11th Symposium on Neural Network Applications in Electrical Engineering, NEUREL-2012
Faculty of Electrical Engineering, University of Belgrade, Serbia, September 20-22, 2012

Radial Basis Function Network Based Feature Extraction for Improvement the Procedure of Sourcing Neolithic Ceramics

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***Abstract*— Modern studies of a cultural heritage objects are increasingly multidisciplinary. A variety of analytical techniques supported by pattern recognition methods can help in answering about the origin, dating or authenticity. Results of sourcing ceramics from three Neolithic sites in Serbia are shown in this paper. The procedure based on radial basic function networks (RBFN) was employed in ceramic characterization. The results obtained were tested in previously established procedure for origin of production determination.**

***Index Terms*—Radial basis function network, Feature extraction, Dimension reduction, Pattern recognition, Classification.**

I. Introduction

ARCHAEOLOGICAL ceramics can be studied in the context of origin of production or production technologies, as well as the distribution of specific ware types or whole assemblages [1]. Such studies have at their disposal an arsenal of different techniques, both analytical [2] and statistical [3], to arrive at answers to archaeological issues. One of the non-destructive techniques that have been most commonly used is energy dispersive X-ray fluorescence (EDXRF). During the past ten years the use of portable XRF (PXRF, pXRF), field-portable (FPXRF) or handheld XRF spectrometers has increased significantly [4]. Such instruments (and consequently technique) become affordable for many applications that generate fast results which imply almost immediate interpretation and decision. On the other hand, different supervised as well as unsupervised multivariate statistical methods are widely and successfully used in archaeometric data analysis. Multivariate statistical methods can be used in provenience studies of artefacts, as well as for the recognition of local ceramic production and its characterisation, distinguishing from objects of possible trading activities, production dating, etc. The objective of this research was to examine the possibility of improving the existing decision-making procedure [5], in the sense of *in-situ* working conditions and working in real or semi-real time. The procedure was derivate to use the information obtained by pEDXRF spectrometry to classify ceramics, excavated at three Neolithic sites: Vinča-Belo Brdo near Belgrade, Pločnik near Prokuplje, and Bubanj near Niš, all in Serbia, according to elemental compositions and well-known provenance.

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II. Algorithm for Sourcing Ceramic

A. Structure of the algorithm

An automated decision-making procedure has been designed to reach the answers about origin of ceramic production. The methodology is based on the characteristics of the ceramic paste (elemental content obtained by pEDXRF spectrometry analysis) and statistical pattern recognition methods (dimension reduction and classifier design based on the desired output). The entire procedure is structured as algorithm (Fig. 1) enabling rapid, simple and effective decision-making. The procedure can have an important role as a support tool by decision-makers.

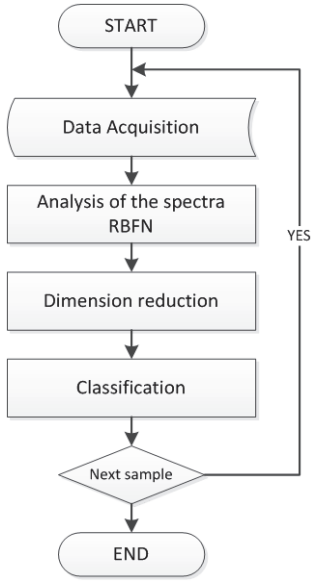

Fig. 1. Structure of the algorithm for decision-making procedure.

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B. Data Acquisition

Decision about origin of ceramic production is based on the elemental content of ceramic body which has been obtained as the result of non-destructive analysis using portable EDXRF spectrometer. The whole methodology is based on the non-destructive and non-invasive approach in the analysis which can easily be performed directly on the archaeological sites. Data acquisition can be performed within 100s, to reach the satisfactory counting statistics. This is of significant importance, due to *in-situ* measurement conditions. After a 100s of measuring time viable information about ceramic object characteristics is available for further processing.

The ceramic sample is exposed to X-rays emitted from cathode tube exciting characteristic X-rays spectra in material, which has been detected using SiPIN X-Ray detector associate with preamplifier, digital pulse processor and multi-channel analyzer or spectra acquisition. In 2048 channels all received impulses has been registered.

