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Optimization of the Algorithm for Searching for the Most Reliable Implementations of a Geological Model

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Оптимизация алгоритма поиска наиболее достоверных реализаций геологической модели

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One of the most important tasks in the oil and gas industry is to predict the values of geological parameters of productive formations in the interwell space. The accuracy of estimating the effective oil-saturated thickness or the values of filtration and capacity properties at the locations of the project well stock directly affects the efficiency of oil and gas assets development and economic indicators.
The task of predicting the values of geological parameters is complicated by the fact that the geological environment has been studied by wells in fragments, and sources of information about the interwell space, despite continuous technological progress, have limited accuracy. In addition, the real geological structure in most cases is much more complex than our understanding of it. The vertical and lateral heterogeneity of productive formations and the high degree of geological properties variability do not allow the effective use of interpolation methods.
This paper presents the results of testing the author's methodology aimed at finding the most reliable implementations of a three-dimensional lithology model.
The proposed approach is based on the use of Bayesian optimization to determine the most optimal values of variogram ranges along the *X* and *Y* axes during the modeling of a three-dimensional lithology cube. The mean absolute error of the predicted total effective thickness of the reservoir, calculated using cross-validation, was employed as the primary metric to evaluate the reliability of the three-dimensional lithology model. The results demonstrate the advantages of applying Bayesian optimization compared to the classical grid search method for parameter optimization. Firstly, the proposed approach enabled the creation of a three-dimensional lithology model with higher predictive capability. Secondly, the developed methodology significantly reduced the computational resources required for the calculations.

Ключевые слова:
геостатистика, 3D-геологическая модель, аллювиальные отложения, стохастическое моделирование, кросс-валидация, байесовская оптимизация, последовательное индикаторное моделирование, оценка неопределенности.

Одной из важнейших задач в нефтегазодобывающей отрасли является прогнозирование значений геологических параметров продуктивных пластов в межскважинном пространстве. Точность оценки эффективной нефтенасыщенной толщины или значений фильтрационно-емкостных свойств в местах расположения проектного фонда скважин напрямую влияет на эффективность разработки нефтегазовых активов и на экономические показатели.
Задача прогнозирования значений геологических параметров осложняется тем, что геологическая среда изучена скважинами фрагментарно, а источники информации о межскважинном пространстве, несмотря на непрерывный технологический прогресс, обладают ограниченной точностью. К тому же реальное геологическое строение в большинстве случаев значительно сложнее, чем наше представление о нем. Вертикальная и латеральная неоднородность продуктивных пластов и высокая степень изменчивости геологических свойств не позволяют эффективно использовать методы интерполяции.
В данной работе представлены результаты апробации авторской методологии, направленной на поиск наиболее достоверных реализаций трехмерной модели литологии.
Предложенный подход основан на использовании байесовской оптимизации для определения наиболее оптимальных значений рангов вариограмм по осям *X* и *Y* при моделировании трехмерного куба литологии. Средняя абсолютная ошибка прогноза суммарной эффективной толщины пласта, рассчитанная с использованием кросс-валидации, использована в качестве основной метрики, оценивающей надежность трехмерной модели литологии. Полученные результаты демонстрируют преимущества применения байесовской оптимизации относительно классического подхода поиска оптимальных параметров модели с перебором по сетке. Во-первых, примененный подход позволил получить трёхмерную модель литологии с более высокой прогностической способностью. И во-вторых, авторская методология позволила значительно сократить необходимые для расчётов вычислительные ресурсы.

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Introduction

In the early 1960s, the science of geostatistics emerged, which enabled to perform not only spatial modeling of parameters, but also facilitate spatial uncertainty analysis [1–7]. Currently, such modeling methods as Sequential Gaussian Simulation (SGS) for continuous parameters and Sequential Indicator Simulation (SIS) for discrete parameters are widely used in creation of three-dimensional geological models [8–10]. These modeling methods are based on variogram analysis and allow for the generation of multiple equally probable realizations of the geological properties distribution.

However, classical geostatistical methods have a number of disadvantages, such as variogram sensitivity and subjectivity in performing variogram analysis, low adaptability to complex real conditions, high computational complexity, etc. [11–14]. Therefore, a promising direction for the development of geostatistical methods is using hybrid models with artificial intelligence algorithms, as machine learning, neural networks, genetic algorithms, fuzzy logic, etc. [2–7, 10, 15].

