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Classification of Wound Infection Data Based on SVM with a Novel Weighted Gaussian RBF Kernel

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Abstract

Rapid and timely monitoring of traumatic inflammation is conducive to doctors' diagnosis and treatment. It has been proved that electronic nose (E-nose) is an effective way to predict the bacterial class of wound infection by smelling the odor produced by the metabolites, and the classification accuracy of E-nose is influenced strongly by the classifier. To improve the performance of E-nose in predicting the bacterial class of wound infection, an enhanced SVM with a novel weighted Gaussian RBF kernel is proposed in this paper, and the way of setting parameters of this enhanced SVM is also given. Experimental results prove that the classification accuracy of SVM with the novel weighted Gaussian RBF kernel is 95.24%, which is better than other considered classifiers (PLS-DA, RBFNN, SVM with single Gaussian RBF kernel and SVM with traditional weighted Gaussian RBF kernel). All results make it clear that the enhanced SVM proposed in this paper is an ideal classifier when E-nose is used to detect the bacterial class of wound infection.

Keywords*: wound infection; electronic nose; SVM; weighted Gaussian RBF kernel*

1. Introduction

Electronic nose (E-nose) is an expert system which is composed of an array of gas sensors and a corresponding artificial intelligence technique. It is effective in dealing with odor analysis [1-2], and has been introduced to many fields such as food engineering [3-5], environmental control [6-7], food safety [8], disease diagnosis [9-12] and so on.

Wound is a big pubic hazard in the world, and it takes long time for the traditional bacteriological diagnosis to confirm infection and the treatment is often delayed. Rapid and timely monitoring of traumatic inflammation is conducive to doctors' diagnosis and treatment. But it is difficult for doctor to distinguish clinical infection in the early stage. The wounds infected by bacteria have a variety of special smell before the obvious metabolin appears, if this smell can be discriminate, then it will be conductive to rapid and timely diagnosis of wound infection.

Previous works [13-16] have confirmed that it's feasible for E-nose to detect bacteria including investigation of bacterial volatile organic compounds (VOCs). So E-nose is employed to detect the bacterial class of wound infection in our lab.

As a classifier, support vector machine (SVM) is good at distinguishing the nonlinear data set, and it has been applied successfully in many fields [17-20]. But the performance of SVM is influenced strongly by the kernel mapping function when it is used to solve the practical problems. The mapping ability of classical kernel, such as Gaussian RBF kernel, is not very ideal, and some key useful information may be lost during the mapping process. It will cost much computing resource to construct a novel kernel with high performance in mapping ability. Recently, it is popular to construct a good kernel from a

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series of kernels during which the weighted kernel method [21] is the most simple and widely used way to produce a new kernel.

In this paper, a novel weighted Gaussian RBF kernel is proposed to improve the classification ability of SVM. In the rest of this paper, we will firstly introduce the material and odor sampling experiments in section 2, and in section 3, we will briefly introduce the theory of SVM, then the detail information of weighted kernel Gaussian RBF function and the setting way of its parameters will be provided; the classification results will be shown and analyzed in section 4; finally we will draw the conclusion of this paper in section 5.

2. Materials and Experiments

2.1. Sampling Preparation

Three clinical common pathogens, *P. aeruginosa*, *E. coli* and *S. aureus*, are considered in this paper. These three species of bacteria used in our experiment are purchased from the Chinese National Institute for the Control of Pharmaceutical and Biological Products, and the National Center for Medical Culture Collection. All species of bacteria grow in media at 37 ℃ with shaking at 150 rpm in a gyratory incubator shaker for 24 h. The culture medium is ordinary broth medium and the main components include peptone, NaCl, beef extract and glucose. After 3 successive generations of subculture, the purchased bacteria become stable. Then they are inoculated into the test agar slant. Dynamic head-space method is adopted during all gas sampling experiments. The head-space gas in each test slant containing the metabolic products of bacteria is imported into the E-nose for the sampling. The detail information of the three bacteria is shown in Table 1.

