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The application of neural networks in the field of sensors

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1. Introduction :

Humans possess the almost perfect example of a sensor, with the senses continuously supplying real time data to the brain. Using the sensory elements (eyes, ears, skin, nose and tongue), almost all information contained in our environment can be obtained. Then, by signal transducers, this information is filtered and processed in the most wonderful natural computer, the human brain. Finally, depending on the results, humans react.

The two most important parts of this marvelous system are the five sensors and certainly our natural "computer". Using these senses not all properties can be detected (*e.g.* radioactivity, low concentration of impurities in the air, etc.) nor can the natural computer work using pressure signals. The real meaning of these limitations teaches us to adapt the design to the property to be measured and the type of signal to be processed. In the technical field, because of these, the appropriate physicochemical characteristics should be found to quantify the desired properties, and mathematical algorithms should work using adequate information.

Different approaches, which consist of neural networks (NNs) and different types of sensors, have been studied. In particular, four application of NNs in the quantification of the concentrations of chemicals in four different systems have been described: (*i*) ionic liquids (ILs) and hydrocarbons in their aqueous mixtures; (*ii*) Lycopene and β-carotene in food samples;[1-2] (*iii*) poliphenolic compounds in olive oil mill wastewater; (*iv*) glucose, uric and ascorbic acids in biological mixtures.[3-4]

2. Experimental :

2.1 Neural networks :

The supervised NNs used in all described applications is a multilayer perceptron. It consists of several artificial neurons arranged in three layers: input, hidden, and output layers. The topology of the NN is given by the number of layers and number of neurons in each layer. The input layer is used to input data into the NN; the nonlinear calculations are carried out in the other two layers. The calculation process in each neuron of the hidden and output layers consists of transfer and activation

functions. The activation function, eq 1, means that the input data to each neuron are multiplied by a self-adjustable parameter *w*, called weight; the result, x_k, is fed into a transfer function. The algorithm used in all applications described here is the sigmoid transfer functions, eq 2. The calculated value, y_k, is the output of the considered neuron. The NNs used were designed by Matlab version 7.01.24704 software.

$$x_k = \sum_{j=1} w_{jk} \cdot y_j \qquad (1)$$

$$y_k = f(x_k) = \left(\frac{1}{1+e^{-x_k}} \right) \qquad (2)$$

The learning process, which updates the weights to improve the predictive capacity of the NN, is carried out by minimizing the error prediction, eq 3 and using the back-propagation model.[1]

$$E_k = \frac{1}{2} \sum_k (r_k - y_k)^2 \qquad (3)$$

2.2 Sensors :

Sensors are devices which measure physicochemical characteristics and convert them into signals which can be read by an observer, an algorithm or by an instrument. A sensor is considered as adequate if it obeys three main rules *viz.* the sensor should be sensitive to the measured property and insensitive to any other and it should be influenced by neither the sample nor the measured property. In addition, the mathematical relation between the output signal and the measured property value should be linear. However, although this relation would be mathematically linear, several types of deviations can be observed and make the measurement process more difficult. This deviation could have its origin in systematic or random errors. Examples of the former deviations could be hysteresis, long term drift, digitalization error, offset, *etc*.

Among the large number of sensors, an extensive family is formed by *bio*sensors. Their history started with the first reference to these types of sensor which appeared in the 1960s.[5] A biosensor is a measurement system for the detection of an analyte that combines a biological component (enzymes, cell receptors, protein, peptide, *oligo*nucleotide, *etc.*) with a physicochemical detector. This type of sensor is capable of continuous measurement of analytes in biological media such as blood serum, urine, *etc*.[4] Among other applications, it is used to measure *bio*moleculars and/or monitoring biological processes.

3. Results and discussions :

One of the principal problems in accurately quantifying concentration of chemicals from complex mixtures is the chemical signals overlapping. In general, three methods can be used to overcome this, *viz.* the design of a specific measurement system, the application of powerful mathematical algorithms[1] and, depending on the system, both techniques can be applied at the same time.[4] The application of NNs on the four aforementioned chemical systems is shown here.

