advantage of both DADO and DIWO by analysing the density distribution of the minority instances via diversity optimisation.

3 METHODOLOGY

3.1 Cluster based Diversified Over-sampling (CDO)

In this section, we aim to describe our new proposed, Cluster-based Diversity Over-sampling (CDO). The new proposed method aims to provide a more robust algorithm compared to DADO and DIWO by combining the strengths of both approaches. A clustering algorithm is used to analyse and learn the density distribution of minority instances. For instances that are compact and similar to each other using density clustering method, DADO is applied. For instances that are widely distributed, DIWO is applied.

Our preferred choice of clustering method is DBSCAN as it is more efficient in comparison to partition-based or hierarchical-based clustering methods when the problem requires us to determine the arbitrary shaped clusters (Ester et al., 1996). DBSCAN was first introduced in 1996 (Ester et al., 1996). It is a non-parametric density-based clustering algorithm and it works by enhancing the grouping of instances which are closely located to each other and simultaneously identifying points which are placed in low-density areas (points whose nearest neighbours are relatively far away). Additionally, we choose DBSCAN over all other clustering methods due to the reason that unlike our typical clustering problem, our objective is to identify instances which are close together and not clustering all the data points. We also note the advantage of DBSCAN which allows the user to select the desired level of similarity required.

The algorithm of CDO is shown in Algorithm 1. It requires the following Epsilon (*eps*), and Border Point (*p*) parameters for clustering. As *p* is a binary pair of parameter values, if it is true, border points are assigned to clusters.

3.2 Diversity Optimisation

The choice of the proposed CDO algorithm for diversity optimisation is the extended form of NOAH's algorithm (Ulrich & Thiele, 2011), as shown in Algorithm 2.

Algorithm 2 contains 3 stages and requires the following input parameters: population size (*n*), number of generations to optimise objective function (*g*), number of instances remaining in the population after bound adaptation (*r*), percentage improvement of bound (*v*) and finally, the stopping criterion diversity maximisation (*c*). The above implies that if the population diversity does not improve for *c*

generations, convergence of the diversity maximisation is achieved. The whole algorithm terminates if the bound does not improve for *c* generation. To further optimise the objective function, Algorithm 2 has also incorporated the usage of Genetic Algorithm (GA), as it is the most popular evolutionary algorithm. Mutation and crossover concepts are utilised to create new instances. Instances which objective functions are better than bound value (*b*) are kept (Algorithm 2, lines 5 and 14). For DADO, the objective function (*f*) is the average of distance from all instances in the minority class. For DIWO, the objective function (*f*) is the distance to each instance.

3.3 Diversity-based Selection

The preferred measure of diversity is Solow-Polasky measure. There are 3 main properties which are required of a diversity measure, which are namely 1) monotonicity in variety, 2) monotonicity in distance and 3) twinning. The first property implies that the diversity measure will increase or at least be non-decreasing when an individual element currently not present in the dataset is added. The second property requires that the diversity between a particular set *S* (i.e. instances) should not be smaller to another set *S'*, if all pairings within *S* are of the distance of all the pairings within *S'*. The third property ensures the diversity measure remains the same when additional element, already in the set, is added. Solow-Polasky measure can be expressed in the following equation (1), where *M* represents the distance matrix. The Euclidean distance between elements of set *S* are denoted as $d(s_i, s_j)$. Thereafter, our diversity measure is derived and computed by the summation of all inverse matrix of $(M^{-1} = [m_{ij}]^{-1})$.

$$D(S) = \sum M^{-1} = \sum_i \sum_j e^{-d(s_i, s_j)} \quad (1)$$

To obtain the best diversity amongst all the instances, the ideal scenario would be to generate all possible permutation of subsets. However, this cannot be achieved as it would be computationally infeasible and expensive. As an alternative methodology, we propose the use of a greedy approach which would filter out instances which have the least contribution to the diversity of our dataset. Our definition of contribution is defined as the difference in diversity for our dataset with and without the instance. As proven in this study (Ulrich & Thiele, 2011), the difference can be expressed in the following formula:

$$\sum M^{-1} - \sum A^{-1} = \frac{1}{\bar{c}} (\sum \bar{b} + \bar{c}) \quad (2)$$