C. Analysis of the spectra

The common approach in analysis of the spectra is to convert the obtained data into elemental concentrations (expressed as weighted percentage or in ppm) which significantly increases the time necessary to obtain the results due to measurements of standard referent material and performing appropriate corrections.

Following the demand that decision-making procedure have to be rapid, it is recommended to use the so-called raw spectra data. ADMCA is one of the commonly used software for the analysis of the EDXRF spectra. The software enables setting regions of interest (ROI), computing ROI information (centroid, total area, net area-NPA, FWHM, as shown in Fig. 2) which was used to generate input *n*-dimensional vector for dimension reduction purpose. The procedure of ROI settings is extremely dependent on operator experience. It is the only one not automated step in the decision-making algorithm implying not only the dependence of human experience, but significant time consumption in the decision making.

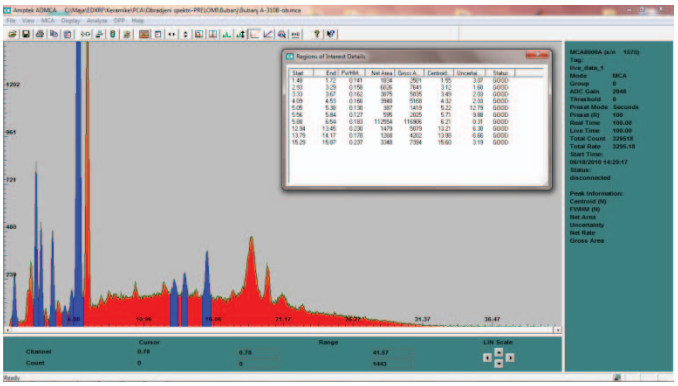

Fig. 2. Generating the *n*-dimensional vector that describes the measurement using ADMCA software package.