When using geostatistical modeling algorithms, it is important to consider not only the results of variogram analysis, but also to assess the predictive ability of each model. In some works [16–20] several quantitative criteria are proposed for assessing the quality of three-dimensional lithology parameter models and selecting optimal modeling parameters. The proposed criteria enable to estimate the predictive ability of each three-dimensional lithology model implementation with most reliable ones.

The calculation in the above-mentioned works was based on the theory of experimental design. The authors determined the variation range for the modeling parameters and the step of each parameter changes. Consequently, the experiment included a full set of possible combinations for lithology modeling parameters. According to the experiment results the most reliable implementations were selected using the values of quantitative criteria. Calculations of lithology cubes were performed by a stochastic algorithm with a variation of the variogram rank values along the X and Y axes [16–20].

One of the three proposed criteria is the D_{skv}, calculated by well-based cross-validation using the leave-one-out method for each combination of variogram ranks. The criterion is necessary for assessing the predictive ability of the model and is calculated using the formula:

$$D_{skv} = \sum_{i=1}^{n} \frac{\left(H_{ef} - H_{ef}^{m}\right)}{n}, \quad (1)$$

where D_{skv} is the deviation from the true value of the effective reservoir thickness, m; H_{ef} – actual value of the effective reservoir thickness in the well, m; H_{ef}^{m} – model value of effective reservoir thicknesses obtained after excluding the given well, m; n – number of wells.

In machine learning, the approach described above is called grid search, commonly applied using cross-validation as the method for assessing the reliability of each model. The main drawback of the proposed approach is the huge computational load considering all possible combinations of variogram ranks and using full well-based cross-validation to calculate the D_{skv} criterion. The number of the three-dimensional lithology parameter was calculated as the product of the hyperparameter combination number and the wells number. In some cases, the number of three-dimensional lithology parameter calculations was more than 10,000, and the time required to compute the entire ensemble was over a day.

Table 1

Main geological and physical characteristics of the object

Parameter	Total thickness, m	Effective thickness, m	Weighted average value of K_p, unit fraction	Number of permeable intervals in wells, unit
Min	7.59	3.56	0.15	1
Mean	16.56	9.12	0.22	3
Max	33.59	22.55	0.25	8
Std	5.69	3.66	0.02	2

Another limitation of the proposed approach is the variation of only two lithology modeling parameters: variogram ranks along the X and Y axes. When examining all possible combinations of variogram ranks, most models are anisotropic, meaning they have different rank values. Meanwhile, the azimuth value is always fixed at 0°. This assumption is justified by computational constraints, since including the azimuth parameter in the variogram experiment will significantly increase the number of implementations.

The aim of this work is to develop an improved algorithm that enables the efficient automated search for the most reliable implementations of a geological model without calculating a full ensemble of models.

Object of Study

The object of the study is a terrigenous layer of alluvial genesis in the X field, located within the Volga-Ural oil and gas province (OGP). The main geological and physical characteristics of the object, determined according to geophysical logging data in 62 wells, are presented in Table 1.

Alluvial deposits are heterogeneous both laterally and vertically, which significantly complicates the task of predicting geological parameters in the interwell space [21–24].

The study area is covered by 3D seismic surveys, the interpretation results of which were used for both structural imaging and lithological modeling.

Three-Dimensional Geological Model Description of the Object

Since the studied interval of the X field is characterized by regular bedding, a proportional type of three-dimensional grid with a lateral cell size of 50×50 m was used in this work. The average vertical size of the cell is 0.26 m, and the total number of active cells amounted to over 3 million. Such detailed grid division is connected, firstly, with the presence of thin siltstone interlayers in the flooding sand facies, and secondly, with the need for maximum correspondence of the averaged well data to the initial data for more effective calculations.

The 3D lithology cubes were modeled using the SIS geostatistical algorithm. A combination of trends was used, including the 1D trend, which is the geostatistical distribution (GSD) of the reservoir proportion for each grid layer, and the 2D trend, as the sandiness map, obtained by dividing the forecast effective thickness map by the total formation thickness map.

The forecast map of effective thicknesses was calculated based on data from dynamic analysis using 3D seismic methods with a multivariate forecast of reservoirs [25, 26].