Algorithm 1: Cluster-based diversity over-sampling algorithm (CDO).

```

/* Step 1: Clustering minority instances */
1  C = 0
2  for each point M in minority class do:
3    if M is labelled then next
4    if M is not labelled then
5      NeighborPts ← return all points within eps neighbourhood of M (incl. M)
6      if size of NeighborPts = 1 then label(M)= NOISE next
7      C = C + 1
8      label(M)= C
9      for each M' in NeighborPts do:
10     if label(M')= NOISE and p = True then label(M') = C next
11     if M' is labelled: next
12     label(M') = C
13     NeighborPts' ← return all points within eps neighbourhood of M' (incl. M')
14     if size(NeighborPts') > 1 then NeighborPts ← NeighborPts U NeighborPts'
15   end for
16 end for
/* Step 2: Perform diversity algorithm for each cluster and NOISE points */
17 for each C do:
18   PDADOC ← NOAH(n, g, r, c, v, f)
19 end for
20 for each minority instances M marked as NOISE do:
21   PDIWOM ← NOAH(n, g, r, c, v, f)
22 end for
/* Step 3: Combine generated datasets */
23 P = PDADOC U PDIWOM

```

Algorithm 2: Diversity optimisation algorithm (NOAH).

```

Input: n, g, r, c, v
Output: a diverse set of instances S
1  S = Null; b = ∞; i = 0
2  while i < c do
/* Step 1: Optimising the objective function */
3    P ← Generate a population with n instances
4    for g generations do
5      P' ← Generate new n instances via mutation and crossover from P with objective values better than b
6      P ← Select n best instances from P ∪ P'
7    end for
/* Step 2: Bound adaptation */
8    P ← Select r best instances from P ∪ S
9    b' ← Put the objective value of rth best instance in P ∪ S
10   if DIWO and b - b' < v × b then i ← i + 1 else i ← 0
11   b ← b'
/* Step 3: Diversity maximisation */
12   j = 0
13   while j < c do
14     P" ← Generate new r instances via mutation and crossover from P with objective values better than b
15     P∴ ← Select r best diverse instances from P" ∪ S
16   end while
17   if diversity of P∴ is more than S then S ← P∴ else j ← j + 1
18 end while

```

where A is the distance matrix of the set without that particular instance, $M = \begin{bmatrix} A & b \\ \bar{b}^T & c \end{bmatrix}$, $M^{-1} = \begin{bmatrix} \bar{A} & \bar{b} \\ \bar{b}^T & \bar{c} \end{bmatrix}$, c and \bar{c} are single elements, b and \bar{b} are vectors and b^T and \bar{b}^T are their transpose.

4 VALIDATION OF SYNTHETIC DATASET

4.1 Evaluation Method

The learning classifiers used to evaluate the generated data are Naïve Bays (NB), Decision Tree (DT), k-Nearest Neighbour (KNN), and Support Vector Machine (SVM), and Random Forest (RF). We choose KNN and RF as they are sensitive to imbalanced data based on their model assumptions (Muñoz et al., 2018). DT works based on developing decision regions which are influenced by re-sampling methods (Chawla, 2010). SVM with radial kernel is effective to classify classes which are not separable linearly.

We measure the performance of the classifiers on test data using F1-score, G-means, and PR-AUC as classification accuracy is not an appropriate measure for imbalanced data.

To calculate F1-score (5), we need to measure recall and precision shown as (3) and (4). Recall is the proportion of correctly predicted positive instances to all instances in the positive class. Precision is the proportion of correctly predicted positive instances to all predicted positive instances.

$$Recall = \frac{TP}{TP+FN} \quad (3)$$

$$Precision = \frac{TP}{TP+FP} \quad (4)$$

$$F1 = \frac{2 \times Recall \times Precision}{Recall + Precision} \quad (5)$$

PR-AUC denotes the area under the Precision Recall curve, is a suitable measure for classifiers' performance especially in the situation of imbalanced data and is independent of the decision boundary.

The G-means (7) is the geometric mean of true positive rate (TPR), as (6) and true negative rate (TNR), which is $1 - FPR$.

$$TPR = \frac{TP}{FN + TP} \quad (6)$$

$$G - means = \sqrt{TPR \times TNR} \quad (7)$$

4.2 Synthetic Dataset

To examine our proposed methods under different scenario, 4 2-dimensional datasets are created. There

is an equal split (2) of datasets with an imbalanced ratio (IR) of 10% and IR of 5%. These datasets are used in our initial experiments to assist in hyper-parameter selections. Table 1 provides a summary of these datasets (DS1-4). There is a varying amount of cluster within each DS, ranging from 0 (randomly distributed data points) in DS3 to 5 in DS1. For each of the 4 synthetic datasets, instances are randomly divided into training and test datasets with a 75:25 split. DADO, DIWO and our proposed method CDO are utilised to balance our training datasets. Learning classifiers are applied onto the balanced training datasets. Performance of these constructed learning classifiers is then assessed using the test datasets. Performance measures (F1, G-Means, and PR-AUC) are computed for the best performing classifier. The above process is repeated 30 times.

Table 1: Synthetic datasets characteristics.

