УДК 504.06+004.032.26

M.I. Horbiychuk, R.I. Khrabatyn, V.V. Bandura, N.C. Pasyeka, L.V. Samaniv

Mathematical and Computer Modeling of Soil Contamination in Halych District Based on the Theory of Neural Networks

Разработан метод математического моделирования загрязнения грунта на базе теории нейросистем. Метод опробован на фактическом материале, полученном вследствие геохимических исследований загрязнения территории Галичского района. В результате получено семейство линий изоконцентраций, нанесенных на ландшафтную карту территории.

The mathematical modeling method of the soil contamination based on the neural networks theory is developed. The method was tested based on the facts received during the geochemical research of the Halych district contamination. As the result of mathematical modeling, the isoconcentration lines are developed and drawn on the landscape map of the area.

Розроблено метод математичного моделювання забруднення грунтів на базі теорії нейромереж. Метод випробувано на фактичному матеріалі, отриманому внаслідок геохімічних досліджень забруднення території Галицького району. У результаті отримано сімейство ліній ізоконцентрацій, нанесених на ландшафтну карту території.

Problems setting. The mathematical modeling methods of soil contamination in Halych district, offered by us, is based on neural networks theory to provide more precise estimation of elements content in soil in any point of the district. Among the values of such estimates the main values are the concentration or abnormality coefficients of the chemical elements, the percentage abundance of elements, summary contamination values etc.

The main research material

Average percentage abundance of elements in crust is called clark. But in every separate region, depending on the geological structure, soil type, geographical zones and other factors, there will be their own specific percentage abundances of elements. These specific values are called regional background. Therefore, only the concentrations which exceed the clarks and background can be abnormal, and hazardous for normal geoecosystems progress.

Abnormal concentration of the elements in, for example, soil, is calculated using formula:

$$C_a = C_i - C_k - C_f, \qquad (1)$$

where C_k – average abundance of element in crust; [1]; C_f – average element background.

Formula (1) contains undefined variable C_i – concentration of element in soil for specified area. To calculate the value of C_i in any point of the chosen region we need to approximate the research results with mathematical dependence

$$C_i = f(\mathbf{X}, Y), \qquad (2)$$

where X and Y – the location coordinates of sampling points.

The analysis of existing approximation points showed that we should pay attention to the functional approximation method using the neural network theory [2].

As the result of representation $C_i = f(X, Y)$ it is necessary to provide the production of appropriate signals according to the samples and possible signals which were not included in the sample. The second condition makes the sample generating very complex. In general, this problem is not solved, but in every single case we can find the particular solution.

The solution of the function approximation problem (2) is grounded on the Hecht–Nielsen Theorem, proving the possibility of an experimental data approximation by a function of many variables, possibility of quite a general view through a two-layer network with full direct links. Such a network has n neurons in the input layer, $2n+1$ neurons in the hidden layer with pre-known activation functions and m neurons in the output layers with the unknown activation functions.

This theorem is non-constructive, as it defines only presentation of any multivariate function of several variables, using neural networks of fixed size. The characteristics of the activation function of hidden layer and the type of activation function of output layer neurons still remain unknown.

In practice, the requirements of Hacht–Nielsen theorem to the activation functions are satisfied in the following way. In hidden layer neurons the sigma activation functions are used, and for the output layer the linear activation functions are used. During the training the parameters of every single neuron are specified.

One of the possible problems during the training of neural network is non-perception. The problem is when the neural network is good enough for training sample and the standard deviation between the network output and the experimental data is pretty small, but when the new data which are not in the training sample are presented, the error becomes larger. One of the methods to avoid non-perception is to increase network. The other is to regularize the network [2]. Research showed that regularization decreases the non-perception of network, but increases the training time.

The radial basis networks are more effective to avoid non perception [3], because they require more neurons than back propagation neural networks.

In [4] the possibilities of neural networks as the approximators of dependences (2) were analyzed. This analysis was based on the precision of functional dependences $f(x)$ reproduced by neural network. We did the analysis of neural networks, taking into account the non-perception of network, therefore the network was trained on the given approximation nodes; then the $f(x)$ values were calculated in nodes different from the training samples. As the result of such analysis there was made the conclusion that the general regression network from radial basis networks class is the best choice. Fig. 1 shows the results of dependence (2) approximation using the radial basis neural network. The inputs were represented with samples coordinates, which were given as dimensionless quantities using the following formulas:

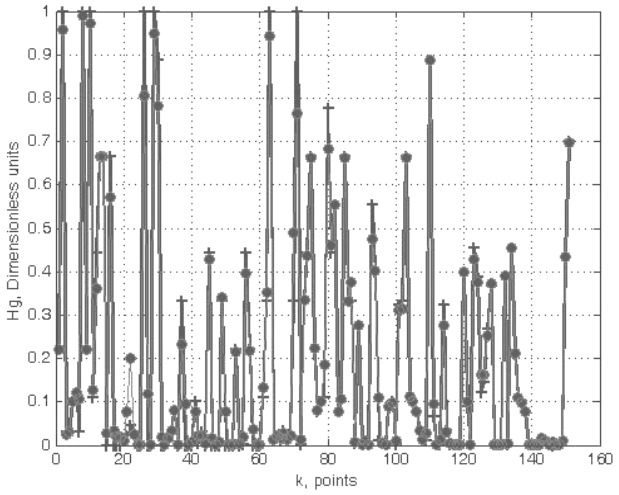
$$x_i = \frac{X_i - X_{\min}}{X_{\max} - X_{\min}}, \qquad (3)$$