Table 1. Pathogens in Wound Infection and Their Metabolites

Pathogens	Metabolites
P. aeruginosa	Butanol, Dimethyldisulfide, Dimethyltrisulfide, Esters, Methyl ketones, Isobutanol, Isopentanol, Isopentyl acetate, Pyruvate, Sulphur compounds, Toluene, 1-Undecene, 2-Aminoacetophenone, 2-Butanone, 2-Heptanone, 2-Nonanone, 2-Undecanone
E. coli	Acetaldehyde, Acetic acid, Aminoacetophenone, Butanediol, Decanol, Dimethyldisulfide, Dimethyltrisulfide, Dodecanol, Ethanol, Formaldehyde, Formic acid, Hydrogen sulfide, Indole, Lactic acid, Methanethiol, Methyl ketones, Octanol, Pentanols, Succinic acid, 1-Propanol
S. aureus	Acetic acid, Aminoacetophenone, Ammonia, Ethanol, Formaldehyde, Isobutanol, Isopentyl acetate, Isopentanol, Methyl ketones, Trimethylamine, 1-Undecene, 2,5-Dimethylpyrazine isoamylamine, 2-Methylamine

2.2. E-nose for Bacteria Detection and Measurement

During the sampling experiments, the head-space gas of each bacteria is sampled by an electronic nose (Airsense-model PEN 3, Airsense Analytics, Schwerin, Germany), equipped with 10 different thermo-regulated (150~500 ℃) sensors (S) made of metal oxide semiconductors (MOS). The sensors which are positioned in a gas chamber (1.8 mL of volume), are sensitive to different classes of chemical compounds, and the detail information is shown in Table 2.

Table 2. Response Characteristics of Sensors

No.	Sensors	Response
S1	W1C	aromatic
S2	W5S	broadrange
S3	W3C	aromatic
S4	W6S	hydrogen
S5	W5C	arom-aliph
S6	W1S	broad-methane
S7	W1W	sulphur-organic
S8	W2S	broad-alcohol
S9	W2W	sulph-chlor
S10	W3S	methane-aliph

The schematic diagram of experimental system is shown in Figure 1. PEN 3 is just used to sample the odor of different bacteria, and the feature extraction and pattern recognition is realized on a computer. The practical E-nose system of this paper is shown in Figure 2.