Dataset	Number of Clusters	Data Points	Imbalance Ratio
DS1	5	200	10%
DS2	2	300	10%
DS3	0	300	5%
DS4	1	300	5%

4.3 Parameter Selection

The distance measures chosen for both objective function and diversity measure are the optimal distance measure based on experimental results (Khorshidi & Aickelin, 2021). Euclidean distance measure (D_{Eu}) is chosen for DADO, and Canberra (D_c) is chosen for DIWO.

$$D_{Eu}(x, y) = \sqrt{\sum_i (x_i - y_i)^2} \quad (8)$$

$$D_c(x, y) = \sum_i \frac{|x_i - y_i|}{|x_i| + |y_i|} \quad (9)$$

Next, we aim to determine the optimal values for 2 hyper-parameters for DBSCAN, Epsilon (ϵ) and Border Point (p). We examine the ϵ using 10 different parameter values, ranging from 0.05 to 50. A binary pair ("T", "F") of p is also examined. Based on parameter testing result on datasets (DS1, DS2, DS3, DS4), $\epsilon = 0.05$ and $p = "T"$ are selected.

4.4 Synthetic Experiment Results

CDO is compared alongside DADO and DIWO on synthetic datasets. In total, there are 4 synthetic datasets available and the performance of each of the 3 algorithms are evaluated. 12 different results are summarised in Table 2. CDO performs better than

Table 2: Performance results of mean and standard error for each measure across synthetic datasets. Bold numbers indicate the mean of method performance is the best among all comparable methods.

	DADO	DIWO	CDO
DS 1			
F1	0.3516 (\pm 0.131)	0.4586 (\pm 0.176)	0.4601 (\pm 0.179)
G-means	0.6341 (\pm 0.194)	0.8498 (\pm 0.080)	0.8456 (\pm 0.084)
PR-AUC	0.9439 (\pm 0.030)	0.9594 (\pm 0.026)	0.9603 (\pm 0.026)
DS 2			
F1	0.1805 (\pm 0.067)	0.4219 (\pm 0.116)	0.4244 (\pm 0.105)
G-means	0.4012 (\pm 0.182)	0.8342 (\pm 0.048)	0.8158 (\pm 0.042)
PR-AUC	0.9516 (\pm 0.019)	0.9786 (\pm 0.024)	0.9792 (\pm 0.023)
DS 3			
F1	0.1333 (\pm 0.047)	0.1092 (\pm 0.063)	0.1092 (\pm 0.063)
G-means	0.0693 (\pm 0.176)	0.4733 (\pm 0.216)	0.4638 (\pm 0.250)
PR-AUC	0.9706 (\pm 0.020)	0.9684 (\pm 0.022)	0.9687 (\pm 0.021)
DS 4			
F1	0.8623 (\pm 0.107)	0.8632 (\pm 0.113)	0.8679 (\pm 0.099)
G-means	0.9861 (\pm 0.014)	0.9926 (\pm 0.007)	0.9907 (\pm 0.009)
PR-AUC	0.9973 (\pm 0.011)	0.9974 (\pm 0.011)	0.9974 (\pm 0.011)

