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«ҚАЗАҚСТАН РЕСПУБЛИКАСЫ
ҰЛТТЫҚ ҒЫЛЫМ АКАДЕМИЯСЫ» РҚБ
«ХАЛЫҚ» ЖҚ

ХАБАРЛАРЫ

ИЗВЕСТИЯ

РОО «НАЦИОНАЛЬНОЙ
АКАДЕМИИ НАУК РЕСПУБЛИКИ
КАЗАХСТАН»
ЧФ «Халық»

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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. Webof 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.

ЧФ «ХАЛЫҚ»

В 2016 году для развития и улучшения качества жизни казахстанцев был создан частный Благотворительный фонд «Халык». За годы своей деятельности на реализацию благотворительных проектов в областях образования и науки, социальной защиты, культуры, здравоохранения и спорта, Фонд выделил более 45 миллиардов тенге.

Особое внимание Благотворительный фонд «Халык» уделяет образовательным программам, считая это направление одним из ключевых в своей деятельности. Оказывая поддержку отечественному образованию, Фонд вносит свой посильный вклад в развитие качественного образования в Казахстане. Тем самым способствуя росту числа людей, способных менять жизнь в стране к лучшему – профессионалов в различных сферах, потенциальных лидеров и «великих умов». Одной из значимых инициатив фонда «Халык» в образовательной сфере стал проект Ozgeris powered by Halyk Fund – первый в стране бизнес-инкубатор для учащихся 9-11 классов, который помогает развивать необходимые в современном мире предпринимательские навыки. Так, на содействие малому бизнесу школьников было выделено более 200 грантов. Для поддержки талантливых и мотивированных детей Фонд неоднократно выделял гранты на обучение в Международной школе «Мирас» и в Astana IT University, а также помог казахстанским школьникам принять участие в престижном конкурсе «USTEM Robotics» в США. Авторские работы в рамках проекта «Тәлімгер», которому Фонд оказал поддержку, легли в основу учебной программы, учебников и учебно-методических книг по предмету «Основы предпринимательства и бизнеса», преподаваемого в 10-11 классах казахстанских школ и колледжей.

Помимо помощи школьникам, учащимся колледжей и студентам Фонд считает важным внести свой вклад в повышение квалификации педагогов, совершенствование их знаний и навыков, поскольку именно они являются проводниками знаний будущих поколений казахстанцев. При поддержке Фонда «Халык» в южной столице был организован ежегодный городской конкурс педагогов «Almaty Digital Ustaz.

Важной инициативой стал реализуемый проект по обучению основам финансовой грамотности преподавателей из восьми областей Казахстана, что должно оказать существенное влияние на воспитание финансовой грамотности и предпринимательского мышления у нового поколения граждан страны.

Необходимую помощь Фонд «Халык» оказывает и тем, кто особенно остро в ней нуждается. В рамках социальной защиты населения активно проводится работа по поддержке детей, оставшихся без родителей, детей и взрослых из социально уязвимых слоев населения, людей с ограниченными возможностями, а также обеспечению нуждающихся социальным жильем, строительству социально важных объектов, таких как детские сады, детские площадки и физкультурно-оздоровительные комплексы.

В копилку добрых дел Фонда «Халык» можно добавить оказание помощи детскому спорту, куда относится поддержка в развитии детского футбола и карате в нашей стране. Жизненно важную помощь Благотворительный фонд «Халык» оказал нашим соотечественникам во время недавней пандемии COVID-19. Тогда, в разгар тяжелой борьбы с коронавирусной инфекцией Фонд выделил свыше 11 миллиардов тенге на приобретение необходимого медицинского оборудования и дорогостоящих медицинских препаратов, автомобилей скорой медицинской помощи и средств защиты, адресную материальную помощь социально уязвимым слоям населения и денежные выплаты медицинским работникам.

В 2023 году наряду с другими проектами, нацеленными на повышение благосостояния казахстанских граждан Фонд решил уделить особое внимание науке, поскольку она является частью общественной культуры, а уровень ее развития определяет уровень развития государства.

Поддержка Фондом выпуска журналов Национальной Академии наук Республики Казахстан, которые входят в международные фонды Scopus и Wos и в которых публикуются статьи отечественных ученых, докторантов и магистрантов, а также научных сотрудников высших учебных заведений и научно-исследовательских институтов нашей страны является не менее значимым вкладом Фонда в развитие казахстанского общества.

С уважением,
Благотворительный Фонд «Халык»!

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STUDY OF THE EFFICIENCY OF MACHINE LEARNING ALGORITMS BASED ON DATA OF VARIOUS ROCKS

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Abstract. Absolute permeability is an important transport property of a porous medium that requires determination on special equipment, so its determination is an important task. This article examines the effectiveness of machine learning regression algorithms for predicting the absolute permeability of various rocks. The performance of algorithms such as Random Forest, Gradient Boosting, Support Vector, Lasso, k-Nearest Neighbors, and Gaussian Process was compared based on data set of 266 sub-samples of carbonate and sand rocks, as well as artificial sand packing. Properties of each sub-sample such as pore radius, pore throat radius, coordination number, porosity, specific surface area, tortuosity and absolute permeability are extracted using pore-network simulation of the single-phase fluid flow through each sub-sample. The influence of the training/testing data subset (70/30 and 80/20) and the number of features of input data set on the performance of each of the above algorithms was investigated. The results showed that for the considered data set, the Random Forest algorithm was the most suitable for predicting absolute permeability with high accuracy. The highest predictive

accuracy was R^2=0.83, and it was obtained using 5 out of 6 features of input dataset. The Gradient Boosting algorithm also showed good predictive ability for absolute permeability, although it chose almost one feature (porosity) as important. Its highest accuracy was R^2=0.73 at 80/20. The results of the study also showed that all algorithms except Random Forest predicted significantly higher minimum permeabilities. Also, all algorithms, except of Support Vector and k-Nearest Neighbors, predicted the mean permeability with the minimal errors.

