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Prediction levels of heavy metals (Zn, Cu and Mn) in current Holocene deposits of the eastern part of the Mediterranean Moroccan margin (Alboran Sea)

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Abstract: *The Alboran basin is part of the bético Rif chain and represents a point of exchange through the Strait of Gibraltar between the Atlantic Ocean to the west and the Algerian-Balearic Basin to the east.*
The purpose of this work is placed in the prediction of levels of heavy metals (Zn, Cu and Mn) in the Holocene to current deposits in the eastern part of the Moroccan Mediterranean margin of the Alboran sea, using the Artificial Neural Networks MLP-type RNA (Multi Layer Perceptron) non recurrent and supervised learning.
Various tests of robustness as: Akaike Information Criteria, Root Mean Square Error, and Maximum Average Percentage Error, allow the choice of the architecture of the neural network. The backpropagation algorithm is used to determine the weights and biases of the neural network. Based learning and test consists of 50 samples (observations) of sediment analyzed at four sampling stations. The independent variables are sedimentological, mineralogical and geochemical parameters. These parameters are: bathymetry, depth levels in carrots,% of sand, the fine fraction <40 microns,% CaCO3,% illite, % Smectite and %Kaolinite + % chlorite. The dependent variables (to predict), which are three in number, are the heavy metal contents (Zn, Cu and Mn) of the sediment. A comparative study has been established between the neural prediction model MLP type and conventional statistical models that is multiple linear regression MLR. The performance of ANN-MLP model clearly shows themselves higher than those established by multiple linear regression MLR.
Keywords: *Prediction, Neural Networks MLP type, robustness tests, Multiple Linear Regression, heavy metals, Alboran Sea.*

I. INTRODUCTION

Neural networks have found great success in the simulation and prediction of environmental parameters. Indeed, Perez et al. (2001), [1] suggested providing the concentration of NO2 and nitric oxide NO in Santiago based on environmental variables and using the method of linear regression and neural networks. Another example of application of these networks is the prediction of the concentrations of heavy metals in Moroccan river sediments from a number of physico-chemical parameters [2]. Recently, in our study, El Hmaidi et al. (2013) [3] found very good results using the method of neural networks for the prediction of organic carbon in the Pleistocene deposits - Holocene of the Alboran Sea from sedimentological, mineralogical and geochemical parameters.

Adopting the same approach, the present work attempts to use artificial neural networks in the development of mathematical models for stochastic modeling of heavy metal contents in the Holocene deposits to current. This focuses on four samples of type "Box Cores" intersected in the Mediterranean continental margin Moroccan on one hand, and secondly of Al Hoceima Bay located south of the Alboran Sea.

This is the prediction of the contents based on sedimentological, mineralogical and geochemical parameters using Artificial Neural Networks ANN MLP type (Multi Layer Perceptron) non-recurrent and supervised learning. The data used come from previous work in the Alboran Sea [4]. The study was performed in order to see the distribution of heavy metals in the first 50 cm of the sediment column to determine firstly the degree of anthropogenic contamination based on Cu, and Zn and on the other hand Mn was chosen because of its oxides play an important role in determining trace metals.

The expected results should lead to equations and models that specify the relationships between levels of heavy metals and other environmental parameters and therefore to modelize and predict these levels in Holocene to existing deposits in the study area.

II. PRESENTATION OF THE STUDY AREA

The study area is located in the southern part of the Alboran Sea at the Moroccan Mediterranean margin between longitude 3 ° 00 'W and 4 ° 00' W (Fig. 1 and 2). The geology of the backcountry is characterized from the West to the East by three major areas of the Rif orogeneese bético [5, 6]. Thus, areas of flyshs are represented by tablecloths equipment marly limestone or sandstone of Cretaceous to Cenozoic. The internal zones are formed of metamorphic basement, tablecloths Paleozoic material and limestone ridge. The external zones are composed of a complex allochthonous group, marl schistose dominance (Fig. 1).

The morphology of the study area is characterized mainly by the presence of the Alboran Ride [7]. It is a complex area anticlinal oblique to the coast. It consists of a number of benches submerged at shallow depth (<100m) separated by deeper areas. It defines in the South western basin a narrow furrow which expands to the east towards the Algerian-Provencal basin.

