N E W S
OF THE NATIONAL ACADEMY OF SCIENCES OF THE REPUBLIC OF KAZAKHSTAN
SERIES CHEMISTRY AND TECHNOLOGY
ISSN 2224-5286 **https://doi.org/10.32014/2019.2518-1491.78**
Volume 6, Number 438 (2019), 86 – 98

UDC 550.42:004.89

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DESIGN OF NEURAL NETWORK FOR FORECAST ANALYSIS OF ELEMENTS-CONTAMINANTS DISTRIBUTION ON STUDIED TERRITORIES (ON EXAMPLE OF PAVLODAR CITY, KAZAKHSTAN)

Abstract. In the article we are presenting results of development appropriate method including neural network for creating predictive map of elements-contaminants distribution (on example of Cr) on the territory of Pavlodar city (Kazakhstan). Obtained method allows to get widen data. The data from 15 points were spread out into 500 points. The average relative error at verification process was 9.45%. Architecture of well working model of neural network is perceptron with one input neuron, which takes values of distances between given point and several nearest points, 10 hidden neurons, and 1 output neuron, which gives value of element concentration in specified point. Obtained data were used in QGIS for creation of IDW interpolated map, which visualizes the information about concentration distribution.

Keywords: neural network, contaminants, distribution, forecasting, modelling, GIS, environmental.

1. Introduction

The search for ways of solving environmental problems and developing scientific methodological approaches to studying the complex consequences of the anthropogenic activities of enterprises involves the study of the ecological state of the region [1–3]. Environmental researches now have special significance because environmental safety and rational use of nature resources are the most important factors, determinant prospective of successful development of economics and social sphere.

The Pavlodar city is the large industrial city on the North of Kazakhstan. It is known, that the main sources of environment contamination of the city and Pavlodar region are different waste of chemical-technological processes [4]. These can be products of related processes and by-reactions not used in subsequent processes. Also, it can be intermediates of reactions and polymerization processes, filer materials, industrial waste water, not reacted gases (Cl_2, NH_3 etc.) [5, 6]. Moreover, environmental contamination occurs as a consequence of mechanical losses of raw material and products due to leakages from equipment and communications. Effect of every kind of contaminant directly depends on its physical-chemical properties. Many gaseous chemicals can react in atmosphere with water vapor, oxygen, as well be affected under radiation converting into other more toxic substances.

Finding of borders of studied territory and identification of danger sources leading to damage are an initial and important stage in the process of assessment of environmental risks. A new approach in this field is to assess impact of factors affecting the environment of region through analysis of territorial distribution of contaminants with creation of maps. Map allows visualizing of effects of contaminants, to understand origin sources of the contaminants, to predict ways of distribution and meanings for prevention of negative consequences from various factors.

In the article we are describing a new approach for creating such kinds of maps using methods of computer modelling, in particular neural network. New ways of data analysis allow to obtain new generated data and are often used for solving problems when it is required to expand weak analytical data and get on output full picture of demanded information [7–9].

Neural network receives input information and analyses it in the way analogous to our brain. During the analysis network is trained (generates some new knowledge) and gives a new output information based on previous experience [10–12]. The main task of analyst using neural network for solving some problem is to design the most effective architecture of network. Namely, correctly choose the sort of neural network, algorithm of training, number of neurons and kinds of relations between them. This work has no formalized procedures and requires deep understanding of different architectures of neural networks, it includes lots of research and analytical work and can take quite much time [13–15]. The most common usages of neural networks are:

- classification – allocation of data by parameters;
- forecasting – possibility to predict following steps;
- recognition – determination of objects in a stack.

The computational item of neural network is neuron. It receives an information, makes simple calculations with it and pass it later. There are three types of neurons with specified functions – input, hidden and output. The principal scheme of simple neural network with two input neurons, two hidden and one output neuron is shown on the figure 1.

