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Determination of cobalt concentration using nonlinear regression and Monte Carlo simulation in Zafarghand Region, Isfahan

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Abstract:

Contamination of heavy metals can change the properties of the soil, biological reduction activity of soil nutrients, also, by entering the food chain, it is considered dangerous for humans. Considering the importance of pollution in the environment, in this research, it has been tried to introduce an estimator to determine the concentration of Co element. In this research, Zafarghand exploration area is considered as a case study (Central Iran, Northeast of Isfahan). There were lithogeochemical data of 184 samples collected and analyzed for major and trace element concentration by ICP-MS. In the first step, nonlinear regression was used to create a model and estimate the concentration of Co element. In the next step, Co concentration value was simulated with the help of the created model and the Monte Carlo simulation method. The results obtained from the combination of nonlinear regression and Monte Carlo simulation show the accuracy and acceptable efficiency of this simulation, so that the mean value of Co concentration was close in the modeling to the values measured in the laboratory. According to the obtained result, the level of Co element in the studied area was in the range of (0.45-0.75) (mg/kg) with a confidence level of 90 percent. This value is below the background limit (less than 1.3010). In addition, in this research, sensitivity analysis was used to determine the most effective input parameter in determining the concentration of Co. Based on the obtained results, the most influential variable in this estimate is the amount of iron It should be noted that the use of this methodology is recommended for determining other heavy metal concentrations in different study areas.

Keywords: Cobalt; Regression; Simulation; Monte Carlo

1. Introduction

The food supply of the population at the growing world is one of the most important issues, according to the limited resources of land and so that it will affect the environment industrial activity and the production of pollutants such as heavy metals is one of the most serious and increasing problems of the present age. There are two sources of heavy metal pollution: human sources and natural sources. heavy metals is one of the natural resources, these entering through the erosion of soil materials. fertilizers and chemicals in agriculture, mining, waste burning are very important sources of heavy metals entering the water and environment (Yalcin et al., 2007; Zeynoldini et al., 2017; Nazari et al., 2023). Weathering of ophiolitic rocks and mining operations on these rocks can cause dispersion and intensification of heavy metals and pollution. Since heavy metals are deposited on the surface of the soil or sediment, they are very suitable tracers for showing the level of environmental pollution (Kelly and Thornton, 1996). Compared to organic pollutants, heavy metals cannot be destroyed through chemical and biological processes. These metals accumulate locally and are transferred to long distances (Merian et al., 2004). Heavy metal pollutions affect the physical and chemical properties of soil, biological reduction activity of soil nutrients. Also, they are considered the risk to human health by entering the food chain and environmental security by infiltrating the underground water (Boisson et al., 1999).

The ophiolitic regions of Iran with relatively long length and variable width are known along the folds of Zagros in the east, north and center of Iran. Ophiolite is a collection of mafic, ultramafic rocks and sediment units that may be regular or layered or mixed together due to tectonic stresses. The ophiolite complex has the distribution of Co, Ni and

Cr elements, mining operations on these rocks can cause dispersion and intensification of heavy metals and pollution (Khaledi and Mohammadzadeh, 2012).

Heavy metal pollution is caused by human activities that are the main cause of pollution, mainly from metal mining (Briffa et al., 2020). Different characteristics of the soil have an effect on the availability of these elements in the soil. For example, the solubility of Co and Ni, like other rare elements, decreases with increasing pH. Heavy metals, with the exception of arsenic, boron and selenium, refer to a number of metals that often have a density higher than 6 (g/cm^3). The concentration of these elements is usually within the safe geochemical background values, but when they reach abnormal values and the highest allowed amount, they should be taken into consideration, and if they reach the threshold, the environment should be cleaned of them (Adriano, 2001).

The purpose of this research is to introduce a combined method to check the concentration of Co element in the Zafarghand exploration area in northeast of Isfahan and southeast of Ardestan as a case study, which was predicted using statistical methods - non-linear regression probabilities and Monte Carlo simulation in confidence level of 90 percent.

