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On reliability of neural network sensitivity analysis applied for sensor array optimization

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ABSTRACT

Sensor arrays are nowadays first choice solution for low-cost and portable gas mixtures analysis systems. The key issue in construction of such systems is selection of sensors. The authors try to apply neural network sensitivity analysis for this task. The algorithm starts from huge set of sensors, which provides satisfying operation of the system, and then detects the most redundant elements, which may be removed without significant decrease of system accuracy. Eventually the small but efficient array of sensors is obtained. Authors present the method, propose some modifications and discuss problems with its application. Results of sensitivity analysis approach are compared with exhaustive search for the best set of sensors. The case study is quantitative analysis of volatile organic compounds mixtures by means of commercial, tin dioxide, TGS 800 series sensors characterized in in-house developed gas chamber.

1. Introduction

Gas mixtures analysis, both qualitative and quantitative, performed with electronic sensors, became the significant research domain which nowadays involves quite interdisciplinary knowledge, with chemistry, solid state electronics, metrology, data processing and system theory included. Two main fields of research could be distinguished here – the first one concerning the technology of sensors fabrication, and the second one concerning sensor systems construction. In the latter case, matrices of sensors applied together with neural processing became the dominating solution elaborated during the last two decades by several research teams. The series of quite successful constructions described in the literature [1–9] disregard, however, optimal selection of sensors. It was caused by the character of research (which was rather preliminary at that stage), and the lack of reasonable and efficient methods of sensors selection. The second stage of electronic noses development may be recognized by common understanding that each redundant sensor applied in the matrix increases the cost of both fabrication and operation of prospective system. Several methods of sensors selection or reduction were proposed. Perhaps the most simple one could be the analysis of correlation ratio of sensors responses and eliminating sensors giving the same information. There are problems however with correlation ratio, which will be discussed in further sections. In [10,11] the reverse approach is proposed – the search for sensors reacting in different way for various compounds. The method seems quite effective but it relies on sensors selectivity, the feature which is not common among popular semiconductor gas sensors. Another classic approach is PCA (Principal Component Analysis) [12,13]. It may be used for both sensors responses preprocessing and for evaluation of sensors array feasibility for specific task. The PCA however is strongly related with classification and hence cannot say much about sensors capability for quantitative analysis. Another troublesome feature is that PCA estimates the performance of a whole set of inputs/sensors, rather than individual elements of array. Perhaps for these reasons some authors apply the PCA for rough evaluation only and relay more on exhaustive search eventually [14], others try to apply clusterization technique to sensors rather then responses [15] or to use Genetic Algorithms [16,17]. In [18] it is shown that two tasks – sensor fabrication and selection, may be integrated into a single process of development of optimal set of gas sensors.

This paper starts from the assumption that preliminary version of a sensor system providing acceptable accuracy of measurements is available (thanks to *huge enough* sensor array). Thus the task consists in the elimination of redundant sensors. For this purpose the authors apply the neural networks sensitivity analysis [19–21]. It derives from both classic neural processing theory and general sensitivity analysis approach [22]. The utilisation of neural networks is somewhat unusual there. Instead of permanent placement in the

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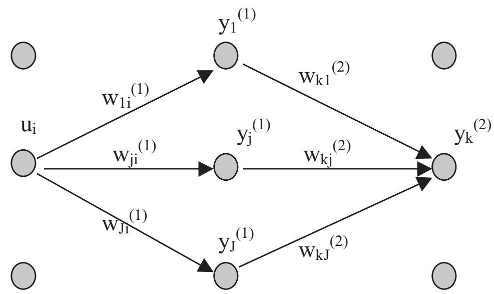

Fig. 1. Feedforward neural network outline.

system, they are temporarily used at preliminary stages of system configuration to provide the information about particular sensors influence on the system response. This way the most redundant sensors are found and removed one after another. After selection of the optimal set of sensors the appropriate algorithm (which may be neural network again) providing sensor matrix responses processing is constructed. When using the neural network sensitivity approach for reduction of sensor matrix [23,24], authors noticed that sometimes the results of its application are confusing. These observations encouraged to perform series of experiments, targeting in finding weak points of the method and a way to improve it. The results are presented in this paper, organized in the following way: Section 2 outlines the method. Section 3 provides an example of its application for sensor array reduction. Section 4 contains the key considerations on the reliability of sensitivity analysis and its comparison with experimental exhaustive search for the best set of sensors. Final conclusions are presented in Section 5.