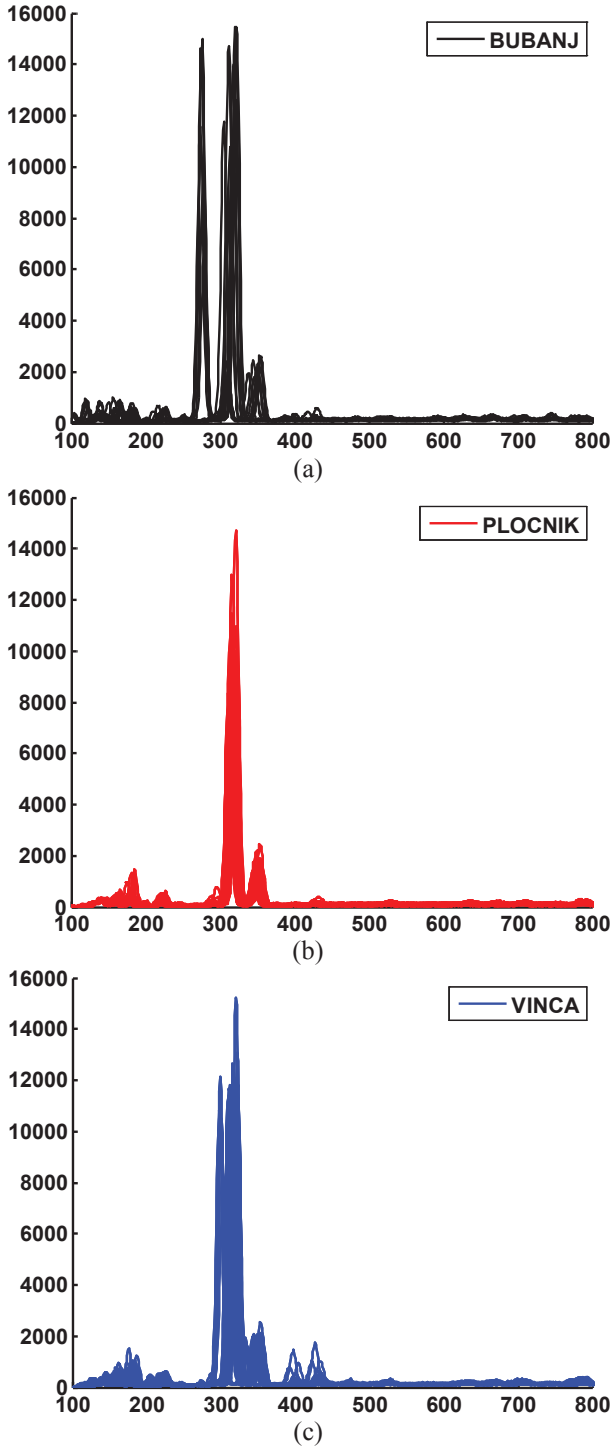

Fig. 3. Measured spectra of samples with different origin. Each subfigure represents spectra of all samples from one location. Neolitic site of: (a) Bubanj, (b) Plocnik, (c) Vinca

D. Dimension reduction

As the dimension reduction of the original space is only one step in the procedure whose goal is classification, the scattering matrices-based dimension reduction method was used proven to be the most appropriate choice [5]. The main advantage of dimension reduction performed in such way as to preserve class membership is two-fold. First, in low-dimensional space it is possible to visualize the classification results and choose the appropriate classifier design approach.

Second, it is possible to identify the important measurements with regard to classification. Dimension reduction consists of finding a transformation matrix A

$$Y = A^T X$$

which will reduce the original data space (X) dimensionality in the new (Y) one, considerably lower dimensionality. The optimal transformation matrix A is the explicate solution of the optimization criterion

$$J = tr(S_w^{-1} S_b)$$

obtained as the solution for the generalized singular value decomposition of the matrix $S_w^{-1} S_b$ (where S_w and S_b represent the within-class scatter matrix and between-class scatter matrix, respectively). The m eigenvectors correspond to the m largest eigenvalues form the matrix A [6]. Two-dimensional projection is the most desirable, allowing examination of the classification results in terms of recognition ability (percentage of members of the training set correctly classified) and prediction ability (percentage of members of the test set correctly classified using the rules developed during the training).

E. Classification

Following dimension reduction, it becomes possible to classify the reduced vector (newly formed vector $Y = [y_1 \; y_2]^T$), into one of the classes. The choice of the most proper classifier is dependent on the dimension reduction, since it was performed in that manner to preserve class separability as much as it is possible. Also, the visualization in two (or three) dimension allows choosing the proper classifier type in order to achieve the best classification results in the terms of prediction and recognition ability.

It is of importance to perform the testing of the classification that was achieved. Several approaches are available for that purpose.

III. Radial Basis Function Network

The radial basis function network (RBFN) [7] has the architecture of the instar-outstar model (Fig. 4) and uses the hybrid unsupervised and supervised learning scheme, unsupervised learning in the input layer and supervised learning in the output layer.

The purpose of the RBFN is to pave the input space with overlapping receptive fields. For an input vector x lying somewhere in the input space, the receptive fields with centres close to it will be appreciably activated. The output of the RBFN is then the weighted sum of the activations of these receptive fields.

The RBFN is designed to perform input-output mapping trained by examples, pairs of inputs and outputs (x, y). The hidden nodes in the RBFN have normalized Gaussian activation function:

$$z_q = g_q(x) = \frac{R_q(x)}{\sum_k R_k(x)} = \frac{\exp\left(-\frac{|x - m_q|^2}{2\sigma_q^2}\right)}{\sum_k \exp\left(-\frac{|x - m_k|^2}{2\sigma_k^2}\right)}$$

where x is the input vector and z_q output of hidden layer. m_q and σ_q are the mean (an m-dimensional vector) and variance of the q-th Gaussian function in hidden layer.