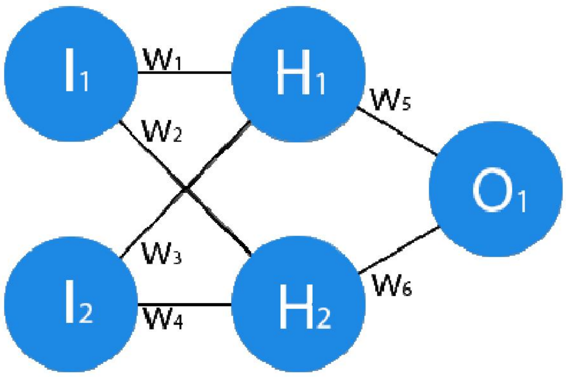

Figure 1 - The scheme of simple neural network

“W” on the figure are “weights”, which are parameters of the network. They are adjusted during the training stage for the network could be able to give correct values. In our work we use neural network for forecasting of distribution of elements-contaminants on the studied territory. The forecast is based on the data obtained with x-ray spectral elemental analysis of the soil samples taken from given locations. The aim of the work was to design appropriate model of neural network for obtaining at least 500 predicted values of element concentrations in 500 given coordinates on the territory of Pavlodar city.

2. Methods and materials

2.1 Sampling of soil

Sampling was carried out for estimation of quality and quantity analysis of elemental content of soils on the territory of Pavlodar city. Sampling was carried out according to requirements of conventional documents “GOST 17.4.4.02-84. Nature protection. Soils. Methods for sampling and preparation of soil for chemical, bacteriological, helmintological analysis”, “GOST 17.4.3.01-83. Nature protection. Soils. General requirements for sampling”, “GOST 5180-84. Soils. Laboratory methods for determination of physical characteristics”. The positions of sampling sites are shown on the figure 2 and specified in the table 1.