2. Materials and methods

2.1 Geology of the studied area

The Zafarghand exploration area is a part of Iran-Central structural zone, and more precisely, it is located in Urmia-Dokhtar volcanic belt (Ghannadpour et al., 2023). Urmia-Dokhtar tectono-magmatic belt is an Andean magmatic arc that was formed due to the subduction of the Neotethys oceanic crust under the southern edge of central Iran along the continental margin of central Iran, during the Alpine uplift. It is also, the studies done on Urmia-Dokhtar belt confirm the existence of subduction zone in this region (Barbarin, 1990). Based on the various studies done in the Urmia-Dokhtar belt in the Eocene, there were calc-alkaline and submarine eruptions, and the volcanic rocks of Urmia-Dokhtar are a mixture of basalt, dacite and less sand. They show lavas along with tuffs and pyroclastics. In the Upper Eocene, the composition of the lavas tends towards alkaline and hyperalkaline. So, in the south of Nain, the potassic series of shoshonite with analsymdia and the hypersedic series around Kashan, and in the north of Shahr-e-Babak city, the potassic series including leucite-bearing phonolite and basanite were formed. At the end of the Tertiary, calc-alkaline lavas have changed and transformed into sub-alkaline and alkaline types, and as a result, potassium-rich alkaline lavas have been formed. In the Eocene volcanisms of Iran, the mixing of acid and basic magmas is a widespread phenomenon that is effective in the production of magma with moderate composition, sometimes with calc-alkaline geochemical characteristics (Ghannadpour et al., 2024). According to the revised geological map of the studied area, the rock units in the area could be divided based on their geological age as shown in Fig 1.

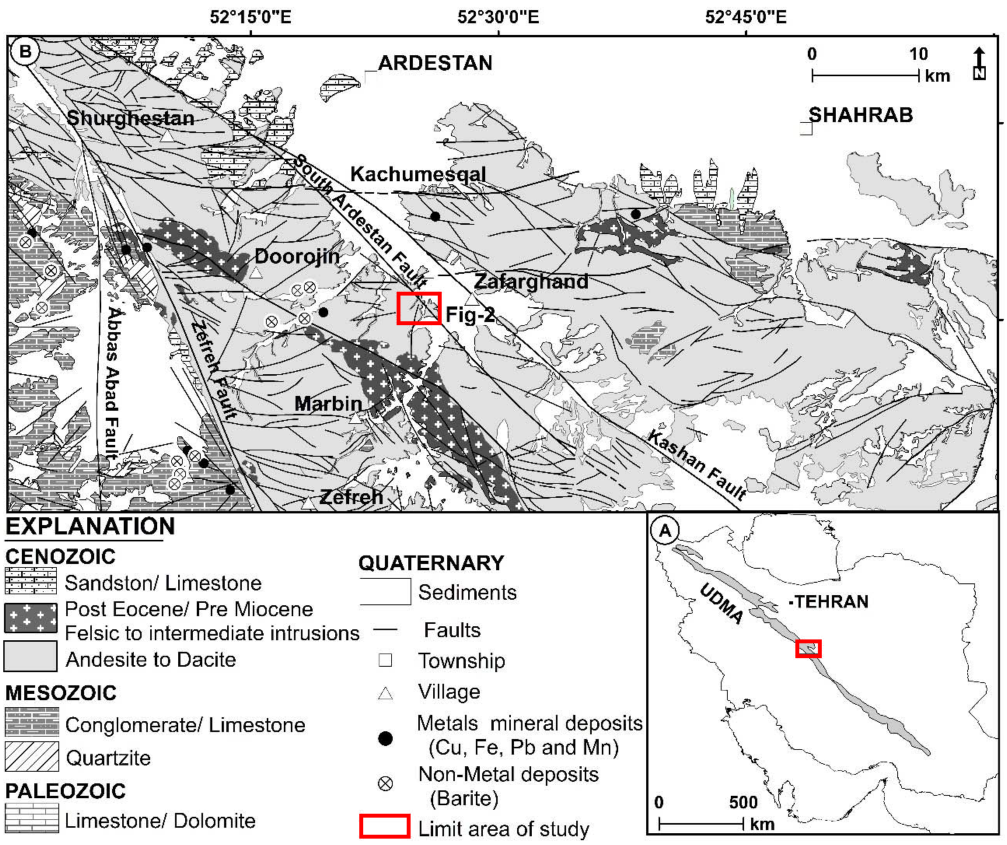

Figure 1. Modified geological map according to the lithology of the studied area rocks (Modified after (Alaminia et al., 2016)).

2.2 An overview of the employed methods

2.2.1 Nonlinear regression model

Statistical models such as regression are better implemented for small sample size and when theory and experiment show a principled relationship between independent and dependent parameters (Razi and Athappilly, 2005). Nonlinear regression is a statistical method that is applied to fit nonlinear random functions on the collected data. The purpose of this method is to randomly fit one of the twenty available functions on the collected data in order to reach the maximum value of the coefficient of determination. After determining the objective function, this stochastic function is expanded on the relationships between independent and dependent variables by searching and different resumes to find the best combination. Nonlinear regression has been used by many researchers (Iliadis and Maris, 2007) to estimate various parameters.