Keywords: machine learning, permeability prediction, microcomputed tomography, sub-sample, pore-scale modeling

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ӘРТҮРЛІ ТАУ ЖЫНЫСЫНЫҢ ДЕРЕКТЕРІ НЕГІЗІНДЕ МАШИНАЛЫҚ ОҚУ АЛГОРИТМДЕРІНІҢ ТИІМДІЛІГІН ЗЕРТТЕУ

Аннотация. Абсолютті өткізгіштік арнайы жабдық көмегімен анықталатын кеуекті ортаның маңызды тасымалдау қасиеті, сондықтан оны анықтау маңызды мәселе болып табылады. Бұл мақалада әртүрлі тау жыныстарының абсолютті өткізгіштігін болжау үшін машиналық оқытудың регрессиялық алгоритмдерінің тиімділігі қарастырылады. Random Forest, Gradient Boosting, Support Vector, Lasso, k-Nearest Neighbors және Gaussian Process сияқты алгоритмдердің өнімділігі карбонатты және құмды жыныстардың, сондай-ақ жасанды құмды орамның 266 мини-үлгілерінің деректері негізінде салыстырылды. Осы мини-үлгілердің әрқайсысының кеуек радиусы, кеуек мойнының радиусы, координациялық саны, кеуектілігі, бетінің меншікті ауданы, бұралу және абсолютті өткізгіштігі сияқты қасиеттері бір фазалы сұйық ағынын кеуекті-желілік модельдеу арқылы алынды. әрбір шағын үлгі арқылы. Оқытушы және сынақтаушы деректер жинағы арақатынасының (70/30 және 80/20) және деректер жиынындағы белгілер санының жоғарыда аталған алгоритмдердің әрқайсысының өнімділігіне әсері зерттелді. Нәтижелер қарастырылған деректер жиыны үшін жоғары сенімділікпен абсолютті өткізгіштікті болжауға ең қолайлы Random Forest алгоритмі екенін көрсетті. Болжамның ең жоғары сенімділік коэффициенті R^2=0.83 құрады және ол деректер жиынындағы 6 белгінің 5-ін пайдалану нәтижесінде алынды. Gradient Boosting алгоритмі де абсолютті өткізгіштікті жақсы болжау қабілетін көрсетті, дегенмен ол бір ғана дерлік белгіні (кеуектілікті) маңызды деп таңдады. Оның болжауының ең жоғарғы сенімділік коэффициенті R^2=0.73 құрады және ол 80/20 үшін алынды.

Зерттеу нәтижелері сонымен қатар Random Forest басқа барлық алгоритмдер айтарлықтай жоғары минималды өткізгіштіктерді болжағанын көрсетті. Сондай-ақ Support Vector және k-Nearest Neighbors басқа барлық алгоритмдер орташа өткізгіштікті ең аз қателікпен болжады.

Түйін сөздер: машиналық оқыту, өткізгіштікті болжау, микрокомпьютерлік томография, мини-үлгілер, кеуекті масштабта модельдеу

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ИССЛЕДОВАНИЕ ЭФФЕКТИВНОСТИ АЛГОРИТМОВ МАШИННОГО ОБУЧЕНИЯ НА ОСНОВЕ ДАННЫХ РАЗЛИЧНЫХ ГОРНЫХ ПОРОД

Аннотация. Абсолютная проницаемость является важным транспортным свойством пористой среды, требующая определение на специальных оборудованиях, поэтому ее определение является актуальной задачей. В настоящей статье изучается эффективность регрессионных алгоритмов машинного обучения для прогнозирования абсолютной проницаемости различных пород. Сравнены производительности таких алгоритмов как Random Forest, Gradient Boosting, Support Vector, Lasso, k-Nearest Neighbors и Gaussian Process на основе данных 266 мини-образцов карбонатных и песчаных пород, а также исскуственной песчаной упаковки. С каждого из этих мини-образцов извлечены их такие свойства как радиус пор, радиус горловины пор, координационное число, пористость, удельная площадь поверхности пор, извилистость и абсолютная проницаемость с помощью поросетевого моделирования течения однофазной жидкости сквозь каждого мини-образца. Было исследовано влияние соотношения обучающего и тестового набора данных (70/30 и 80/20) и количества признаков в наборе данных на производительность каждого из выше рассмотренных алгоритмов. Результаты показали, что для рассматриваемого набора данных алгоритм Random Forest являлся наиболее подходящим для прогнозирования абсолютной проницаемости с высокой достоверности. Наибольший коэффициент достоверности прогноза составил R^2=0.83, и он был получен при использовании 5 из 6 признаков в наборе данных. Алгоритм Gradient Boosting тоже показал хорошую прогнозирующую способность абсолютной проницаемости, хотя он выбирал практически одного признака (пористости) как важным. Его наибольший коэффициент составил R^2=0.73 при 80/20. Результаты исследования также показали, что все алгоритмы, кроме Random Forest, предсказали существенно завышенные минимальные проницаемости. А также все алгоритмы, кроме Support Vector и k-Nearest Neighbors, предсказали среднее значение проницаемости с наименьшими погрешностями.

Ключевые слова: машинное обучение, прогноз проницаемости, микрокомпьютерная томография, мини-образец, поромасштабное моделирование

Introduction

Absolute permeability is an important macroscopic transport characteristic of a porous medium, on which the production of hydrocarbons during field development, the performance of filters in indoor air purification, separation of gas-liquid systems and in catalytic systems, etc. depend. Permeability is usually determined experimentally in the laboratory using special equipment. Laboratory measurements usually take a long time and are expensive. Therefore, its determination in alternative ways based on available analytical and experimental data on porous media is an urgent task.

With the development of machine learning methods, they began to be used to analyze data and predict important characteristics in many areas such as medicine (Rajalingam, Priya, 2018), economics (Cicceri et al., 2020; Yoon, 2021), geophysics (Gholami et al., 2012; Tembely et al., 2020; Waszkiewicz et al., 2019), etc. When predicting absolute permeability, images of real rocks or synthetic porous media obtained using microcomputed tomography (Tembely et al., 2020; Wu et al., 2018) and digital data extracted in one way or another from these images are used (Al Khalifah et al., 2020; Rabbani & Babaei, 2019). Well logging data is also used to predict absolute permeability (Rezaee & Ekundayo, 2022; Waszkiewicz et al., 2019).

Two-dimensional images of synthetic porous media combined with the lattice Boltzmann method were used to predict porosity, tortuosity and absolute permeability in (Rabbani & Babaei, 2019). Synthetic porous media are obtained by randomly distributing square particles, representing a solid rock matrix, in a square area. The authors used convolutional neural networks to determine the relationship between the structure and basic characteristics of synthetic porous media. And using the lattice Boltzmann method, flow fields were found for further calculation of tortuosity and permeability. They argued that convolutional neural networks showed high predictive ability of the underlying features. A similar study was carried out in (Wu et al., 2018), where it was also said that convolutional neural networks showed high performance in predicting absolute permeability. Thambley et al. (Tembely et al., 2020) used high spatial resolution micro-computed tomography images of over 1000 rock samples to build a predictive permeability model based on machine learning and deep learning techniques. They showed that permeability models based on machine learning and deep learning methods predicted permeability with confidence of 88 and 91%, respectively. They also showed that the use of artificial intelligence methods can reduce the time of calculating permeability by three orders of magnitude compared to traditional methods. Prediction of absolute rock permeability based on well logging data using machine learning methods is given in (Rezaee & Ekundayo, 2022; Waszkiewicz et al., 2019).