Table 2

Main descriptive statistics of the D_{skv}* criterion for two calculation options

Calculation option	No obs.	Average	Median	Min.	Max.	Dispersion	St. dev.	Coeff. var.	Asymmetry	Excess
Option 1	100	1.093	1.083	0.923	1.360	0.0092	0.0957	8.758	0.6797	0.0652
Option 2	100	1.061	1.033	0.839	1.452	0.0188	0.1372	12.934	0.6853	-0.0128

Methodology

The basis for developing the author's algorithm was the works described above [16–20]. The aim of this study is to automatically select hyperparameters to minimize the error without calculating all possible model variants. An example of such an approach is the gradient descent method in a neural network [27, 28], in which the weights of neurons are adjusted to minimize the forecast error tends.

The algorithm development can be divided into several steps. The aim of the first step was to reduce the number of calculations for the model reliability metric. At the second step, optimization algorithms were selected that allow for the automatic adjustment of the model's hyperparameters – in this case, the values of the variogram ranks – so that the error is minimized.

The quantitative metric for assessing the reliability of each calculated implementation of the three-dimensional lithology model was the D_{skv}* criterion (mean absolute error) found with the formula

$$D_{skv}^{*} = \sum_{i=1}^{n} \frac{\left| H_{ef} - H_{ef}^{m} \right|}{n}. \quad (2)$$

Unlike the D_{skv} criterion described above (1), which can reach a value close to zero when averaging negative and positive error values, the D_{skv}* criterion is not sensitive to the error and can serve as a basis for optimization by global and local minima.

Cross-Validation

The task of reducing the calculation number for the quality criterion D_{skv}* was accomplished by using a more representative "training" sample with a smaller number of "training" cycles. Instead of using leave-one-out cross-validation method to calculate the D_{skv}* criterion, jackknife cross-validation was applied, dividing the initial well data into several equal parts in terms of quantity and coverage density of the sample area.

In this paper, the initial well data are randomly divided into five equal-sized samples. During each calculation of the lithology cube, 20 % of the wells were excluded, followed by the calculation of model effective thickness deviation from the actual one for each excluded well. In the second cycle, the next 20 % of wells were excluded during the calculation of the lithology cube. Thus,over five cycles, the deviation of the model effective thickness from the actual one was calculated for all available wells. The mean absolute value of all calculated deviations serves as the quality criterion D_{skv}*. The size of the test sample can be determined by the user; however, 20 % is considered an optimal value in many machine learning tasks [29, 30].

To evaluate the effectiveness of the proposed cross-validation method, an experiment was conducted in this work to calculate an implementation ensemble of three-dimensional lithology cubes using the method proposed in works [16–20] (option 1) and using the method described above, with the well data divided into five equal samples (option 2).

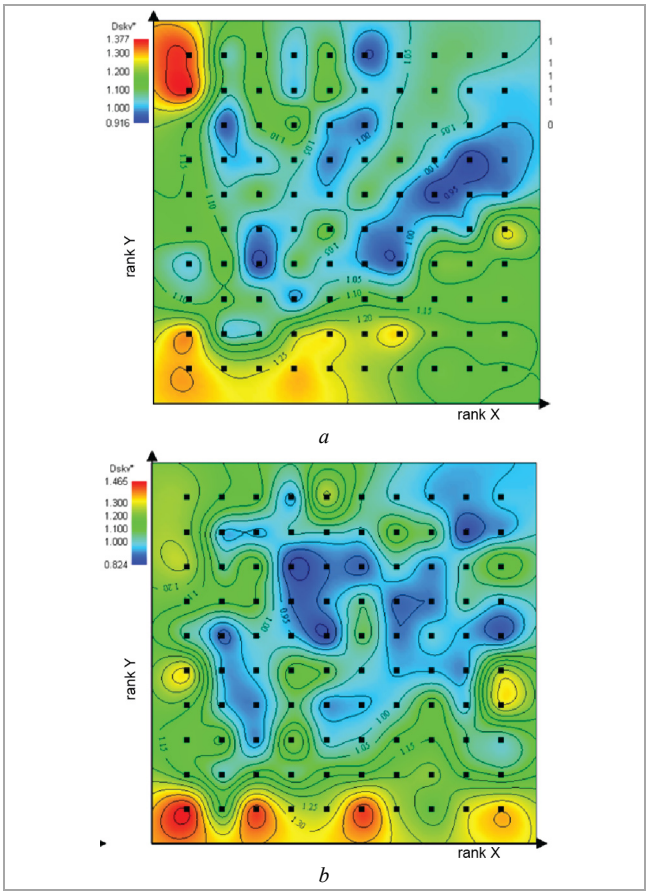

Fig. 1. Response surfaces obtained by *leave-one-out* cross-validation (*a*) and jackknife cross-validation methods (*b*)

