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ИЗВЕСТИЯ

РОО «НАЦИОНАЛЬНОЙ
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NAS RK is pleased to announce that News of NAS RK. Series of geology and technical sciences scientific journal has been accepted for indexing in the Emerging Sources Citation Index, a new edition of Web of Science. Content in this index is under consideration by Clarivate Analytics to be accepted in the Science Citation Index Expanded, the Social Sciences Citation Index, and the Arts & Humanities Citation Index. The quality and depth of content Web of Science offers to researchers, authors, publishers, and institutions sets it apart from other research databases. The inclusion of News of NAS RK. Series of geology and technical sciences in the Emerging Sources Citation Index demonstrates our dedication to providing the most relevant and influential content of geology and engineering sciences to our community.

Қазақстан Республикасы Ұлттық ғылым академиясы «ҚР ҰҒА Хабарлары. Геология және техникалық ғылымдар сериясы» ғылыми журналының Web of Science-тің жаңаланған нұсқасы Emerging Sources Citation Index-те индекстелуге қабылданғанын хабарлайды. Бұл индекстелу барысында Clarivate Analytics компаниясы журналды одан әрі the Science Citation Index Expanded, the Social Sciences Citation Index және the Arts & Humanities Citation Index-ке қабылдау мәселесін қарастыруда. Web of Science зерттеушілер, авторлар, баспашылар мен мекемелерге контент тереңдігі мен сапасын ұсынады. ҚР ҰҒА Хабарлары. Геология және техникалық ғылымдар сериясы Emerging Sources Citation Index-ке енуі біздің қоғамдастық үшін ең өзекті және беделді геология және техникалық ғылымдар бойынша контентке адалдығымызды білдіреді.

НАН РК сообщает, что научный журнал «Известия НАН РК. Серия геологии и технических наук» был принят для индексирования в Emerging Sources Citation Index, обновленной версии Web of Science. Содержание в этом индексировании находится в стадии рассмотрения компанией Clarivate Analytics для дальнейшего принятия журнала в the Science Citation Index Expanded, the Social Sciences Citation Index и the Arts & Humanities Citation Index. Web of Science предлагает качество и глубину контента для исследователей, авторов, издателей и учреждений. Включение Известия НАН РК. Серия геологии и технических наук в Emerging Sources Citation Index демонстрирует нашу приверженность к наиболее актуальному и влиятельному контенту по геологии и техническим наукам для нашего сообщества.

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INTELLIGENT METHODS FOR CLASSIFYING ROCKS BASED ON THEIR CHEMICAL COMPOSITION

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Abstract. Automation of rock classification by chemical composition is an important task in geology, ecology, mining and construction. Traditional methods based on visual characteristics and field studies are not effective enough to process large amounts of data. The paper describes the development of a model for classifying rocks based on their chemical composition using logistic regression. The dataset used was a dataset of key oxide concentrations of different rock types. The quality of the model was assessed using the accuracy, recall, precision and F1-score metrics, as well as visualization of the results using confusion matrices and heat maps of rock distribution by geographic zones. The model effectively used chemical features to identify these rocks. However, for rare or similar rocks (diorite,

granodiorite, rhyolite), the accuracy was lower, indicating the need for further work to improve the model. Heat map of rock distribution by region (Washington, Oregon) demonstrates the correlation between rock type and geological features (volcanic activity, subduction). The model has proven effective in classifying common rock types. The results can be applied in practice to speed up and improve the accuracy of geological studies, especially when processing large amounts of data, for example, to automate the analysis of drilling results and determine rock types over large areas. The obtained data on the distribution of rocks in a region can help in understanding geological history and predicting possible mineral deposits.

Keywords: rock classification, machine learning in geology, analysis of oxides in rocks, classification accuracy, model evaluation metrics, importance of features.