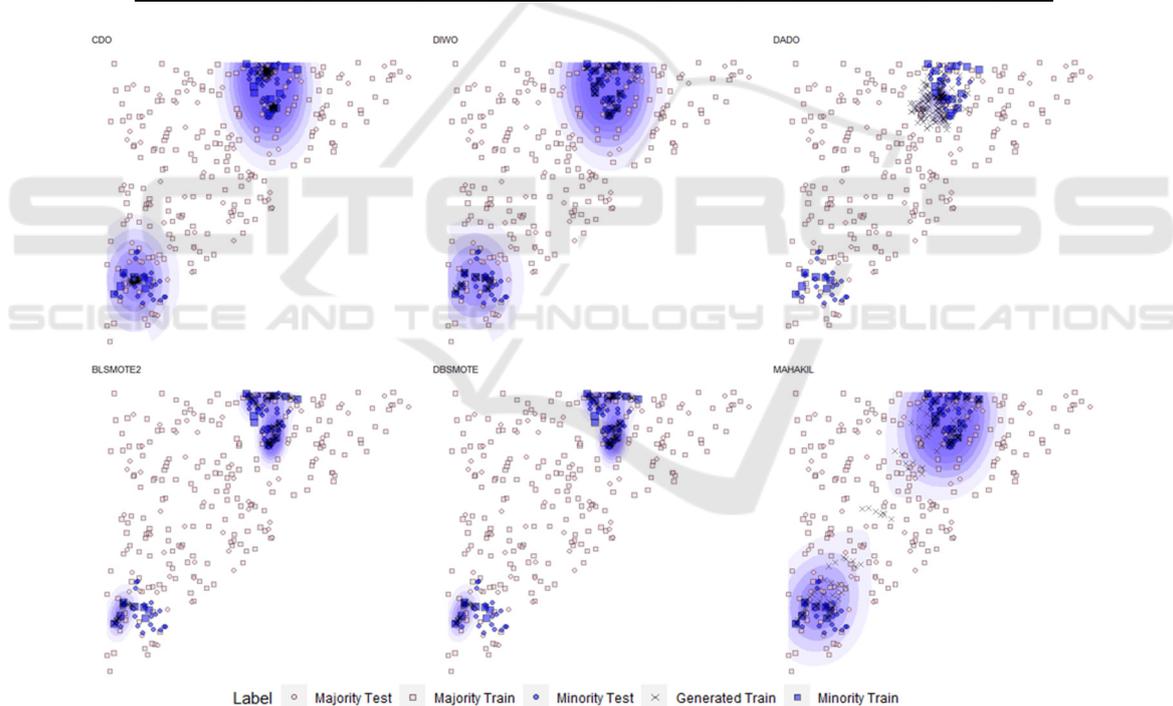


Figure 1: Plots for synthetic datasets, blue area indicates minority generation density.

DADO in all evaluation metrics over 3 of 4 datasets. CDO performs better in 2 of 3 evaluation metrics to DIWO, when 2 or more clusters are detected (DS1 and DS2). CDO outperforms in 1 of 3 evaluation metrics for DS 3, and 2 of 3 evaluation metrics for DS4, where datasets have less than 2 clusters

4.5 Graphical Representation

To provide a graphical representation of the synthetic datasets generated by CDO and its 5 comparable methods (BL-SMOTE, DB-SMOTE, DIWO, DADO and MAHAKIL), we created a separate synthetic dataset with two clusters, 5% imbalanced ratio in testing data with a balanced ratio in training data. The

generated minority data for each algorithm is displayed in Figure 1. We observe that the region of synthetic generated instances for CDO, DIWO and MAHAKIL is relatively similar. However, CDO stands out for its ability to cover all the data points of the minority test data with the narrowest region. MAHAKIL created synthetic data points between the 2 clusters, which occupies a larger region and could result in over-generalisation and higher false positive rate. For DADO, BL-SMOTE and DB-Smote, the region of generated data does not cover all of minority test data points, which could result in higher false negative rate.

5 VALIDATION

We validate the proposed CDO algorithm against an assortment of 10 imbalanced datasets, with varying dimensions. The datasets and their characteristics are described in Table 3, and “Ratio” is used to indicate the original proportion of majority to minority instances. To replicate the scenarios with low and extremely low imbalanced ratio, we reduce the imbalanced ratio to 5% and 10 absolute count of minority instances.

The data within each of the real-world datasets are randomly divided into train and test datasets using a 75:25 split respectively. This process is repeated for 30 iterations, resulting in 30 unique variations of training datasets and accompanying test datasets for each of the 10 real-world datasets. After the initialisation step, we apply our proposed method, CDO, alongside with existing methods in the literature, namely BL-SMOTE, DB-SMOTE and

MAHAKIL to evaluate algorithm performance. Six learning classifiers (GLM, NB, DT, KNN, SVM, NN) are then constructed on each of the training datasets ($n=30$). Subsequently, the trained classifiers are applied onto test datasets.

For each real-world datasets, the best performing classifier is selected, and we compute the mean and standard error of the performance measures as F1, AUC and G-mean. Additionally, we examine the statistical significance of differences for the performance measures obtained from CDO, BL-SMOTE, DB-SMOTE and MAHAKIL using a non-parametric test, Mann-Whitney test.

5.1 Experimental Results

The mean and standard error (stated in parenthesis) of our proposed method (CDO) and its comparable methods (BL-SMOTE, DB-SMOTE and MAHAKIL) are presented in Table 4 and 5, with 5% imbalanced ratio and 10 minority instances.

By looking at the performance metrics for 5% imbalanced ratio (Table 4), it can be concluded that CDO shows encouraging result as it outperformed its comparable algorithms in terms of F1 score and G-Means in 5 out of the 10 datasets. Additionally, CDO outperformed other comparable methods in 6 out of the 10 datasets based on PR-AUC.

By looking at the performance metrics for 10 minority instances (Table 5), CDO shows promising result as it outperformed its comparable algorithms in terms of F1 score in 4 out of the 10 datasets. It outperformed other comparable methods in 5 out of the 10 datasets based on PR-AUC. CDO performed equivalently well to MAHAKIL in G-Means.

Table 3: Real-word Data Description.

