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Research article

Application of resampling algorithms in the imbalanced geochemical data classification: Case study; Geochemical data of Qayen 1:100000 sheet

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Keywords

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RUS algorithm
OSS algorithm
SMOTE-Tomek algorithm
ADASYN-CNN algorithm
Qayen Sheet

English Extended Abstract

Summary

The geochemical data exhibit an imbalance, with a high number of samples belong to the low-grade or background class, and a low number of samples in the high-grade or anomaly class. This imbalance in the dataset can lead to the development of a biased model, decreasing the likelihood of new samples belonging to classes with fewer representations and resulting in reduced accuracy and precision of the model. This paper introduces oversampling techniques such as SMOTE and ADASYN, undersampling methods like RUS and OSS, and hybrid-sampling approaches such as SMOTE-Tomek and ADASYN-CNN to address this data imbalance. The performance of these algorithms on geochemical data from the Qayen sheet is evaluated using SVM and ANN classification methods. The results demonstrate that data balancing leads to a significant increase in metrics such as accuracy, sensitivity, specificity, precision, F-score, F-value, G-mean, and AUC by 10 to 50 percent, while reducing error metrics by about 10 percent. The oversampling, hybrid-sampling, and undersampling algorithms exhibit high performance levels in improving the classification results, respectively. The geochemical anomaly maps generated with the help of these balancing algorithms show a greater number of anomaly areas in the study area, effectively aligning with mineralized rock units. Notably, oversampling techniques like SMOTE and ADASYN, followed by the hybrid-sampling method ADASYN-CNN, demonstrate superior performance in this regard. Therefore, this paper recommends oversampling and then hybrid-sampling algorithms before classifying exploration data to enhance model accuracy and better identify geochemical anomalies in the target area.

Introduction

Classification is a supervised machine learning technique that seeks to build a model from a dataset comprising multiple classes by analyzing the statistical relationships between them, determining the probability of a new sample belonging to each class. The accuracy of model estimation heavily relies on the distribution of samples within the dataset. A balanced dataset indicates an equal distribution of samples across different classes. However, in real-world data, we often encounter imbalanced datasets. Various approaches have been proposed to address the issue of classifying imbalanced datasets, including data sampling, algorithmic modification, and cost-sensitive learning methods [1,2]. This paper focuses on the algorithms associated with the first approach. To achieve this, geochemical data from the 1: 100,000 Qayen sheet in South Khorasan Province were utilized, employing support vector machine (SVM) and artificial neural network (ANN) classification methods.

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Methodology and Approaches

In a two-class training dataset with n samples, if the number of samples in the first class (n1) significantly exceeds the number of samples in the second class (n2) such that n1≫n2 and n=n1+n2, we are faced with the challenge of classifying an imbalanced dataset. The majority class is represented by the first class while the second class is considered the minority class, and the ratio n1/n2 is referred to as the imbalance ratio. Three approaches have been suggested to address this issue: oversampling techniques, undersampling techniques, and hybrid methods. This study introduces oversampling methods such as SMOTE and ADASYN, undersampling techniques like RUS and OSS, as well as hybrid-sampling approaches including SMOTE-Tomek and ADASYN-CNN, in order to achieve dataset balance [3,4,5]. Furthermore, the performance of these methods on the geochemical data of stream sediments from the Qayen sheet has been examined using SVM and ANN classification methods. Accuracy, sensitivity, specificity, precision, F-score, F-value, G-mean, and AUC metrics have been employed to assess the confusion matrix of the classification techniques [6,7].

Results and Conclusions

Initially, the dataset is randomly split into two parts: training data (comprising approximately 80 percent of the data, specifically 450 samples from the majority class and 71 samples from the minority class, totaling 521 samples) and testing data (comprising around 20 percent of the data, which equates to 113 samples from the majority class and 18 samples from the minority class, totaling 131 samples). The classification outcomes of the imbalanced dataset reveal that despite the high average classification accuracy in both methods, approximately 87 percent, the classification accuracy of the minority class is notably low. Consequently, there is a necessity to balance the training data. Tables 1 and 2 exhibit the classification outcomes of the testing data using balanced models and the metrics from the confusion matrix, respectively. These tables illustrate that data balancing has succeeded in enhancing the value of all metrics and diminishing the error metric's value. Overall, the ADASYN-CNN algorithm within the SVM method and the SMOTE algorithm within the ANN method can be recommended as the top methods, as they possess the highest cumulative metric values.