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ТАУ ЖЫНЫСТАРЫН ХИМИЯЛЫҚ ҚҰРАМЫНА ҚАРАЙ ЖІКТЕУДІҢ ИНТЕЛЛЕКТУАЛДЫ ӘДІСТЕРІ

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Аннотация. Тау жыныстарын химиялық құрамы бойынша жіктеуді автоматтандыру геология, экология, тау-кен өнеркәсібі және құрылыстағы маңызды міндет болып табылады. Көрнекі сипаттамалар мен далалық зерттеулерге негізделген дәстүрлі әдістер үлкен көлемдегі деректерді өңдеуде

тиімді емес. Мақалада логистикалық регрессияны қолдана отырып, тау жыныстарын химиялық құрамына қарай жіктеу моделінің дамуы сипатталған. Деректер ретінде әртүрлі тау жыныстарының негізгі оксидтерінің концентрациясы туралы мәліметтер жиынтығы қолданылды. Модельдің сапасы дәлдік, толықтық, нақтылық және F1 Өлшем көрсеткіштері, сондай-ақ қате матрицалары мен тау жыныстарының географиялық аймақтар бойынша таралуының жылу карталары арқылы нәтижелерді визуализациялау арқылы бағаланды. Модель осы жыныстарды анықтау үшін химиялық белгілерді (Al_2O_3 , FeO, P_2O_5) тиімді пайдаланды. Алайда сирек кездесетін немесе құрамы ұқсас тау жыныстары үшін (диорит, гранодиорит, риолит) дәлдік төмен болды, бұл модельді жақсарту үшін одан әрі жұмыс істеу қажеттілігін көрсетеді. Тау жыныстарының аймақтар бойынша таралуының жылу картасы (Вашингтон, США; Орегон, США) тау жыныстарының түрі мен геологиялық ерекшеліктері (вулкандық белсенділік, субдукция) арасындағы корреляцияны көрсетеді. Модель жалпы тау жыныстарының түрлерін жіктеуде тиімділікті көрсетті. Нәтижелерді мысалы, бұрғылау нәтижелерін талдауды Автоматтандыру және үлкен аумақтардағы тау жыныстарының түрлерін анықтау секілді іс жүзінде геологиялық зерттеулердің дәлдігін жеделдету және жақсарту үшін қолдануға болады, әсіресе үлкен көлемдегі деректерді өңдеу кезінде, Аймақтағы тау жыныстарының таралуы туралы алынған мәліметтер геологиялық тарихты түсінуге және пайдалы қазбалардың ықтимал кен орындарын болжауға көмектеседі.

Түйін сөздер: тау жыныстарының жіктелуі, геологиядағы Машиналық оқыту, тау жыныстарындағы оксидтерді талдау, жіктеу дәлдігі, модельді бағалау көрсеткіштері, белгілердің маңыздылығы.

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ИНТЕЛЛЕКТУАЛЬНЫЕ МЕТОДЫ КЛАССИФИКАЦИИ ГОРНЫХ ПОРОД НА ОСНОВЕ ИХ ХИМИЧЕСКОГО СОСТАВА

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Аннотация. Автоматизация классификации горных пород по химическому составу является важной задачей в геологии, экологии, горнодобывающей промышленности и строительстве. Традиционные методы, основанные на визуальных характеристиках и полевых исследованиях, недостаточно эффективны для обработки больших объемов данных. Статья описывает разработку модели классификации горных пород на основе их химического состава, используя логистическую регрессию. В качестве данных использовался набор данных о концентрациях ключевых оксидов различных типов горных пород. Качество модели оценивалось с помощью метрик точности, полноты, точности и F1-меры, а также визуализацией результатов с помощью матриц ошибок и тепловых карт распределения пород по географическим зонам. Модель эффективно использовала химические признаки (Al_2O_3 , FeO, P_2O_5) для идентификации этих пород. Однако для редких или сходных по составу пород (диорит, гранодиорит, риолит) точность была ниже, что свидетельствует о необходимости дальнейшей работы по улучшению модели. Тепловая карта распределения пород по регионам (Вашингтон, Орегон) демонстрирует корреляцию между типом породы и геологическими особенностями (вулканическая активность, субдукция). Модель показала эффективность в классификации распространенных типов горных пород. Результаты могут быть применены на практике для ускорения и повышения точности геологических исследований, особенно при обработке больших объемов данных, например, для автоматизации анализа результатов бурения и определения типов пород на больших территориях. Полученные данные о распределении пород в регионе могут помочь в понимании геологической истории и прогнозировании возможных залежей полезных ископаемых.