Dataset	Name	Dim	Size	Ratio	Dataset	Name	Dim	Size	Ratio
D1	Wisconsin	9	683	65-35	D6	Glass (0,1,2,3 vs 4,5,6)	9	214	76-24
D2	Diabetes	8	768	65-35	D7	Haberman	3	306	74-26
D3	Ecoli (0,1 vs 5)	6	240	90-10	D8	New Thyroid	5	215	84-16
D4	Ecoli 2	7	336	85-15	D9	Pima	8	768	65-35
D5	Ecoli 3	7	336	90-10	D10	Wine Red Low vs High	11	280	75-25

Table 4: Performance results of mean and standard error across datasets with 5% imbalance levels. Bold numbers indicate the mean of method performance is the best among all comparable methods.

	F1			
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	0.9528 (± 0.022)	0.9443 (± 0.023)	0.9487 (± 0.022)	0.9494 (± 0.023)
D2	0.4834 (± 0.067)	0.4639 (± 0.125)	0.4987 (± 0.096)	0.5964 (± 0.054)
D3	0.9091 (± 0.089)	0.8860 (± 0.095)	0.9113 (± 0.101)	0.9158 (± 0.086)
D4	0.8529 (± 0.091)	0.8467 (± 0.070)	0.8635 (± 0.074)	0.8221 (± 0.111)
D5	0.6441 (± 0.103)	0.6788 (± 0.083)	0.6600 (± 0.081)	0.6365 (± 0.109)
D6	0.8515 (± 0.065)	0.8004 (± 0.084)	0.8181 (± 0.081)	0.8378 (± 0.070)
D7	0.4327 (± 0.127)	0.2555 (± 0.151)	0.3747 (± 0.133)	0.4084 (± 0.139)
D8	0.9628 (± 0.046)	0.9458 (± 0.056)	0.9551 (± 0.043)	0.9571 (± 0.041)
D9	0.4845 (± 0.065)	0.4582 (± 0.120)	0.4888 (± 0.097)	0.5964 (± 0.054)
D10	0.6600 (± 0.105)	0.4915 (± 0.165)	0.5763 (± 0.127)	0.6317 (± 0.117)
	G-Means			
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	0.9681 (± 0.014)	0.9616 (± 0.017)	0.9646 (± 0.016)	0.9668 (± 0.015)
D2	0.5890 (± 0.050)	0.5690 (± 0.102)	0.6025 (± 0.073)	0.6861 (± 0.034)
D3	0.9521 (± 0.066)	0.9109 (± 0.087)	0.9415 (± 0.086)	0.9552 (± 0.065)
D4	0.9260 (± 0.041)	0.9130 (± 0.049)	0.9285 (± 0.043)	0.9108 (± 0.048)
D5	0.8890 (± 0.045)	0.9068 (± 0.053)	0.8841 (± 0.064)	0.8907 (± 0.042)
D6	0.8916 (± 0.059)	0.8378 (± 0.077)	0.8578 (± 0.075)	0.8854 (± 0.060)
D7	0.5883 (± 0.085)	0.3963 (± 0.132)	0.5541 (± 0.090)	0.5767 (± 0.082)
D8	0.9847 (± 0.023)	0.9581 (± 0.047)	0.9762 (± 0.028)	0.9789 (± 0.026)
D9	0.5885 (± 0.050)	0.5671 (± 0.098)	0.5966 (± 0.073)	0.6861 (± 0.034)
D10	0.7450 (± 0.089)	0.5874 (± 0.144)	0.6760 (± 0.115)	0.7442 (± 0.099)
	PR AUC			
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	0.9821 (± 0.062)	0.9778 (± 0.067)	0.9801 (± 0.065)	0.9815 (± 0.061)
D2	0.8279 (± 0.062)	0.8437 (± 0.062)	0.8268 (± 0.067)	0.8175 (± 0.065)
D3	0.9981 (± 0.003)	0.9978 (± 0.003)	0.9985 (± 0.002)	0.9981 (± 0.003)
D4	0.9803 (± 0.039)	0.9769 (± 0.039)	0.9796 (± 0.036)	0.9798 (± 0.038)
D5	0.9934 (± 0.004)	0.9927 (± 0.005)	0.9924 (± 0.005)	0.9925 (± 0.006)
D6	0.9559 (± 0.094)	0.9662 (± 0.068)	0.9614 (± 0.082)	0.9560 (± 0.094)
D7	0.8391 (± 0.056)	0.8222 (± 0.060)	0.8182 (± 0.060)	0.8238 (± 0.064)
D8	0.9990 (± 0.001)	0.9988 (± 0.002)	0.9989 (± 0.001)	0.9989 (± 0.001)
D9	0.8291 (± 0.062)	0.8433 (± 0.062)	0.8259 (± 0.067)	0.8175 (± 0.065)
D10	0.9578 (± 0.057)	0.9488 (± 0.066)	0.9517 (± 0.059)	0.9571 (± 0.056)

Table 5: performance results of mean and standard error across datasets with 10 minority instances. Bold numbers indicate the mean of method performance is the best among all comparable methods.