$$y_i = \frac{Y_i - Y_{\min}}{Y_{\max} - Y_{\min}}, \qquad (4)$$

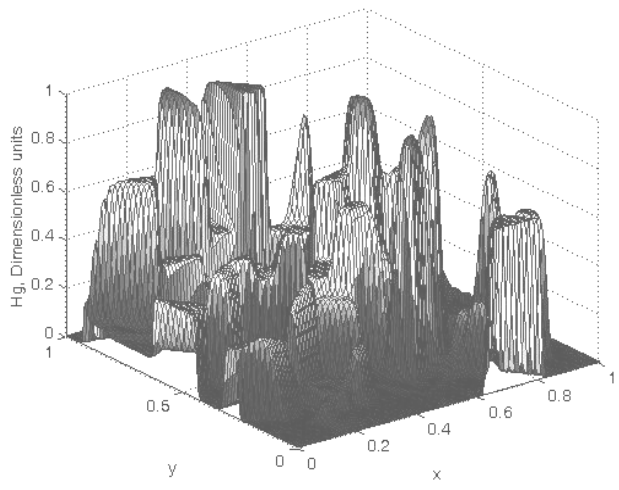
where X_i, Y_i – coordinates of i – th sample, $i = \overline{1, N}$; $X_{\min}$, $Y_{\min}$ – minimal values of X_i and Y_i; $X_{\max}$, $Y_{\max}$ – maximum values of X_i and Y_i; N – sample size.

As the training sample the values of quicksilver concentration in soil $C_{Hg}^{(i)}$, calculated as the results of sample analysis in coordinates X_i, were used. This results were given as dimensionless quantities as well:

$$z_i = \frac{C_{Hg}^{(i)} - C_{Hg}^{(\min)}}{C_{Hg}^{(\max)} - C_{Hg}^{(\min)}}. \qquad (5)$$



a



b

Fig. 1. Results of mathematical modeling of quicksilver concentration in Halych district soils

The last stage of the model construction was the adequacy testing, which consists of the given model testing for usability to solve the problem using the final result. As the adequacy criteria the correlation coefficient was used [5]:

$$K_{zz} = \frac{\sum_{i=1}^{N} z_i^* z_i}{\sqrt{\sum_{i=1}^{N} \left(z_i^*\right)^2 \sum_{i=1}^{N} z_i^2}},$$

where z_i^*, z_i – are the results of modeling and the real values of quicksilver concentration (in relative values) for point i.

The threshold of correlation coefficient is when the $z_i = z_i^*$ is equal to 1. For the given case which shows the high degree of the experimental data equality to the modeling results (Fig 1, *a*). Quicksilver concentration change (in relative values) as the function of coordinates x and y is shown on Fig 1, *b*, which shows that space surface has signified peaks, which tells us about the heterogeny of the quicksilver distribution in soils of Halych district.

The trained general regression neural network gives an opportunity to calculate the quicksilver concentration in the soil in any part of Halych district. To do this we need to calculate the coordinates using the map and calculate the non-dimensional values x_i and using formulas (3) and (4). The results are given to the neural network inputs. As the output of the network we receive the quicksilver concentration z_i^* in non-dimensional quantities. Using formula (5), we can calculate the quicksilver concentration in soil in dimensional quantity (mg/kg)

$$C_{Hg}^{(i)} = C_{Hg}^{(\min)} + z_i^* \left(C_{Hg}^{(\max)} - C_{Hg}^{(\min)} \right).$$

The received value $C_{Hg}^{(i)}$ gives a possibility to calculate the abnormal quicksilver concentration in chosen region of Halych district using formula (1).

The developed method can be used to calculate the abnormal concentration of other elements in soil (Pb, As, Cu, F , Mg etc.).

To estimate the usability of soils to breed the pollution-free production the eco-techno-geochemical maps [6] of specified element dispersion can be recommended. They are built by drawing the harmful chemical elements is concentration lines on the area map. The weak point of this method is that it gives just an average concentration values calculated with the certain step.

The more detailed is the map, the less is the step of isoconcentrations and the bigger is the volume of the real material required for the construction. Also there is the danger to miss the concentration altitudes and this can cause the distorsion of eco-techno-geochemical maps.

Conclusions

The developed method of chemical elements concentration estimation in soils gives an opportunity for automation of mathematical modeling process by construction of real concentration isolines, not their average values. The amount of such lines is unlimited. This makes possible to calculate more precise and fairer eco-techno-geochemical maps. As the example, Fig. 2 shows the quicksilver isoconcentration lines drawn on the Halych district map.

Fig. 2. Isoconcentration lines in Halych district soils

1. *Vinogradov A.P.* The average content of elements in the earth's crust. // Geochemistry. – 1962. – N 7. – P. 555–557.
2. *Kruglov V.V.*, *Borisov V.V.* Artificial neural networks. Theory and practice. – M.: Hotline – Telecom, 2001. – 382 p.
3. *Osovsky S.* Neural networks for information processing. – M.: Finance and Statistics, 2004. – 344 p.
4. *Horbiychuk M.I.*, *Kohutiak N.I.*, *Kuznetsov E.A.* Identification of static characteristics of technological objects based on neural networks. // Measuring and computing in industrial processes. – 2002. – **2**, N 9. – P. 139 – 145.
5. *Handbook* of standard simulation programs. / A.G. Ivakhnenko, U.V. Kopp, V.S. Stepashko et al. / Ed. Ivakhnenko A.G. – K.: Technique, 1980. – 184 p.
6. *Adamenko O.M.*, *Rud'ko G.I.*, *Konsevych L.M.* Ecological mapping. – Ivano-Frankivsk: Polumya, 2003. – 584 p.

Поступила 30.12.2014

E-mail: *ksm@nung.edu.ua*, *romankhr@yahoo.com*, *vikaban@gmail.com*, *leuro@list.ru*