3.1 Determination of an ionic liquid and toluene concentrations in aqueous solutions :

In recent years, although ILs are being measured using reliable techniques, these are not adequate to measure/control on-line extraction processes because these require a relatively long sample

preparation time. Given the importance of this process, an analytical technique with a sample preparation time less than the sampling time of the process is necessary. Given that the imidazolium ring of the IL is UV active and the UV-visible spectroscopy fulfilled all mentioned conditions, this analytical technique was proposed. When the intention is to measure the concentration of aromatic chemicals and imidazolium ILs simultaneously, given that the aromatic compounds are also active in the UV region, the use of powerful chemometric tools to solve signal overlapping is required. A NN/UV has been optimized and validated using the absorbance at 191, 205 and 260 nm of several aqueous solutions of 1-ethyl-3-methylimidazolium ethylsulfate IL ([emim][$C_2H_5SO_4$]) and toluene between 0 and 5 ppm. The mean difference between the real and predicted values of the concentration of these compounds is less than 1%. Therefore, the NN/UV can be adapted to deconvolute the contribution of each chemical. And as result, in the ionic liquid field, the NN/UV is very interesting for further applications to digital control, or measurement devices.

3.2 Determination of lycopene and β-carotene concentrations in food samples :

Carotenoids are widespread in nature being the main group of pigments with important metabolic functions. Due to its antioxidant activity, these chemicals show a strong correlation between carotenoid intake and a reduced risk of some diseases, such as cancer, atherogenesis, bone calcification, eye degeneration and neuronal damages. Lycopene and β-carotene chemicals belong to this family. Given that these chemicals are active in UV/vis spectroscopy, their determination by classical methods is not adequate. In order to use this simple analytical technique, a nonlinear algorithm has been applied on the UV absorbance data (absorbance at 446 and 502 nm). Applying NN/UV-Vis spectroscopy, the Lycopene and β-carotene chemicals concentrations are estimated with a mean prediction error fifty times lower than classical models. This improvement in the results is extremely valuable for its application to a fast and reliable lycopene and β-carotene evaluation in food samples.

3.3 Determination poliphenolic compounds concentrations in olive oil mill wastewater :

In the manufacture of extra virgin olive oil, waste is produced and this has a serious environmental impact due to its high content of organic substances (sugars, tannins, polyphenols, polyalcohols, pectins and lipids, etc.) It is known that caffeic acid (CA) and catechol (CT) are two of the major contributors to the toxicity of these wastes. Given the electrochemical characteristics, laccase biosensor (LB) is commonly used to determine CA and CT. Because of the similarities in the produced oxidized species, the amperometric signal overlapping in the reduction voltammograms is high, and therefore, a powerful tool is required to solve this signal. Given that the mean difference between real and estimated values of CA and CT concentrations is less than 0.5 %, the integrated NN/LB system is an adequate approach to estimate both hazardous chemicals.

3.4. Determination of glucose, uric and ascorbic acids in biological mixtures :

The major obstacle for the amperometric detection of glucose in real samples is the interference arising from electrooxidizable substances such as ascorbic and uric acids existing in a measured system. Here an amperometric biosensor based on a colloidal gold - cysteamine - gold disk electrode with an enzyme glucose oxidase and a redox mediator, tetrathiafluvalene, co-immobilized atop the modified electrode, was used for the simultaneous determination of glucose, ascorbic and uric acids, in mixtures. Analytical data obtained from cyclic voltammograms generated by the biosensor were processed using a NN, and the separate quantification of the analytes over a range of 0.1 to 1 mM was performed without any *pre*treatment. In all cases the correlation coefficients obtained were higher than 0.99 and the mean prediction error was less than 1.7 %.

4. Conclusions :

In the light of the aforementioned results, tools based on NNs are suitable in the treatment of information from sensors. One of the most important factors to achieve reliable models requires the determination of the most characteristic information to describe the system to be modeled. Although every application should be previously tested, these successful results are extremely promising for other types of sensors.

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References

(1) Industrial and Engineering Chemistry Research, 2007, 46, 3787.
(2) Journal of Agricultural and Food Chemistry, 2008, 56, 6261.
(3) Journal of Agricultural and Food Chemistry, 2007, 55, 7418.
(4) Journal of Chemometrics, 2008, 22, 46.
(5) Annals of the New York Academy of Sciences, 1962, 102, 29.