Table 1. Classification results of testing data with balanced models using the SVM and ANN methods

		Predicated samples							
Type of data		SMOTE				ADASYN			
		SVM		ANN		SVM		ANN	
		Background	Anomaly	Background	Anomaly	Background	Anomaly	Background	Anomaly
True samples	Background	102	11	111	2	100	13	112	1
	Anomaly	1	17	2	16	1	17	3	16
	Accuracy	90.3	64.4	98.2	89.9	88.5	94.4	99.1	89.9
		RUS				OSS			
True samples	Background	88	25	95	18	89	24	99	14
	Anomaly	۴5	13	2	16	5	13	2	16
	Accuracy	77.9	72.2	84.1	89.9	78.8	72.2	87.6	89.9
		SMOTE-Tomek				ADASYN-CNN			
True samples	Background	93	20	107	6	101	12	110	3
	Anomaly	1	17	1	17	1	17	2	16
	Accuracy	82.3	94.4	94.7	94.4	98.3	94.4	97.3	89.9

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Table 2. Values of the confusion matrix metrics for the testing data

Method		Type of data						
		Imbalanced	Balanced					
			SMOTE	ADASYN	RUS	OSS	SMOTE-Tomek	ADASYN-CNN
SVM	AC	0.809	0.908	0.893	0.771	0.779	0.839	0.901
	ER	0.191	0.092	0.107	0.229	0.221	0.161	0.099
	S	0.867	0.903	0.885	0.885	0.779	0.823	0.983
	SP	0.444	0.994	0.994	0.994	0.722	0.994	0.994
	P	0.907	0.990	0.990	0.946	0.947	0.989	0.990
	F-Score	0.887	0.945	0.935	0.914	0.855	0.898	0.986
	F-Value	0.889	0.971	0.967	0.933	0.908	0.951	0.989
	G-Mean	0.620	0.923	0.914	0.914	0.750	0.934	0.963
	AUC	0.656	0.923	0.915	0.750	0.755	0.884	0.919
ANN	AC	0.855	0.969	0.977	0.847	0.878	0.947	0.962
	ER	0.145	0.031	0.023	0.153	0.122	0.053	0.038
	S	0.903	0.982	0.991	0.841	0.876	0.947	0.973
	SP	0.555	0.899	0.899	0.899	0.899	0.944	0.899
	P	0.927	0.982	0.974	0.979	0.980	0.991	0.982
	F-Score	0.915	0.982	0.982	0.905	0.925	0.969	0.977
	F-Value	0.922	0.982	0.977	0.948	0.957	0.982	0.981
	G-Mean	0.708	0.939	0.943	0.870	0.887	0.945	0.935
	AUC	0.729	0.936	0.912	0.865	0.882	0.946	0.931

In the following, models generated from a balanced dataset utilized to produce a composite geochemical anomaly map of the study area. To achieve this, we employed the inverse square distance method to estimate the concentration of each element in 500×500 m cells. The Qayen sheet comprises a total of 12221 cells, resulting in a data matrix of 27×12221. Figures 1 and 2 display the geochemical anomaly map of the study area generated using SVM and ANN classification methods, utilizing imbalanced and balanced datasets, respectively. The anomaly zones in the SVM and ANN maps cover approximately 16 and 50.25 km2, respectively. Figure 1 highlights that the identified geochemical anomalies exhibit limited overlap with the igneous rock units within the study area. The balancing algorithms utilized in modeling the geochemical anomaly maps expanded the anomaly areas and effectively aligned them with mineralized rock units. Furthermore, oversampling algorithms such as SMOTE and ADASYN, followed by the hybrid ADASYN-CNN algorithm, demonstrated superior performance in achieving this outcome.