This paper examines the prediction of absolute permeability based on data from various rocks whose actual permeability is very different from their average statistical permeability. An analysis of the literature showed that when studying the effectiveness of machine learning methods, data from synthetic porous media and real rocks with slightly changing characteristics were mainly used. During the study, 6 machine learning methods were considered, the effectiveness of which was studied for different ratios of the training and test data sets.

Materials and methods

Typically, machine learning methods use a dataset with various features as input. For this purpose, digital models of 266 mini-samples from ready-made models of various breeds were prepared. Each mini-sample has 7 features as feature (input) data. Larger finished digital models of 8 different real rocks and 1 artificial rock (packed with sand particles) were taken from the open access library of Professor M. Blunt's research group at Imperial College London, which are shown in Figure 1. Note that the above digital models have already been filtered and segmented. As can be seen from Figure 1 The pore spaces of sandy rocks are formed by voids between sand granules and have a more uniform distribution throughout the sample compared to the structures of carbonate rocks. These models were obtained by scanning rocks using a microcomputed tomograph with a spatial resolution of about 3 μm.

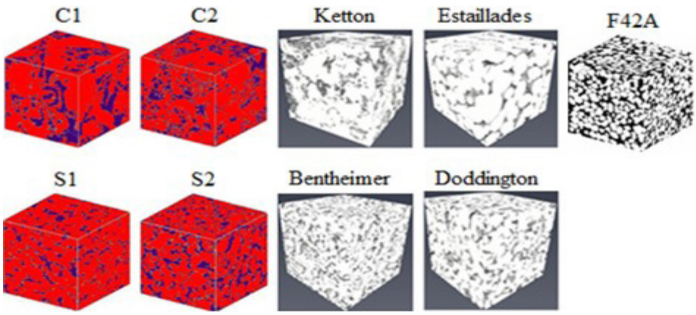


Figure 1. Digital models of samples of various rocks

In order to increase the amount of input data into machine learning methods, the resulting digital rock models were divided into different pieces (mini-samples) of smaller size (Figure 2). Thus, a total of 266 mini-samples were prepared, the sizes of which varied from 0.125 mm to 3 mm.

The permeability of mini-samples is given in Table 1. As can be seen from this table, the considered samples have significantly different permeability. Separately, we can highlight a sample of packed sandstone, which has relatively high permeability. As can be seen from Table 1, carbonate rocks have relatively heterogeneous and low permeability compared to sandy rocks. A comparison of the minimum, maximum and average permeability values shows that the carbonate mini-samples generally have permeability close to the minimum, while the sandy mini-samples other than Bentheimer and Doddington have more uniform permeability distributions. And mini-samples of F42A sand packaging have almost the same permeability.

Table 1 – Permeability of mini-samples

Sample/ rock type	Carbonate				Sandy				Sand packaging
	C1	C2	Ketton	Estaillades	S1	S2	Bentheimer	Doddington	F42A
Minimum	0,097	0,012	0,0033	0,0019	0,45	1,81	0,04	0,001	7,42

Maximum	4,95	4,24	16,05	85,4	3,59	7,84	15,1	9,24	104,3
Average	1,65	0,87	3,08	4,09	1,36	4,44	2,53	2,16	66,0

The main and difficult stage of the entire process was the collection of data from the already prepared mini-samples, since most parameters of the porous medium, such as the average pore radius, average pore throat radius, average tortuosity, average coordination number and absolute permeability, will be found only by simulating the flow fluids through these porous media. The data set contains porosity (ϕ), average pore radius (r_p, in μm), average pore throat radius (r_t, in μm), tortuosity (r), coordination number (N_c), specific pore surface area (S_s, in 1/μm) and absolute permeability (k, in μm2) for each mini-sample. In this work, fluid flow in porous media was simulated using pore network modeling using special Avizo software, during which a pore network of the microstructure of mini rock samples is first constructed based on the allocated pore space (Figure 3), then the pore network will be modeled on it. the flow of the fluid itself based on the law of conservation of mass.

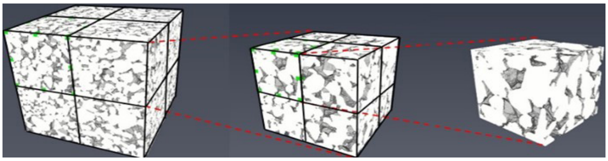


Figure 2. Breaking samples into smaller mini-samples

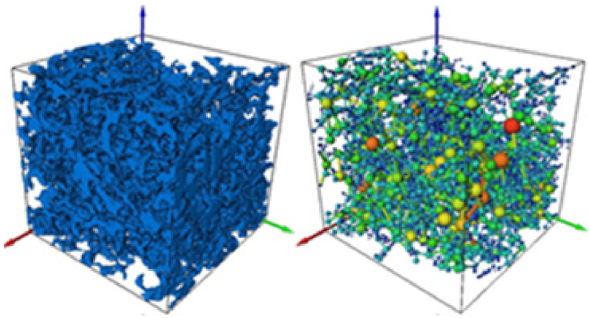


Figure 3. Pore space and pore network of the sub-sample

A pore network is a collection of individual pores and pore throats, which in turn are presented in the form of spheres and cylinders. The construction of the pore network is based on the maximum ball algorithm, in which pores are replaced by spheres and pore throats by cylinders. Accordingly, the radii of spheres and cylinders are the radii of the pores and pore throats. The pore network provides information about the distribution of pores and pore throats according to their sizes; accordingly, we can find the average radii of pores and pore throats. The pore network also allows one to determine the number of connections of a particular pore with other pores connected to it, which means this gives the coordination number of the network. The specific pore surface area is one of the important parameters of a porous medium, since it affects the absolute permeability and the degree of dissolution of rock with different acid compositions.