If the relationship between the independent and dependent variables is in the form of a nonlinear function with respect to the parameters, the estimation of the model parameters can be obtained with the help of nonlinear regression. Usually, in this case, the model is displayed as below;

$$y \sim f(X,\beta) \quad (1)$$

This method of representation states that there is a relationship between the vector y as the dependent variable and the vectors of the independent variables such as f according to the parameters X and β. In statistics, nonlinear regression is one of the methods of multivariate analysis. In this method, the data is modeled by a nonlinear function of parameters.

2.2.2 Monte Carlo simulation method

Simulation means creating an artificial environment and using a theoretical model to estimate the behavior of a system in the real world. An artificial environment is a real or virtual space in which the analyst tries to model the system in the real world. Depending on the purpose of simulation and what limitations exist in its application, four types of simulation can be distinguished from each other, which are: productive simulation (sampling), analytical or technical simulation, strategic simulation, and mental or intuitive simulation (Eskandari et al., 2004). The first type of simulation, i. e. generative simulation (sampling), is used when, for some reason, it is not possible to obtain data for the variable under investigation, which is either not recorded or sampling is not economical. This type of simulation can also be used for prediction through regression models containing random disturbances The Monte Carlo simulation method is included in the first type of simulation types (Klimentos, 1991).

Monte Carlo stochastic simulation method is based on sampling and probabilistic symbols and is mostly used in the analysis of unchanging random trends with time (Banks and Carson, 1986). The Monte Carlo method is based on: In the following expression, whenever T tends to infinity, the mean tends to the Expected Value ($Ef[h(X_i)]$).

$$\frac{1}{T}\sum_{i=1}^{T} h(X_i) \quad (2)$$

$h(X_i)$ is Probability density function, (X_i) is the random parameters and T is the number of times each state is observed. Monte Carlo simulation steps (Hoffman, 1998):

1- Creating a parametric model, firstly should be created a relation between independent parameters.

2- Creation random output, in this step is generated random data sets.

3- Model evaluation, finally should be evaluate output of model.

Some of the studies that have been investigated using the Monte Carlo simulation method are: to analyze the quality of groundwater, determine the noncarcinogenic risk factors as a result from the concentration of nitrate and fluoride ions, and analyze the sensitivity using Monte Carlo method (Morovati et al., 2024). In the study of Feng and Yu, the probabilistic health risk assessment results based on Monte Carlo simulation showed that 17.52 percent of children and 1.99 percent of adults exceeded the maximum (Feng and Yu, 2024). In another study, the occurrence of potentially toxic elements (PTEs), was evaluated in groundwater in the copper mining and smelter area of Bor city (south Carpathian, eastern Serbia). Veskovic et al employed the Monte Carlo method to estimated potential human health risks due to exposure to these toxic substances. The study underscores the need for stringent environmental management measures (Veskovic et al., 2024). Liu et al conducted a comprehensive investigation in the Zijiang River (ZR). The concentration range of As was specificd, (11.42-74.53 mg/kg, 1.36-6.23 μg/L, and 1.26-130.68 μg/L). Based on Monte Carlo simulation results, the possibility of As pollution in sediments is low. but in the middle stream (Liu et al., 2023). In another study, to reduce the uncertainty of pollution and the risk of assessment, the Monte Carlo simulation method was used to assess the level of pollution (Lian et al., 2022).

3. Estimating the concentration of Co in the study area

3.1 Input data structure for modeling

Almost regular sampling grid has been executed in the Zafarghand exploration district. There were lithogeochemical data of 184 samples that were collected and processed for trace and major element values by ICP-MS at Amdel Mineral Laboratories, Adelaide, South Australia (for 43 elements). Figure 2 illustrates the sampling location and also the lithology of this samples. The samples placed in the areas of the sediments were collected from trenches having access to rock or from rock outcrops that shared the lithology of their adjacent igneous units. The analyzed elements along with their detection limits are listed in Table 1.

For modeling in this article, the corrected data set contains 184 data, which is divided into two parts (Saqib et al., 2014; Ghannadpour et al., 2017): data for building the model (70% of 184 data randomly) and test data (30% of 184 data randomly) were divided to estimate the concentration of Co. Among the analysis of 43 elements obtained, those that have a closer relationship with the Co element are considered as input data, which include four independent variables: Fe, Li, Cr and Ni. Correlation matrix was used to check the relationship between the input parameters and the output

Table 1. Analyzed elements with detection limit.