In both calculation options, only the variogram rank values along the *X* and *Y* axes were varied. Based on the density and uniformity of the well placement and the size of the study object, the step for changing the parameters was set at 500 m, with a variation range from 500 to 5000 m. Thus, 100 combinations of variogram ranks were used for the calculations. In the first case, the forecast ability of each model was assessed using the D_{skv}* criterion through well-based cross-validation *using the leave-one-out method* [16–20]. Since the number of wells was 62, the total volume of the calculated three-dimensional cubes amounted to 6200 (62 for each set of variogram ranks). In the second case, the forecast ability of the models was estimated by calculating the D_{skv}* criterion using the jackknife cross-validation dividing the sample into five equal parts. The number of calculations for the three-dimensional lithology cube was 500 (five calculations for each set of variogram ranks). Fig. 1 shows the final response surfaces of the D_{skv}* criterion calculated with the *leave-one-out* cross-validation (*a*) and the jackknife cross-validation with the sample divided into five equal parts (*b*).

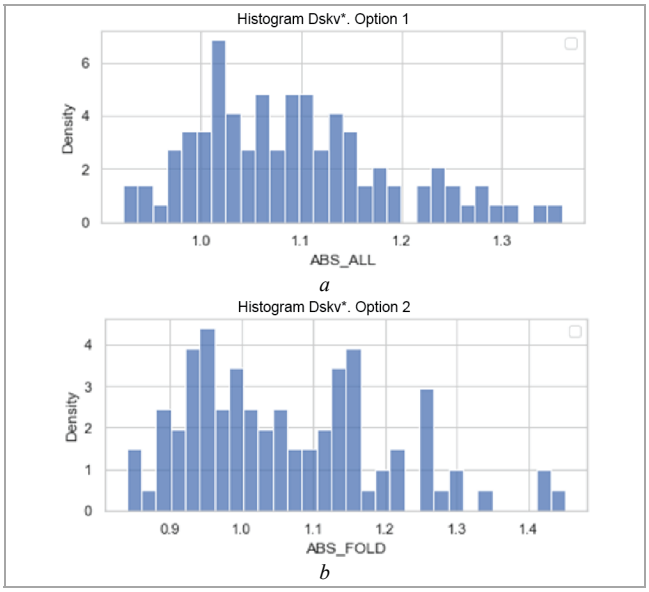

Fig. 2. Histograms of the D_{skv}* criterion distribution obtained by *leave-one-out* cross-validation (*a*) and the jackknife method (*b*)

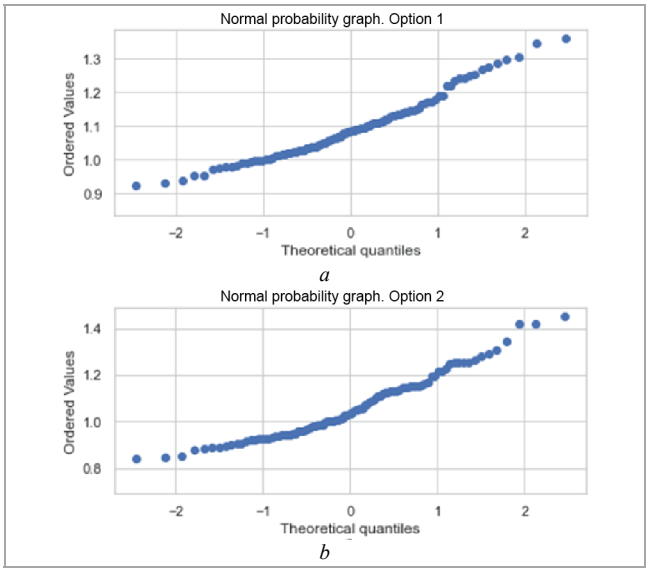

Fig. 3. Normal probability graphs for the D_{skv}* criterion obtained with leave-one-out cross-validation (*a*) and the jackknife method (*b*)

Table 3

Result of statistical criteria calculations

Statistical criterion	Criterion value	p< 0.05
Shapiro – Wilk	0.952	0.001
Kolmogorov – Smirnov	0.799	0.0001
t-criterion	2.94	0.0041
Wilcoxon test	2.91	0.0036

Visually, both response surfaces show similarities, however, for a more substantiated comparison, the analysis of the two approaches was performed. Table 2 presents the main descriptive statistics for the D_{skv}* criterion obtained from two calculation options: option 1 – using well-based *leave-one-out* cross-validation method, option 2 – using jackknife cross-validation with five equal samples.