Ключевые слова: классификация горных пород, машинное обучение в геологии, анализ оксидов в породах, точность классификации, метрики оценки модели, важность признаков.

Introduction. Rocks are the main material of the Earth's crust and are formed as a result of complex geological processes such as magmatic activity, metamorphism

and sedimentary deposits. Each type of rock has unique chemical, mineralogical and physical properties that determine their role in the lithosphere and influence on natural processes (Filina, et al., 2023). The correct identification of rocks plays an important role in such industries as geology, ecology, mining and construction (Golik, et al., 2023).

Rock classification has historically been based on visual characteristics, mineralogical composition, and field studies. However, with the development of big data processing and machine learning technologies, it has become possible to automate this process using quantitative chemical composition data and other parameters. This is especially important in the context of increasing amounts of data collected from various geological objects, including mountain ranges, volcanic zones and mineral deposits (Podgornyj, et. al., 2024; Kachurin, et. al., 2021).

One of the most effective approaches for classifying rocks is the analysis of their chemical composition. Elements such as oxides of aluminum, iron, silicon and other elements can play a key role in the identification of rock types (Tananykhin, et. al., 2021; Tananykhin, 2024). The use of such data makes it possible to more accurately divide samples into classes, which is an important step in geological research.

The purpose of this study is to create a model for classifying rocks based on their chemical composition, which will improve the accuracy and speed of analysis of geological data.

Research methods. To perform the classification of rocks, data on the chemical composition of various types of rocks were used. The dataset includes information on concentrations of key oxides, which are important parameters for determining the geochemical characteristics of rocks. Each entry in the dataset is a rock sample with an indication of its type and concentrations of chemical elements (Martyushev, 2014). The collected data underwent a preprocessing stage, including the removal of missing values and normalization of numerical features to improve the performance of the model (Golik, Kachurin, et. al., 2022; Golik, Gabaraev, et. al., 2019). Normalization was carried out in order to eliminate the influence of differences in the magnitude of chemical elements and to ensure a more uniform contribution of each feature to the model (Kukartsev, et al., 2023).

A logistic regression model was used to classify rocks, which is one of the machine learning methods for solving classification problems. Logistic regression was chosen due to its ability to interpret the contribution of each feature to the final classification and its relative ease of implementation and interpretation. The logistic regression model estimates the probability of assigning a sample to each of the rock classes based on the chemical composition (Panfilova, et al., 2024). The final decision is made based on the probability threshold (by default, 0.5). This allows you to divide the samples into several classes and determine which breed the sample belongs to.

The assessment of the quality of the model was carried out using the following metrics:

1. Accuracy: The percentage of correctly classified samples among all.
2. Recall: the ability of the model to correctly identify all instances of a given class.
3. Precision: the ability of the model to correctly classify only those samples that actually belong to this class.
4. F1-score: the harmonic mean between accuracy and completeness, which allows you to take into account both false positive and false negative classifications.

Visualization methods such as the confusion matrix, which shows the success and classification errors for each type of breed, were used to analyze and interpret the results (Kravtsov, et al., 2024; Degtyareva, et al., 2024; Fedorova, et al., 2024). Curves of dependence of accuracy and completeness for each class of rocks were also used, which makes it possible to assess the quality of the model at different thresholds. The heat map of the distribution of rock samples by geographical feature made it possible to visualize how different types of rocks are distributed in the space (Panfilov, et al., 2024).

Results and discussion. During the study, a heat map was developed (Fig. 1), which shows the distribution of rock samples by type in the geographical region under study. The different colors represent different types of rocks, and each circle on the map corresponds to a separate rock sample that has been classified by the model.