Element	Detection limit*	Element	Detection limit*	Element	Detection limit* Element
Cr	1	Au	1	Th	0.5
Al	10	Cs	0.5	Sr	2
Fe	100	Cu	1	Te	0.2
Ca	100	La	1	Sn	0.5
Mg	100	Li	1	Ti	10
K	100	Mn	5	Tl	0.2
Na	100	As	0.5	U	0.5
Ag	0.1	Nb	1	V	2
Mo	0.5	Ni	1	Y	0.5
Ba	2	P	10	W	0.5
Bi	0.2	Pb	1	Yb	0.2
Be	0.2	Rb	1	Zr	5
Cd	0.1	S	50	Zn	1
Co	1	Sb	0.5		
Ce	1	Sc	0.5		

*The detection limit unit of all elements except gold is in milligrams per kilogram, and for the gold element it is micrograms per kilogram.

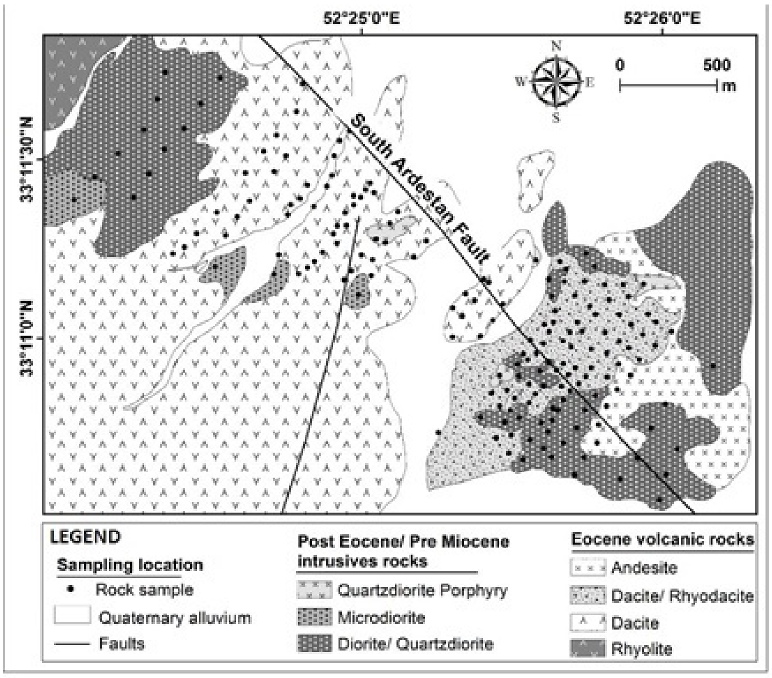

Figure 2. Simplified geological map of the Zafarghand exploration region (modified after (Alaminia et al., 2016)).

variable, in such a way that the correlation of the available parameters with the Co element was checked and according to that, the highest correlation and relationship between the input parameters and the Co element was determined. Finally, the information of the most relevant parameters was used to estimate the concentration of Co element.

According to geological studies, the investigated range includes two groups: 1- Intermediate mafic rock (olivine gabbro, gabbro, diorite and quartzdiorite) and 2- felsic (granodiorite, granite, alkaline feldspar granite), Correlation of Co, Fe, Li, Cr, Ni elements is gabbroic (mafic) units due to their same origin. Table 2 shows the correlation of input and output parameters.

3.2 Data pre-processing and statistical indicators to evaluate model performance

For data modeling and input, it is mostly necessary that the ranges of data changes are similar to each other, which

Table 2. Correlation of the variables used in the simulation.

Elements	Fe	Co	Cr	Li	Ni
Fe	1				
Co	0.89	1			
Cr	0.69	0.81	1		
Li	0.73	0.85	0.89	1	
Ni	0.68	0.82	0.97	0.92	1

is called data normalization. The importance of data normalization to improve data quality and subsequently model performance has been presented in many studies (Singh and Singh, 2020). Normalization of input data including values (Ni, Cr, Li, Fe) in this study is done by Equation 3.

$$P_n = \log(P_i) \tag{3}$$

where in: P_n is the normalized data, P_i is the real data. Also, in this article, the MSE (Mean Square Error) and R^2 (correlation coefficient) have been used to evaluate the performance of the model. These statistical indices are shown in Equations 4 and 5.

