



Enhancing electronic nose performance based on a novel QPSO-RBM technique

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ABSTRACT

A novel classification technique for bacteria detection termed quantum-behaved particle swarm optimization-based restricted Boltzmann machine (QPSO-RBM) based on electronic nose technology is proposed in this paper. In order to improve the performance of the QPSO-RBM technique, three training objective functions have been adopted in the training process of RBM respectively. A new synchronous optimization method is adopted in QPSO-RBM to ensure it research the best performance. By comparing classification performance of the three training objective functions, we have found discriminative training objective has better effect than the other two ways. Four kinds of features extracted from the time and frequency domains have been developed to demonstrate the effectiveness of this classification technique for four different classes of wounds. When wavelet coefficients are adopted as features, QPSO-RBM performs best. Then the link between the number of hidden nodes in RBM and recognition rate of the model has been explored. In the end, QPSO-RBM is compared with four existing classifiers: radical basis function neural network (RBFNN), support vector machine (SVM), k-nearest neighbor (KNN) and linear discriminant analysis (LDA). The results have shown that QPSO-RBM outperforms the four classifiers.

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1. Introduction

An electronic nose (E-nose) is a system used to recognize gas and odor, which is designed like the biological olfactory system [1–3]. It consists of a gas sensor array and a series of related intelligent algorithms. Through the gas sensor array, E-nose obtains response curves of the sensors to the target gas, then using relevant intelligent algorithms to deal with response curves so as to identify the gas or odor which includes a single component or complex components [4,5]. Recently, the research of E-nose has made rapid progress and E-nose has been generally used in many fields, such as environment protection [6,7], public health [8–12], quality control of food industry [13–15], odor analysis, and explosives detection [16–18]. This paper mainly concerns wound infection detection.

A timely determination of the bacterial type of wound infection can help doctors diagnose and select appropriate treatment options to facilitate recovery. However, traditional diagnostic methods, which over reliance on the doctor's clinical experience, are prone to miscarriage of justice and delay treatment. Consequently, there has been a resurgence of interest in developing techniques for wound

infection detection. Our previous work has proved that the use of E-nose for wound infection detection has obvious advantages in non-invasive and rapid wound detection [19,20].

The intelligent algorithms applied to E-nose can be divided into three parts: feature extraction, pattern recognition and parameters optimization [21–23]. Feature extraction is the first step of the sensor signal processing, which plays an important role in the subsequent pattern recognition. At present, the feature extraction methods used in electronic nose can be divided into three categories [24,25]. The first type is basic feature extraction method based on the original response curve [26], such as maximum values, minimum values, corresponding time coordinates of maximum and minimum, slope, integral, and so on. The maximum response reflects the final steady-state information of the sensor response, which is the most common feature to be used and an important feature to distinguish gas species and concentration. Due to the steady-state response of the sensor, a good classification of pathogenic bacteria could not be achieved. Therefore, feature extraction also calls for dynamic responses, which have specific physical meaning. For example, the integral represents the cumulative sum of the changing degrees of reaction and the slope represents the reaction rate. The second type is feature extraction method based on curve fitting [27]. It refers to using appropriate model to fit the response curve of sensors and extracting model

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Table 1
Pathogens in wound infection and their metabolites.

Pathogens	Metabolites
<i>P. aeruginosa</i>	Pyruvate, 2-nonanone, 2-undecanone, toluene, 1-undecene, 2-aminoacetophenone, esters, dimethyl disulfide, 2-heptanone, methyl ketones, dimethyl trisulfide, butanol, 2-butanone, sulphur compounds, isopentanol, isobutanol, isopentyl acetate
<i>E. coli</i>	Ethanol, decanol, dodecanol, methanethiol 1-propanol, indole, methyl ketones, lactic acid, succinic acid, formic acid, butanediol, dimethyl disulfide, octanol, dimethyl trisulfide, acetaldehyde, hydrogen sulfide, formaldehyde, acetic acid, aminoacetophenone, pentanols
<i>S. aureus</i>	Isobutanol, isopentyl acetate, ethanol, ammonia, 1-undecene, methyl ketones, 2-methylamine, 2,5-dimethylpyrazine, isoamylamine, trimethylamine, formaldehyde isopentanol, aminoacetophenone, acetic acid

parameters as features. The common models include polynomial model, exponential model, fractional function model and S function model, etc. The third one is based on the transform domain [28,29], which conducts appropriate transform to original response curve and extracts transform coefficients as features, such as Fourier transform and wavelet transform. Fourier transform decomposes the original response into a superposition of DC component and different harmonic components. By using the amplitudes of these components as features, qualitative analysis as well as quantitative analysis can be realized. Wavelet transform is an extension of Fourier transform, which maps signals into a new space with basic functions quite localizable in time and frequency space [30]. It bears a good anti-interference ability for the following pattern recognition.