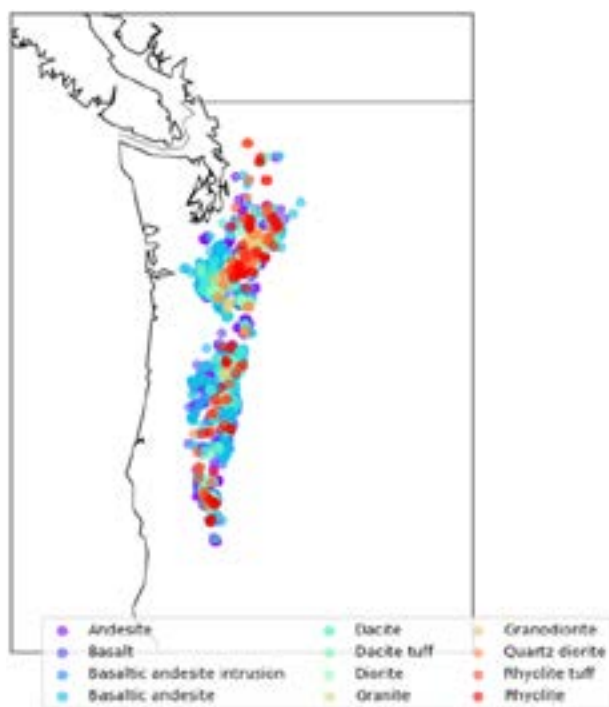


Fig. 1. Heat map of rock distribution of rocks

The distribution of rocks in Washington and Oregon is closely related to the features of the geological structure of the region, including active volcanic activity and subduction processes. Rocks such as basalt and andesite are found in significant volumes due to their origin as a result of volcanic activity (Boyko, et al., 2023). These igneous rocks are the product of volcanic eruptions, which are characteristic of the region due to their location along the Cascade Mountains. Basalt, as one of the most common volcanic rocks, is formed by the rapid cooling of lava, which leads to its extensive distribution in areas of active volcanism, as observed in Washington and Oregon. Andesite, which is formed by slower cooling of magma with a high silicon content, is also widely represented in this region due to frequent volcanic eruptions (Larichev, et al., 2024).

Other rocks, such as rhyolite and granite, are less common and have a different origin. Rhyolite is formed during volcanic activity, but at a higher concentration of silica, which makes it typical for more viscous magma. This explains its lower distribution compared to basalts (Ilyushin, Pervukhin, Afanasieva, Afanasyev, Kolesnichenko, 2016; Ilyushin, Pervukhin, Afanasyeva, Klavdiev, Kolesnichenko, 2016). Granite and granodiorite, on the contrary, are deep igneous rocks formed as a result of slow cooling of magma in the depths of the earth’s crust (Golik, et al., 2023). Their rare distribution on the map is due to the fact that these rocks do not form on the surface, but manifest themselves in regions where erosion or tectonic processes occur, exposing the deep layers.

Thus, the rocks on the heat map reflect the diversity of geological processes occurring in the states of Washington and Oregon. Large volumes of basalt and andesite are associated with frequent volcanic activity, while rarer rocks such as granite, rhyolite and diorite are formed as a result of deep magmatic processes and manifest themselves in places of tectonic activity or erosion. This distribution of rocks allows for a deeper understanding of the volcanic and tectonic history of the region, as well as the formation features of each rock (Ilyushin, Kivayev, Novozhilov, 2017; Ilyushin, Pervukhin, Afanaseva, 2019).

During the study, a logistic regression model was developed to classify rocks based on their chemical composition. The model showed satisfactory accuracy, reaching 76%, which indicates its ability to correctly classify most types of rocks. The classification report is shown in Fig. 2.

	precision	recall	f1 score	support
Andesite	0.79478	0.87728	0.83604	1913
Basalt	0.96476	0.88371	0.92156	1333
Basaltic andesite	0.79474	0.8994	0.84913	2179
Basaltic andesite intrusion	0.0	0.0	0.0	37.0
Diorite	0.64331	0.73529	0.68893	34.0
Diorite tail	0.0	0.14286	0.10513	14.0
Diorite	0.33333	0.07143	0.11765	28.0
Granite	0.66667	0.00000	0.76923	22.0
Granodiorite	0.98333	0.00000	0.80000	38.0
Quartz diorite	0.0	0.0	0.0	35.0
Rhyolite	0.39442	0.45455	0.41967	11.0
Rhyolite tail	0.0	0.18182	0.30000	11.0
avg/total	0.76335	0.76335	0.76335	0.76335
macro avg	0.79685	0.86136	0.85007	993.0
weighted avg	0.79964	0.86335	0.77988	993.0