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y-y')^2}{\sum_{i=1}^{N}(y-\bar{y})} \tag{4}$$

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - y_i')^2 \tag{5}$$

where N represents the number of data points, $\bar{y}$ is the mean of data, y_i is the actual value, and y_i' is the predicted value. It is necessary to explain that the criterion of correlation coefficient indicates the conformity between the measured and predicted values, the best case is where its value is one, and if it is zero, it means that the performance of the model for prediction it is very weak. The *MSE* measure also expresses the *MSE* between the values of estimated and measured, and the lower its value, the more reliable the model's performance.

3.3 Estimation of Co concentration using nonlinear multivariate regression method

In this part, multivariable nonlinear regression methods are used to estimate the Co concentration from the correlations between the elemental analysis of the collected samples and the desired parameter. In this study, four normal nonlinear regression methods including: polynomial, logarithmic, power, and exponential nonlinear regression have been used to estimate the concentration of Co. In order to find the optimal equation of each of the mentioned methods, more than 50 equations have been analyzed in the STATISTICA software, among which the 6th equation had the highest correlation in the modeling phase, which will be further analyzed in this model. According to the equation obtained from the logarithmic function, the determination coefficient R^2 value for the teaching data was 0.8.

$$Co = \exp(0.89 \times Fe - 0.15 \times Cr + 0.41 \times Li + 0.39 \times Ni - 3.6) \tag{6}$$

Fig 3 and Fig 4 show the results of the equation analysis obtained for the teaching and test data. Also, to evaluate the performance of the statistical index model, correlation coefficient and mean square error were calculated. The result obtained is shown in Table 3.

3.4 Estimation and simulation of Co concentration using Monte Carlo simulation method

In the previous part, an optimal equation was obtained using nonlinear regression to estimate the concentration of Co. In this part, due to the uncertainty in the data, the parameters of Co element have been simulated using the Monte Carlo method using the obtained equation. In addition, the most effective parameters in the estimation of this element have been determined using this method. In this modeling, the type of data distribution function was determined using the Kolmogorov-Smirnov and Chi-squared tests (Ghannadpour and Hezarkhani, 2022; Ozonur et al., 2021). Fe, Ni, Li and Cr variables are defined with normal function. Fig 5 shows the frequency distribution of each of the input variables used in the simulation (values are defined based on logarithms). The characteristics of input data functions are also listed in Table 4.

Table 3. Performance of the regression model for the analyzed data.

Teaching data		Test data	
MSE	R^2	MSE	R^2
0.4	0.83	0.2	0.73

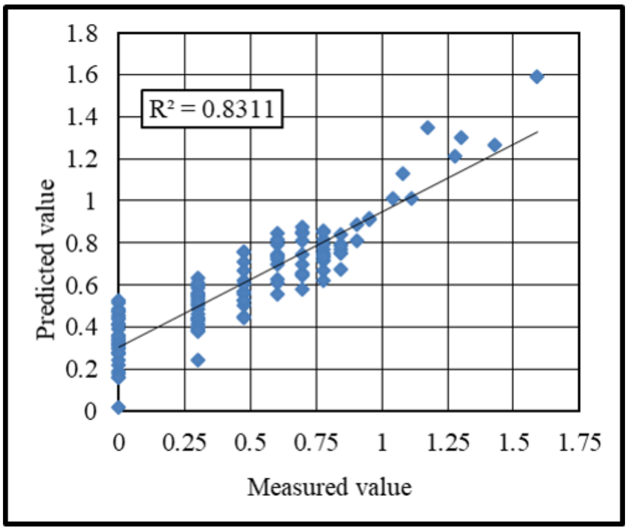

Figure 3. Correlation of Co concentration values for teaching data.

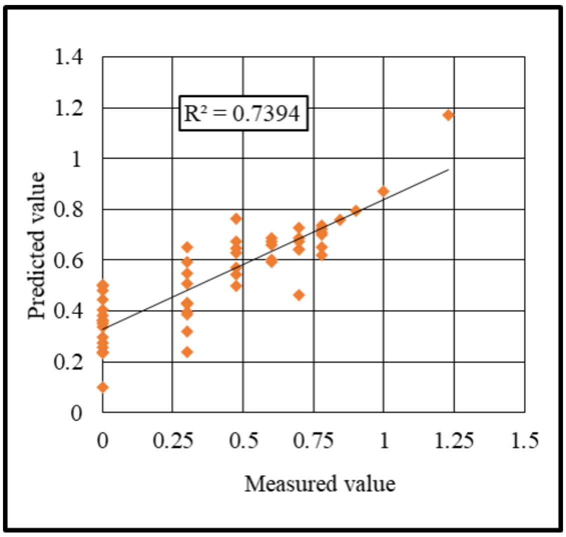

Figure 4. Correlation diagram of Co concentration values for test data.