	F1			
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	0.9465 (± 0.021)	0.9358 (± 0.029)	0.9453 (± 0.024)	0.9417 (± 0.025)
D2	0.3799 (± 0.085)	0.2176 (± 0.111)	0.3818 (± 0.081)	0.4434 (± 0.148)
D3	0.8490 (± 0.115)	0.8571 (± 0.105)	0.8725 (± 0.119)	0.8548 (± 0.130)
D4	0.8586 (± 0.082)	0.8438 (± 0.075)	0.8617 (± 0.077)	0.8330 (± 0.089)
D5	0.6509 (± 0.086)	0.6828 (± 0.093)	0.6763 (± 0.076)	0.6456 (± 0.101)
D6	0.8549 (± 0.070)	0.8187 (± 0.089)	0.8240 (± 0.081)	0.8672 (± 0.062)
D7	0.4398 (± 0.108)	0.2822 (± 0.121)	0.3788 (± 0.116)	0.4114 (± 0.118)
D8	0.9753 (± 0.029)	0.9510 (± 0.063)	0.9672 (± 0.037)	0.9716 (± 0.035)
D9	0.3980 (± 0.078)	0.2125 (± 0.114)	0.3846 (± 0.078)	0.4389 (± 0.141)
D10	0.6769 (± 0.074)	0.5128 (± 0.137)	0.6413 (± 0.091)	0.6525 (± 0.099)
	G-Means			
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	0.9625 (± 0.014)	0.9514 (± 0.027)	0.9588 (± 0.019)	0.9580 (± 0.020)
D2	0.5267 (± 0.062)	0.3454 (± 0.159)	0.5372 (± 0.055)	0.6261 (± 0.062)
D3	0.9128 (± 0.101)	0.8908 (± 0.094)	0.9073 (± 0.106)	0.9194 (± 0.096)
D4	0.9301 (± 0.044)	0.9122 (± 0.057)	0.9332 (± 0.042)	0.9188 (± 0.045)
D5	0.8918 (± 0.044)	0.8955 (± 0.060)	0.8975 (± 0.053)	0.8905 (± 0.051)
D6	0.8882 (± 0.066)	0.8516 (± 0.080)	0.8597 (± 0.074)	0.9029 (± 0.049)
D7	0.5905 (± 0.079)	0.4327 (± 0.107)	0.5432 (± 0.078)	0.5765 (± 0.080)
D8	0.9927 (± 0.011)	0.9675 (± 0.055)	0.9787 (± 0.030)	0.9889 (± 0.018)
D9	0.5310 (± 0.064)	0.3476 (± 0.156)	0.5364 (± 0.054)	0.6258 (± 0.061)
D10	0.7691 (± 0.068)	0.6105 (± 0.119)	0.7135 (± 0.071)	0.7467 (± 0.088)
	PR AUC			
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	0.9937 (± 0.004)	0.9855 (± 0.015)	0.9911 (± 0.008)	0.9919 (± 0.007)
D2	0.8099 (± 0.063)	0.7950 (± 0.071)	0.8131 (± 0.055)	0.8064 (± 0.059)
D3	0.9903 (± 0.023)	0.9888 (± 0.024)	0.9894 (± 0.023)	0.9882 (± 0.027)
D4	0.9838 (± 0.029)	0.9817 (± 0.028)	0.9825 (± 0.027)	0.9826 (± 0.028)
D5	0.9902 (± 0.020)	0.9901 (± 0.017)	0.9908 (± 0.016)	0.9893 (± 0.021)
D6	0.9609 (± 0.092)	0.9655 (± 0.075)	0.9625 (± 0.084)	0.9625 (± 0.086)
D7	0.8233 (± 0.065)	0.8139 (± 0.063)	0.8094 (± 0.069)	0.8127 (± 0.067)
D8	0.9923 (± 0.032)	0.9925 (± 0.030)	0.9923 (± 0.031)	0.9923 (± 0.032)
D9	0.8134 (± 0.062)	0.7963 (± 0.070)	0.8139 (± 0.054)	0.8085 (± 0.059)
D10	0.9586 (± 0.054)	0.9449 (± 0.064)	0.9535 (± 0.057)	0.9563 (± 0.053)

Table 6: performance results of Mann-Whitney test across datasets with 5% imbalance levels. Each figure reports the frequency that the selected method is significantly better than its comparable methods within the same dataset ($p < 0.05$).