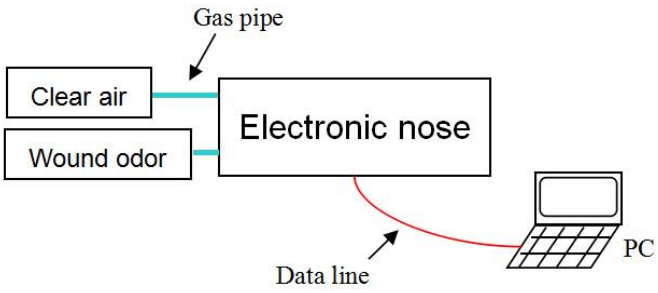

Figure 1. Schematic Diagram of Experimental System

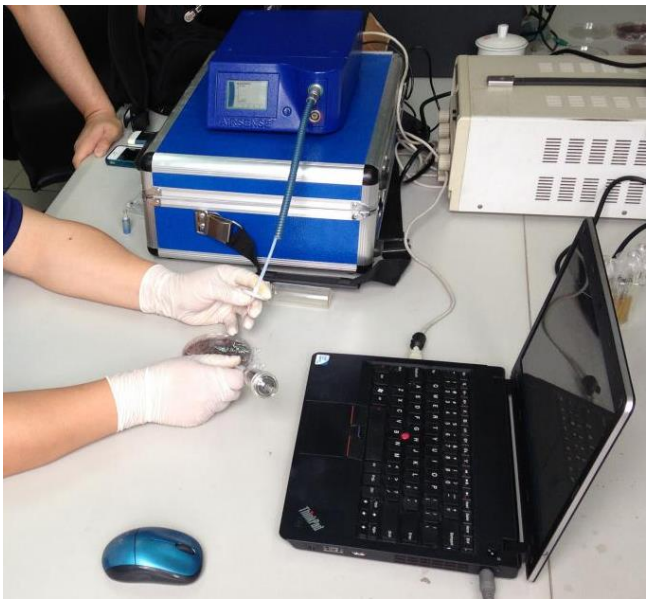

Figure 2. Practical E-Nose System

Before the measurement starts, the system (gas pipe and sensor array chamber) is cleaned by a cycle of 300 s, using filtered air (zero-air: air filtered on active carbon), to ensure the absence of the residual odor molecules and to report sensors to the baseline. The flow rate of the sampling gas is 300 mL/min, the sampling frequency is 1 Hz, and one sampling experiment lasts 60 s. The response curves of 10 sensors on one culture medium with *E. coli* are shown in Figure 3. One can find the obvious rise of each response curve appears when the gas containing VOCs of *E. coli* begins to pass over the sensor array, which is the result of cross sensitivity.

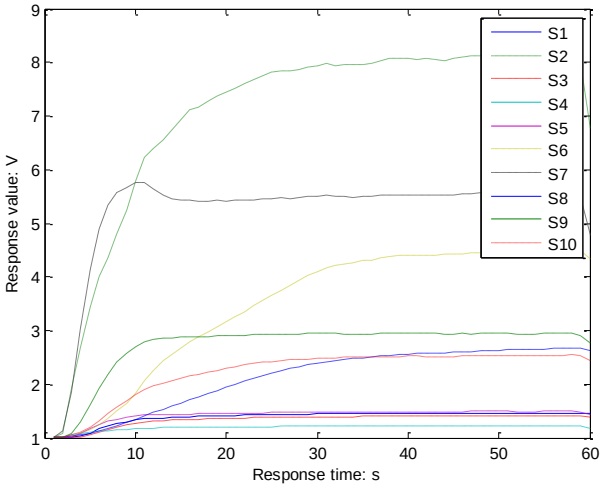

Figure 3. Response of E-Nose on One Wound Infected With *E. Coli*

The maximum value of each sensor's response will be extracted to build the feature matrix of wound infection bacteria, and we define this matrix as matrix **X** during which there are 84 samples and the dimension of each sample is 10. A detail introduction is available in Figure 4.

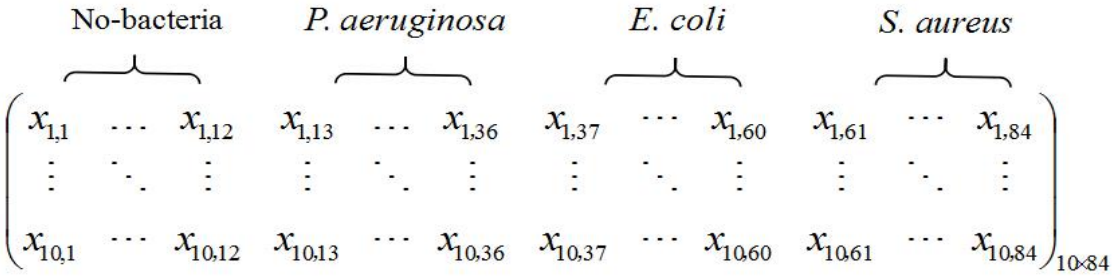

Figure 4. Data Structure of the Feature Matrix

To research the response of 10 sensors when they are used to sample the head-space odor of different wound infection bacteria, the radar map is employed in this paper (shown in Figure 5). It is clear that the radar map of the three bacteria are different from each other, which indicates that PEN 3 can be used to detect the bacteria of wound infection.