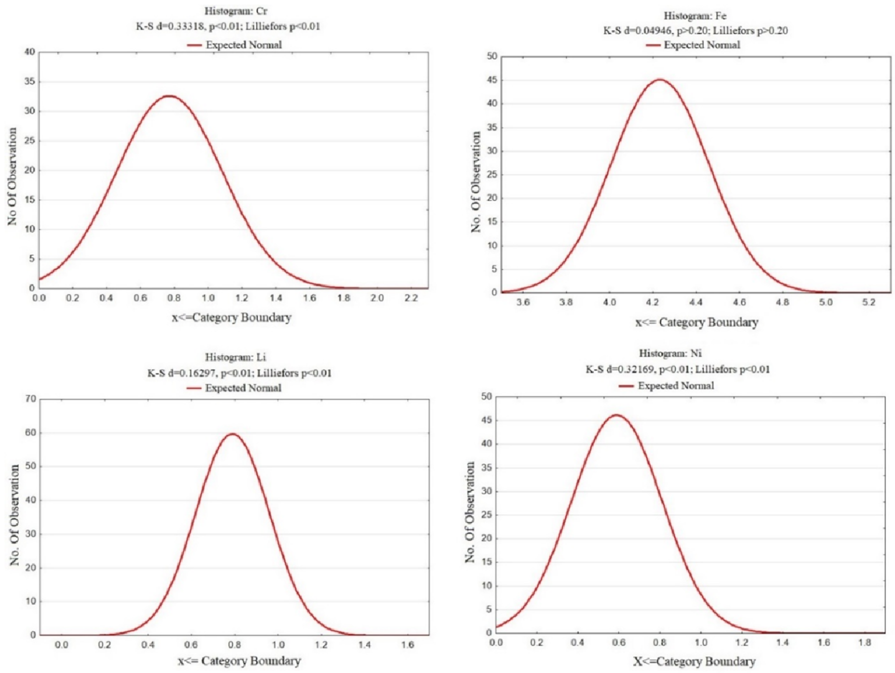

Figure 5. Frequency distribution of input variables used in simulation.

Table 4. . Probability distribution functions of each of the input variables used in the simulation.

Input variables	Distribution functions
Fe element	normal (4.2 , 0.22)
Li element	normal (0.79 , 0.17)
Cr element	normal (0.77 , 0.31)
Ni element	normal (0.58 , 0.22)

In this research, @RISK software is used for simulation. Several studies in prediction with high confidence level have been done with @risk software. For example, in 2016, Bouayed used Monte Carlo simulation with @risk software to predict project risk and cost (Bouayed, 2016). Weishaar predicted the impact of resource delays on the critical path of a construction project using Monte Carlo simulation and @risk software (Weishaar, 2018), also Abramov employed @risk software to identify and evaluate the impact of risk factors on the operations of building companies in the performance of enterprise projects. In this research, the success of construction companies increased significantly (Abramov and AlZaidi, 2023).

The risk software analyzes the input parameters by using the Monte Carlo simulation method and generating random numbers and presents the output values along with its probability distribution functions. To improve the performance of Monte Carlo Simulation, the correlation matrix of the analyzed data is used. Then, according to the equation explained in the previous part, the most suitable function was selected in terms of correlation with the analyzed and tested values to estimate the concentration of Co in Monte Carlo simulation. The logarithmic Equation 6 was chosen as the output of Monte Carlo Simulation. Table 5 shows the statistical description of the variables.

Table 5. Statistical parameters of each of the input and output variables used in the simulation.

Statistical information of the input and output (mg/kg)				
Parameters		The lowest	The most	Mean
Inputs	Lithium	0.47	1.66	1
	Iron	3.07	4.8	4.3
	Chromium	0.6	2.5	1.13
	Nickel	0.4	2.1	0.95
Output	Cobalt	0	1.3	0.66

In this method, the number of random numbers is determined by calculating the mean result from the output distribution function. Therefore, more than 8000 numbers were simulated in this research, Table 6 shows the number of random numbers along with the mean distribution function of each random data set. According to the obtained result, after producing 5000 numbers, the mean value of a fixed number equal to 0.69 (mg/kg) was obtained. Therefore, the number considered for this modeling is

Table 6. Number of random numbers generated for simulation.

