

SMOTE: Synthetic Minority Over-sampling Technique

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Abstract—Class imbalance in datasets has been one of the greatest challenge in classification tasks in machine learning. Often times the most important samples are the ones which is least represented. This results in an inherent bias towards the majority class while learning the classifier, resulting in a higher rate of mis-classification of minority class samples to majority class. Our work provides a study of the class imbalance in datasets and reviews ways in which the problem has been dealt with. Furthermore, we implement an algorithm “SMOTE”, which tackles this problem by generating synthetic samples from the minority class samples and augmenting it to the dataset. We plot the ROC Curve for classification using Decision Trees, Naive Bayes and k-Nearest Neighbor classifiers and compare the performance of our algorithm with the help of ROC Convex Hull (ROCCH) and Area-Under-the-Curve (AUC) metrics.

Index Terms—Imbalanced class datasets, minority over-sampling, ROC, Convex Hull, AUC

1 INTRODUCTION

THE seminal work, “SMOTE: synthetic minority over-sampling technique” [1] deals with the fundamental problem of imbalanced class data-sets in machine learning, where, data points of one class are in majority over data points of another class. A number of times the data points belonging to the minority class are more important than the majority class. This majority-minority skew in the data-set leads to classification in favor of majority class samples when one uses standard classification techniques like Naive Bayes or Decision Trees. In several cases, the penalty for mis-classifying these minority classes are much higher than mis-classifying the majority class. For example, the problem of classifying images of mammograms for cancerous cell detection is very sensitive and mis-classification may lead to disastrous outcomes. Still, the number of positive class samples is way outnumbered by the number of negative class samples with the majority (negative) class sample constituting 98% of total samples.

The authors in [1] propose a new algorithm to augment the minority samples in a data-set by creating synthetic data points for minority class in the feature space, to even the data distribution between majority and minority classes. They compare the result obtained by this new technique with the results of plain under-sampling the majority samples, as well as over-sampling the minority samples as previously done in other works dealing with the problem. The results show that their method leads to learning of better classifiers. Further, they show that the classifiers improve with near equal representation from all class in training data. The authors use Receiver Operating Characteristics (ROC) curves as their performance measure. ROC curves provide trade-off between true positive (TP) vs. false positive (FP) which is much more suited to the class imbalance problem than the error rate (accuracy) metric. Area Under

the Curve (AUC) and convex hull of ROC curve are used for the experiments as they provide good comparison of the classifiers’ performance in class imbalance scenarios both quantitative and qualitatively.

In our project, we learn to deal with the challenges of class imbalanced data-sets and how to overcome them. We reproduce the work done in [1] and understand the problem by going over the previous works cited in this paper. Additionally, we summarize the various techniques researchers came up to deal with this issue in Section 2. We overview the performance metrics used in this paper and explain why the authors chose to use these metrics, as well as how are they relevant to this particular problem in Section 3. We then move on to the implementation of the algorithm SMOTE proposed in the paper, along with two more approaches which was used to emphasize the novelty of this technique in Section 4. We replicate the experiments section on 3 of the 9 datasets listed in the paper, using Decision Trees, Nearest Neighbours and Naive Bayes classifiers to learn classification models in Section 5. We also use the prediction results from these models to plot ROC curves, and taking AUC and convex hull of the curve as evaluation metric, compare our plots with the plots obtained in the paper and provide a detailed discussion on the results in Section 6. Finally, we conclude our work with an overview of future works in Section 7.

2 PREVIOUS WORKS

Most of the cases of imbalanced dataset is dealt in two ways, viz. under-sampling the majority class samples or over-sampling the minority class samples. Different domain requires different techniques for the same based on their requirement. When it comes to under-sampling the majority class, Kubat et al [12] [13] experimented with the same. In Kubat and Matwin [12], the majority class is selectively under sampled while the minority class sampling remains fixed. The performance metric used for the classifier is geometric mean which is not as expressive as a ROC curve

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and corresponds to just one point on it. Related to the above, the SHRINK system of Kubat et al [13] classified the overlapping reasons of both majority and minority classes as positive, leading to a "best positive region" classification.