The main macroscopic parameter of a porous medium is its permeability – it shows the ability of a porous medium to pass liquids through itself and depends on many factors, such as porosity, tortuosity, specific pore surface area, etc. But it has not yet been specifically established which parameters influence it most. The absolute permeability of the medium is determined by Darcy's law. From the digital model of each mini-sample, 7 of its parameters were extracted, such as the average pore radius, the average pore throat radius, tortuosity, coordination number and absolute permeability, which are shown in Figure 4. In the table in Figure 3, each line means a data set of 7 parameters (not including the name) for each mini-sample. This data is the initial information when analyzed using machine learning methods. This dataset has a target variable: 'k' and input variables: 'r_p', 'N_c', 'r_t', 'ϕ', 'S_s', 'r'. Statistics of the characteristics of the mini-samples used are given in Table 2.

	Samples/Parametrs	Input data (input parameters/layers)						Output data (must to predict)
2		Mean Radius (pores) [μM]	Mean Coordination Number	Mean Radius (throats)[μM]	Connected Porosity	Specific surface area [1/μm]	Tortuosity	k [μm^2]
3	Full Size C1	31,382	5	15,064	0,21	0,050	1,809	1,277
4	C1-1	18,235	4	10,160	0,14	0,023	1,596	0,097
5	C1-2	19,583	5	11,921	0,25	0,026	1,779	4,056
6	C1-3	19,745	3	13,590	0,16	0,025	2,053	0,387
7	C1-4	30,996	4	14,737	0,17	0,023	1,569	0,729
8	C1-5	29,190	4	14,091	0,19	0,025	1,337	1,069
9	C1-6	30,269	5	13,718	0,26	0,030	1,675	0,749
10	C1-7	21,431	5	11,523	0,18	0,025	1,800	1,503
11	C1-8	34,897	5	17,082	0,33	0,033	1,646	4,951
12	Full Size C2	47,434	4	20,461	0,14	0,014	1,888	0,081

Figure 4. Data set from digital models of mini-samples

Table 2 – Statistics of characteristics of mini-samples

Parameter	Minimum	Maximum	Average	Standard deviation
r_p(μm)	11,70	188,32	77,33	26,73
N_c	1,71	7,48	4,13	1,18
r_t (μm)	10,11	73,85	27,27	11,08
ϕ	0,02	0,34	0,19	0,067
S_s (1/ μm)	0,0014	0,050	0,013	0,005
r	1,05	2,66	1,51	0,19
k (μm ^{2})	0,001	104,3	9,38	21,98

When studying the data, methods such as random forest, gradient boosting, support vector machines, LASSO, K-nearest neighbors, and Gaussian process were used.

The Random Forest (RF) method is a machine learning algorithm based on an ensemble of decision trees. In this method, each tree solves the problem independently of other trees, and at the end the answers of all trees are averaged. RF uses many parameters to control the optimization of the solution such as n_estimators, max_depth, max_features, etc. (Rezaee & Ekundayo, 2022). Their values used in this work are given in Table 3. We selected the best parameters for this method using the GridSearchCV library (Erofeev et al., 2019), which will help simplify the selection of parameters.

The first important parameter in the RF method is n_estimators - meaning the number of trees, the more trees, the better the quality, but the setup and operation time of RF also increases proportionally. The second important parameter is max_features, when increased, the forest construction time increases, and the trees become "more uniform". The third parameter is max_depth (tree depth), which increases the quality of training sharply. When using shallow trees (i.e., with small max_depth), changing the parameters associated with limiting the number of objects in a leaf and for division does not lead to a significant effect.

Gradient Boosting (GB) is a method for transforming poorly trained models into well trained ones. This method is based on minimizing the loss function using gradient descent (Erofeev et al., 2019). Due to the similarity with the random forest method, this method has almost the same control parameters as in the random forest method. Control parameters and their values are given in Table 3.

Table 3 – Methods and their control parameters

Method	Control options	Value
Random Forest	max_depth	41
	max_features	1
	n_estimators	15
	bootstrap	Actual
	criterion	MSE
Gradient Boosts	n_estimators	19
	learning_rate	0.9
	max_depth	1
	criterion	friedman_mse
Support vector machines	kernel	linear
	epsilon	0.5
	C	10
	gamma	1e-07
LASSO	alpha	0.01
	max_iter	11
K-nearest neighbors	n_neighbors	86
	p	1
	weights	distance
Gaussian process	alpha	0.001
	kernel	DotProduct (sigma_0=0.1)

The Support Vector (SV) method (regressor) is a version of the support vector machine for use in regression problems. This regressor is based on finding a continuous (linear or nonlinear) function that maximally approximates the input data inside a given tube with a sufficiently small diameter based on support vectors (Gholami et al., 2012). This method also has its own control parameters, which are given in table. 3.

LASSO is a method originally designed for linear regression that provides variable selection and regularization to improve forecast accuracy. The control parameters of this method are given in Table 3.

The K-Nearest Neighbors (k-NN) method is a method for solving classification and regression problems based on searching for the nearest objects with known values of the target variable.

Gaussian Process (GP) regression is a general-purpose non-parametric supervised learning method designed for solving regression (Rodríguez-Rodríguez et al., 2021). Lasso, k-NN and GP algorithms are considered to compare the prediction results of other algorithms with their results.

Results and discussions

The collected data was analyzed using the above machine learning techniques. First, we will show the connections between features (parameters of porous media), which is visualized in the form of a correlation matrix (Figure 5). This matrix shows how good or bad connections each pair of features has – the larger the coefficient in the matrix, the higher the correlation between the selected features. A coefficient of 1 means perfect correlation. The seaborn library was used to display the correlation matrix. Seaborn is essentially a higher level API based on the matplotlib library. Seaborn contains more appropriate default chart design settings. The library also has quite complex visualization types that would require more code in matplotlib. As can be seen from Figure 5, all input variables (features), except specific surface area and tortuosity, have a high correlation with the target variable.

