Kernel density estimation-based sampling for neural network classification

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Abstract—Imbalanced data occurs in a wide range of scenarios. The skewed distribution of the target variable elicits bias in machine learning algorithms. One of the popular methods to combat imbalanced data is to artificially balance the data through resampling. In this paper, we compare the efficacy of a recently proposed kernel density estimation (KDE) sampling technique in the context of artificial neural networks. We benchmark the KDE sampling method against two base sampling techniques and perform comparative experiments using 8 datasets and 3 neural networks architectures. The results show that KDE sampling produces the best performance on 6 out of 8 datasets. However, it must be used with caution on image datasets. We conclude that KDE sampling is capable of significantly improving the performance of neural networks.

Index Terms—imbalanced data, KDE, neural networks, kernel density estimation, deep learning, sampling

I. INTRODUCTION

Imbalanced data refers to skewed distribution of the target variable in the dataset. It occurs in a range of fields including medical diagnostics, cybersecurity, fraud detection, text categorization, and many others. Imbalanced data can cause bias in machine learning classifiers [16]. Since the objective of a classifier is to minimize the overall error rate it focuses on correctly classifying the majority class subset at the expense of the minority class. However, the minority class data is often of more importance than the majority class set. For instance, although only a minority of credit card transactions data is fraudulent identifying such transactions is critical. A commonly employed approach to combat imbalanced data is resampling the original data. Concretely, oversampling the minority set points is often used to achieve a balanced dataset. In this paper, we analyze the effectiveness of a recently proposed sampling technique based on KDE in the context of artificial neural networks.

The KDE sampling is carried out by first estimating the underlying distribution of the existing points and then generating the new minority points from the estimated distribution. As a result, KDE offers an effective and natural way to sample new points. The KDE sampling was originally proposed in [5] where the authors demonstrated the effectiveness of the sampling method on k-nearest neighbors, support vector machines, and multilayer perceptron classifiers. Our goal is to conduct a more in-depth analysis of the performance of the KDE sampling with neural networks.

We employ neural networks of various depths to analyze the performance of the KDE sampling. We train and test the neural networks on 8 different datasets from a range of applications. We also employ two standard sampling approaches as benchmarks against the KDE sampling. The results demonstrate that the KDE sampling is effective in the majority of cases achieving the highest overall F_1 -scores on 6 out of 8 datasets. We conclude that the KDE method can be a valuable tool in dealing with imbalanced data when using neural network classifiers.

II. LITERATURE SURVEY

Imbalanced data occurs in a range of machine learning applications. In [3], the authors study various sampling techniques in the context of cancer data. In [17], the authors use generative adversarial networks (GAN) to balance machinery vibrations data. GANs are applied to train and generate artificial readings of faulty machinery states. Sampling techniques are evaluated in the context of software detection in [13]. The authors of the study compare the performance of sampling and cost sensitive approaches to imbalanced learning using 12 NASA datasets. Oversampling is used to balance traffic incident data in [14]. The authors use SMOTE to preprocess highway traffic dat to develop an accident predicting intelligent model.

There exists a number of sampling approaches to deal with imbalanced data. A survey of the existing sampling methods can be found in [10]. Sampling approaches can be grouped into two categories: undersampling and oversampling. Undersampling involves sampling from the majority subset to achieve the same size as the minority subset. In [12], the authors propose two undersampling methods where the majority points are divided into the same number of clusters as the number of the minority points. In the first approach, the new majority points are taken as the centers of the clusters whereas in the second approach the new majority points are taken as the nearest neighbors of the clusters. Oversampling

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involves generating new minority points to achieve the same number as the majority set. One of the popular oversampling methods SMOTE creates new points along the line segment joining a pair of neighboring minority points [2]. More recently, a Gamma distribution-based oversampling approach was introduced in [6]. The authors generate the new points along the straight line between two existing minority points using the Gamma distribution. Oversampling for multiclass data is explored in [8]. The authors propose to generate new data samples in the regions of space with sparse mutual class distribution.

Sampling has been used to address the issue of imbalanced data in the context of neural networks. In [15], the authors employed the SMOTE algorithm to balance the data before using backpropagation neural network to analyze credit card data. In [4], the author evaluate the performance of ROS and RUS with deep learning in the context of Medicare fraud detection.

III. METHODOLOGY

A. Sampling methods

KDE is a well-known nonparametric density estimator used in number of applications [7], [9]. The KDE-based sampling approach is based on estimating the underlying distribution of the minority data. Given a set of existing minority points $x_1, x_2, ..., x_n$ the underlying density distribution f can be approximated by

$$\tilde{f}(x) = \frac{1}{n} \sum_{i=1}^{n} K_h(x - x_i),$$
(1)

where K is the kernel function, h is the bandwidth parameter, and $K_h(t) = \frac{1}{h}K(\frac{t}{h})$. The optimal bandwidth value can be determined numerically through cross-validation. It is done by applying a grid search method to find the value of h that minimizes the sample mean integrated square error:

$$MISE_n(h) = \frac{1}{n} \sum_{i=1}^n (\tilde{f}(x_i) - f(x_i))^2.$$
 (2)

Default values of h exist under certain assumptions about the underlying density function f. A standard approach to calculating the optimal value of h is given by Scott's rule:

$$h = n^{-\frac{1}{5}} \cdot s, \tag{3}$$

where s is the sample standard deviation.