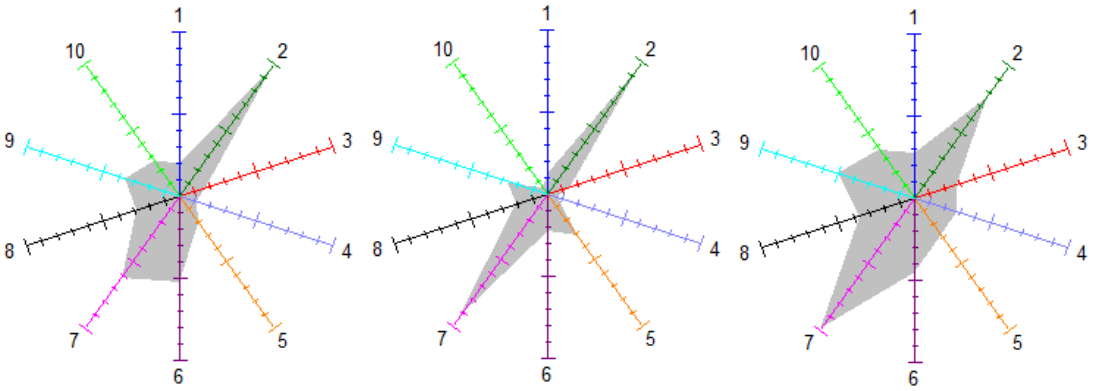

Figure 5. Radar Map of the Three Bacteria

3. SVM with a Novel Weighted Kernel Function

3.1. Overview of SVM

SVM has been known as an ideal technique for classification. It adopts structural risk minimization principle to get the best generalization ability according to the limited sample information. The target of SVM is to find an optimal separating hyper-plane $y = \mathbf{w} \cdot \mathbf{x} + b$ for samples.

For linearly separable two classes' data $\{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$, where $\mathbf{x}_i$ is the sample of which the label is +1 or -1, and the dimension is d, y_i is the label of $\mathbf{x}_i$, and n is the number of samples in training data set. As is shown in Figure 6, **H** is the optimal hyper-plane which is found by SVM to separate the samples from different classes. Multi-class problems can be achieved by constructing a multiple SVM.

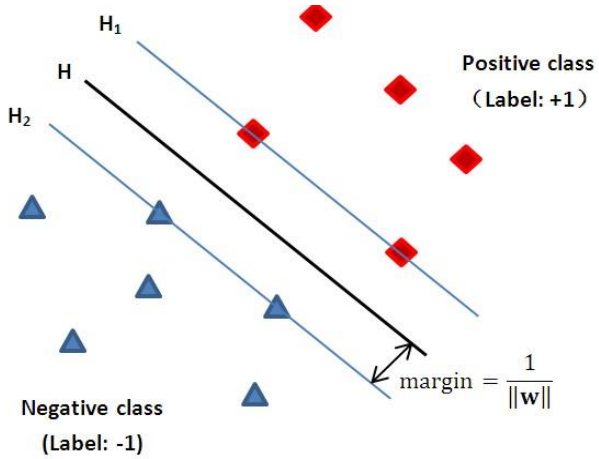

Figure 6. SVM Separation of Linearly Separable Two Classes' Data

The problem of finding the optimal separating hyper-plane can be formalized as follows:

$$\begin{aligned} &\min \frac{1}{2} < \mathbf{w}, \mathbf{w} > + C \sum_{i=1}^{n} \xi_i, \\ &\text{s.b.} < \mathbf{w}, \mathbf{x}_i > + b \geq +1 - \xi_i, \text{for } y_i = +1, \\ &\quad < \mathbf{w}, \mathbf{x}_i > + b \leq -1 + \xi_i, \text{for } y_i = -1 \\ &\quad \xi_i \geq 0, \forall i \end{aligned} \tag{1}$$

where ξ_i is called the slack variable, and C is the penalty factor. By using Lagrange multiplier techniques, Eq. (1) can be changed to the following dual optimization problem:

$$\begin{aligned} &\max \sum_{i=1}^{n} \alpha_i - \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j < \mathbf{x}_i, \mathbf{x}_j >, \\ &\text{s.b.} \sum_{i=1}^{n} \alpha_i y_i = 0, \alpha_i = [0, C] \end{aligned} \tag{2}$$

Using Lagrange multipliers, the optimal desired weight vector of the discriminant hyper-plane is:

$$w = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i \ . \tag{3}$$

So the best discriminant hyper-plane can be derived as:

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i < \mathbf{x}_i, \mathbf{x} > + b, \tag{4}$$

where b is the bias of the discriminant hyper-plane.