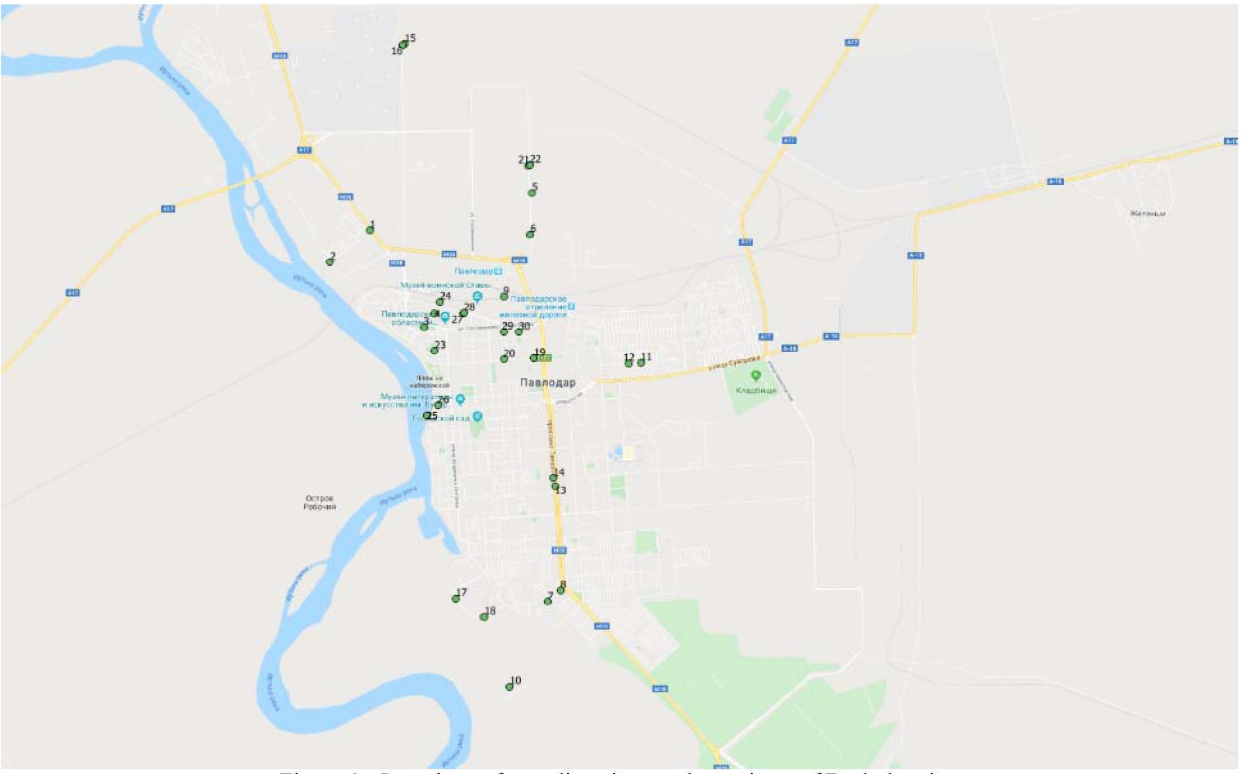

Figure 2 - Locations of sampling sites on the territory of Pavlodar city

Table 1 – Coordinates of positions of sampling sites

Number of sample	Name	X	Y
1	Lesozavod 1	76.919125	52.313194
2	Lesozavod 2	76.9083333333	52.3077777778
3	Constitution square 1	76.9338888889	52.2966666667
4	Constitution square 2	76.9367	52.2989166667
5	CHP2 1 (TEC2 1)	76.9630916667	52.3196361111
6	CHP2 2 (TEC2 2)	76.9625833333	52.3125277778
7	Zhayau Musa str. 1	76.9673194444	52.2497555556
8	Zhayau Musa str. 2	76.9707611111	52.2516555556
9	Railway Station 1	76.9552861111	52.3018861111
10	Railway Station 2	76.9570277778	52.235275
11	Narkodispancer 1	76.9926	52.2906138889
12	Narkodispancer 2	76.9894055556	52.290475
13	Gulliver TH 1	76.96925	52.2695777778
14	Gulliver TH 2	76.9688638889	52.27085
15	PNCP 1	76.9285722222	52.3449916667
16	PNCP 2	76.9279916667	52.3448638889
17	Usolka riv. 1	76.942475	52.2503555556
18	Usolka riv. 2	76.9501694444	52.2471638889
19	Lermontov str. 1	76.9636111111	52.2913888889
20	Lermontov str. 2	76.9553111111	52.2911972222
21	PTP 1	76.9619861111	52.3242555556
22	PTP 2	76.962475	52.3243888889
23	Satpayev str. 1	76.936725	52.292625
24	Satpayev str. 2	76.938175	52.3009916667
25	Naberezhnaya str. 1	76.9345222222	52.2815777778
26	Naberezhnaya str. 2	76.9375833333	52.2833
27	Mir str. 1	76.9444111111	52.2990027778
28	Mir str. 2	76.9447	52.2991111111
29	Toraigyrov str. 1	76.9552861111	52.2959166667
30	Toraigyrov str. 2	76.9594861111	52.2958333333

* Coordinate system EPSG:4326 - WGS 84 - Geographic

2.2 Elemental analysis of soil samples

The catalyst samples were studied on a low-vacuum scanning electron microscope with a thermal emission cathode (LaB6) JSM-6610LV from JOEL. The device is equipped with an energy dispersive microanalysis system (EDM), a wave dispersive microanalysis system, a backscattered electron diffraction analysis system with a reflected electron detector, an Everhart-Thornley secondary electron detector, a low-vacuum secondary electron detector and sample preparation equipment. Elemental analysis was performed using energy dispersive x-ray fluorescence spectroscopy on an energy dispersive microanalysis system INCA Energy 450. Spectra were obtained three times with the calculation of the average value.

2.3 Neural network designing

For creation of neural network Brain.js library was used. Brain.js is an opened JavaScript library that allows implementation of neural networks with different architectures right in the browser or with using Node.js. Simple browser program was prepared for implementation of developed neural net. The program allows to input initial data for training, verification and forecasting from text file with data written in CSV-like manner, columns are divided with commas. Moreover, average relative divergence is calculated after verification process, as well diagram of convergence of forecast with original data is created automatically using the Graph.js library. Using neural network based on initial data about element concentration from 30 input points, 500 points were predicted after calculations. These 500 points were used for plotting on the map.

2.4 Creating of element distribution map

Free geographic information system with open code QGIS 3.8.3-Zanzibar was used. QGIS is an open source, user-friendly geographic information system (GIS) distributed under the GNU General Public License. QGIS is a project of the Open Source Geospatial Foundation (OSGeo). It works on Linux, Unix, Mac OSX, Windows and Android, supports many vector and raster formats, databases and has many features. Input data were added as a layer with coordinate system EPSG:4326 - WGS 84 – Geographic. For better visualization of information data analysis with IDW interpolation method has been implemented. In the IDW (Inverse Distance Weighting) interpolation method, the sample points are weighted during interpolation such that the influence of one point relative to another declines with distance from the unknown point you want to create [16, 17]. The figure 3 demonstrates the principle of the IDW method.