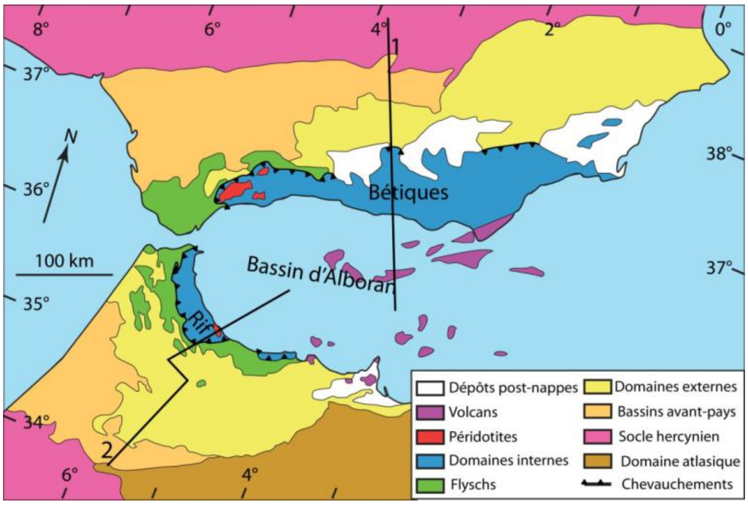

Fig. 1. Simplified geological map of the Betic-Rif chain ([5] modified by [6]).

III. MATERIALS AND METHODS

Four samples were taken from both sides of the Al Hoceima Bay with a core large section type "Box Cores" when oceanographic mission Albosed II in 1986 [4]. The "Box" B11 and B12 were taken respectively 400m and 300m depth on a very narrow north and south of the bench Xauen continental shelf. In addition to the East, Box B07 and B08 were performed successively 230m and 600m depth off the Bay Betoya on a broad continental shelf of about 15 km (Fig. 2). The geographical coordinates of the samples are summarized in Table 1.

Tab. 1. Geographical coordinates of samples studied.

Box	Latitude N	Longitude W	Depth (m)	Lenght (cm)
B07	35° 21' 77''	03° 19' 11''	230	25
B08	35° 27' 48''	03° 21' 55''	600	40
B11	35° 18' 01''	04° 20' 52''	400	40
B12	35° 25' 57''	04° 20' 10''	300	25

After opening carrots, samples were collected in thin slices of 2 cm. $CaCO_3$ contents were made by Bernard calcimetry on gross sediment finely milled. Separation of sand and pelitic fractions was performed by sieving the water on sieve 40µm. The clay minerals were analyzed by X-ray diffractometry from deposit focused on blades. The diffractometer used is a 1729 copper anticathode Philips. The geochemical study focused on the fine fraction (<40µm).

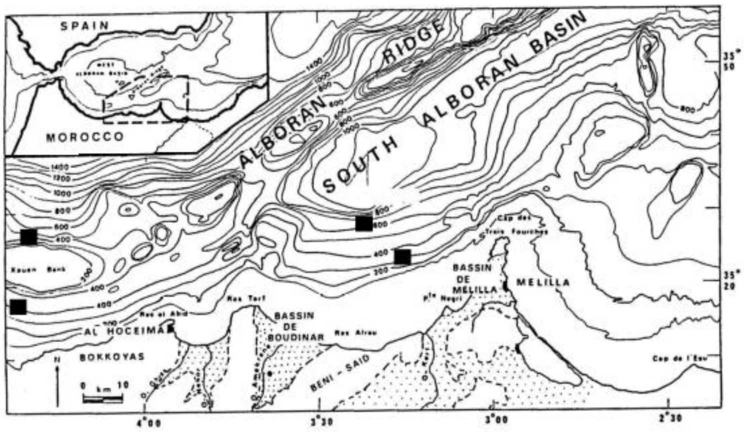

Fig.2. Bathymetry of the eastern part of the Moroccan Mediterranean margin, with positions of Box Cores studied.

