Neural Networks 33 (2012) 204–215

Contents lists available at SciVerse ScienceDirect

Neural Networks

journal homepage: www.elsevier.com/locate/neunet

Performance evaluation of multilayer perceptrons for discriminating and quantifying multiple kinds of odors with an electronic nose

Gao Daqi *, Yang Zeping, Cai Chaoqian, Liu Fangjun

Department of Computer Science, State Key Laboratory of Bioreactor Engineering, East China University of Science and Technology, Shanghai 200237, China

ARTICLE INFO

Article history:
Received 2 January 2012
Received in revised form 14 May 2012
Accepted 23 May 2012

Keywords:
Perceptrons
Local learning
Local generalization
Discrimination
Quantification
Odors

ABSTRACT

This paper studies several types and arrangements of perceptron modules to discriminate and quantify multiple odors with an electronic nose. We evaluate the following types of multilayer perceptron. (*A*) A single multi-output (SMO) perceptron both for discrimination and for quantification. (*B*) An SMO perceptron for discrimination followed by multiple multi-output (MMO) perceptrons for quantification. (*C*) An SMO perceptron for discrimination followed by multiple single-output (MSO) perceptrons for quantification. (*D*) MSO perceptrons for discrimination followed by MSO perceptrons for quantification, called the MSO-MSO perceptron model, under the following conditions: (*D*1) using a simple one-against-all (OAA) decomposition method; (*D*2) adopting a simple OAA decomposition method and virtual balance step; and (*D*3) employing a local OAA decomposition method, virtual balance step and local generalization strategy all together. The experimental results for 12 kinds of volatile organic compounds at 85 concentration levels in the training set and 155 concentration levels in the test set show that the MSO-MSO perceptron model with the D3 learning procedure is the most effective of those tested for discrimination and quantification of many kinds of odors.

1. Introduction

There exist many kinds of odors in the natural world, and their components as well as concentrations are changeable. The purpose of electronic noses is to sense odors by using gas sensor arrays and to make decisions by means of appropriate pattern recognition methods (Gardner & Bartlett, 1999; Liran & David, 2007; Pearce, Schiffman, Nagle, & Gardner, 2003).

Neural networks are one of the most popular pattern recognition models used in electronic noses (Alizadeh, 2010; Burlachenko, Snopok, Capone, & Siciliano, 2011; Falasconi, Pardo, Sberveglieri, Riccò, & Bresciani, 2005; Vito, Piga, Martinotto, & Francia, 2010; Widyanto, Kusumoputro, & Hirota, 2008), and most of them are multilayer perceptrons (MLPs) using a back-propagation (BP) learning algorithm. They are mainly employed for the discrimination (Brezmes, Llobet, Vilanova, Saiz, & Correig, 2000; Li, Heinemann, & Sherry, 2007; Panigrahi, Balasubramanian, Gu, Logue, & Marchello, 2006) and quantification (Gulbag, Temurtas, Tasaltin, & Ožtuřk, 2007; Leis et al., 2010; Llobet, Brezmes, Vilanova, Suerias, & Correig, 1997; Orts, Llobet, Vilanova, Brezmes, & Correig, 1999) of odors. An advanced electronic nose will have to work well with a wide variety of odors over large concentration ranges, as a chromatography instrument does, in order to implement complicated discriminative and quantitative tasks. These tough conditions are a challenge for neural networks (Cho, Katahira, Okanoya, & Okada, 2011; Jaiyen, Lursinsap, & Phimoltares, 2010; Jeong & Lee, 2012; Kohler & Mehnert, 2011; Razavi & Tolson, 2011; Rubio, Angelov, & Pacheco, 2011; Trenn, 2008; Wilamowski & Hao, 2010).

In order to simultaneously discriminate and quantify many kinds of odors using neural networks, the divide-and-conquer strategy is brought to mind as expected (Horner & Hierold, 1991; Huang & Leung, 2007; Llobet et al., 1997; Orts et al., 1999). Unfortunately, neural networks have only been applied to limited kinds of odors, limited concentration levels and limited samples, up to now (Cho, Kim, Na, & Jeon, 2008; Llobet et al., 1997; Orts et al., 1999). Orts et al. (1999), for example, first used an MLP with two output nodes to recognize two kinds of odors, methane and ethanol, with only 54 training patterns, and then utilized two MLPs, each of which has three output units, to determine three concentration levels of each odor. Similarly, Llobet et al. (1997) employed the same type of MLPs for quantifying three kinds of odors, ethanol, toluene and o-xylene, with only 36 training patterns in total, each of which with only three concentration levels of 25, 50 and 100 ppm. Because a concentration point is taken for a class, the employed MLPs cannot handle the situation where a sample is located just in or close to the middle of two known concentrations.