2. Neural networks and sensitivity analysis

The operation of a feedforward neural network may be presented as shown in Fig. 1 (for clarity only the most important elements were outlined). For the construction with single hidden layer it may be described by:

$$y_k^{(2)} = f\left(\sum_{j=0}^{J} w_{kj}^{(2)} \cdot f\left(\sum_{i=0}^{I} w_{ji}^{(1)} \cdot u_i\right)\right) \tag{1}$$

where $y_k^{(2)}$ is the response of the k-th output of the network, u_i is the i-th input value, $w^{(1)}$ and $w^{(2)}$ are the appropriate weights associated with neurons from the first (hidden) and the second (output) layer respectively, I is the number of input units, J is the number of neurons in the hidden layer. The $f(x)$ is activation function, which may be sigmoid, described by (2).

$$f(x) = \frac{1}{1+e^{-x}} \tag{2}$$

After the training process all the weights are fixed to the appropriate values and neural network gains the unique approximation capabilities. In a sensor system, neural network transforms sensors responses u to the series of outputs $y^{(2)}$, which represent desired information, either qualitative or quantitative, depending on the target application.

The k-th neural network output sensitivity for selected input u_i is defined as a differential coefficient:

$$s_{ki} = \frac{\partial y_k^{(2)}}{\partial u_i} \tag{3}$$

which for the presumed construction (1) gives

$$s_{ki} = f'(x_k^{(2)}) \sum_{j=1}^{J} (w_{kj}^{(2)} \cdot f'(x_j^{(1)}) \cdot w_{ji}^{(1)}) \tag{4}$$

Sensitivity factor is calculated for each output–input pair and for each input pattern $u^{(p)}$. Concerning patterns, a global sensitivity for the whole data set (containing patterns indexed by $p = 1\ldots P$) is calculated using e.g. the Euclidean formula (5) or by finding the maximum absolute value. This way sensitivity matrix is obtained with two dimensions associated with inputs and outputs. Further analysis may involve the min–max procedure which reduces this matrix to a vector. Each coefficient of the vector describes neural networks sensitivity to the particular input, generalized for all the outputs and all patterns. The inputs (i.e. the sensors in our context), with lower values of sensitivity shall be considered as the candidates to remove.

$$S_{ki} = \sqrt{\sum_{p=1}^{P} (s_{ki}^{(p)})^2} \tag{5}$$

Described procedure was originally proposed for pruning of the redundant inputs of neural network with a single hidden layer [20]. Our own experience with construction of neural networks for gas sensor arrays responses processing, point to the need of applying two hidden layers for the highest performance. And sensitivity analysis applied to neural networks of poor quality may lead to wrong results. This poor quality may be caused by the architecture, too scant to mimic the target function well or by insufficient (too short) training. Concerning the latter issue – we have observed that at early stages of neural network training, relations between sensitivity factors may change. Seems like the task performed by weights in neural network is not only to mimic a function but also to discriminate useless inputs. A poor quality neural network performs both these tasks in a very bad manner. Thus it is necessary to train the network well and simultaneously extend the original sensitivity formula for neural networks with more hidden layers. Starting from (6), describing neural network with two hidden layers, where u_h and $y_k^{(3)}$ denote selected input and output, and the $w^{(1)}$, $w^{(2)}$ and $w^{(3)}$ with the appropriate indexes are weights of the appropriate neurons in layers 1, 2 and 3, the sensitivity is given by (7).

$$y_k^{(3)} = f\left(\sum_{j=0}^{J} w_{kj}^{(3)} \cdot f\left(\sum_{i=0}^{I} w_{ji}^{(2)} \cdot f\left(\sum_{h=0}^{H} w_{ih}^{(1)} \cdot u_h\right)\right)\right) \tag{6}$$

$$s_{kh} = \frac{\partial y_k^{(3)}}{\partial u_h} = f'(x_k^{(3)}) \sum_{j=0}^{J} \left[f'(x_j^{(2)}) \cdot w_{kj}^{(3)} \cdot \sum_{i=0}^{I} w_{ji}^{(2)} \cdot f'(x_i^{(1)}) \cdot w_{ih}^{(1)} \right] \tag{7}$$

Generalized sensitivity formula may be described in more elegant way, by the recurrence defined in formulae (8) and (9), where $s_{ki}^{(1)}$ is the sensitivity of neural network with single hidden layer and the sensitivity of neural network with L layers $s_{ki}^{(L)}$ is calculated as a weighted sum of sensitivities of a network containing *L–1* hidden layers.

$$s_{ki}^{(1)} = \frac{\partial y_k^{(1)}}{\partial u_i} = f'(x_k^{(1)}) w_{ki}^{(1)} \tag{8}$$

$$s_{ki}^{(L)} = \frac{\partial y_k^{(L)}}{\partial u_i} = f'(x_k^{(L)}) \sum_{j=1}^{J} (w_{kj}^{(L)} \cdot s_{ji}^{(L-1)}) \tag{9}$$

This kind of neural network sensitivity calculation algorithm was implemented in the software prepared by authors.

3. Application example

Sensitivity analysis was applied for the reduction of gas sensor array providing quantitative analysis of acetone and chloroform