Another study on under-sampling of dataset was performed by Japkowicz et al [14]. In her study, she explored different sampling techniques on artificial 1D data for better evaluation of concept complexity. Her exploration involved under-sampling as well as resampling of data. Both strategies involved two different methods, viz. random and focused. Random resampling used samples from minor class to be sampled randomly until they matched major class samples, while focused resampling used only the boundary points between minor and major class. In random under-sampling, the samples from majority class were removed randomly to match the minority class samples, in contrast to focused under-sampling which under sampled majority class samples lying further away. Her study revealed the efficacy of both the sampling techniques but did not provide any clear advantage in the domain considered.

While under sampling approach works, other works uses under-sampling of majority class samples along with over-sampling of minority class samples for learning a better classifier. Ling and Li et al [15] uses lift analysis to measure classifier's performance in the domain of marketing analysis problem. They ranked the test examples by confidence measures and used lift as the evaluation criteria. In one of the experiments they performed, they under sampled the majority class and observed that the best lift index is obtained when there is equal representation of the classes. In another experiment, they over-sampled the minority samples with replacement to match the negative samples but could not prove the same as significant. The work present in this paper is similar in strategy, but the over-sampling techniques is different. Another work which uses the idea of under-sampling as well as over-sampling of data to overcome class imbalance problem is Solberg and Solberg et al [16]. They use SAR imagery dataset obtained for classification of oil slicks which is heavily biased towards look-alike data compared to oil slicks (98%-2%). They created a new dataset by over-sampling the oil slicks data randomly and under-sampling the look-alike data to create equal class distribution. As a result, on learning a classification tree on the balanced dataset they obtained better error rates on both classes compared to training on imbalanced dataset. Domingos et al [17] also take the same approach to deal with class imbalance by introducing a "metacost" term to under-sampling as well as over-sampling. The work shows the metacost improves over either, and proves that under-sampling of majority class does better than over-sampling of minority class.

Other researchers (DeRouin et al [18]) tried to use the same on feed-forward neural networks which is not able to learn to discriminate between classes sufficiently due to the same class imbalance problem. The learning rate of the neural network was adapted according to the class distribution in the data set. Experimenting over artificial as well as real-world training data with multi-class problem provided better classification accuracy for minority class. In information retrieval domain, document classification is one of the challenging problems which is affected by this class

	Predicted Negative	Predicted Positive
Actual Negative	True Negative (TN)	False Positive (FP)
Actual Positive	False Negative (FN)	True Positive (TP)

TABLE 1
Confusion Matrix

imbalance. Creating a simple bag-of-words model results in interesting words samples as a minority due to very limited instances of such words in the document. Thus, in IR domain, the performance metric is replaced from error rates and instead, precision and recall terms are used for performance measurements.

$$recall = \frac{TP}{TP + FN}$$

$$precision = \frac{TP}{TP + FP}$$

We will see what we mean by the terms True Positive (TP), False Positive (FP) and False Negative (FN) in the next section. In the same domain, Mladenic and Grobelnik [19] proposed a feature subset selection approach to deal with class imbalance. They found out that using odd ratio along with Naive Bayes classifier performs best in the domain. Odds ratio incorporates target class information giving better result over information gain which is computed per word for each class. In [20], Provost and Fawcett introduced the ROC convex hull method for performance evaluation of the classifier in which ROC space is used to separate classification performance from class and cost distribution.

3 EVALUATION CRITERIA AND PERFORMANCE METRICS

Confusion matrix, shown in Table 1, is one of the most common method in machine learning used to evaluate performance of a (2-class) classification problem for imbalanced class datasets. As shown in the table, the columns are predicted class and the rows are actual class. Over a dataset of finite samples, the count of correctly classified negative samples is termed as True Negative (TN), while the count of incorrectly classified negative samples is termed as False Positive (FP). Similarly, the count of incorrectly classified positive sample is termed as False Negative (FN), while the count of correctly classified positive sample is termed as True Positive (TP).