Number	Mean of simulated data at each step
1000	0.69
2000	0.70
3000	0.68
4000	0.68
5000	0.69
6000	0.69
7000	0.69
8000	0.69

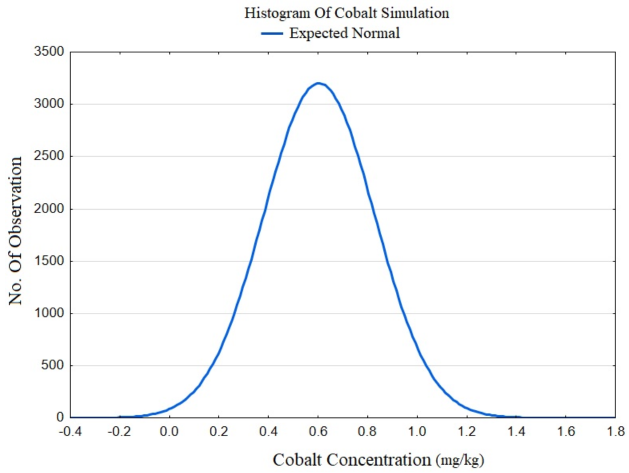

Figure 6. The result of describing the optimized model of the logarithmic value of Co concentration.

5000 random numbers and the distribution function of this number was used to predict the confidence interval of Co element. According to the obtained distribution function, the mean concentration of Co element in the studied area is 0.66 (mg/kg). Compared to statistical methods, the mentioned distribution function gives a better insight into the changes of Co concentration and instead of a single number, it can provide engineers with a range of changes. Based on the output from the distribution function, the confidence interval at the 90% confidence level of Co (0.45, 0.75) (mg/kg) was obtained based on logarithm Fig 6.

Metal Contamination factor (CF):
The relation CF is the ratio of the average amount of heavy metals to its amount in the background. Equation 7 shows this ratio;

$$CF = \frac{\text{HM content in soil}}{\text{HM content in background}} \tag{7}$$

Hakanson (1980) classified the pollution coefficient in four categories has:
$CF < 1$category one with low contamination, $1 < CF < 3$ category two with contamination Medium, $3 < CF < 6$ category three with significant contamination and $CF \geq 6$ category four with Very high pollution.

Pollution load index (PLI):
Pollution load index for each sampling by the method suggested by (Tomlinson et al., 1980) has been determined. Based on the output from the distribution function, the confidence interval at the 90% confidence level of Co was obtained based on logarithm (0.45, 0.75) (mg/kg).

$$PLI = n\sqrt{CF_1 \times CF_2 \times \ldots \times CF_n} \tag{8}$$

$$CF_1 = 0.45/0.66 = 0.68$$

$$CF_2 = 0.75/0.66 = 1.13$$

$$PLI = 2\sqrt{0.68 \times 1.13} = 1.74$$

In this equation, CF is the coefficient of heavy metals and n is the number of samples. PLI close to 1, It shows the

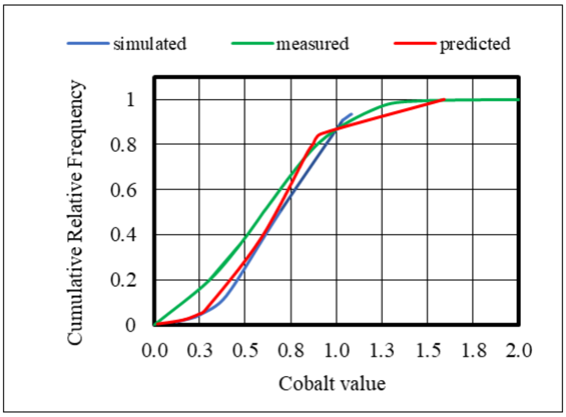

Figure 7. Comparison of density functions of predicted, simulated and measured values.

concentration of heavy metals close to natural conditions While more than 1 indicates metal deposition in the area. Considering that the value obtained is higher than 1, the study area is contaminated Co with metal.
In addition, in this research, a comparison has been made between the simulated, predicted and measured values, and the results of this comparison can be seen in Fig 7. The results of this comparison show that statistical-probability methods can be a useful and efficient estimator in the field of geochemistry.