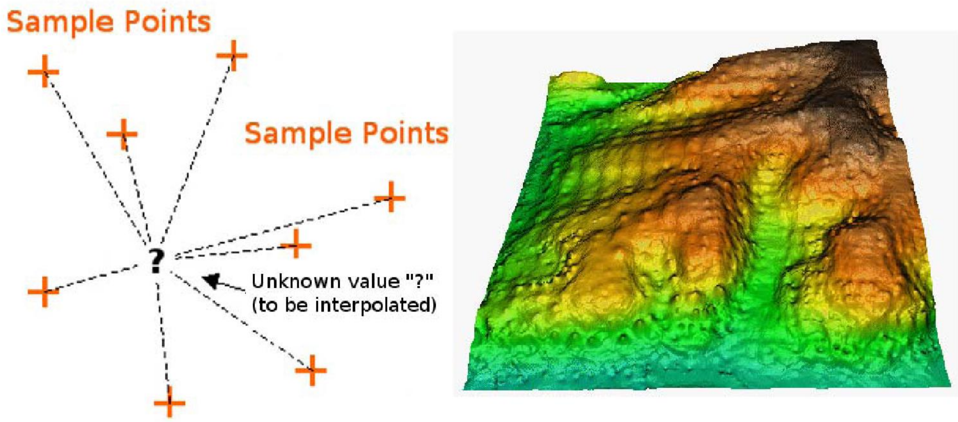

Figure 3. Inverse Distance Weighted interpolation based on weighted sample point distance (left).
Interpolated IDW surface from elevation vector points (right).
(Image Source: Mitas, L., Mitasova, H. (1999),
url: https://docs.qgis.org/2.18/en/docs/gentle_gis_introduction/spatial_analysis_interpolation.html)

Interpolation was visualized as a gradient of colors, monochannel pseudocolor mode of image was used. For map of chromium distribution following table of color distribution in dependence on concentration was assigned (table 2).

Table 2 – Distribution of colors in dependence on concentration in the method of interpolation visualization

Threshold concentration, %	Color	Color name	RGB color
0.00326683		blue	43,131,186
0.082261464		green	171,221,164
0.161256098		yellow	255,255,191
0.240250732		orange	253,174,97
0.319245366		red	215,25,28

3. Results and discussion

When we are describing distribution of concentrations of elements on the territory, practically we have to consider the data in three-dimensional space, where X and Y represent coordinates and Z is a third parameter – concentration in our case. Thus, we have to find the dependence between coordinates and concentration. First approach for creation of neural net, which could reveal that dependence is to give into input layer two parameters X and Y and get from output layer the value of concentration. In order to try the effectivity of developed neural network we have to find appropriate model with similar parameters. The convenient, simple and available model is some picture in gray scale. In this case a picture has its X and Y coordinates, when we are considering it as a matrix of pixels, and graduation of gray color is similar to concentration. Graduation of gray color lies in the range from 0 to 255 in RGB scheme [18].

So, the first picture we have chosen is quite simple and has dense relatively uniform sites of different shades of gray color (figure 4).

Figure 4 - Model image №1 for development of neural network

For this model we have taken 35 points as training data. The architecture of neural network included 2 neurons of input layer (X, Y coordinates), 3 hidden layers with 10, 20 and 4 neurons accordingly, 1 neuron on output layer (figure 5).

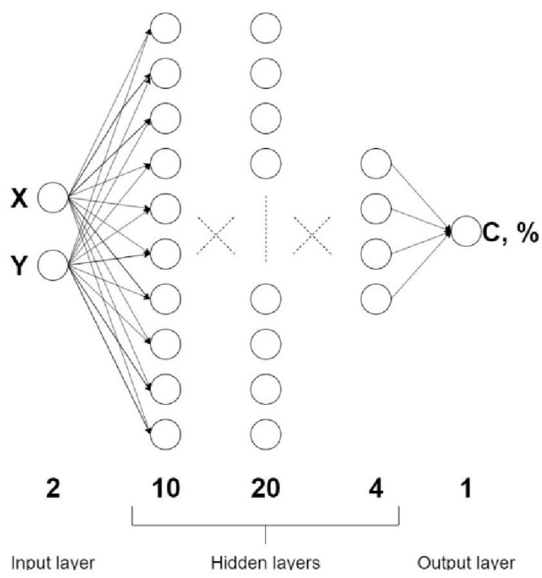

Figure 5 - Architecture of neural network model №1

Activation function was used sigmoid (1), because this function is widely used for neural networks aimed in prediction some values between 0 and 1 [19–22]. Graphical represent of the sigmoid function is showed on the figure 6.