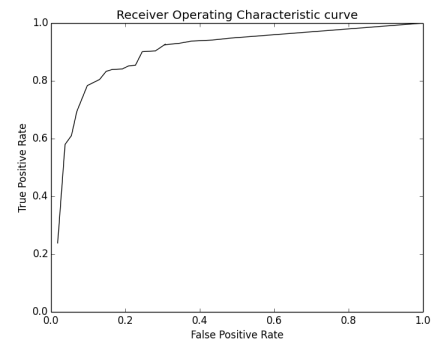


Fig. 1. Example of an ROC Curve

For any classification task, predictive accuracy is defined as the total number of correctly classified samples over total number of samples. Mathematically, it is given by,

$$Accuracy = \frac{TP + TN}{TN + FP + FN + TP}$$

In machine learning, we evaluate the performance of a classifier by its error rate which is given by,

$$ErrorRate = 1 - Accuracy$$

This performance measure works well for balanced class data sets, but for imbalanced datasets a much wider used metric is the Receiver Operating Characteristics (ROC) curves.

A typically ROC curve is a plot of percentage True Positive vs percentage False Positive. One such curve is shown in Figure 1. We have %ge FP on the X-axis given by,

$$\%ge FP = \frac{FP}{TN + FP}$$

and %ge TP on the Y-axis given by,

$$\%ge TP = \frac{TP}{TP + FN}$$

As evident from the definition, the ideal point on the curve will be (0, 100), signifying that all positive examples are classified correctly while no negative samples are misclassified as positive. The Area Under the Curve (AUC) can be taken as a good metric for comparing different classifiers, but these can be suboptimal for some specific cost and class distributions. Thus, the convex hull of ROC curve, being potentially optimal, is also taken as one of the performance metrics.

4 IMPLEMENTATION

In this section we provide the details of the various approaches we implemented from the paper. Using the “mam-mography” dataset [3], we show the effectiveness of SMOTE in this class imbalanced scenario. The dataset consist of 11,183 samples of which 10,923 are negative samples while we have only 260 positive samples. The dataset has 6 attributes, while we learn the classifier on 2 attributes, by decomposing the dataset using PCA, for better visualization. In Figure 2, we show the decision boundaries in the feature space, created by classifying 10% of the total data containing 18 positive samples and 1,100 negative samples. We have used the classifiers implemented in Scikit Learn library [2] with codes written in Python 2.7.1. The codes and dataset are provided in the supplementary material.

4.1 Over-sampling with replacement

Learning a classifier on the imbalanced class data gives us a biased classification towards the majority class samples (red circles). From Figure 2a, we observe that the classification decision boundary using the original data is not very accurate. Many minority class samples (blue circles) are classified under majority class (red region) resulting in decrease in true positive rate. The decision boundary is more general and spread away from minority (positive) class samples too.

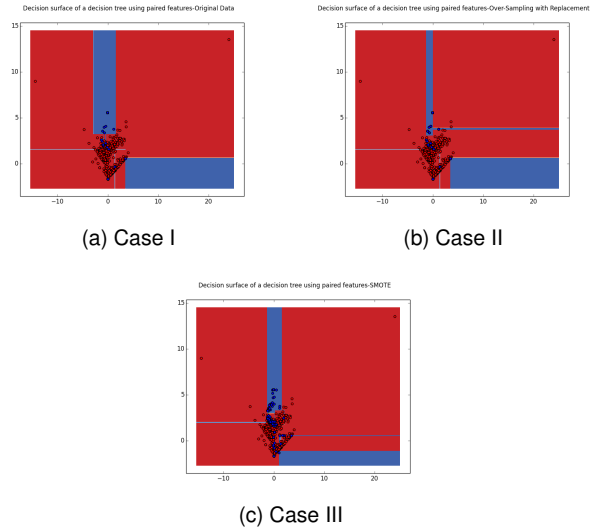


Fig. 2. Comparison of classification using Decision Trees on (a) Original dataset (b) Minority Over-sampling with replacement dataset, and (c) Over-sampling using SMOTE 500% dataset.