We benchmark the performance of KDE sampling against two standard sampling techniques: random oversampling (ROS) and random undersampling (RUS). The ROS technique balances the data by randomly selecting with replacement from the existing minority points. The main disadvantage of the ROS is overfitting. Since the ROS selects points with replacement it essentially replicates the minority set multiple times creating points of high concentration. The RUS technique randomly selects a subset of the majority set to match the size of the minority set. The main disadvantage of the RUS is the loss of information since only a portion of the available data is utilized.

B. Experimental Data

We employ 8 different imbalanced datasets in our numerical experiments. The datasets are available through the imblearn library [11] or the UCI repository [1]. The details of the datasets are provided in Table I. The imbalance ratio in the datasets ranges from 9.3 : 1 to 42 : 1. The datasets include a diverse areas of application including medical, meteorology, computer vision, and others.

TABLE I: Details of the experimental datasets.

Name	Ratio	#Samples	#Features
abalone	9.7:1	4177	10
letter_img	26:1	20,000	16
libras_move	14:1	360	90
mammography	42:1	11183	6
ozone_level	34:1	2536	72
satimage	9.3:1	6435	36
spectrometer	11:1	531	93
wine_quality	26:1	4898	11

C. Neural network classifiers

The performances of the KDE sampling and the benchmark methods are tested on 3 different neural network architectures with 1, 2, and 3 hidden layers. Deeper networks would be redundant due to the relatively small size of the datasets used in our experiments. The details of the three neural networks are presented in Table II.

TABLE II: Details of the neural networks used in the experiments.

Classifier	Layer 1	Layer 2	Layer 3	Activation	Optimizer
MLP-1 MLP-2 MLP-3	64 32 64	8 32	- - 4	Relu, sigmoid (output layer)	RMSprop

As noted earlier, the classifier performance on the minority labeled data is often of far more importance than the majority data. For instance, in medical diagnostics it is crucial to identify the positive cases even if occasionally producing false positive results. Similarly, in network intrusion detection catching malicious attacks is the primary concern even if they comprise only a small portion of network traffic. Therefore, the accuracy on the minority set must play an important role when measuring the performance of the sampling methods. In our experiments, the performance of the neural networks is measured with the macro average F_1 -score which is well suited for imbalanced datasets. The macro average F_1 -score of the majority and minority labeled data

$$F_1^{\text{macro}} = \frac{F_1^{\text{major}} + F_1^{\text{minor}}}{2}.$$
 (4)

As a result, it properly reflects the performance on the minority set.

IV. RESULTS

The detailed results of the experiments are provided in Figures 1-3. As can be seen from the figures, the KDE-based approach outperforms the benchmark methods. The KDE sampling performs particularly well on the *abalone*, *libras_move*, *mammography* and *wine_quality* datasets. On the other hand, it does not perform well on image recognition tasks and the corresponding datasets *letter_image* and *satimage*.

In the experiments using a 1-layer neural network, the KDE sampling method performs well in all but two datasets (Figure 1). It achieves either the best or nearly the best results. The only datasets with poor performance are the image datasets letter_image and satimage. In the abalone dataset, the KDE sampling outperforms the benchmarks but lags behind the original imbalanced dataset. In the experiments using a 2layer neural network, the KDE sampling method performs well in all but one dataset (Figure 2). As above, it achieves either the best or nearly the best results. The only dataset with poor performance is the image dataset *letter_image*. Note that the performance is good on the second image dataset satimage. The experiments with a 3-layer neural network yield mixed results (Figure 3). The KDE sampling achieves the best F_1 -score on the three datasets *abalone*, *libras move* and ozone_level. It is tied with the ROS method on the spectrometer.



Fig. 1: Macro average F_1 -score for MLP with 1 hidden layers.



Fig. 2: Macro average F_1 -score for MLP with 2 hidden layers.



Fig. 3: Macro average F_1 -score for MLP with 3 hidden layers.

To obtain the overall comparison of the sampling methods we averaged the F_1 -scores for each dataset over the three neural networks. A summary of the overall results is presented in Table III. As shown in the table, the KDE sampling achieves the best overall score on 6 out of 8 datasets and tied on 1 dataset. Furthermore, we observe that the KDE sampling method performs poorly on the image datasets *letter_image* and *satimage*. The poor performance on the image datasets is not surprising as the process of generating new image samples must take into account the internal structure of image files. Small changes in the values of an image file can easily result in a nonsensical image. As a result the new samples would be unhelpful.

TABLE III: Summary of averaged the F_1 -scores for each dataset over the three neural networks.