$$S(x) = \frac{1}{1+e^{-x}} \tag{1}$$

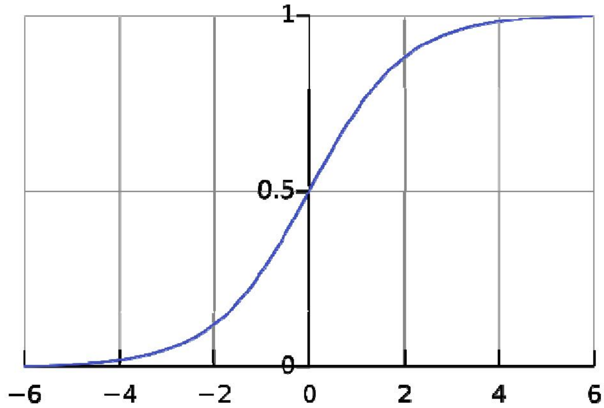

Figure 6 - Curve of sigmoid function

Using neural network model №1 after training we have obtained forecast for 10 points with average relative error 13.35%. The diagram of convergence of predicted data with original data is presented on the figure 7.

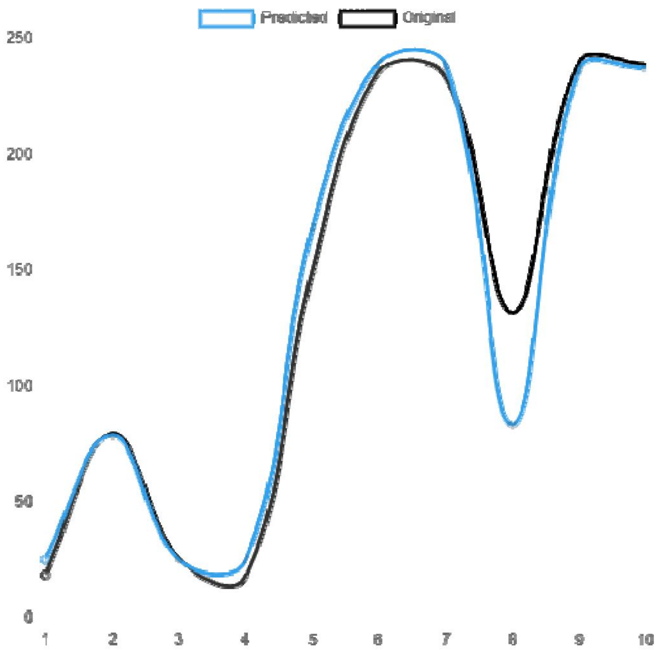

Figure 7 - The diagram of convergence of predicted data with original data on the neural network model №1
(x axis – number of verify point, y axis – shade of gray color in RGB)

Thus, neural network model 1 has shown good results with the first picture, so we have tried to use it with the second picture, which is more complicated and more similar to landscape distribution of some parameter: height, depth or may be the concentration of some element (figure 8). This picture is in the gray scale as well.

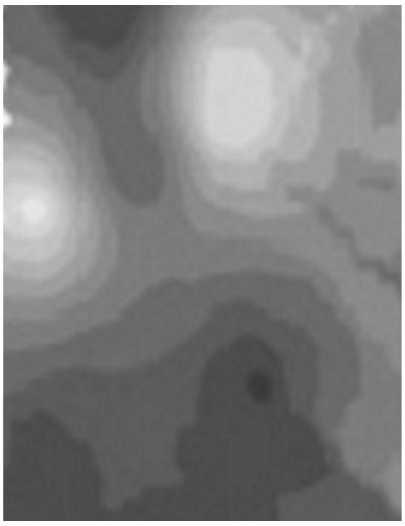

Figure 8 - Model image №2 for development of neural network

With the second model picture and using the previous architecture of neural network we have obtained the value of average relative error 20.49%. The diagram of convergence of predicted data with original data is presented on the figure 9.