As can be seen in option 2, the minimum and average values of the D_{skv}* criterion are slightly lower than in option 1. At the same time, in option 2, the maximum value of the D_{skv}* criterion and the variance are slightly higher.

To compare two samples, it is necessary to determine whether their distributions are normal. For this purpose, histograms and normal probability graphs for the two samples of the D_{skv}* criterion were constructed (Fig. 2, 3).

The histograms and normal probability graphs show that the distributions in both optons are close to normal, but in the areas of low and high values, the deviation of actual frequencies from the normal distribution increases. The calculation of the Shapiro-Wilk and Kolmogorov-Smirnov statistical criteria also showed that the distributions of the D_{skv}* parameter in both variants differ from normal. However, since the deviation from normality is insignificant, both parametric and nonparametric criteria were used for sample comparison (Table 3).

The obtained p-values from the t-criterion and the Wilcoxon criterion calculation are slightly below the significance level of 0.05. The results of the sample comparison are ambiguous and do not allow us to assert statistically significant differences between the results of applying the two different cross-validation methods.

For more substantiated conclusions, it is necessary to conduct a regression analysis for the two sets of the D_{skv}* criterion. The scatter graph with the regression line is shown in Fig. 4.

Regression equation:

$$D_{skv}2^* = 0.898 \cdot D_{skv}1^* + 0.0799, \quad (3)$$

where $D_{skv}1^*$ is a criterion calculated by *the leave-one-out cross-validation method*; $D_{skv}2^*$ is a criterion calculated using the jackknife method; the correlation coefficient was $r = 0.62$; the determination coefficient was $r^2 = 0.39$; $p = 0.0001 < 0.05$.

The result of the regression analysis demonstrates a high degree of linear correlation between the two sets of D_{skv}* criteria. The visual similarity of the response surfaces also indicates that there is a statistically significant relationship between the two sets of D_{skv}* criteria calculated using different cross-validation methods.

Summarizing the selection and justification of the cross-validation method, the following conclusions can be drawn:

– the response surfaces show visual similarity, and there is a statistically significant relationship between the two sets of D_{skv}* criteria, revealed by regression analysis;

– despite the fact that three-dimensional lithology models constructed by jackknife cross-validation are based on significantly fewer well data compared to those constructed by leave-one-out cross-validation, the forecast capability of such models is not less. Moreover, the average accuracy metric of D_{skv}* is even slightly lower in option 2;

– calculations using the jackknife cross-validation method are significantly less time-consuming and computationally intensive. The difference increases with the number of wells. In this study, the full cycle of calculations with the jackknife cross-validation was found to be 12.5 times faster than calculations using the leave-one-out cross-validation;

– one of the reasons for the impracticality of applying leave-one-out cross-validation is the stationary noise inherent in most geostatistical algorithms [8].

Depending on the calculation sequence, which is determined by the random number of project seed, the result of forecast error calculation may vary [10, 31]. Using cross-validation with the leave-group-out method helps to minimize the impact of forecast unpredictability and stationary noise on the models.

Thus, it can be concluded that jackknife cross-validation is no less effective in terms of assessing the forecast ability of lithology models and more effective in terms of computation speed. In the next stage of research, which aims to test the algorithm for automatically selecting variogram rank values, jackknife cross-validation will be used, dividing the well dataset into five equal samples.

Bayesian Optimization

The optimal values of the model hyperparameters are such values of the hyperparameters (the ranks of the variograms along the X and Y axes) at which the forecast error (metric D_{skv}*) tends to zero. The task of finding a global minimum is complicated as stochastic geostatistical algorithms, such as Sequential Indicator Simulation, Sequential Gaussian Simulation, etc., are influenced by stationary noise. It means that the value of the forecast error will depend not only on the model settings, but also to some extent on the random component (random path) [10].