Trace metals (Zn, Cu, and Mn) were dosed using an atomic absorption spectrometer; model Philips SP 9000 using the selected method recommended by several authors [8, 9]. For each sample, 1 g of sediment was mineralised at 140 °C for 30 min in the presence of aqua regia (a mixture of 25% HNO3 and 75% HCl). The mineral deposit is taken by successive rinsing with ultra-pure and filtered through a membrane of 0.45 microns and filled to a volume of 50ml water. The Zn, Cu and Mn are given in mg / g.

The modeling approach for the prediction of heavy metal contents in the current Holocene deposits is the formal or artificial neural networks [10, 11]. The database consists of 50 samples. For each sample, 8 parameters sedimentological, mineralogical and geochemical were considered (bathymetry, depth levels in carrots,% of sand,% of the fine fraction <40µm,% CaCO3,% illite, % smectite and% kaolinite + % chlorite).

IV. RESULTS

IV.1 Normalization and data pre-processing

In general, the database must undergo pre-processing to be adapted to the network inputs. The basis of learning consists of eight vectors x1, x2, ..., x8, independent and normalized between 0.1 and 0.9 [12] that are bathymetry, depth levels in carrots,% of sand, the fine fraction <40 microns,% CaCO3,% illite, % Smectite and% kaolinite + %chlorite.

$$x_{i\ new}^{k} = 0,8 * \frac{x_{i\ old}^{k} - \min(x_i)}{\max(x_i) - \min(x_i)} + 0,1$$

The database is composed of 50 vectors, and each vector is to dimension eight. Therefore, the size of the network inputs is eight.

IV. 2 Development of models of artificial neural network MLP

Neural networks are powerful techniques of nonlinear data processing, which have proven themselves in many fields. Therefore, the artificial neural networks have been applied in various fields' prediction.

The various models of artificial neural network used in this work have been developed and implemented with the programming language C + + on a machine I3 PC, 2.4 GHz and 3 Gb of RAM.

The artificial neural network consists of an input layer, a hidden layer and an output layer. The input variables X = (x1, x2, ..., x8) independent and standardized between 0.1 and 0.9 and then presented to the input layer of the neural network that contains eight. They are first multiplied by the weight IW, and then added to IB bias that exists between the input layer and the hidden layer. Neurons in the hidden layer receive the weighted signals. After addition, they transform them by using a nonlinear sigmoid function S (.). Given by the equation:

$$S(n) = \frac{1}{1 + \exp(-n)}$$

The following mathematical model S (IW * X + IB) is presented to the input of the output layer. This model will be multiplied by the weight LW then added to the bias LB that exist between the hidden layer and output layer, and finally transformed by a nonlinear sigmoid function S (.).

Finally, we obtain the mathematical model of artificial neural network as follows:

S {LW * S (IW * X + IB) + LB}

The backpropagation algorithm was used to train the artificial neural network in a fast and robust manner. The analysis was restricted to networks that contain a single hidden layer, since this architecture is able to predict all outputs.

IV. 3 - Robustness tests

To choose the "best" architecture of neural network, several statistical tests are commonly used; in our case we used statistical tests Root Mean Square Error RMSE, Maximum Average Percentage Error MAPE and Akaike Information Criteria. This last criterion that seeks to minimize proposed by Akaike (1973) [13] is derived from the theory of information, and is based on the measurement of Kullback et al., (1951) [14]. It is a model selection criterion that penalizes models for which the additions of new variables do not provide enough information to the model. These tests are given respectively by the following equations:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{i=N}(E_{pi} - E_{ai})^2}{N}}$$

$$MAPE = \frac{1}{N}\sum_{i=1}^{N}\frac{|E_{pi} - E_{ai}|}{E_{ai}} * 100$$

$$AIC = \ln\left(\frac{N}{2} * L_F\right) + \frac{2N_w}{N}$$

With: LF is the cost function (mean square errors).

$$L_F = \frac{1}{N}\sum_{i=1}^{i=N}(E_{pi} - E_{ai})^2$$

Ea and Ep are the values of the target vector and prediction vector of output neuron of the network. N represents the number of test samples studied, and Nw is the total weight and bias used for each architecture. Figures (3-5) RMSE, MAPE and AIC-after 4500 iterations for different number of neurons in the hidden layer, give the possibility to choose 8 neurons to the hidden layer. We then get the 8-8-3 architecture as "best" configuration of the neural network for its good predictive ability.