One of the earliest ways suggested by researchers to overcome this issue is over-sampling the minority class samples, in order to reduce the bias towards the majority class. We implement the over-sampling approach by duplicating the minority class samples. The degree of over-sampling in our implementation is 500%, i.e. if the dataset had 18 positive class samples and 1,100 negative class samples, as is the case in Figure 2, we upsample the positive class sample to 90. As a result, we see the decision boundary for minority class samples (blue region) shrink to enclose each individual positive sample. In other words, the data starts overfitting towards the positive class samples as more and more leaf nodes are added to the decision tree leading to very specific decision boundaries in the feature space. We see the same happening in Figure 2b with the 6 positive samples in the region around (0, 5).

4.2 SMOTE

Over-sampling of minority samples provides better accuracy but increases the complexity of classifier learnt manifolds. Moreover, the results does not generalize well as the decision region become very specific to the few minority samples present in the feature space leading to increase in false negatives. To overcome these issues a new over-sampling technique is proposed which augments the minority class samples by adding “synthetic” data. The algorithm works in the feature space of minority data samples. For a given degree of over-sampling rate, say 200%, the algorithm finds k-nearest neighbors of a minority sample and generates 2 random points on the line joining any 2 of the k-nearest neighbors found. We use nearest neighbors class implementation from scikit-learn library to find the nearest neighbor of each data point in the minority feature space. Algorithm 1 gives the steps to generate “SMOTED” data.

Figure 2c compares the effect of over-sampled data using SMOTE by 500%, with original data (Figure 2a) and replaced data (Figure 2b). It is clear from the plot that synthetic data

obtained using SMOTE helps classifier to generalize well over minority samples by providing better synthetic data to overcome the class imbalance. The decision region becomes larger and less specific as is the case with over-sampling by replacement, at the same time reducing mis-classification by creating better decision boundary which is seen in the case of classification using original data.

4.3 SMOTE with under-sampling

Over-sampling minority class samples with the help of SMOTE helps in increasing the percentage of minority samples, but still doesn't help overcoming the effect of grossly skewed data perfectly. To overcome this bias towards majority class sample, we under-sample the majority samples in addition to SMOTing the dataset. The under-sampling is done to a degree with respect to the number of minority class samples. We first SMOTE the dataset and obtain the final number of minority class samples and then under-sample the majority class sample to get the desired degree of under-sampling. For example, in the above example, we have 18 minority samples and 1,100 majority samples. SMOTing the dataset by 500% results in an increase in minority samples to 90. Now, under-sampling the dataset by a degree of 200% means drawing out *half the samples of minority class samples, at random, from the total majority class samples*, i.e using 45 samples from the 1,100 majority (negative) class samples along with the 90 minority (positive) class samples to train the classifier.

Data: #Minority Samples T; Degree of SMOTE N%;
#nearest neighbor k

Result: synthetic[[]] := (N/100)*T synthetic minority samples

initialization:= original[[]]; nIdx=0; nAttr;

if N < 100 **then**

 T = (N/100) * T;

 N = 100;

end

N = (int) (N/100);

for i := 1 to T **do**

 nnArray := compute k nearest neighbor;

while N != 0 **do**

 nn := random(1, k);

for attr := 1 to nAttr **do**

 dif = original[nnArray[nn]][attr] - sample[i][attr];

 gap = random(0, 1);

 synthetic[nIdx][attr] = sample[i][attr] + gap*dif;

end

 nIdx++;

 N--;

end

end

Algorithm 1: Steps to perform over-sampling using SMOTE to generate synthetic minority data

5 EXPERIMENTS

We experiment with our implementation of plain under-sampling and under-sampling with SMOTE under varying

Datasets	#Minority (+ve) Class	#Majority (-ve) Class
Mammography	260	10,923
SatImage	626	5,809
Pima Indian	268	500

TABLE 2
Class Distribution in Datasets Used

degrees of under-sampling and SMOTE combinations. Our aim is to tackle the class imbalance problems in datasets, thus, we test the algorithm on 3 different dataset with different class distributions. We use Decision Trees, Naive Bayes and k-NN classifiers with varying under-sampling and SMOTE degrees to (i) analyze the effectiveness of SMOTing data, and (ii) compare the classifiers learning the best decision boundaries. We plot the ROC curves and use ROC Convex Hull (ROCCH) and Area Under the Curve (AUC) as our metrics to draw our conclusions.