In the process of searching for a suitable algorithm, several popular optimization methods were tested. However, only the algorithm based on Bayesian optimization turned out to be relatively effective.

Bayesian optimization is an effective method for finding the extrema of complex functions, particularly those influenced by random noise. It treats the objective function as a realization of a Gaussian process, establishing probabilistic relationships between function values at different points. The algorithm iteratively builds a Gaussian process model that incorporates all previously obtained results. It employs an acquisition function to select the next set of model parameters. Initially, the acquisition function divides the search space into large hypercubes, calculating a quality metric (in this case, the average absolute error D_{skv}*) for each. The hypercube with the lowest error is chosen, which is then subdivided into smaller hypercubes for further evaluation. This method allows for a focused search in the most promising areas of the parameter space, thereby accelerating the optimization process [32–37].

The scheme of the optimization process is presented in Fig. 5.

The first stage involves initialization, which includes defining the objective function, the range of hyperparameter variation, and the stopping criterion for optimization. In our case, the objective function is the calculation of five iterations of a three-dimensional lithology parameter, with the average absolute error for all wells (D_{skv}* criterion) by jackknife cross-validation. The hyperparameters are the variogram ranks along the X and Y axes. The range of variogram ranks varies from 500 to 5000 meters. The stopping criterion in our case is the completion of 100 iterations.

After initialization and selection of variogram rank, the objective function is calculated. In the initial optimization iterations, the values of the variogram ranks along the X and Y axes are selected randomly. The objective function calculation involves generating three-dimensional lithology parameters using the SIS method with the average absolute forecast error (D_{skv}*) assessed with jackknife cross-validation method.

Then, the result of the objective function calculation is saved in the database, and the approximation model is updated. Using the acquisition function, the principles of which are described above, the next set of hyperparameters is determined. The optimization process is repeated for a specified number of cycles or until the user-defined conditions are met.

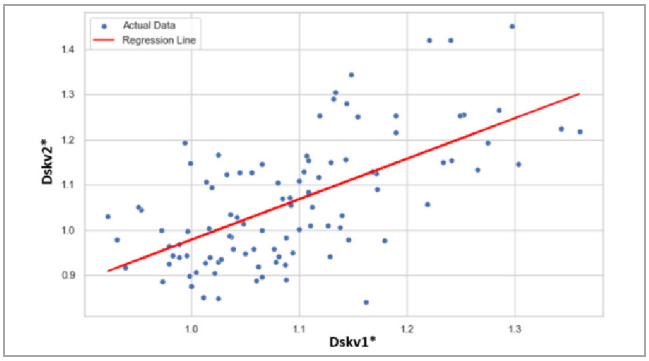

Fig. 4. The dependence between the $D_{skv}1$* criterion calculated with the leave-one-out cross-validation and the $D_{skv}2$* criterion calculated with the jackknife method

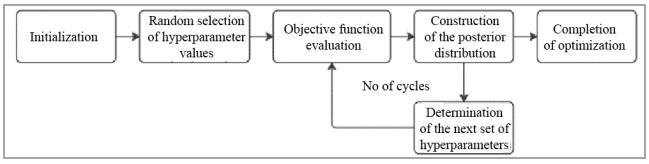

Fig. 5. Flowchart of the algorithm for finding optimal hyperparameters values

Below are the response surfaces calculated earlier by varying the variogram ranks on the grid using the jackknife cross-validation method. To demonstrate the efficiency of the optimization process, the D_{skv}* parameter calculation using Bayesian optimization are plotted on the response surfaces (Fig. 6).

Low values of the D_{skv}* parameter are marked in blue, high values in red, and average values in green. In Fig. 6, it can be observed how the results of the Bayesian optimization calculation tend to local minima on the response surface of the D_{skv}* parameter, while the local maxima are "avoided" by the function. It can also be stated that the search space has been explored relatively uniformly. The uniformity is achieved by dividing the search space into hypercubes and calculating the quality metric for each.

In most cases, the anisotropy of properties is not clearly expressed in terrigenous layers of alluvial genesis in the Volga-Ural oil and gas province, and the ratio of variogram rank values is usually no more than 1:2. Therefore, the optimization algorithm focus on exploring search areas where the rank values along the X and Y axes do not differ by more than twice also indicates the validity of applying Bayesian optimization technology for geological modeling.