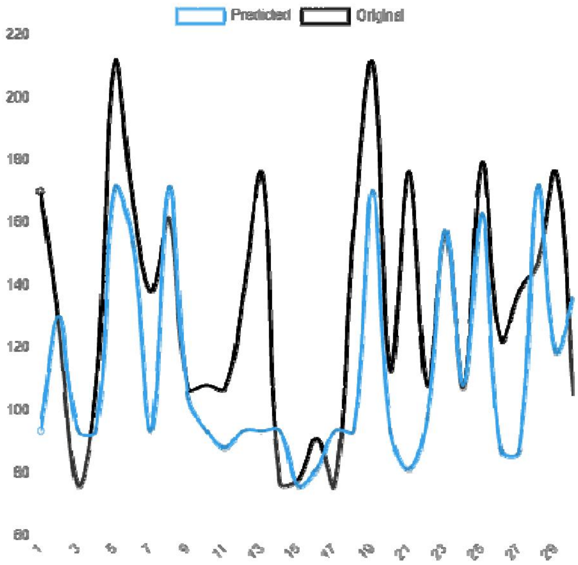

Figure 9 - The diagram of convergence of predicted data with original data on the neural network model №1 with picture 2
(x axis – number of verify point, y axis – shade of gray color in RGB)

On the diagram we can see that convergence in this case is much lover. Thus, it can be concluded, that the model №1 of neural network is appropriate just for simple characters of parameter distribution. That is why we are developed the second model of neural network and changed the approach for data analysis.

In the second model we used the interpolation method IDW for obtaining of demanded parameter value [23, 24]. But the calculations were made by neural network. This architecture has one neuron on input layer, which receives the values of distances between demanded point and each of 3 closest point. The distances were calculated by formula (2)

$$D = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2} \quad (2)$$

In accordance to this approach we have to get training data for each demanded point and train neural network for every point to prediction. However, taking into account the fact that training data contain only 3 input values it allows to simplify the model of neural network itself, so the second model of neural network has 1 neuron in input layer, 10 neurons in single hidden layer, and 1 output neuron. On the figure 10 we can see the convergence diagram for this case with picture №2.

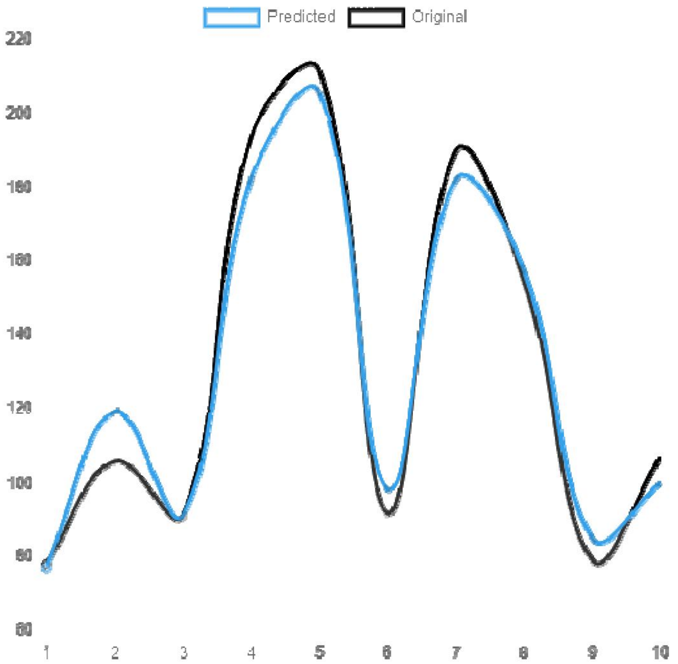

Figure 10 - The diagram of convergence of predicted data with original data on the neural network model №2 with picture 2 (x axis – number of verify point, y axis – shade of gray color in RGB)

In this situation we have obtained the value of average relative error 4.97% unless the picture was more complicated. Thus, this model of neural network was selected for using in analysis of concentration distribution of elements-contaminants on the studied territory.

Content of Cr in soils of studied territory was estimated using X-ray spectral microanalysis (table 3). These data were given into input of the neural network for training. On the figure 11 we can see the convergence diagram for verification process using model of neural network №2. The value of average relative error was 9.45%.