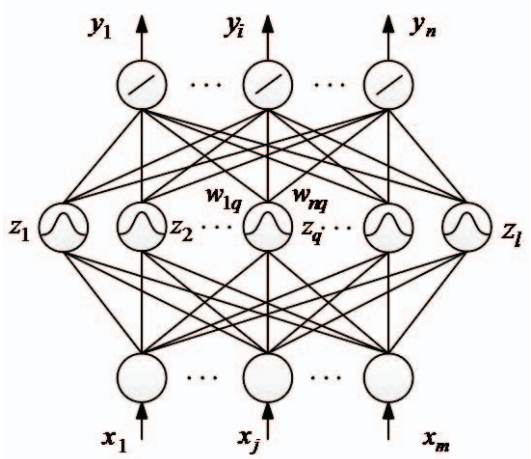

Fig. 4. Radial basis function network structure, with m inputs, l nodes in hidden layer, and n outputs

The output of the RBFN is simply the weighted sum of the hidden node output:

$$y_i = a_i\left(\sum_{q=1}^{l} w_{iq} z_q + \theta_i\right)$$

where a_i (.) is the output activation function, generally linear function, and θ_i is the threshold value.

The weights in the output layer can be updated simply by using the delta learning rule (supervised learning). The unsupervised part of the learning involves the determination of the receptive field centres m_q and widths σ_q, q = 1, 2, ..., l. The proper centres m_q can be found by unsupervised learning rules such as the vector quantization approach, competitive learning rules, or simply the Kohonen learning rule.

Another learning rule for the RBFN with node-growing capability is based on the orthogonal least squares learning algorithm [8].This procedure chooses the centres of radial basis functions one by one in a rational way until an adequate network has been constructed, or maximal number of nodes is reached.

The RBFN offers a viable alternative to the two-layer neural network in many applications of signal processing, pattern recognition, control, and function approximation. It has been shown that the RBFN can fit an arbitrary function with just one hidden layer[9], but they cannot quite achieve the accuracy of the back-propagation network. Although, RBFN can be trained several orders of magnitude faster than the back-propagation network, and this is very important advantage in real or semi real time applications.

A. Application of the RBFN for feature extraction

This paper presents a procedure for chemical spectrum estimation and extraction of features based on the application of RBFN. For purposes of determining the origin of pottery, it is extremely important to accurately determine the concentration of individual chemical elements that are of interest. Using pXDRF is not possible, in the measurement and data acquisition phase due to instrument construction and measurement procedure, to get the individual chemical elements as a single line in the spectrum. Each element is obtained as the range of values with the Gaussian distribution, and centre around the expected value for a given element. From this it can be concluded that the entire range of analysed materials can be described as the sum of the corresponding normal distribution function, with corresponding centres, and the amplitudes representing concentration of element in material.

This led the authors to conclude that the training of RBFN can obtain a neural network which can approximate measured chemical spectra with high accuracy and minimum deviation. It is now possible to extract features that efficiently describe the unknown material, i.e. uniquely determine the vector of characteristics of a given sample. This feature vector will be composed of pairs that describe each node in the hidden layer, i.e. its position in the spectrum (m_q) and weight of the output neuron w_{1q}, which represents the energy of the individual components in the spectrum (amplitude of corresponding radial function). The number of such pairs is determined by the desired accuracy that is needed to describe the corresponding chemical spectra. Increasing the number of pairs (ie, adding a number of chemical elements in analysis) increases the accuracy of the approximation with RBFN in given input range.

Variance of the Gaussian functions in hidden layer, is determined by the instrument characteristics and measuring procedure for the particular instrument. This value is obtained at the beginning of the procedure, and then it was set to a constant value. This step significantly speeds up the training of neural network. Number of nodes in the hidden layer is determined on the basis of previous experience [5], where was determined what the chemical elements affect efficient separation of classes. In this paper, we adopt that the number of nodes is 15, i.e. feature vector consists of 15 values, which describe the concentration of individual, pre-defined chemical elements.

Such efficient and fast procedure (Fig. 5) eliminates the human factor in the determination of the chemical composition on the based on the measured spectra, and thus a significant source of error. It is important to note that determining the threshold value θ_1 in the output layer, instruments offset and fon environment is automatically compensated, and thus increases the accuracy of the procedure.