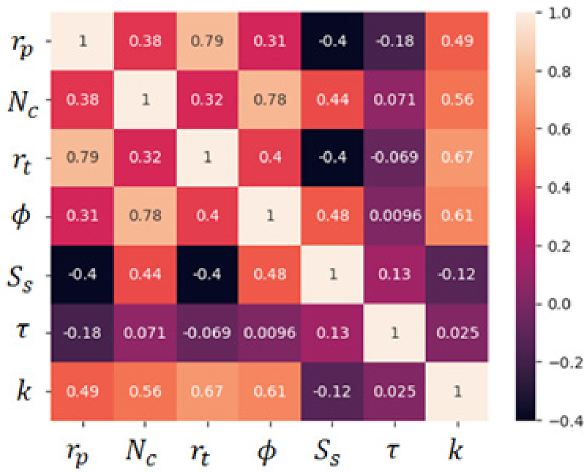


Figure 5. Correlation matrix for visualizing connections between features

Impact of training/test data splitting on algorithm performance

After choosing a machine learning algorithm, the first priority is to determine the list of input data (features) that are most important when building a predictive model

(Otchere et al., 2021). To do this, each algorithm has the feature_importances_ property, with which you can see the weight (importance) of each feature in the final predictive model. The importance of dividing the input data set into training and testing is that the training set contains the known output data from which the model learns. In this paper, the data set was split 70/30 and 80/20.

The results of permeability prediction using the machine learning algorithms discussed above are shown in Figure 6-8 and Table. 4. Figure Figure 6 shows which of the 6 independent input data were selected as the most important when building a predictive permeability model using different machine learning algorithms. Note that for comparison purposes here and below, the importance of the feature is normalized by the maximum importance value for each algorithm. As the diagrams show, the RF, SV and GP algorithms turned out to be resistant to changes in the share of the training data set – when using these algorithms, the number of important features and their importance practically did not change. RF and GP selected 5 out of 6 features as important, while SV considered only 2 features to be most important. Increasing the proportion of the training dataset significantly influenced the selection of important features by the Lasso and k-NN algorithms. If the Lasso algorithm at 70/30 identified only 2 important features, then for 80/20 important features increased to 5, and for k-NN the number of important features increased from 3 at 70/30 to 6 for 80/20. All this shows the sensitivity of the considered algorithms to the amount of training data.

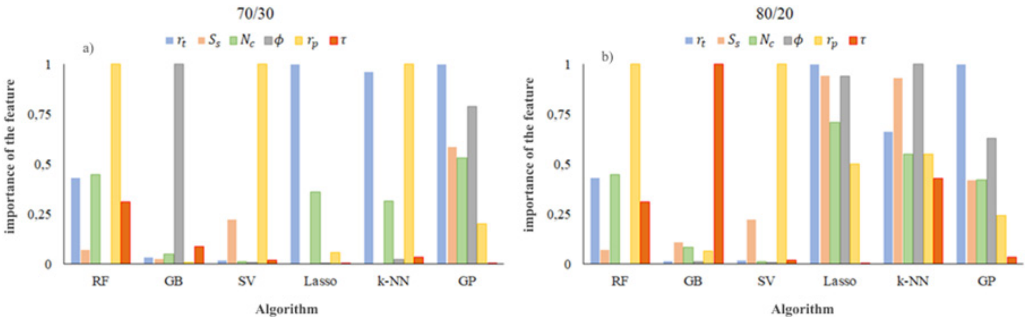


Figure 6. Importance of a feature when splitting data in a ratio of 70/30 (a) and 80/20 (b)

After the considered algorithms were trained, their predictive ability was tested on test data by comparing their results with the actual data. The comparison results are shown in Figure 7, where the symbols of different shapes correspond to different algorithms, and the solid line means the perfect correlation between the predicted and actual permeability values. Here and further, in all graphs, the actual and model permeability are located on the abscissa and ordinate axis, respectively.

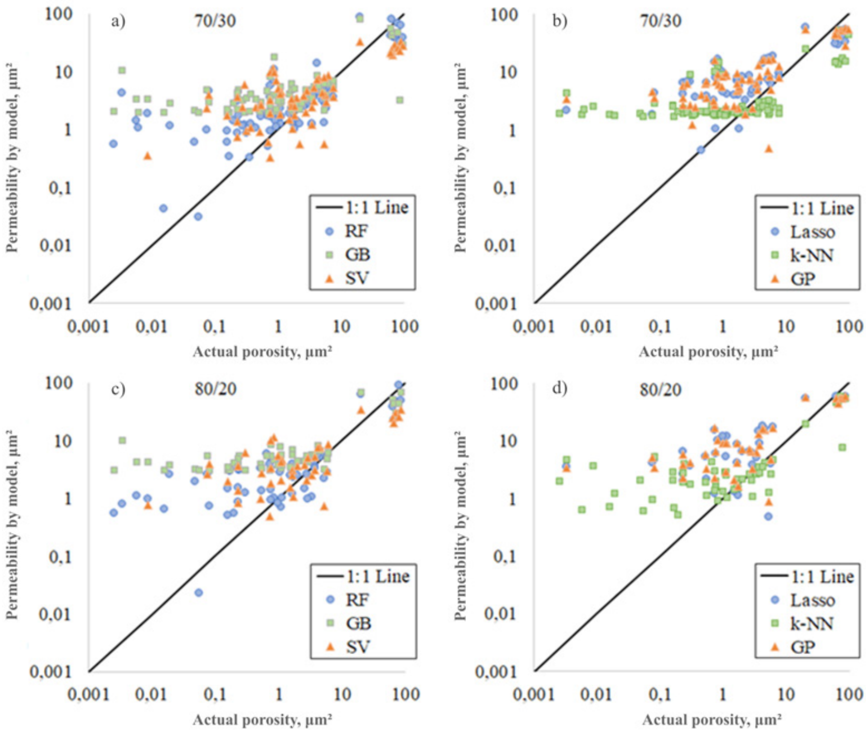


Figure 7. Predicted permeability using different algorithms compared to actual permeability when splitting the data in a ratio of 70/30 (a, b) and 80/20 (c, d)