Fig. 2. Classification report

The model successfully copes with the classification of the main types of rocks, such as basalt and andesite, due to their pronounced chemical characteristics. For these breeds, the model showed high levels of accuracy, completeness and F1-score, which indicates its ability to distinguish between these types of breeds with minimal errors. However, for rocks such as diorite, granodiorite and rhyolite, the accuracy is much lower, indicating difficulties in their classification. This may be due to the fact that these rocks have chemical similarities with other types of rocks, which makes it difficult to distinguish them (Orlov, et al., 2023). The model also showed low accuracy for rare rock types such as tuff and quartz diorite, which may be due to insufficient data for these classes.

A diagram of the importance of the features is shown in Fig. 3.

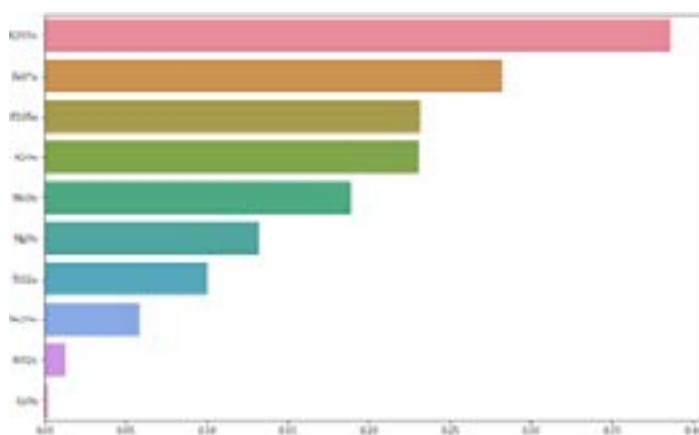


Fig. 3. Importance of feature. The Y axis indicates the feature, and the X axis indicates the absolute value of the coefficient.

This graph shows the importance of various chemical features of rocks based on the absolute values of the logistic regression coefficients. Each feature is represented on the vertical axis, and the horizontal axis shows the absolute value of the coefficient, which is interpreted as the importance of the feature for the model.

Al₂O_{3n} (aluminum oxide) is the most significant feature with the highest coefficient, which indicates its high contribution to the classification of rocks. FeO*n (iron oxide) and P₂O_{5n} (phosphorus oxide) also have a significant impact, ranking second and third in importance. The signs K₂On (potassium oxide) and MnOn (manganese oxide) occupy the middle positions in importance. The least contribution to the classification is made by such features as CaOn (calcium oxide) and SiO_{2n} (silicon dioxide), which indicates their lesser importance in the model.

Thus, the logistic regression model relies most heavily on the content of Al₂O_{3n}, FeO*n and P₂O_{5n} to accurately classify rocks, whereas features such as CaOn and SiO_{2n} play a less significant role.

Figure 4 shows the confusion matrix.