IV. Results and Discussion

Using RBFN fifteen features were extracted from the 2048 data derived during measurements. In such manner 67 fifteen-dimensional vectors were generated to describe all samples within three classes. After scattering matrix based dimension reduction performed on 15-dimensional vectors, 67 new two-dimensional vectors were created as it can be seen in Fig. 6. Next step that follows dimension reduction is classification. A hierarchical classification method based on one sequentially chosen class out of two classes has been performed since the three classes presented in Fig. 6 are not quite separable from each other (especially the classes representing the sites of Pločnik and Vinča). The third class (representing the site of Bubanj) is separated from the other two in such a way that it is possible to determine the linear segments which differentiate from the two patterns without any classification error. In this case proper classification has been achieved by designing a linear classifier, based on the desired output ($h_1(Y)$).

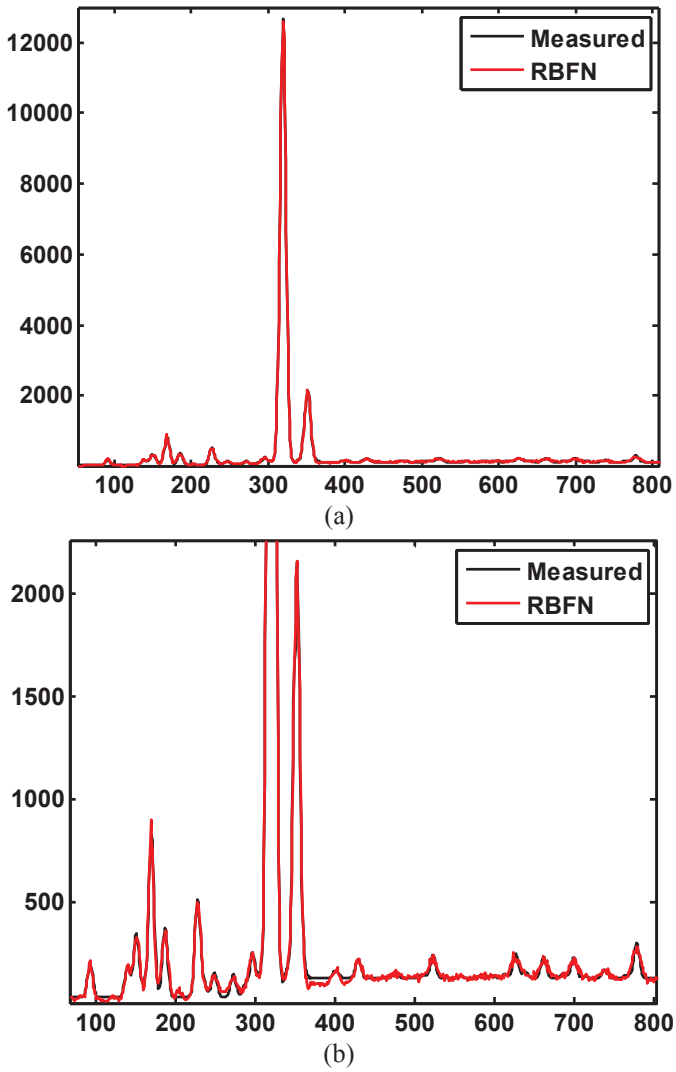

Fig. 5. Radial basis function network approximation of measured spectra: (a) original spectra, (b) magnified

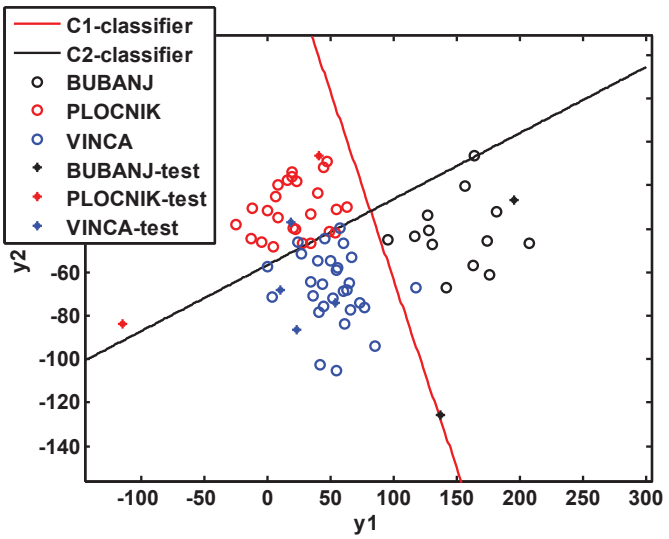

Fig. 6. Classification results: linear classifiers and test samples shown together with classified training samples

