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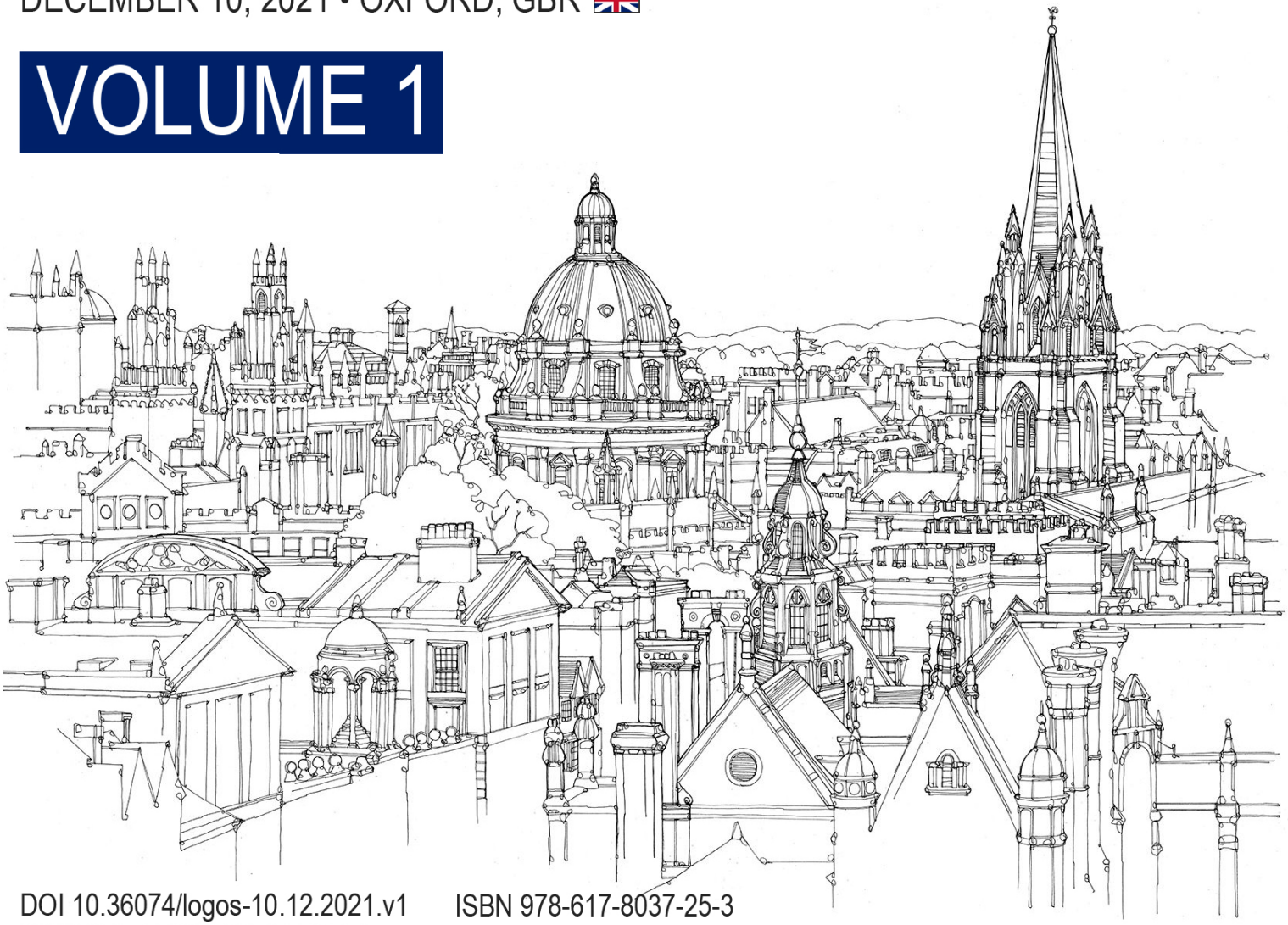
DECEMBER 10, 2021 • OXFORD, GBR

VOLUME 1



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SECTION XII. CHEMISTRY, CHEMICAL ENGINEERING AND BIOENGINEERING

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COMPARISON OF ARTIFICIAL NEURAL NETWORKS AND TRADITIONAL CLUSTERING METHODS

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Actuality. Classification of objects proceeding from their numerical characteristics is considered to be the main tool of modern qualitative chemical analysis. Classification is widely used to extract useful information from multivariate experimental data for foodstuff, drugs, environmental objects, materials, substances, industrial wastes, etc. Artificial neural networks have received much attention recently. Thanks to their adaptive structure and learning capability, they are success fully used to solve classification, identification and prediction tasks [1, 2].

Theoretical details. A new clustering procedure based on the combination of the unsupervised Kohonen and supervised probabilistic artificial neural networks (PNN) was created like M-script program in the software package MATLAB 7.11b. The approach has been demonstrated to be efficient for the classification of a large set of solvents. The additional use of the leave-one-out cross-validation procedure has improved the results. The final solvent classification is meaningful and chemically interpretable [3]. The main steps of the proposed procedure are as follows:

1) to classify objects with the use of the Kohonen neural network at different assigned numbers of classes;

2) to reveal groups of objects which were assigned to the same classes independently of the prescribed number of classes; these objects form the first set for training the PNN;

3) to form testing sets of approximately equal sizes from the remaining objects;

4) to classify objects from each testing set (handled in turn) with the use of PNN; to include classified objects from the testing set into the training set;

5) to verify the obtained classification with the use of a leave-one-out cross-validation procedure.

The aim of this work was to compare effectiveness of proposed procedure with effectiveness of popular clustering methods [4] like hierarchical cluster analysis and k-means. Capability of discussed methods has been demonstrated for the data sets for testing clustering and classification algorithms: data with two-level hierarchical structure, iris flower data set, wine data set (http://archive.ics.uci.edu/ml/datasets). For clustering these data sets number of neurons from 3 till 9 was used.

The unreliability of clustering was calculated based on the percentage of samples classified wrongly as follows:

$$P = \frac{n}{N} \times 100\%,$$

where n is the number of wrongly classified samples, N is the total number of samples.

Results. The unreliability of clustering of three data sets resulting from use proposed algorithm, different algorithms of hierarchical cluster analysis, k-means and fuzzy k-means algorithms are shown in Table 1.

Summary. Proposed procedure is more effective than widely used clustering methods, namely, k-means, fuzzy k-means, different types of hierarchical cluster analysis. The approach based on the combination of the Kohonen neural network and probabilistic neural network can be considered a prospective tool for the solution of ill-posed chemical classification tasks.

Table 1

Results of clustering

Data set	*P*, %									
	Algorithm of hierarchical cluster analysis							Algorithm of k-means		Proposed procedure based on combination of artificial neural networks
	intergroup relations	intragroup relations	single linkage	complete linkage	centroid method	median method	Ward's method	standard algorithm	fuzzy k-means	
Wine samples	49.9	37.6	69.1	32.5	49.4	33.1	32.6	35.95	32.6	29.2
Data with two-level hierarchical structure	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	13.5	0.0
Iris flower samples	49.4	16.7	32.6	15.3	32.0	10.0	9.3	11.3	10.2	2.6

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