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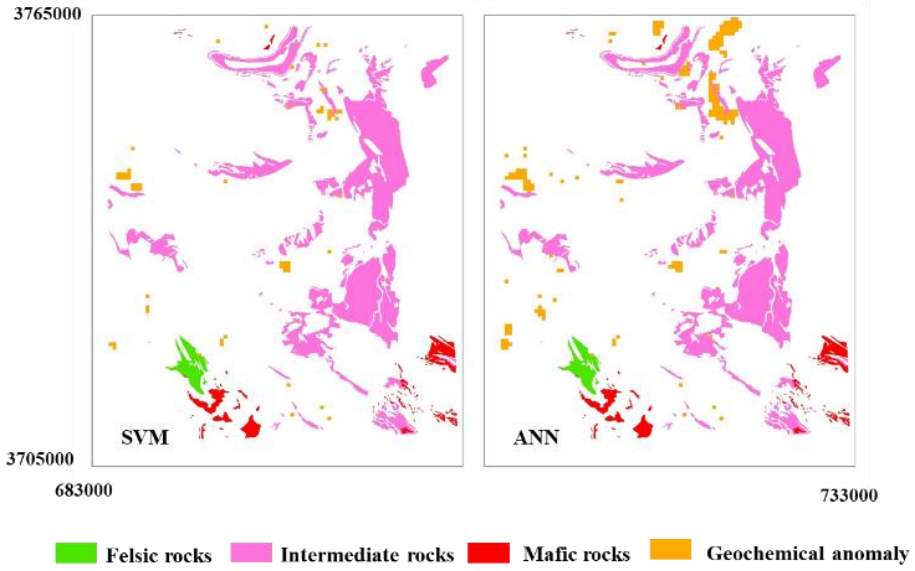
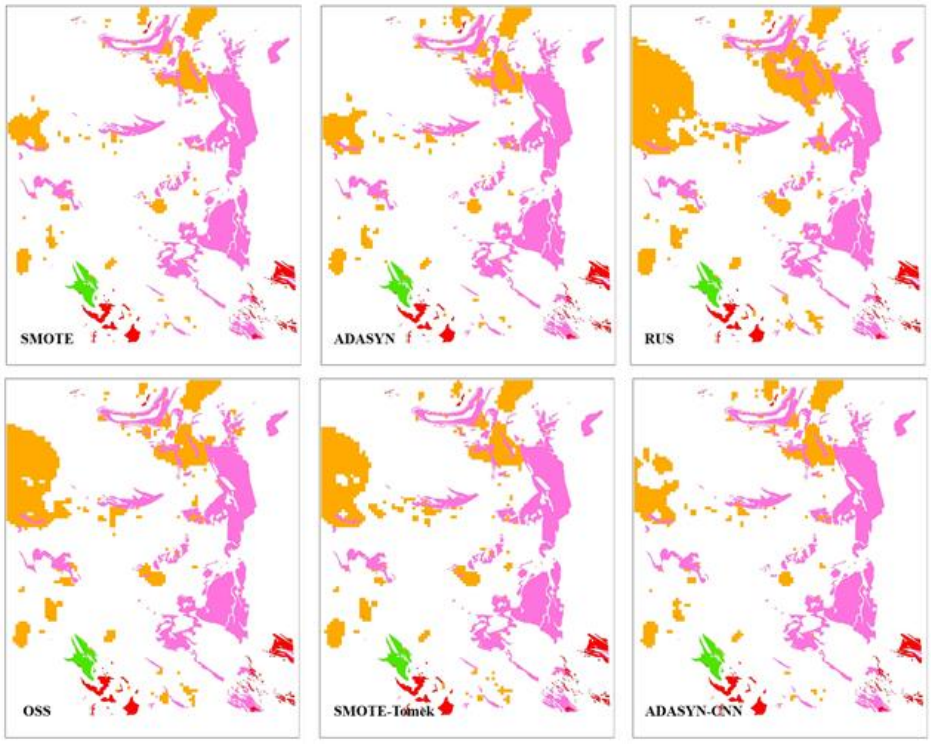


Fig. 1. Map of composite geochemical anomalies estimated with the imbalanced dataset along with the location of igneous rock units in the study area



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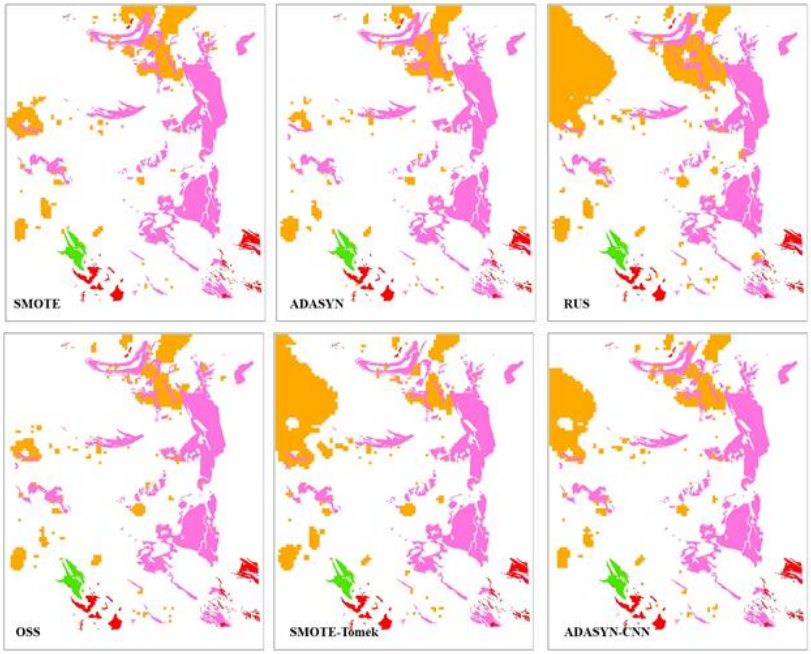

Fig. 2. Map of composite geochemical anomalies estimated with the balanced dataset (Legend is the same as in Fig. 1)

Hence, this paper recommends balancing the dataset before classification to enhance the accuracy, precision, and efficiency of the classification model. Additionally, another suggestion outlined in this paper is to utilize oversampling algorithms followed by hybrid-sampling algorithms prior to classifying the exploration data.

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