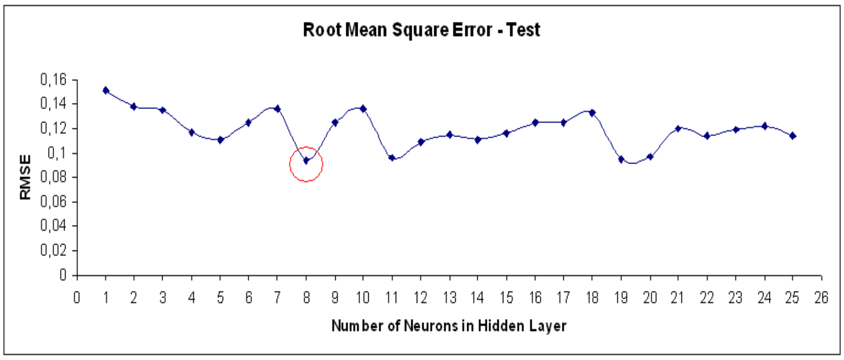

Fig.3. Robustness test: Root Mean Square Error.

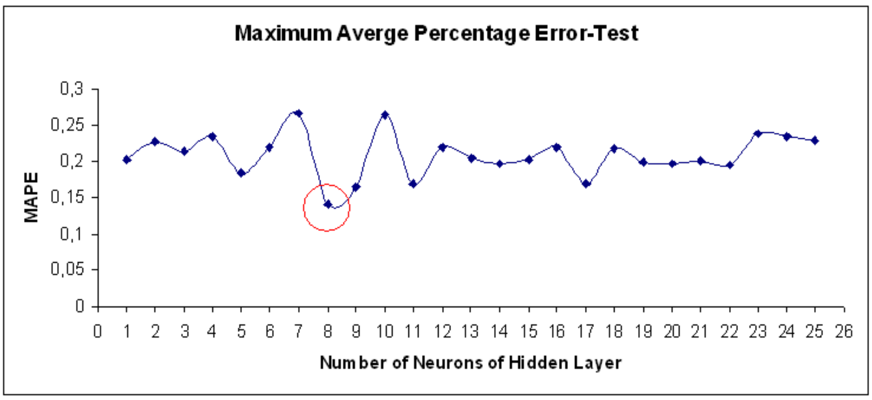

Fig.4. Robustness test: Maximum Average Percentage Error.

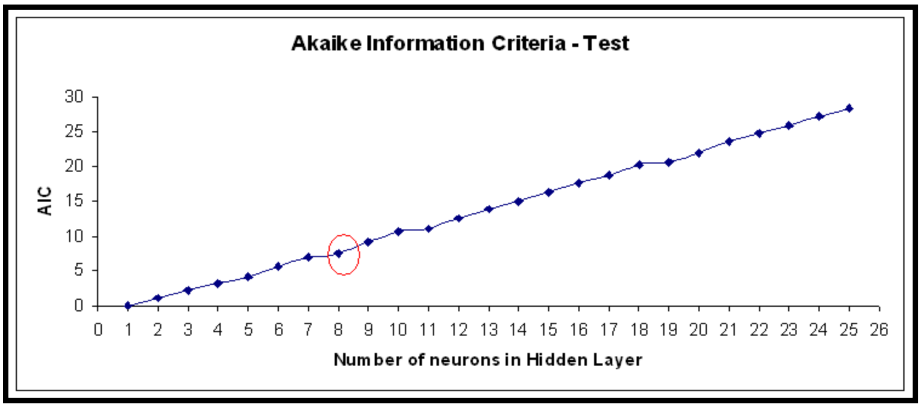

Fig.5. Robustness test: Akaike Information Criteria.

IV.4 Learning and validation

The artificial neural network MLP "Multi Layer Perceptron" consists of an input layer containing eight neurons, a hidden layer containing eight neurons and an output layer containing three neurons (Figure 6).