The hyper-plane determined by Eq. (4) is linear and can solve the linearly separable classification problem. The nonlinear problem can be mapped to a new space by a nonlinear transformation with the help of the kernel function. Suppose $\Phi(\mathbf{x})$ is a map function, then the algorithm only depends on the data through dot products in high-dimensional feature space. Define k is such a kernel function as follow:

$$k(\mathbf{x}_i, \mathbf{x}_j) = < \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) > \ . \tag{5}$$

In Eq. (5), the dot product in high-dimension space can be expressed as a kernel function. Similar to Eq. (4) in the linear problem, there is also a discriminant function for this nonlinear problem:

$$f(\mathbf{x}) = \sum_{i=1}^{n} \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b. \tag{6}$$

3.2. A Novel Weighted Kernel Function

Support

$$\Phi(\mathbf{x}) = p\Phi_1(\mathbf{x}) + (1-p)\Phi_2(\mathbf{x}), \tag{7}$$

so Eq. (5) can be translated as:

$$\begin{aligned} k(\mathbf{x}_i, \mathbf{x}_j) &= < \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) > \\ &= < (p\Phi_1(\mathbf{x}_i) + (1-p)\Phi_2(\mathbf{x}_i)), (p\Phi_1(\mathbf{x}_j) + (1-p)\Phi_2(\mathbf{x}_j)) > \\ &= p^2 < \Phi_1(\mathbf{x}_i), \Phi_1(\mathbf{x}_j) > + (1-p)^2 < \Phi_2(\mathbf{x}_i), \Phi_2(\mathbf{x}_j) > + 2p(1-p) < \Phi_1(\mathbf{x}_i), \Phi_2(\mathbf{x}_j) > \\ &= p^2 k_1(\mathbf{x}_i, \mathbf{x}_j) + (1-p)^2 k_2(\mathbf{x}_i, \mathbf{x}_j) + 2p(1-p) k_{1,2}(\mathbf{x}_i, \mathbf{x}_j) \end{aligned} \tag{8}$$

Gaussian RBF kernel is used as the base kernel in this paper, so k_1 and k_2 are in the form as follows:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\left\|\mathbf{x}_i - \mathbf{x}_j\right\|^2}{\sigma^2}\right). \quad (9)$$

It has been proved $k_{1,2}(\mathbf{x}_i, \mathbf{x}_j)$ can be computed if $\Phi_l(\mathbf{x})$ can be formulated as $k_l^{\frac{1}{2}}(\mathbf{x}, \mathbf{z})$ which is a function of $\mathbf{z}$ and belongs to space L_2 [22]. Using the definition of inner products in space L_2, kernel function can be defined as:

$$\begin{aligned} k_{l,l'}(\mathbf{x}_i, \mathbf{x}_j) &\equiv < \Phi_l(\mathbf{x}_i), \Phi_{l'}(\mathbf{x}_j) > \\ &\equiv \int k_l^{\frac{1}{2}}(\mathbf{x}_i, \mathbf{z}) k_{l'}^{\frac{1}{2}}(\mathbf{x}_j, \mathbf{z}) d\mathbf{z} \end{aligned}. \quad (10)$$

Using the self-similarity property of Gaussian distributions, the square root of a radial basis kernel is:

$$k_l^{\frac{1}{2}}(\mathbf{x}, \mathbf{z}) = \left(\frac{4}{\pi\sigma_l^2}\right)^{\frac{n}{4}} \exp\left(-\frac{2\|\mathbf{x} - \mathbf{z}\|^2}{\sigma_l^2}\right). \quad (11)$$