* Correspondence to: Department of Computer Science, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, China. Tel.: +86 21 6425 3780; fax: +86 21 6425 2984.

E-mail addresses: gaodaqi@ecust.edu.cn (D. Gao), yangzeping@ecust.edu.cn (Z. Yang), av15fire@gmail.com (C. Cai), lfj529@163.com (F. Liu).

0893-6080/$ – see front matter © 2012 Elsevier Ltd. All rights reserved.
doi:10.1016/j.neunet.2012.05.009

Along with the increasing numbers of classes, concentration levels and samples of odors, such problems as slow learning speeds and complicated structures of MLPs will unavoidably arise (Bishop, 1995; Huang, Zhou, Ding, & Zhang, 2012; Huang, Zhu, & Siew, 2006; Trenn, 2008). However, the learning algorithms suitable for the small-scale problems cannot be simply generalized to large-scale ones (Aizenberg, 2010; Castro & Zuben, 2011; Jesús & Hagan, 2007; Ludermir, Yamazaki, & Zanchettin, 2006; Oong & Isa, 2011; Romeroa & Alquézar, 2012; Sun, Todorovic, & Goodison, 2010; Vito, Martinelli et al., 2010). Modular MLPs are thus especially attractive because they are relatively effective for the large-set discrimination tasks (Alex, Zurada, Laiping, & Jian, 2007; Anand, Mehrotra, Mohan, & Ranka, 1995; Connolly & Labib, 2009; Gao, Li, & Yang, 2007; Jesse, Bernhard, Geoff, & Eibe, 2011; Justin, Qiang, & Sayan, 2011; Juyang & Wey-Shiuan, 2007; Seiichi, Asim, & Dmitri, 2009; Shenguei, Chunyu, & Tsengee, 2007). Unfortunately, MLPs of this type unavoidably run up against the problem of "imbalanced data", which often results in huge computational load and low generalization accuracy (He & Edwardo, 2009; Khoshgoftaar, Hulse, & Napolitano, 2010; Malof, Mazurowski, & Tourassi, 2012; Micheloni, Rani, Kumar, & Foresti, 2012; Ou & Murphey, 2007).

There are several such kinds of solution to implement the discriminative and quantitative analysis of many kinds of odors using MLPs. (A). By treating the task as a pure discrimination problem and a concentration point as a class, we can utilize either a single multi-output (SMO) perceptron or an SMO perceptron followed by multiple multi-output (MMO) perceptrons (Llobet et al., 1997; Orts et al., 1999) to solve it. (B). By looking upon the task first as a single multi-class discrimination and then as multiple quantification problems (Horner & Hierold, 1991), we can employ an SMO perceptron and multiple single-output (MSO) perceptrons to accomplish it. (C). By regarding the task first as multiple two-class discrimination and then as multiple quantification problems, we can use MSO perceptrons followed by MSO perceptrons to perform it (Gao, Liu, & Wang, 2012; Gao, Sun, & Li, 2007; Gao, Yang, & Sun, 2008). In our previous work (Gao & Chen, 2007), the task was first decomposed into multiple many-to-one regression tasks and then solved by multiple many-to-one regression model ensembles. The members in an ensemble may be a multivariate logarithmic regression model, a multivariate quadratic logarithmic regression model, an MLP, a support vector machine, and others. However, this type of ensemble is only suitable for implementing small-scale quantification tasks.

This paper focuses on evaluating the structural complexity, learning and generalization performance of several MLPs (Esmeir & Markovitch, 2011; Giovanni, Nicolò, & Claudio, 2011) in order to effectively recognize many kinds of odors and predict their concentrations as well. The rest of this paper is organized as follows. Section 2 specifically describes four types of single-hidden-layer perceptrons and their learning strategies. In Section 3, we give the experimental results for discriminating and quantifying 12 kinds of volatile organic compounds (VOCs) with different concentrations. Finally, Section 4 comes to our conclusions.