5.1 Datasets

The 3 dataset we use are Mammography Dataset [3], Pima Indian dataset [4] and SatImage dataset [5]. The class distribution of the datasets are provided in Table 2. We have provided the codes to convert raw data file into comma separated file format (CSV), which is the input dataset file format in our implementation and experiments code, in the supplementary material.

Each datasets are multi-dimensional, with mammography dataset consisting 6 attributes, Pima Indian having 8 attributes and SatImage datasets having 36 attributes. Wherever needed, we reduce the dimensionality of dataset using PCA for preserving maximum information, faster computation and visualization of decision boundary in 2-D feature space.

5.2 Classifiers

Our main classifier for testing the algorithm implementation is **Decision Trees**. In the paper, the authors use C4.5 variant of Decision Trees to test the classification quality. We have used the implementation of Decision Trees provided by scikit-learn library, which is an optimized version of C4.5 algorithm called Classification and Regression Trees (CART) algorithm. As stated in the documentation [6], "CART is very similar to C4.5, but it differs in that it supports numerical target and does not compute rule sets. CART constructs binary trees using the feature and threshold that yield the largest information gain at each node."

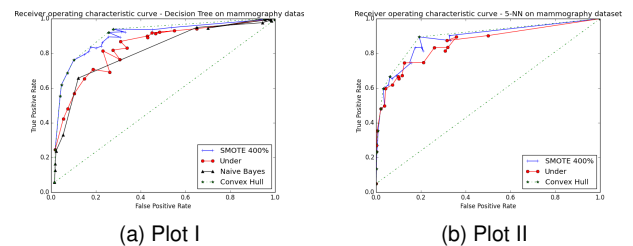


Fig. 3. ROC Curve plots for Mammography dataset.

Datasets	Under	SMOTE 100	SMOTE 200	SMOTE 300	SMOTE 400	SMOTE 500
Mammography	0.7220	0.7290	0.7776	0.7919	0.7918	0.7752
SatImage	0.7866	0.7881	0.8259	0.8318	0.8380	0.8283
Pima Indian	0.6581	0.6567	0.7014	0.7145	0.7207	0.7327

TABLE 3

AUC of the ROC Curve for plain under-sampling and varying degree of minority over-sampling using SMOTE (100%, 200%, 300%, 400% & 500%)

In addition to decision tree classifiers, we compare the performance of the same algorithms on **Naive Bayes** classifier with varying minority class priors. The paper also uses Ripper classifier to compare the performance, but we failed to locate any existing implementation of Ripper classifier in a 3rd party library in Python. Instead we use **k-Nearest Neighbor** classifier with a fixed value of k for comparison with Decision Tree classifier, and varying values of k for comparison amongst k-NN classifiers. Our change in classifier is guided by the intuition that the algorithm augments data in the feature space, and since k-NN classification works directly in the feature space, it should provide a better classification accuracy. The value of k in all k-NN a implementation is 5 for all our experiments.

5.3 ROC Curves and Cross-Validation

In order to evaluate the performance we plot the Receiver Operating Characteristics (ROC) curves for varying parameters of classification. ROC curves are essentially a plot of False Positive Rate (FPR) on x-axis vs True Positive Rate (TPR) on y-axis which measures a classifier's performance in more detail than a simple accuracy measure. This granularity is of great use in a class imbalance scenario because it gives an idea about the degree of mis-classification in both positive as well as negative class. Ideally, we will like a low False Positive Rate and a high True Positive Rate, resulting in a shift in ROC curve towards the (0, 100) point. As the curve goes nearer to this point, the classification gets better.