F1									
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL	Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	3	0	0	1	D6	2	0	0	2
D2	0	0	1	3	D7	3	0	1	1
D3	0	0	0	0	D8	0	0	0	0
D4	1	1	1	0	D9	0	0	0	3
D5	0	3	0	0	D10	2	0	1	1
G-Means									
	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL	Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	2	0	0	1	D6	2	0	1	2
D2	0	0	1	3	D7	2	0	1	1
D3	0	0	1	1	D8	3	0	1	1
D4	1	0	1	0	D9	0	0	1	3
D5	0	3	0	0	D10	2	0	1	1
PR-AUC									
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL	Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	1	0	1	1	D6	0	0	0	0
D2	1	3	1	0	D7	3	0	0	0
D3	0	0	0	0	D8	0	0	0	0
D4	0	0	0	0	D9	1	3	1	0
D5	0	0	0	0	D10	0	0	0	1

Table 7: performance results of Mann-Whitney test across datasets with 10 minority instances. Each figure reports the frequency that the selected method is significantly better than its comparable methods within the same dataset ($p < 0.05$).

F1									
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL	Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	1	0	1	0	D6	2	0	0	2
D2	1	0	1	3	D7	3	0	1	2
D3	0	0	2	0	D8	2	0	1	1
D4	2	0	2	0	D9	1	0	1	3
D5	0	2	2	0	D10	1	0	1	1
G-Means									
	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL	Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	2	0	1	0	D6	2	0	0	2
D2	1	0	1	3	D7	2	0	1	2
D3	0	0	1	1	D8	2	0	0	2
D4	2	0	2	0	D9	1	0	1	3
D5	0	0	0	0	D10	2	0	1	1
PR-AUC									
Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL	Dataset	CDO	BL-SMOTE	DB-SMOTE	MAHAKIL
D1	1	0	1	1	D6	0	0	0	0
D2	1	0	0	0	D7	3	0	0	0
D3	0	0	0	0	D8	0	0	0	1
D4	1	0	0	0	D9	1	0	0	0
D5	0	1	1	0	D10	0	0	0	0

The Mann-Whitney test is performed for each pairing of all 4 comparable methods. This implies that there are 6 total combinations of pairings available. Table 6 and 7 displays the results from the test, where each figure represents the frequency that the specified

method is statistically better than its comparable method.

From Table 6, CDO performs the best across 10 datasets where there is a 5% imbalanced ratio. It statistically outperforms its comparable algorithms on 11 occasions based on F1, 12 occasions based on

G-Means and 6 occasions based on PR-AUC. MAHAKIL comes next in line in terms of performance, where it statistically outperforms its comparable methods on 11 occasions based on F1, 13 occasions based on G-Means and only 2 occasions based on PR-AUC. Both BL-SMOTE and DB-SMOTE only statistically outperform their comparable methods on 4 occasions using F1. DB-SMOTE performs significantly better when evaluated using G-Means, where it outperformed its comparable methods on 8 occasions. BL-SMOTE comes last as it only statistically outperformed its comparable methods on 3 occasions based on G-Means and on 6 occasions based on PR-AUC.

From Table 7, CDO is the best performing algorithm for 10 minority instances. It statistically outperformed its comparable algorithms on 13 occasions based on F1, 14 occasions based on G-Means and 7 occasions based on PR-AUC. For the remaining algorithms, MAHAKIL is the 2nd best performing algorithm as it statistically outperformed its comparable methods on 12 occasions using F1, 14 occasions using G-Means and 2 occasions using PR-AUC. DB-SMOTE comes 3rd, as it statistically outperformed its comparable methods on 12 occasions using F1, 8 occasions using G-Means and 2 occasions using PR-AUC. BL-SMOTE comes last as it barely outperformed other methods (2 occasions using F1, 0 occasion on G-Means and 1 occasion on PR-AUC).

6 DISCUSSIONS

As shown in the statistical test results, although CDO outperforms MAHAKIL in most cases, CDO and MAHAKIL have superior performance results when compared to BL-SMOTE and DB-SMOTE. This can be explained by their better ability to capture more information when constructing minority generation region. Both CDO and MAHAKIL consider the entire minority class distribution and generating instances within the boundaries of the identified data generation region diversely. In contrast, SMOTE-based methods typically create synthetic instances using linear interpolation.