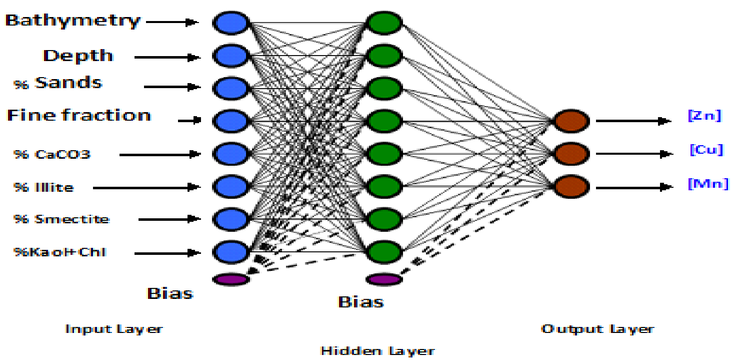

Fig.6. Neural network (architecture 8-8-3).

The basis learning consists of eight vectors x1, x2, ..., x8, independent and normalized between 0.1 and 0.9 are: bathymetry, depth levels in carrots,% sand, the fine fraction <40 microns,% CaCO3,% illite, %Smectite and% kaolinite + %chlorite respectively.

The learning base of the neural network consists of 30 samples. The weights and biases of the network were readjusted using the backpropagation algorithms. Once the architecture, weights and biases of the neural network have been set, you need to know if this neural model is capable of being generalized.

Validation of neural architecture [8-8-3] is therefore to assess its ability to predict the concentrations of heavy metals (Zn, Cu and Mn) sediments using the weights and biases calculated during the training for applying them to another tests database composed by 20 sample which means 40% of the total data.

The ANN model [8-8-3] gave a correlation coefficient for the testing and validation of 0.882073, which is equivalent to a mean square error of 0.09407 and 7.475 for AIC.

Figures (7-9) show the results of prediction of the contents of heavy metals (Zn, Cu and Mn) in the Late Quaternary deposits of the eastern part of the Mediterranean Moroccan margin of the Alboran Sea, it is remarkable based on these figures that the test data that consists of 20 samples are perfectly modeled.

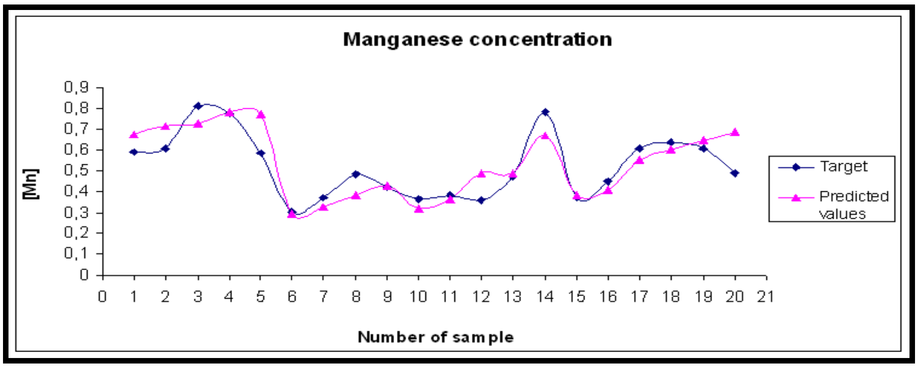

Fig.7. Test result of predicting the model Manganese content of RNA-MLP [8-8-3].

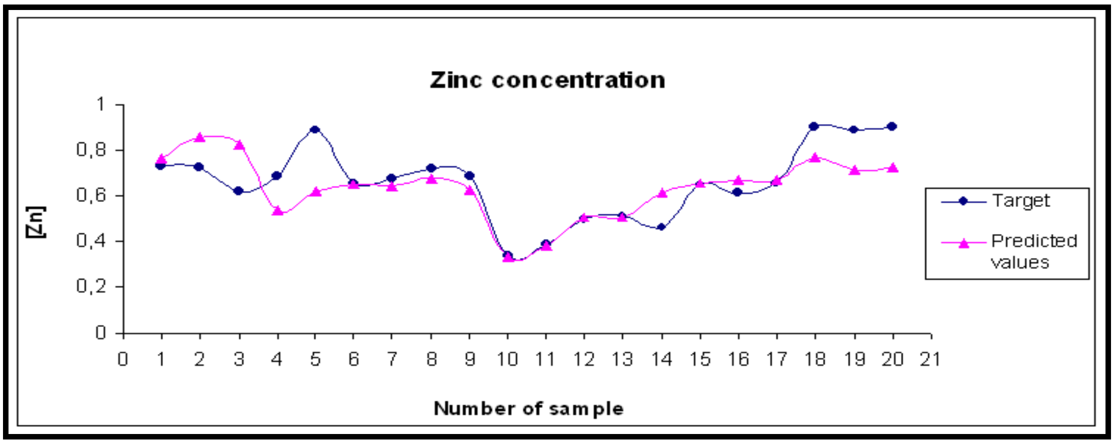

Fig.8. Test results for predicting the content of Zinc Model RNA-MLP [8-8-3].