2. Structures and learning strategies of perceptrons

Each perceptron has a single hidden layer, and the BP algorithm is employed as the basic learning algorithm. The sigmoid activation functions of all the hidden and output neurons are set to be $f(x) = (1 + \exp(-x))^{-1}$, and the input variables are scaled in proportion to the real range [0.0, 1.0]. Correspondingly, the target or expected outputs for discrimination are coded in binary {0, 1}, and those for quantification are scaled to the real value (0.05, 0.95).

The input matrix of the original training set is expressed as $\boldsymbol{X} \in R^{N\times m}$, where N is the number of patterns and m the number

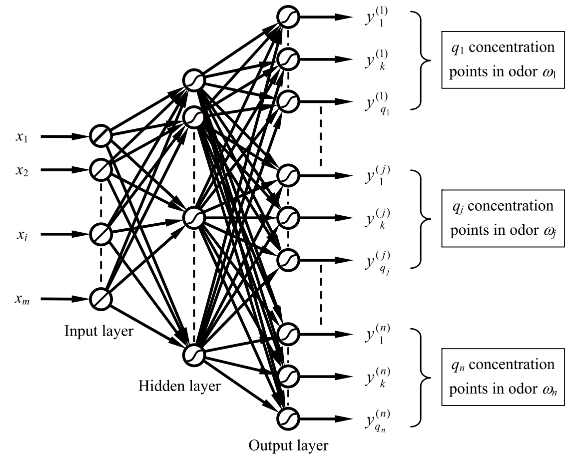

Fig. 1. A single multi-output perceptron.

of input dimensions or gas sensors. Let the real and target values of the jth output node of a perceptron at the τth iteration epoch for the pth pattern $\boldsymbol{x}_p = (x_{p1}, x_{p2}, \dots, x_{pm})^T$ be $y_p^{(j)}(\tau)$ and $t_p^{(j)}$, the root-mean-square (RMS) error of the perceptron is given by

$$E(\tau) = \sqrt{\frac{1}{2nN}\sum_{p=1}^{N}\sum_{j=1}^{n}\left(t_p^{(j)} - y_p^{(j)}(\tau)\right)^2}, \quad (1)$$

where n is the number of output nodes or kinds of odors. For the purpose of differentiation, sometimes $t_p^{(j)}$ is written as $d_p^{(j)}$, and $y_p^{(j)}(\tau)$ is written as $z_p^{(j)}(\tau)$, which is self-evident and needs no elaboration.

2.1. Structures of perceptrons

2.1.1. A single multi-output perceptron

An SMO perceptron looks upon a concentration point as a class. If there are n kinds of odors and q_j concentration levels in each, there are $q_1 + q_2 + \cdots + q_j + \cdots + q_n$ output units. Fig. 1 shows the structure of an SMO perceptron. For a m-dimensional input vector or pattern $\boldsymbol{x}_p = (x_{p1}, x_{p2}, \dots, x_{pi}, \dots, x_{pm})^T$, the SMO perceptron has m input nodes, and makes decisions according to the biggest of all the $q_1 + q_2 + \cdots + q_j + \cdots + q_n$ real output values. The expected output $d_{pk}^{(j)}$ corresponding to the kth concentration level in odor ω_j is coded as 1.0; otherwise 0.0. The SMO perceptron must be trained by all patterns $\boldsymbol{X} \in R^{N\times m}$. Along with the increase in numbers of odor sorts and concentration points, the SMO perceptron will become large and complicated in structure, and slow in learning speed. At the same time, the situation of imbalance between subclasses will tend to be serious. Besides that, what if a certain sample is located in or close to the middle of two known concentration points? One isolated island after another appears. Therefore, this type of perceptron extrapolates (Geoffrey, Janice, Fei, Kaiming, & Houssam, 2012) and has poor generalization performance.

2.1.2. A single multi-output perceptron followed by multiple multi-output perceptrons

A variant of the above SMO model is an SMO perceptron followed by multiple multi-output (MMO) perceptrons, called the SMO–MMO perceptron model, as shown in Fig. 2. The model first considers one kind of odor as a class, and then a concentration level in this kind as a class, too. If there are n kinds of odors and q_j concentration levels in ω_j, there are n output nodes in the former half, i.e., the SMO perceptron, and q_j output neurons in the jth multi-output perceptron in the latter half, i.e., one of the MMO