If we evaluate the statistical significance of CDO's performance, it has better performance compared to MAHAKIL when minority instances become more sparse. This is due to the nature of MAHAKIL algorithm that it only performs well when minority data distribution is convex and when there are sufficient number of minority instances (Khorshidi & Aickelin, 2021). In addition,

MAHAKIL algorithm does not consider clusters within datasets, which results in a broader generation region for minority instances and leads to a higher false positive rate. The main reason for superiority of CDO in comparison with MAHAKIL in terms of PR-AUC is that MAHAKIL generates synthetic instances, even though few, in the majority space (see Figure 1). This leads to lower precision that can be picked up by PR-AUC.

7 CONCLUSIONS

In this study, our key objective is to design an algorithm which generates diversified synthetic instances within the minority class while considering the distribution of the minority data space. We incorporate diversity optimization which optimises both similarity to minority instances and diversity of synthetic instances. The proposed algorithm first utilises clustering technique to identify the boundaries for the generation of minority instances and preserve similarity between minority instances. Subsequently, diversity optimization is incorporated to promote diversity within clusters. The proposed method CDO is evaluated on 10 real-world datasets, and it has statistically superior performance to its comparable methods. Its superior performance can be attributed to its ability to identify the minority space for synthetic data generation and its ability to obtain optimal spread of generated instances due to genetic algorithm. The proposed algorithm is evaluated on 2 class imbalance datasets. For future research, we extend CDO to address multi-class imbalance problems.

REFERENCES

- Ali, A., Shamsuddin, S. M., & Ralescu, A. L. (2013). Classification with class imbalance problem. *Int. J. Advance Soft Compu. Appl*, 5(3).
- Bennin, K. E., Keung, J., Phannachitta, P., Monden, A., & Mensah, S. (2017). Mahakil: Diversity based oversampling approach to alleviate the class imbalance issue in software defect prediction. *IEEE Transactions on Software Engineering*, 44(6), 534-550.
- Chawla, N. V. (2009). Data mining for imbalanced datasets: An overview. *Data mining and knowledge discovery handbook*, 875-886.
- Chawla, Bowyer, K. W., Hall, L. O., & Kegelmeyer, W. P. (2002). SMOTE: synthetic minority over-sampling technique. *Journal of artificial intelligence research*, 16, 321-357.

- Ester, M., Kriegel, H. P., Sander, J., & Xu, X. (1996, August). A density-based algorithm for discovering clusters in large spatial databases with noise. In *kdd* (Vol. 96, No. 34, pp. 226-231).
- Japkowicz, N., & Stephen, S. (2002). The class imbalance problem: A systematic study. *Intelligent data analysis*, 6(5), 429-449.
- Khorshidi, H. A., & Aickelin, U. (2021). Constructing classifiers for imbalanced data using diversity optimisation. *Information Sciences*, 565, 1-16.
- Lim, P., Goh, C. K., & Tan, K. C. (2016). Evolutionary cluster-based synthetic oversampling ensemble (eco-ensemble) for imbalance learning. *IEEE transactions on cybernetics*, 47(9), 2850-2861.
- Muñoz, M. A., Villanova, L., Baatar, D., & Smith-Miles, K. (2018). Instance spaces for machine learning classification. *Machine Learning*, 107(1), 109-147.
- Protopapa, K. L., Simpson, J. C., Smith, N. C. E., & Moonesinghe, S. R. (2014). Development and validation of the surgical outcome risk tool (SORT). *Journal of British Surgery*, 101(13), 1774-1783.
- Sasaki, Y. (2007). The truth of the F-measure. *Teach tutor mater*, 1(5), 1-5.
- Sharma, S., Bellinger, C., Krawczyk, B., Zaiane, O., & Japkowicz, N. (2018, November). Synthetic oversampling with the majority class: A new perspective on handling extreme imbalance. In 2018 IEEE international conference on data mining (ICDM) (pp. 447-456). IEEE.
- Tallo, T. E., & Musdholifah, A. (2018, August). The implementation of genetic algorithm in smote (synthetic minority oversampling technique) for handling imbalanced dataset problem. In 2018 4th international conference on science and technology (ICST) (pp. 1-4). IEEE.
- Thabtah, F., Hammoud, S., Kamalov, F., & Gonsalves, A. (2020). Data imbalance in classification: Experimental evaluation. *Information Sciences*, 513, 429-441.
- Ulrich, T., & Thiele, L. (2011, July). Maximizing population diversity in single-objective optimization. In Proceedings of the 13th annual conference on Genetic and evolutionary computation (pp. 641-648).
- Yang, Y. Y., Akbarzadeh HA Khorshidi, H., Aickelin, U. U., Nevgi, A. A., & Ekinci, E. E. (2021, February). On the Importance of Diversity in Re-Sampling for Imbalanced Data and Rare Events in Mortality Risk Models. In 2021 Australasian Computer Science Week Multiconference (pp. 1-8).