As can be seen from the graphs, all machine learning algorithms predicted overestimated permeability values, especially in the range <1 μm^2, and the average and maximum values lie close to the 1:1 line, which shows that the permeability forecast using the constructed forecast models is close to the actual values (Figure 7a-d). Al-Khalifa et al. (Al Khalifah et al., 2020), when studying carbonate rocks, also found that the quality of prediction by machine learning methods decreases at low permeability values. With increasing proportion of the training data set, almost all algorithms predicted permeability values that are relatively close to the 1:1 line at 80/20 (Figure 7c, d) compared to the 70/30 case (Figure 7a, b). This is confirmed by Figure 8, which provides a quantitative comparison of the predictive ability of the considered machine learning algorithms in the form of the correlation coefficient (R^2) between the predicted and actual permeability. As can be seen from this figure, the correlation between predicted and actual permeability improved for all algorithms as the size of the training dataset increased. Relatively high correlation coefficients were observed for GP (0.75), Lasso (0.77) k-NN (0.784), while for the remaining algorithms this coefficient was 0.687, 0.723 and 0.732, respectively for SV, RF and GB. Obviously, the higher the coefficient R^2, the higher the reliability of the forecast, i.e. the predicted permeability is closer to the actual permeability. Although all algorithms predicted permeabilities that were highly correlated with actual permeability, some algorithms predicted negative permeabilities, which was unacceptable. Table 4 shows the minimum, maximum and average values of actual permeability and permeability predicted using the considered machine learning algorithms. As can be seen from table. 4, when forecasting using the SV, Lasso and GP algorithms, negative minimum permeabilities were obtained. Yun (Yoon, 2021) also obtained negative values using the GB algorithm when forecasting Japan's GDP for 2001-2018. Although GB and k-NN produced positive values, they are three orders of magnitude higher than the actual minimum value. The closest value to the actual value was obtained only by the RF algorithm for both cases of partitioning the input data set. The maximum permeability predicted by the SV, Lasso, k-NN and GP algorithms has a significant difference from the actual permeability. The GB algorithm predicted permeability that was within 20% of the actual value. The maximum permeability predicted by the RF algorithm is quite close to the actual permeability, the relative prediction error is 8.5 and 4.5%, respectively, at 70/30 and 80/20. All algorithms except SV and k-NN predicted values close to the actual permeability. This may be due to the fact that machine learning methods are mainly based on data statistics that reliably predict averages.

Table 4 – Statistics of predicted permeabilities at 70/30 and 80/20

Parameter	Training/Test	Actual	RF	GB	SV	Lasso	k-NN	GP
Minimum	70/30	0,00249	0,03128	1,94	-10,95	-16,37	1,66	-17,10
	80/20	0,00249	0,02273	3,03	-10,79	-16,32	0,52	-18,27
Maximum	70/30	95,91	87,81	80,94	33,44	58,44	51,63	56,39
	80/20	87,07	91,15	68,40	34,18	59,12	58,35	59,36
Average	70/30	9,31	8,22	7,96	4,59	7,64	5,57	8,18
	80/20	8,37	7,72	9,78	4,65	8,60	6,30	8,33

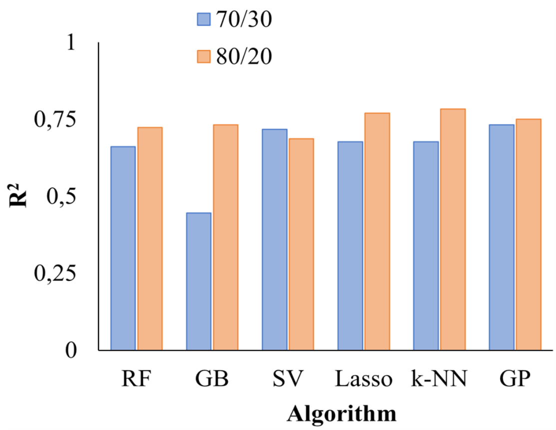


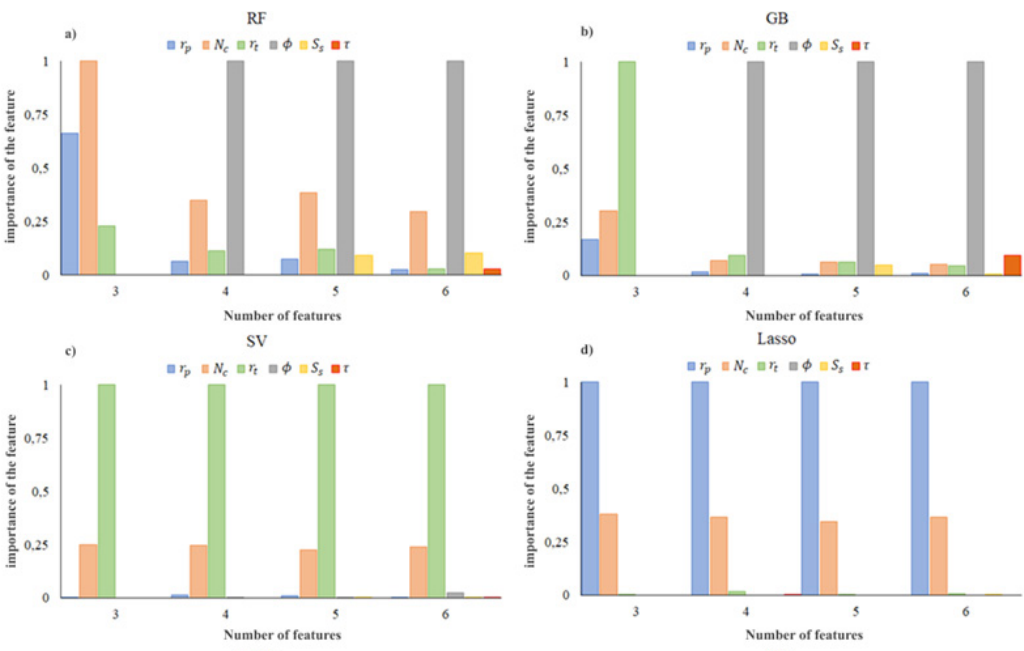
Figure 8. Confidence coefficient of permeability forecast on test data when splitting the data in a ratio of 70/30 (blue columns) and 80/20 (orange columns)

The influence of the number of features on the performance of algorithms

And also the algorithms were trained on a data set in which the number of features varied from 3 to the maximum (i.e. up to 6), and amounted to 'r_p', 'N_c', 'r_t' (3 features), '

'r_p', 'N_c', 'r_t', 'ϕ' (4 features), 'r_p', 'N_c', 'r_t', 'ϕ', 'S_s' (5 features) and 'r_p', 'N_c', 'r_t', 'ϕ', 'S_s', 'r' (6 signs), respectively. At the same time, the ratio of the training and testing data set did not change and was 70/30 in all cases. The purpose of changing the number of features in the input data set is to test the sensitivity of the permeability prediction model to the number of independent variables on which permeability could have a functional dependence. Obviously, it would be better if permeability was calculated using a formula (model) that uses minimal but important parameters (features) without losing accuracy. For example, the empirical Kozeny-Karman equation (Bolysbek et al., 2021), which allows one to find absolute permeability, uses only three characteristics (porosity, specific surface area and tortuosity) and one parametric constant.