In our experiments we draw two plots for each dataset. The first plot contains Decision Tree as the base classifier and we compare the Decision Tree implementation of plain under-sampling of majority class samples at rates varying from 10% to 2000% as described in Section 4.3. For plain under-sampling we do not SMOTE the dataset before under-sampling. We compare the ROC curve obtained by plain under-sampling with that obtained by under-sampling with SMOTE. To obtain the second ROC curve, we over-sample the dataset with varying degrees from 100% to 500%, based on the dataset class distributions. In the same plot we compare Decision Tree classifier with Naive Bayes classifier, by

adding another ROC curve plotted using classification from Naive Bayes with varying class priors of minority class. In the implementation provided by scikit-learn, the class priors are automatically calculated as the frequency of each class samples, as stated in the documentation [7]. Thus, we feed in the data used in plain under-sampling to NB classifier as it varies the ratio between the two class samples. The various class priors used to plot the curve vary for different dataset based on the class distribution ratio of the dataset. We report the class priors at the end, after performing each experiment. In the second plot we replace decision tree classifier with k-NN classifier as the base classifier. We provide a comparison of the classifier with respect to plain under-sampled data and under-sampled data with SMOTE as with previous case.

Each point on the ROC curve is obtained by classifying the training data using a **10-fold cross validation**. In an n-fold cross validation, each dataset is divided into n equal parts randomly, and (n-1) of those parts are use for training while 1 left-out part is used for validation to improve the classifier parameters. This process is iteratively performed n times and classification metric is generated with each prediction. The points are the mean False Positive Rate vs mean True Positive Rate for the 10 different classification with a particular configuration of over-sampling/ under-sampling combination. We followed the ROC curve implementation with cross-validation of scikit-learn library [8], with modification to plot curves as we needed for our particular experiments. Figure 3, 4 and 5 provides the ROC curves we plot with comparison on all 3 datasets and the 3 classifiers we use. The average time taken to plot the ROC curves for Mammography dataset is **91.9 secs**, for SatImage dataset is **297.3 secs** and for Pima Indians dataset is **68.5 secs**.

5.4 Convex Hull and AUC

The performance of the ROC curve is quantified using ROC Convex Hull and AUC metric. Convex Hull gives the boundary of a potential optimal classifier in comparison of multiple ROC curves. ROC Curves themselves may not

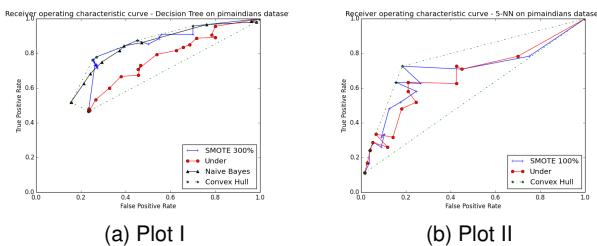


Fig. 4. ROC Curve plots for Pima Indians dataset.

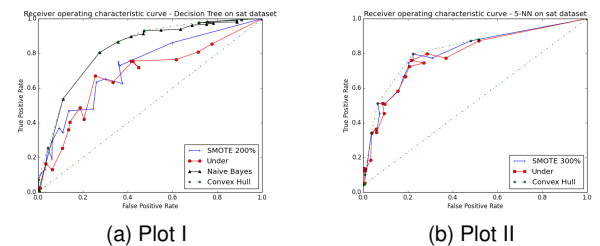


Fig. 5. ROC Curve plots for SatImage dataset.

be optimal at every instance. Thus, we use the hull to find out when a given classifier/method is optimal and when it can be replaced. We have implemented convex hull in all our plots, which should be taken as the perfect classification ROC curve. We construct the hull by first creating an array of all the 2D points on the ROC Curves using all classifier/method combination. Then we call the ConvexHull implementation of Scipy library [9] provided in *scipy.spatial* class, which essentially uses the QuickHull algorithm of [10] [11]. This breaks the decision space into multiple simplices of the convex hull and finally we draw each individual simplex to complete the convex hull of the curves.