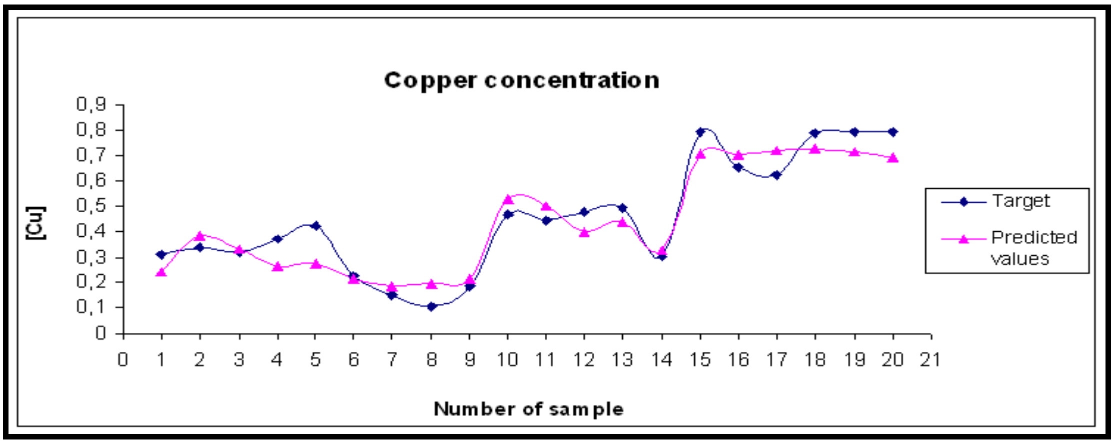

Fig.9. Test results of predicting the copper content of the model RNA-MLP [8-8-3].

We evaluate the quality of prediction of neural architecture [8-8-3] by the correlation coefficient. In our case the correlation coefficient is 88.2073%.

V. COMPARISONS AND DISCUSSIONS

To assess the performance of the method RNA-MLP [8-8-3], we compared this method with other methods namely Multiple Linear Regression MLR.

The correlation coefficient calculated by RNA-MLP [8-8-3] was significantly higher (88.2073%), however, the correlation coefficients calculated by the MLR are lower (between 0.266 and 0.710). On the other hand, the correlation coefficients obtained by testing the validity of the models established by the RNA (88.2073%) are significantly similar to those related to learning (92.2588%), unlike the correlation coefficients of the tests the validity of the models for the RLM, are widely different from those obtained during learning (see Table 2).

Tab. 2. Correlation coefficients obtained by MLR and ANN - MLP [8-8-3] concerning zinc, copper and manganese.

Method	Zn		Cu		Mn	
	Learning	Test	Learning	Test	Learning	Test
RLM	0.677	0.266	0.943	0.689	0.758	0.710
RNA	0,922588	0,882073	0,922588	0,882073	0,922588	0,882073

VI. CONCLUSION

The prediction of levels of heavy metals from sedimentological, mineralogical and geochemical data in the current Holocene deposits of the Alboran Sea was performed using neural networks. Neural networks are used to non-recurring layers, with Levenberg Marquardt algorithm and supervised learning.

The results show a significant capacity for learning and prediction for heavy metal contents with a coefficient of determination of 88.2073% and a very low maximum square error of 0.09407 for the database used in addition to a better choice of the network architecture achieved through statistical tests of robustness.

For multiple linear regression, the results are less significant with a coefficient of determination between 0.266 and 0.710. This shows that the parameters are associated with the levels of heavy metals by a non-linear relationship. For the prediction of heavy metal contents in the current Holocene deposits of the Alboran Sea, the use of a neural model configuration [8-8-3] gave better results.

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