Which features were selected by the considered machine learning algorithms when their number changed are shown in Figure 9. As can be seen from this figure, the SV, Lasso and k-NN algorithms selected the same features, although their number was different in each case (Figure 9c, d, e). At the same time, the importance of the selected features was almost the same. The remaining algorithms tried to select almost all features when their total number changed (Figure 9a, b, f). In addition, the importance of these features was different for the RF, GB and GP algorithms. GP selected the average pore throat radius r_t as the most important feature, regardless of the number of features, and the importance of the remaining features was noticeable as the number of features increased (Figure 9f). And the GB algorithm considered that the most important feature is the porosity of the mini-sample ϕ (Figure 9b). In the case of RF, porosity ϕ and coordination number N_c were considered to be the most important features (Figure 9a).



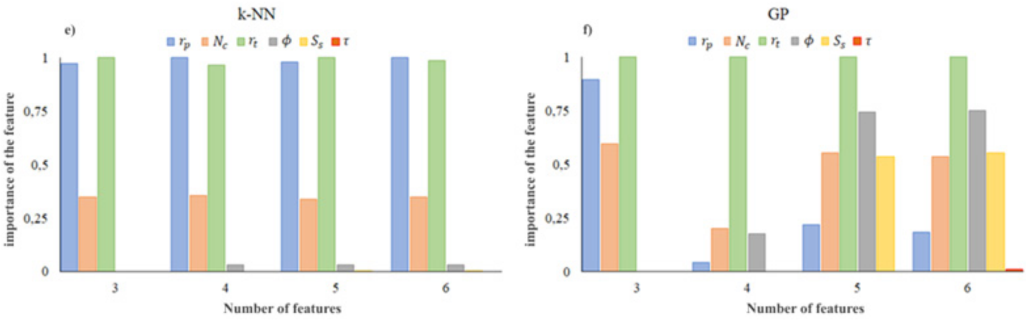


Figure 9. The feature importance with their different numbers in the data set for different machine learning algorithms

The distribution of predicted permeability according to different algorithms in comparison with its actual value is shown in Figure 10. It can be said that all algorithms predicted visually close to the actual permeability value. However, all algorithms were characterized by overpredicted minimum permeabilities, and the maximum and average values were predicted significantly close to the actual permeability (distribution of values around the solid line). Among all the algorithms, RF predicted the closest to the actual permeability in the range of minimum permeabilities (0.001–1 μm^2).

As can be seen from Figure 10, with an increase in the number of features, the predicted permeability by the RF (blue circles in Figure 10a, c, e and g) and GP algorithms (orange triangles in Figure 10b, d, f and h) approached the actual permeability, since these methods selected the largest number of important features (Figure 9a, f).

The parameter characterizing how well or poorly a particular algorithm predicted the permeability of mini-samples is shown in Figure 11. In this figure, the prediction confidence coefficients are distributed when the number of features in the input data set increases. And in the table Figure 5 shows the minimum, maximum and average permeability values obtained using the considered machine learning algorithms depending on the number of important features.

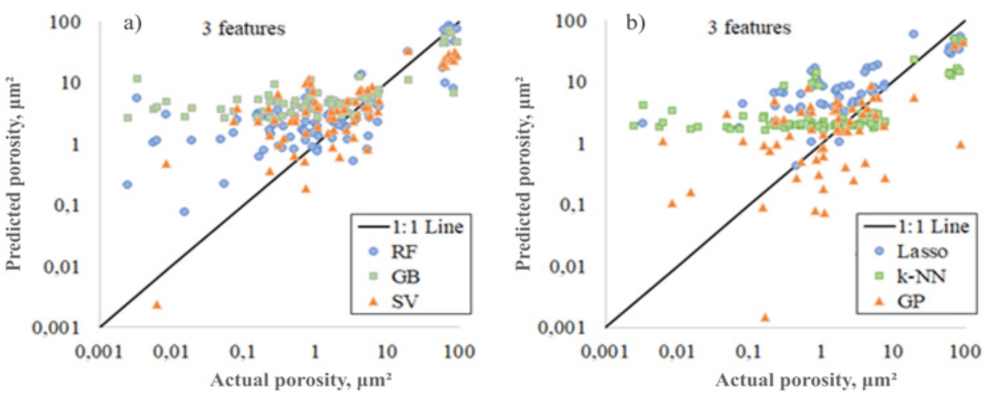
As can be seen in Figure 11, for the SV, Lasso and k-NN algorithms, the forecast reliability coefficient practically did not change with the increase in the number of features in the input data set, although the value of this coefficient is not low. This is due to the choice of almost the same number of features according to their importance (see Figure 9c, d, e). On the other hand, R^2 for other algorithms is sensitive to changes in the number of important features. The RF and GP algorithms tend to increase R^2 with increasing number of features, i.e. these algorithms predict permeability values more accurately when more minisample properties are included in the input data set. On the contrary, the GB algorithm deteriorates the quality of the forecast with an increase in the number of input features. This may be due to the fact that this algorithm considered different features with different numbers to be important (Figure 9b). We also note that the maximum forecast reliability coefficient R^2=0.83 was achieved when using the RF algorithm, and this was obtained with 5 features.

Table 5 collects statistics of key parameters of the predicted and actual permeability values. As can be seen from this table, the SV, Lasso and GP algorithms predicted negative (minimum) permeability values in all cases with the number of features, whereas it should be strictly positive. Moreover, negative permeabilities have large modulus values. Although the minimum permeability by GB and k-NN is positive, it still has a large error from the actual minimum permeability.

Table 5 – Statistics of predicted permeabilities for different numbers of features

Parameter	Features	Actual	RF	GB	SV	Lasso	k-NN	GP
Minimum	3	0,00249	0,07540	2,66	-10,64	-16,37	1,6557	-4,33
	4		0,01001	1,75	-10,94	-16,37	1,6634	-21,50
	5		0,17730	2,40	-10,93	-16,37	1,6633	-17,05
	6		0,03128	1,94	-10,95	-16,37	1,6563	-17,10
Maximum	3	95,91	84,05	71,47	33,25	58,44	50,893	45,63
	4		88,70	78,88	33,26	58,44	50,409	60,02
	5		78,69	72,95	33,23	58,44	50,408	56,54
	6		87,81	80,94	33,44	58,44	51,634	56,39
Average	3	9,31	7,51	8,67	4,627	7,64	5,4628	2,40
	4		9,40	9,10	4,626	7,64	5,3918	7,63
	5		8,04	8,63	4,640	7,64	5,3917	8,29
	6		8,22	7,96	4,589	7,64	5,5671	8,18

The closest to the actual permeability value (exceeding only 4 times) was obtained using the RF algorithm with 4 features. The most distant from the actual maximum permeability values were obtained using the SV, Lasso, k-NN and GP algorithms, which have an error of 37–65 % of the actual permeability. The closest to the maximum actual permeability was the error obtained using the RF algorithm, which was 7.5 %. The permeability predicted by GB is also close to the actual one. The average permeabilities obtained using the RF and GB algorithms are the closest to the actual permeability for 2 features, and their errors from the actual permeability were 2–3 %. Other average permeability values for the remaining number of features are relatively close compared to the results of other algorithms. The farthest averages from the actual permeability values were obtained using SV and k-NN, while the Lasso and GP permeabilities are within the error range of 18–29 % of the actual permeability.