Table 3 – Data on Cr content in soils from sample sites 1-15 obtained using X-ray spectral microanalysis

Number of samples	X	Y	C, %
1	76.919125	52.313194	0.71
2	76.9083333333	52.3077777778	0.25
3	76.9338888889	52.2966666667	0.25
4	76.9367	52.2989166667	0.19
5	76.9630916667	52.3196361111	0.13
6	76.9625833333	52.3125277778	0.3
7	76.9673194444	52.2497555556	0.15
8	76.9707611111	52.2516555556	0.03
9	76.9552861111	52.3018861111	0.05
10	76.9570277778	52.235275	0.15
11	76.9926	52.2906138889	0.06
12	76.9894055556	52.290475	0.06
13	76.96925	52.2695777778	0.31
14	76.9688638889	52.27085	0.30
15	76.9285722222	52.3449916667	0.06

* Coordinate system EPSG:4326 - WGS 84 - Geographic

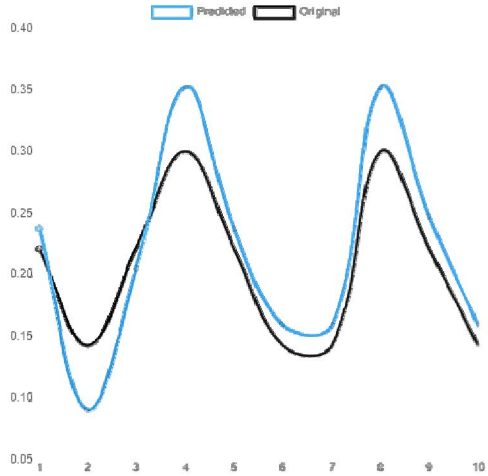

Figure 11 - The diagram of convergence of predicted data with original data on the neural network model №2 with data on Cr content in soils (x axis – number of verify point, y axis – concentration of Cr, %)

For prediction we have taken 500 points according to map represented on the figure 12. The batch process was performed with creation of prediction for every of 500 points. The obtained data with forecast of Cr distribution was plotted on the map in QGIS software. IDW interpolation was used in order to visualize the character of concentration distribution. The obtained interpolated map is represented on the figure 13. From the map it can be seen the large site with higher content of Cr. It is not necessary mean that the level exceeds the MPC level, but it gives the information about areas with higher and lower levels of the metal content. Control about MPC levels was not aimed in this research.

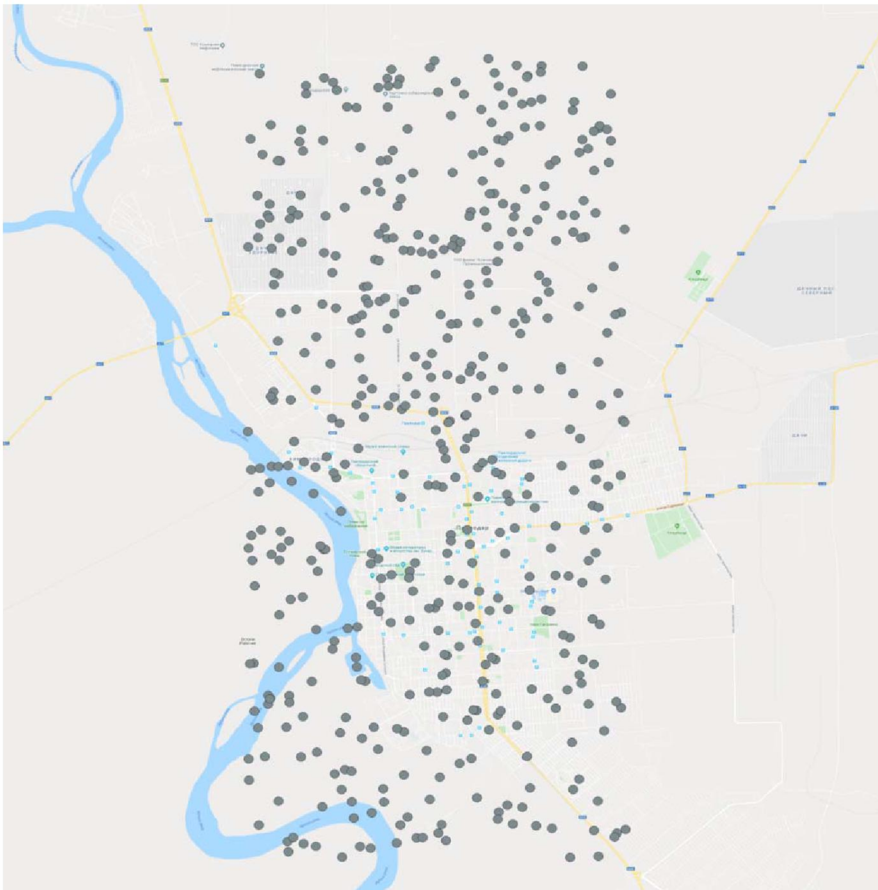

Figure 12 - Points where concentrations were calculated based on developed model of neural network