Area Under-the-Curve (AUC) is another metric which we use to evaluate the performance of each classification. In simple terms, the more the value of AUC, the better the classification as the curve will be nearer to the ideal point (0, 100) to maximize the area. We again use the implementation provided in scikit-learn library to calculate the AUC for each ROC curve. We summarize the average AUC values obtained from 10 runs of the experiment in Table 3. The average time taken to calculate the AUC for Mammography dataset is **17.4 secs**, for SatImage dataset is **88.8 secs** and for Pima Indians dataset is **17.2 secs**.

6 DISCUSSIONS

In Figure 3a, 4a and 5a, we plot the results obtained by SMOTE based minority oversampling with majority under-sampling technique, previous techniques of plain majority under-sampling learnt on Decision Trees and changing minority class priors in Naive Bayes. For mammography dataset, we observe that we obtain optimal results at 400% SMOTE oversampling with varying under-sampling degree. With SMOTE, we obtained better results than Naive Bayes or plain under-sampling which is evident from the convex hull, as most of the points from SMOTE lie on the convex hull. For Pima Indians dataset, we observe that both Naive Bayes with different minority class priors and SMOTE works equally well where each lies partially on the convex hull but even though SMOTE is better because more points on the convex hull comes from SMOTE than Naive Bayes. For SatImage Dataset, Naive Bayes performs better than SMOTE which can be attributed to the higher number of attributes in SatImage. In all the datasets, we observe SMOTE with under-sampling performs way better than plain under-sampling with Decision Trees.

Next in Figure 3b, 4b and 5b, we use nearest neighbor classifier with the same SMOTE with under-sampling and plain under-sampling. Here, we observe that for all three datasets, SMOTE based classifier performed better than plain under-sampling which is in line with our previous results with different classifiers. Most of the points on the convex hull comes from SMOTEd dataset which proves SMOTE classification with SMOTE is most optimal.

Last, we compare Area Under Curve for different degree of SMOTE i.e. 100%, 200%, 300%, 400% and 500% for all the three datasets with plain under-sampling on mammography dataset trained with Decision Tree classifier. We again observe that SMOTE perform better than under-sampling though at different degrees of minority oversampling. As we

can observe from the values, for mammography SMOTing at 300% is the best, for SatImage SMOTing at 400% is best while for Pima Indians SMOTing at 500% is best with maximum area under their respective ROC curves.

These results confirm our intuition that SMOTE with under-sampling perform much better than plain under-sampling. This can be attributed to the fact since we are increasing the minority class samples, the training set has more data to learn better classifier with better class distributions. Again, this over-sampling method is better than replacement because new data points are generated in the feature space, which will again help the classifier generalize well over the dataset. While we can not argue that augmenting the data with SMOTE helps, the degree of SMOTE remains a variable in the implementation. If we specify a lower degree the number of synthetic samples created do not boost the minority class ratio much while if we use very high degree, the high number of minority class sample will start over-fitting the data similar to what we see in over-sampling with replacement. Thus, finding the degree based on the original class distributions such that SMOTing negates the effect of dis-proportionate distribution on learning classifier is a challenge with this approach.

7 CONCLUSION & FUTURE SCOPE

Through this project, we have studied the problem of class imbalance in dataset. We reviewed techniques to overcome this challenge, and went one step ahead by implementing one of the popular techniques used to overcome this problem, SMOTE. We compared our implementation of synthetic over-sampling with over-sampling with replacement and showed that the classifier learnt by our method is more general. Through our experiments, we show that while SMOTE with under-sampling works best for specific classifiers like decision trees and nearest neighbor, comparing classifiers' performance, naive bayes with varying minority class samples can also be used for better classification. While convex hull of ROC curves show that SMOTE is optimal for classification, AUC shows that varying degree of SMOTE helps in improving the classifier further.

Thus, as future works that should be a natural extension of this algorithm is to automatically find the degree of SMOTE to be used for augmenting the minority class sample. The degree should be neither high nor low as at low degrees the algorithm will not be effective, while at higher degree will lead to generation of data specific to training set.

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