In general, the pattern recognition algorithms applied to E-nose can be divided into two major categories [31,32]. One is linear classifier, such as K-nearest neighbor (K-NN) [33,34], least square method (LSM), cluster analysis (CA) [35], partial least square (PLS) [36], and discriminant analysis (DA) [37]. Another is nonlinear classifier, back propagation artificial neural networks (BP-ANN) [38,39], radial basis function (RBF) [40], probabilistic neural network (PNN), self-organizing map (SOM) and adaptive resonance theory (ART) [41] for instance. Besides, fuzzy classification (FC) [42], support vector machine (SVM) [43], and minimal spanning tree (MST) also have been explored in E-nose application. For optimization algorithms, the main algorithms include genetic algorithm (GA) [44], particle swarm optimization (PSO) [45] and quantum-behaved particle swarm optimization (QPSO) [46]. A new integer-based GA approach was used to enhance the performance of E-noses by sensor selection. The PSO was posed to analyze signals of wound infection detection based on an E-nose. Meanwhile, a new feature selection method based on QPSO was proposed to optimize the gas sensor array and reduce the dimensions of the feature matrix.

With the development of E-nose research, a large number of methods in statistical pattern recognition, neural networks, stoichiometry, and biological control have been applied to the data processing of E-nose system. At present, neural networks (NN) and support vector machines (SVM) are used in the research of E-nose most widely. However, researches have proved that restricted Boltzmann machine (RBM) can be used successfully as stand-alone non-linear classifiers alongside classifiers like neural networks and support vector machines.

RBM is a generative stochastic artificial neural network that can learn probability distribution from a set of its inputs. In the past few years, RBMs' applications have been found in dimension reduction, classification, collaborative filtering, feature learning. But so far, there has been no research on the application of RBM to E-nose. Thus, in order to make a further contribution to E-nose research and explore different techniques in the application of E-nose, a novel QPSO-RBM technique is presented for the detection of wound infection gas with an E-nose in this paper. In the novel technique, RBM is adopted as a stand-alone non-linear classifier and a novel syn-



Fig. 1. Sensors array.

chronous optimization algorithm based on QPSO is applied for the better performance of E-nose. In the rest of the paper, materials and experiments are discussed in Section 2. Then an overview of the RBM and the proposed novel synchronous optimization algorithm are discussed in Section 3. The results and discussion are shown in Section 4. Finally in Section 5 we draw our conclusion.

2. Material and experiments

The datasets used in this paper were obtained by a home-made E-nose, whose details can be found in our previous publication [47]. To make the paper self-contained, the system structure and experimental setup are briefly repeated in the following subsections.

2.1. Target gas and experimental setup

Twenty SD (Sprague-Dawley) male rats, 6–8 weeks old and 225–250 g weight, are randomly divided into four groups (five in each group), including one control group and three groups infected by *P. aeruginosa*, *E. coli*, and *S. aureus*, respectively. After the rats are anaesthetized, a small incision (about 1 cm long) is made in the hind leg of each rat. Then 100 mL of bacterial solution (10^9 CFU/mL, *P. aeruginosa*, *E. coli*, or *S. aureus*) is added into the wound described above in the respective infection group. Meanwhile, the same volume of physiological saline (0.9% NaCl solution) is added in the control group. The rats are used for the further experiment after 72 h.

The metabolites in the reproduction process of the three pathogens are shown in Table 1. According to the pathogen metabolites in Table 1 and the sensitive characteristics of gas sensors, fourteen metal oxide sensors and one electrochemical sensor are selected to construct the sensor array (shown in Fig. 1). They are nine TGS sensors (TGS2600, TGS2602, TGS2620, TGS800, TGS822, TGS825, TGS826, TGS813, TGS816), one WSP-2111 XSC sensor, two

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