Dataset	imbalanced	KDE	ROS	RUS
abalone	0.5400	0.6167	0.5800	0.5833
letter_im	0.8667	0.8267	0.9100	0.7833
libras	0.8000	0.8800	0.8533	0.6767
mammo	0.6633	0.6933	0.6567	0.6233
ozone	0.5567	0.6267	0.6233	0.5500
satimage	0.7667	0.7233	0.7633	0.6967
wine	0.4900	0.6167	0.5967	0.5400
spectrometer	0.7533	0.9300	0.9300	0.8000

The KDE sampling algorithm outperforms the benchmark methods due to a more natural approach to sampling. The RUS method reduces the size of the majority set thereby losing valuable information contained in the original set. The ROS method essentially replicates the original minority set multiple times leading to overfitting. The KDE method avoids the above problems associated with the ROS and RUS methods. It samples from the estimated distribution providing an organic sampling procedure.

It is worth noting that, in theory, ROS and RUS are computationally more efficient than KDE sampling. Since ROS and RUS perform simple random sampling of the original dataset the associated algorithmic complexity is very small. The KDE sampling requires estimation of the underlying distribution prior to sampling which requires additional time. Modern implementations of the KDE have linear complexity O(n).

V. CONCLUSION

Imbalanced data occurs in a range of machine learning applications. Sampling is one of the effective approaches to deal with imbalanced data. In this paper, we analyzed the performance of a recently proposed KDE-based sampling method in the context of neural network classifiers. The performance of KDE sampling was compared against two standard benchmark sampling methods as well as the original imbalanced dataset. The results show that KDE sampling achieves the best overall score in 6 of the 8 datasets used in the experiments. However, KDE sampling performs poorly on image data. The underperformance is explained by the internal structure on image files that require a more nuanced approach. We concluded that the KDE sampling offers a viable tool to deal with imbalanced data when using neural network classifiers.

REFERENCES

- [1] Dua, D., & Graff, C. (2017). UCI Machine Learning Repository. Retrieved from http://archive.ics.uci.edu/ml
- [2] Fernandez, A., Garcia, S., Herrera, F., & Chawla, N. V. (2018). SMOTE for learning from imbalanced data: progress and challenges, marking the 15-year anniversary. Journal of artificial intelligence research, 61, 863-905.
- [3] Fotouhi, S., Asadi, S., & Kattan, M. W. (2019). A comprehensive data level analysis for cancer diagnosis on imbalanced data. Journal of biomedical informatics, 90, 103089.
- [4] Johnson, J. M., & Khoshgoftaar, T. M. (2019, July). Deep learning and data sampling with imbalanced big data. In 2019 IEEE 20th international conference on information reuse and integration for data science (IRI) (pp. 175-183). IEEE.
- [5] Kamalov, F. (2020). Kernel density estimation based sampling for imbalanced class distribution. Information Sciences, 512, 1192-1201.
- [6] Kamalov, F., & Denisov, D. (2020). Gamma distribution-based sampling for imbalanced data. Knowledge-Based Systems, 207, 106368.
- [7] Kamalov, F., & Leung, H. H. (2020). Outlier detection in high dimensional data. Journal of Information & Knowledge Management, 19(01), 2040013.
- [8] Krawczyk, B., Koziarski, M., & Wozniak, M. (2019). Radial-based oversampling for multiclass imbalanced data classification. IEEE transactions on neural networks and learning systems, 31(8), 2818-2831.
- [9] Lee, W. J., Mendis, G. P., Triebe, M. J., & Sutherland, J. W. (2020). Monitoring of a machining process using kernel principal component analysis and kernel density estimation. Journal of Intelligent Manufacturing, 31(5), 1175-1189.
- [10] Leevy, J. L., Khoshgoftaar, T. M., Bauder, R. A., & Seliya, N. (2018). A survey on addressing high-class imbalance in big data. Journal of Big Data, 5(1), 1-30.
- [11] Lemaitre, G., Nogueira, F., & Aridas, C. K. (2017). Imbalanced-learn: A python toolbox to tackle the curse of imbalanced datasets in machine learning. The Journal of Machine Learning Research, 18(1), 559-563.
- [12] Lin, W. C., Tsai, C. F., Hu, Y. H., & Jhang, J. S. (2017). Clusteringbased undersampling in class-imbalanced data. Information Sciences, 409, 17-26.
- [13] Malhotra, R., & Kamal, S. (2019). An empirical study to investigate oversampling methods for improving software defect prediction using imbalanced data. Neurocomputing, 343, 120-140.
- [14] Parsa, A. B., Taghipour, H., Derrible, S., & Mohammadian, A. K. (2019). Real-time accident detection: coping with imbalanced data. Accident Analysis & Prevention, 129, 202-210.
- [15] Shen, F., Zhao, X., Li, Z., Li, K., & Meng, Z. (2019). A novel ensemble classification model based on neural networks and a classifier optimisation technique for imbalanced credit risk evaluation. Physica A: Statistical Mechanics and its Applications, 526, 121073.
- [16] Thabtah, F., Hammoud, S., Kamalov, F., & Gonsalves, A. (2020). Data imbalance in classification: Experimental evaluation. Information Sciences, 513, 429-441.

[17] Zhang, W., Li, X., Jia, X. D., Ma, H., Luo, Z., & Li, X. (2020). Machinery fault diagnosis with imbalanced data using deep generative adversarial networks. Measurement, 152, 107377.