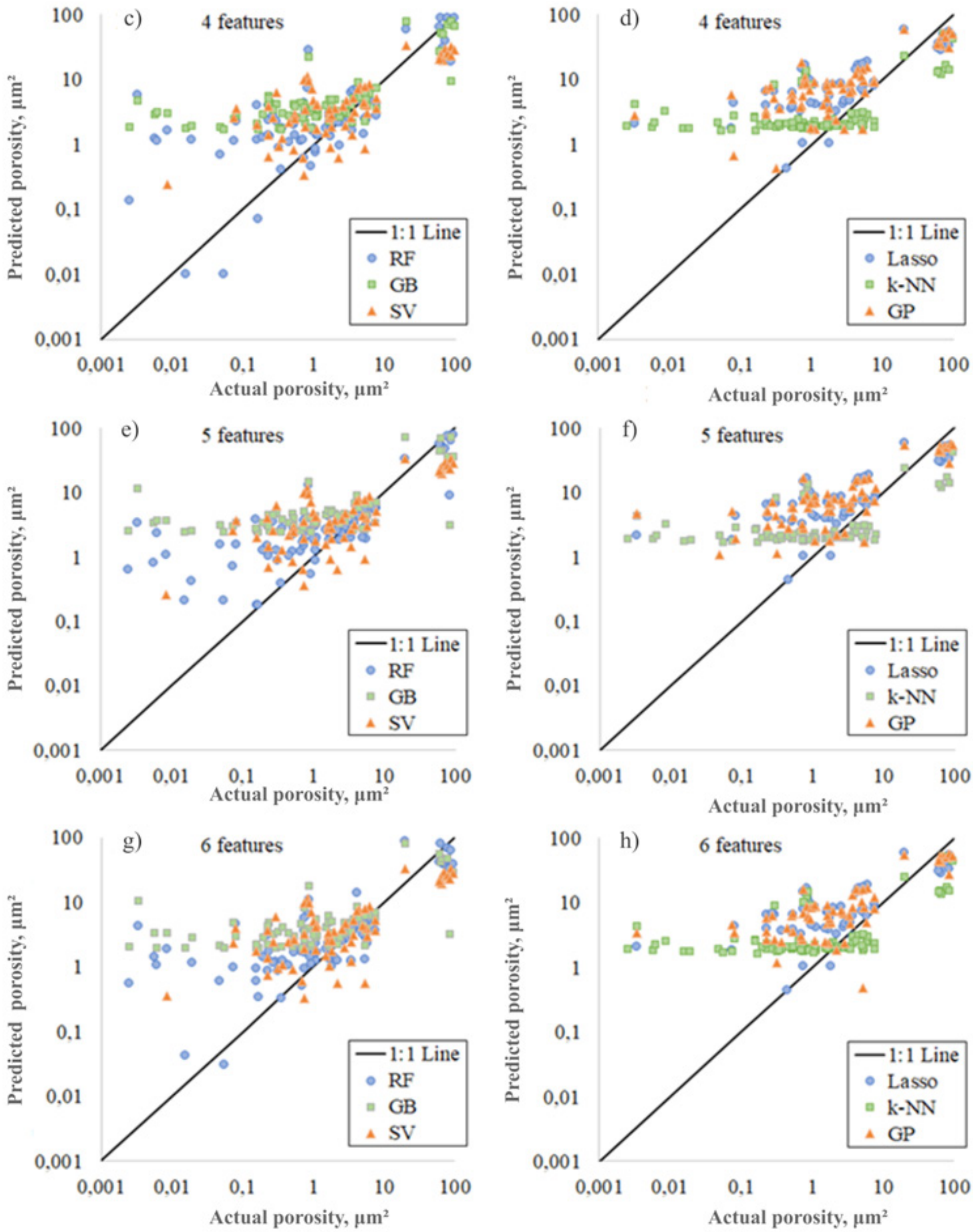


Figure 10. Predicted permeability using different algorithms compared to actual permeability for different numbers of features

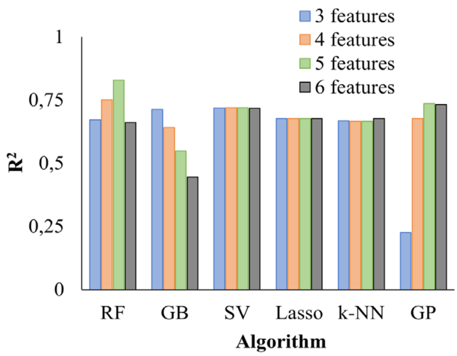


Figure 11. Reliability coefficient of permeability forecast for different numbers of features

Conclusion

This article examines 6 different machine learning methods for analyzing data and predicting the absolute permeability of 266 samples of various rocks ranging in size from 125 μm to 3 mm. Analysis of the complete data set showed a high correlation of permeability with pore throat radius, porosity, coordination number and pore radius. Splitting the full data set into training and testing significantly influenced the results of the GB, Lasso and k-NN methods: with an increase in the share of the training data set, the number of important features for choosing these methods increased. All algorithms overpredicted minimum permeabilities for all data set splits. In addition, the SV, Lasso and GP algorithms predicted negative permeabilities. All algorithms tried to predict the maximum and average values (sand rocks and sand pack) close to the actual permeability value. A comparison of the forecast qualities of all algorithms showed that the RF algorithm is the most suitable for analyzing heterogeneous data, i.e. data from samples of different rocks, the properties of which differ greatly from their average statistical value. The highest prediction reliability coefficient R^2=0.83 was achieved when using the RF algorithm, and this was obtained with 5 features. The algorithms mainly selected pore radius, pore throat radius and porosity as important features (parameters).

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