Then the mixture of two kernel matrix can be changed as:

$$\begin{aligned} k_{1,2}(\mathbf{x}_i, \mathbf{x}_j) &= \int k_1^{\frac{1}{2}}(\mathbf{x}_i, \mathbf{z}) k_2^{\frac{1}{2}}(\mathbf{x}_j, \mathbf{z}) d\mathbf{z} \\ &= \int \left(\frac{4}{\pi\sigma_1^2}\right)^{\frac{n}{4}} \exp\left(-\frac{2\|\mathbf{x}_i - \mathbf{z}\|^2}{\sigma_1^2}\right)\left(\frac{4}{\pi\sigma_2^2}\right)^{\frac{n}{4}} \exp\left(-\frac{2\|\mathbf{x}_j - \mathbf{z}\|^2}{\sigma_2^2}\right) d\mathbf{z}, \quad (12) \\ &= \left(\frac{2\sigma_1\sigma_2}{\sigma_1^2 + \sigma_2^2}\right)^{\frac{n}{2}} \exp\left(-2\frac{\left\|\mathbf{x}_i - \mathbf{x}_j\right\|^2}{\sigma_1^2 + \sigma_2^2}\right) \end{aligned}$$

where σ_1 and σ_2 are called the scale factor.

For SVM, the parameters of kernel function will influence the data structure in the high-dimension space. There are three base kernels in the proposed weighted kernel function, and the numerical relationship of the three scale factors can be described as:

$$\sigma_1^2 < \frac{\sigma_1^2 + \sigma_1^2}{2} < \sigma_2^2, \text{ if } \sigma_1 < \sigma_2. \quad (13)$$

This relationship can map data from different scale to ensure more information of the feature matrix can be considered by SVM during the classification process. The weighted coefficient will also influence the data structure in the high-dimension space. So these parameters must be optimized by some optimization technique to ensure that each method can achieve its best performance.

4. Results and Discussion

First we will verify the effectiveness of SVM in predicting the bacterial class of wound infection. Two other classifiers, partial least square discriminant analysis (PLS-DA) [23] and radial basis function neural network (RBFNN) [24] are also used to predict the class label of wound data besides SVM. The feature matrix which is introduced in section 2.2 is treated by the three classifiers. Leave-one-out (LOO) technique is used to train and test the classifiers. The parameters of all three classifiers are optimized by QPSO [25] to make sure that all classifiers reach their best working state, and the classification results are shown in Table 3.

Table 3. Classification Accuracy of RBFNN and SVM

Classifiers	Classification accuracy of train data set (%)	Classification accuracy of test data set (%)
PLS-DA	81.14	75
RBFNN	100	88.10
SVM (single Gaussian RBF kernel)	100	91.67

We can find from Table 3 that the classification accuracy of PLS-DA is worse than RBFNN and SVM, and the performance of SVM with single Gaussian RBF kernel is the best during all three classifiers. This result proves the effectiveness of SVM in predicting the bacterial class of wound infection. Then we use SVM with different kernel to deal with the data set of wound infection, and the results are shown in Table 4.

Table 4. Classification Accuracy of SVM with Different Kernel Functions

Classifiers	Classification accuracy of train data set (%)	Classification accuracy of test data set (%)
SVM (single RBF kernel)	100	91.67
SVM (traditional weighted Gaussian RBF kernel)	100	92.86
SVM (proposed weighted Gaussian RBF kernel)	100	95.24

Note: the equation of traditional weighted Gaussian RBF kernel function is $k(\mathbf{x}_i, \mathbf{x}_j) = pk_1(\mathbf{x}_i, \mathbf{x}_j) + (1-p)k_2(\mathbf{x}_i, \mathbf{x}_j)$, $p \in (0,1)$.

It is clear that the best result is achieved by the proposed SVM during all three different SVM techniques. This result proves that the novel weighted kernel can map more information of feature matrix to the high-dimension space, and this improves the performance of the proposed SVM in classification of wound infection bacteria.

5. Conclusions

When SVM is employed by E-nose to predict the bacterial class of wound infection, its performance is influenced by the kernel function. An enhanced SVM with a novel weighted Gaussian RBF kernel is proposed in this paper. This weighted kernel can map more useful information of the feature matrix to the high-dimension space. The experimental results show the performance of the novel SVM is much better than that of PLS-DA, RBFNN, SVM with single Gaussian RBF kernel and SVM with traditional weighted Gaussian RBF kernel. Above all, the proposed SVM is an ideal classifier in wound infection detection based on E-nose.

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