Results

In this work, a series of calculations for the three-dimensional lithology parameter were performed using the stochastic algorithm Sequential Indicator Simulation. When calculating the lithology cubes, two parameters were varied: the variogram ranks along the X and Y axes. To assess the predictive ability of each model, the value of the mean absolute error D_{skv}* was calculated. Moreover, it was experimentally proven that jackknife cross-validation method is more optimal than using leave-one-out cross-validation. Initially, grid search approach was used to assess the predictive capability of each model, constructing a response surface that visually indicates the hyperparameters values at which the model is most accurate.

The next step involved calculating a set of three-dimensional lithology parameters, but instead of using

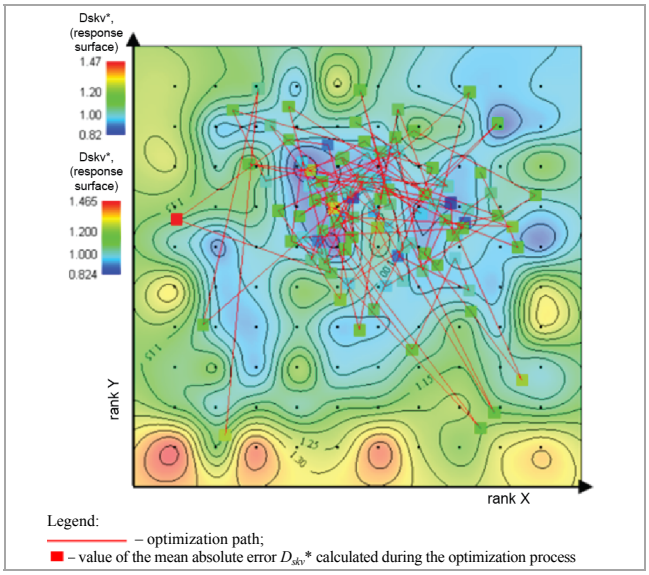

Fig. 6. Response surface of the D_{skv}* parameter with the results of Bayesian optimization

a grid search to vary the hyperparameters, an algorithm based on Bayesian optimization was used. In both cases, the predictive ability of the models was determined as the mean absolute error of the forecast (D_{skv}* criterion) using jackknife cross-validation.

As a result, using the grid search approach, the minimum value of the D_{skv}* criterion was 0.839 m, with the rank values along the X and Y axes being 2000 and 4000 m, respectively. In case of applying Bayesian optimization, the value of the D_{skv}* criterion for the most reliable model was 0.803 m, which is 4.3 % lower than that obtained by grid hyperparameter searching. The variogram rank values for the most reliable model along the X and Y axes were 3895 and 3547 m, respectively.

Thus, the Bayesian optimization algorithm was successfully applied to find the most optimal values of the variogram ranks along the X and Y axes when modeling a three-dimensional parameter of lithology. Bayesian optimization allowed for a more detailed exploration of the search area where the model error values are minimal, moreover, it enabled a more precise selection of model parameters. In contrast, the grid search, due to its fixed step in changing hyperparameters, 'missed' the most suitable hyperparameter values.

Conclusion

The application of modern computational algorithms alongside the classical geostatistical tools significantly enhances the reliability of geological modeling and adapts it for solving a wide range of non-trivial tasks, such as predicting properties in the interwell space and in wells, forecasting reservoir development parameters, and economic indicators [38–46]. The implementation of geological parameters for forecasting tasks is often complicated as the geological environment has a complex and unpredictable structure, and modeling in such conditions has numerous challenges.

In this paper, the object of modeling is a terrigenous layer of alluvial genesis from one of the fields in the Volga-Ural oil and gas province. The results of applying Bayesian optimization to find the most reliable models are demonstrated through the example of modeling a three-dimensional lithology parameter. The key advantage of Bayesian optimization lies in its suitability for black box functions and functions that are subject to noise.

Successful optimization of the process for identifying the most reliable lithology models will allow further complexity in the model by adding hyperparameters and metrics of model reliability.

The author's methodology allows for overcoming a number of limitations with the traditional application of geostatistical tools and provides a more substantiated forecast of the reservoirs distribution in the inter-well space. This is particularly relevant for the task of identifying targets for infill drilling in fields.

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