Figure 13. Map of Cr concentration distribution in soils of Pavlodar city obtained on the basis of calculations of neural network model №2

Conclusion

Thus, during this work two models of neural network were developed. The method of calculating "point by point" using IDW approach and neural network №2 allows to predict complicatedly distributed data, which are usual when we are considering various geographical data: geochemistry, chemistry of environment, geology etc. That complexity is due to territorial distribution is influenced with many factors in very complex dependences. Using the developed method, it was possible to obtain 500 predicted points with values of chromium concentration on the different sites on the territory of Pavlodar city. The developed method allows to diminish level of error up to 9.45% (average relative error). The calculated data were inputted as a layer in QGIS. Based on the layer a new interpolated layer was created using IDW method. Thus, the colored map of chromium distribution on the territory of Pavlodar city was obtained in GIS. It allows to scale the map, get, print and save various views of the map.

Acknowledgments

The research work has been carried out in the frame of the project AP05134022 granted by Ministry of Education and Science of Republic of Kazakhstan.

УДК 550.42:004.89

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ЗЕРТТЕЛЕТІН АУМАҚТАРДА ЛАСТАУШЫ ЭЛЕМЕНТТЕРДІҢ ТАРАЛУЫН БОЛЖАМДЫҚ ТАЛДАУ ҮШІН НЕЙРОНДЫҚ ЖЕЛІНІ ӘЗІРЛЕУ (ПАВЛОДАР ҚАЛАСЫ МЫСАЛЫНДА, ҚАЗАҚСТАН)

Аннотация: Осы мақалада біз Павлодар қаласының аумағында (Қазақстан) ластаушы элементтердің (мысалы, Cr) таралуының болжамдық картасын жасау үшін нейрондық желіні қолданудың тиімді әдісін жасау нәтижелерін ұсынамыз. Әзірленген әдіс кеңейтілген деректерді алуға мүмкіндік береді. 15 нүкте бойынша деректер 500 нүктеде масштабталды. Верификация процесінің орташа салыстырмалы қателігі 9,45% құрайды. Нейрондық желінің жұмыс моделінің архитектурасы берілген нүкте мен бірнеше жақын нүктелер арасындағы қашықтықтың мәндерін қабылдайтын бір кіріс нейронымен перцептронды, жасырын қабаттың 10 нейронын және берілген нүктеде элементтің концентрациясының мәнін беретін 1 шығыс нейронды білдіреді. Алынған деректер концентрацияның таралуы туралы ақпаратты бейнелейтін IDW интерполяцияланған картасын құру үшін QGIS-те қолданылды.

Түйін сөздер: нейрондық желі, ластағыштар, бөлу, болжау, модельдеу, ГАЖ, экологиялық.

УДК 550.42:004.89

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РАЗРАБОТКА НЕЙРОННОЙ СЕТИ ДЛЯ ПРОГНОСТИЧЕСКОГО АНАЛИЗА РАСПРЕДЕЛЕНИЯ ЭЛЕМЕНТОВ-ЗАГРЯЗНИТЕЛЕЙ НА ИССЛЕДУЕМЫХ ТЕРРИТОРИЯХ (НА ПРИМЕРЕ ГОРОДА ПАВЛОДАР, КАЗАХСТАН)

Аннотация. В данной статье мы представляем результаты разработки эффективного метода с использованием нейронной сети для создания прогностической карты распределения элементов-загрязнителей (на примере Cr) на территории г. Павлодар (Казахстан). Разработанный метод позволяет получать расширенные данные. Данные по 15 точкам были масштабированы в 500 точек. Средняя относительная погрешность процесса верификации составляет 9,45

%. Архитектура рабочей модели нейронной сети представляет собой перцептрон с одним входным нейроном, который принимает значения расстояний между заданной точкой и несколькими ближайшими точками, 10 нейронов скрытого слоя и 1 выходной нейрон, который выдает значение концентрации элемента в заданной точке. Полученные данные использовались в QGIS для создания IDW интерполированной карты, которая визуализирует информацию о концентрационном распределении.

Ключевые слова: нейронная сеть, загрязнители, распределение, прогнозирование, моделирование, ГИС, экологический.

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