Following the demand that the decision – making procedure should be rapid, simple and effective in classification of unknown samples, it is reasonable and justifiable to perform the second classification of the Vinča and Pločnik classes using the simplest classifier of the linear discriminatory function type. It is now necessary to decide whether the new vector *Z* belongs to the Bubanj excavation site or not. If it does not belong to Bubanj (h_1 will have a negative value), the next step is to choose between the Pločnik and Vinča excavation sites (h_2 positive value indicates the Pločnik site while the negative value of h_2 indicates that the analysed sample belongs to the Vinča group). The classification results are presented in Table 1. The recognition ability of the classification performed using RBFN for feature extraction is 95.5 %, while it was 89.6 % of correctly classified samples when training data was created using net peak area values.

TABLE 1.
CLASSIFICATION RESULTS

			Predicted Group Membership						
			Bubanj		Plocnik		Vinca		Total
			NPA	RBFN	NPA	RBFN	NPA	RBFN	
TRS	Count	1	13	12	0	0	0	1	13
		2	0	0	22	25	3	0	25
		3	1	0	3	2	25	27	29
	%	1	**100**	**92,3**	0	0	0	7,7	100
		2	0	0	**88**	**100,0**	12	0	100
		3	3,4	0	10,3	6,9	**86,2**	**93,1**	100
Cross validated	Count	1	10	9	1	0	2	4	13
		2	0	0	18	19	7	6	25
		3	1	1	5	6	23	22	29
	%	1	**76,9**	**69,2**	7,7	0	15,4	30,8	100
		2	0	0	**72**	**76,0**	28	24,0	100
		3	3,4	3,4	17,2	20,7	**79,3**	**75,9**	100

	Recognition ability [%]	**Prediction ability [%]**
NPA	89,6	76,1
RBFN	95,5	74,6

The success of the classification model was tested by the leave-one-out cross validation method [10, 11]. Only analysed cases were cross validated, and each case was classified using the functions derived from all cases other than that case. The achieved prediction ability was 74.6 % (comparing to 76.1 % in the case of using NPA values) of cross-validated grouped cases correctly classified.

Another test of the classification model was performed. Two (h_1 and h_2) linear classifiers designed in the training step were used for the classification of the eight vectors belonging to the TDS. The results (Fig. 6) show that only one sample from the TDS was not correctly classified using the model developed during the training process.

V. CONCLUSION

According to the results presented, several conclusions can be drawn. Algorithm of the proposed decision-making procedure enables effective classification of ceramic artefacts based on their elemental compositions determined by pEDXRF spectrometry.

As shown, the data from the first algorithm step, denoted as in-situ data acquisition, can be used as a viable tool for sourcing ceramics.

Application of the RBFN feature extraction, as the next step, has proved to be an extremely powerful tool.This procedure can efficiently obtain the concentration of chemical elemental particles from the chemical spectrum of analysed piece of material. This RBFN aided procedure is fully automated, and thus eliminates the factor of human error in the calculation of the chemical content of a given sample, and that without losing the accuracy. On the contrary, by applying the proposed method can solve the two important issues, namely the appearance of offset and overlap of two close chemical elements, when you need to carry out deconvolution, which is not a simple procedure.

The next step in algorithm, denoted as dimension reduction from 15-dimension space to the 2D space, gave significant results, and it is possible to achieve the initial goal (expressed through the classification of ceramics based on the elemental composition) by a method founded upon dimension reduction, which has scattering matrices as its basis and which takes into account minimal information loss.

According to the results obtained, successful classification is shown, based on RBFN supported feature extraction and scattering matrices dimension reduction. Expressed through prediction and recognition ability, allows the application of this method for the identification of objects based on their well-known provenance and that the proposed decision-making procedure yields satisfactory classification results.

ACKNOWLEDGMENT

This research was supported by Serbian Ministry of Education and Science (Projects TR37021, TR32038 and III42007).

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