3.5 Sensitivity analysis of input parameters using Monte Carlo method

In addition to simulation, the Monte Carlo method also performs sensitivity analysis on the input variables.
In this analysis, the correlation of the simulated input variables is calculated with respect to the output variable, and the range of correlation values can be between -1 and +1. In this research, sensitivity analysis has been used to prioritize the input variables in determining the concentration of Co element. According to the results obtained from Fig. 8, the most influential variables in estimating the concentration of Co element are: Fe, Cr, Ni and Li, respectively. Also, Table 7 shows the prioritization of variables based on the least and the most impact on Co concentration.

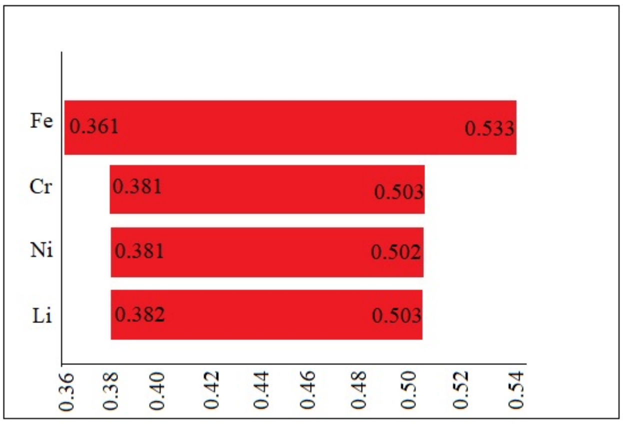

Figure 8. The impact of the input variables on the concentration of Co .

Table 7. Sensitivity analysis of used variables.

Prioritize	Element	The lowest	The most
1	Fe	0.3619223	0.5337161
2	Cr	0.3811466	0.5033239
3	Ni	0.3812542	0.5029207
4	Li	0.3825553	0.5036719

4. Conclusions

Today, with the increasing development of the industry and the extensive activity of the industries, environmental pollution is one of the issues that has caused many concerns. Heavy metals are among the organic pollutants that accumulate in the body tissues of aquatic animals due to their stable structure and affect the Physiological and vital processes cause their poisoning. Since heavy metals are deposited on the surface of the soil or sediment, they are very suitable tracers to show the level of environmental pollution. The concentration of these elements is usually in safe geochemical background values, but when which reached abnormal values and the highest permissible value, should be taken into account and if the threshold is reached, the environment should be cleaned from them. Heavy metal pollution is caused by human activities that are the main cause of pollution, mainly from metal mining. Heavy metals, with the exception of arsenic, boron and selenium, refer to a number of metals that often have a density higher than 6 (g/cm^3). The concentration of these elements is usually within the safe geochemical background values, but when they reach abnormal values and the highest allowed amount, they should be taken into consideration, and if they reach the threshold, the environment should be cleaned of them. The purpose of this research is to estimate the concentration of Co in Zafarghand region of Isfahan province by using statistical methods. For this purpose, after sampling from the study, the information of 43 elements was analyzed, the elements that had more correlation with Co element were used in this research. These elements include Fe, Li, Cr and Ni. 184 data were available, 30% of them were randomly set aside to test the methods and the rest of the data were included in the analysis. After preparing the data by applying nonlinear regression on independent variables including: Fe, Ni, Li and Cr, Co concentration values were calculated. The equation that had the best correlation coefficient was chosen as the appropriate equation for examining the test data. On the other hand, using the Monte Carlo method and the equation that was chosen as the best equation, 5000 data were randomly simulated, then the simulated numbers and the measured numbers, with the corresponding density function the type of distribution function of numbers were compared. Based on the obtained results, the mean value of Co in laboratory measured values is 0.66, in the simulation method it is 0.69 (mg/kg) and in the prediction mode with the nonlinear regression method it is 0.60(mg/kg). Also, the level of Co element in the studied area with a confidence level of 90% was in the range of (0.45, 0.75) (mg/kg).

The results of this comparison show that statistical-probability methods can be a useful and efficient estimator in the field of geochemistry. In addition, in this article, using the Monte Carlo simulation (MCS), sensitivity analysis was performed to determine the most effective input parameter in predicting the concentration of Co element, and the most effective variable in its estimation was found to be Fe element. It should be noted that the use of this methodology is recommended for determining other heavy metal concentrations in the study area. The MCS method can be used for regions with a uniform geological structure. For example, for sedimentary areas that do not have complex geology. or areas that are massive. But it is not very useful in strati-band structures where the changes in the concentration of metals are high.

Authors contributions
Authors have contributed equally in preparing and writing the manuscript.

Availability of data and materials
The data that support the findings of this study are available from the corresponding author, upon reasonable request.

Conflict of interests
The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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