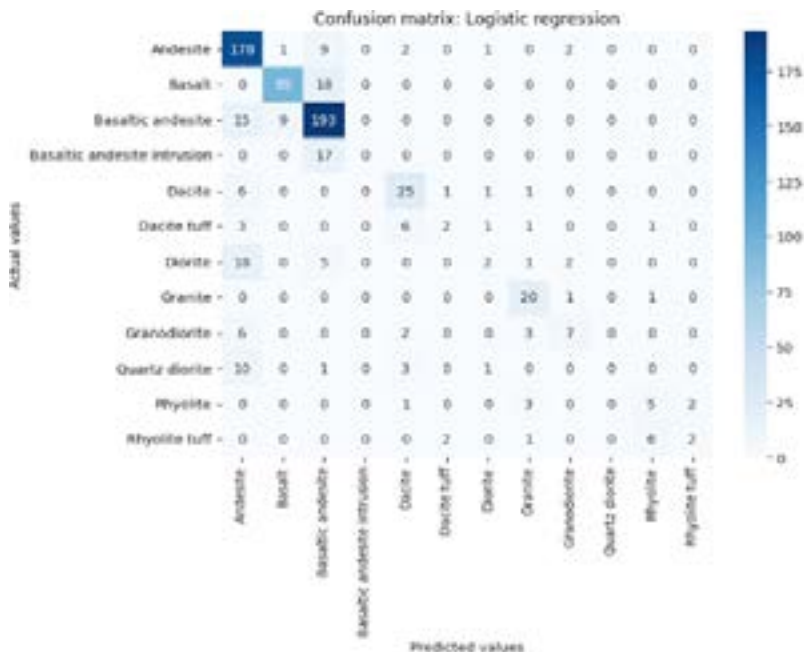


Fig. 4. Confusion matrix.

The confusion matrix shows that the model classified andesite quite successfully, with 178 correct predictions from 193 samples, although some samples were mistakenly attributed to basalt andesite and diorite. For basalt, the model showed a good result: 95 correct classifications out of 113 samples, but 18 of them were attributed to basalt andesite. This also confirms the difficulty of distinguishing these rocks, probably due to their close chemical composition. In the case of basalt andesite intrusions, the model correctly predicted all 17 samples, which shows high accuracy for this type of rock. However, other rocks, such as diorite and granodiorite, showed significantly worse results. For example, for diorite, only 2 of the 28 samples were correctly classified, and the rest were distributed into other categories, including andesite, granite and quartz diorite. Granite and rhyolite also showed mixed results. Granite was correctly classified in 20 out of 22 cases, while rhyolite was classified with errors, and only 3 out of 11 samples were correctly assigned to this class. Rhyolite tuff and quartz diorite were often confused with other rocks, which also indicates the low accuracy of the model for these classes.

In general, the confusion matrix shows that the model does a good job of classifying common rocks such as andesite and basalt, but has difficulties with rare or chemically similar rocks such as diorite, granodiorite and rhyolite.

Thus, the classification results show that the logistic regression model copes well with the definition of common rocks such as andesite, basalt and basalt andesite, which is confirmed by high accuracy and completeness for these classes. This is due to the fact that the chemical characteristics of these rocks are quite pronounced,

which allows the model to easily distinguish them (Klyuev, Kashapov, et al., 2023; Klyuev, Kashapov, et al., 2022). However, when it comes to breeds with more similar characteristics or rare breeds, the model begins to experience difficulties. For example, diorite and granodiorite are often misclassified, indicating their chemical similarity to other rock types in the data. This highlights the importance of increasing the number of samples for rare breeds and possibly applying more sophisticated machine learning techniques that could better capture subtle differences between classes.

However, the low accuracy in some classes indicates the need for further work with the model and data. It is worth considering the possibility of using other machine learning methods. In addition, it is necessary to conduct a more in-depth analysis of the chemical composition of rocks in order to identify additional distinctive features that could improve the quality of classification (Kuznetsov, Klyuev, et al., 2023; Mohammad, et al., 2021).

Thus, the results obtained confirm that logistic regression is a suitable tool for the basic classification of common breeds, but more accurate recognition of rare or similar breeds requires additional research and model improvement.

Conclusion. During the study, a logistic regression model was developed and tested to classify various types of rocks based on their chemical composition (Volneikina, et al., 2023). The model showed good results for common rocks such as andesite, basalt and basalt andesite, which indicates that these rocks have pronounced chemical characteristics that allow the model to successfully distinguish them. However, for less common rocks such as diorite, granodiorite and rhyolite, the classification turned out to be less accurate, due to their chemical similarity to other rocks (Panfilov, et al., 2023; Panfilov, et al., 2023). In conclusion, the developed model has shown its effectiveness in solving the problem of rock classification, but further improvements, such as more complex algorithms and detailed feature analysis, can significantly increase its accuracy and applicability to a wider range of rocks (Panfilov, et al., 2024).

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