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Applications of Adaptive Kalman Filter Coupled with Multilayer Perceptron for Quantification Purposes in Electronic Nose ⋆

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Abstract

This paper proposes a hybrid method of adaptive Kalman filter and multilayer perceptron (MLP) neural network for more accurately estimating the gas concentration from transient response patterns of metal oxygen semiconductor (MOS) sensor array in an electronic nose. Since the gas sensor is easy to be disturbed by environmental background noise which is difficult to be removed in multidimensional nonlinear sensor array system. An adaptive Kalman filter, as a preprocessor, is used to reduce the possible background interference to each gas sensor separately. Besides, as a post-processing method, it is also operated on the outputs (concentrations) of MLP which has been well trained using a large number of gas samples toward reducing the instability of MLP predictor. Take common formaldehyde indoor as an analyte, experimental results demonstrate that the accuracy of MLP concentration predictor has been improved significantly by the adaptive parameters tuning Kalman filter.

Keywords: Adaptive Kalman Filter; Multilayer Perceptron; Electronic Nose; Preprocessing; Post-processing

1 Introduction

The primary focus of this work is the development of an adaptive filtering technique, known as Kalman filtering coupled with multilayer perceptron neural network, for more accurate concentration prediction using multidimensional sensor array in an electronic nose. Sensor array system or commonly called electronic nose system (E-nose), have already been shown to be effective in air quality monitoring application [1]. In [2], Gardner and Bartlett gave a comprehensive overview of these systems, which also contains a concise definition of an electronic nose: "an instrument

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which comprises an array of electronic chemical sensors with partial specificity and an appropriate pattern recognition algorithm". Artificial neural network (ANN) has been widely used for pattern classification and concentration estimation [3, 4]. However, the disadvantage of ANN is its strong sensitivities to very little response variations of sensors result from the environmental disturbance so that the concentration prediction would become unstable and inaccurate.

While numerous filtering techniques can be applied to preprocessing sensor response, only a few successful techniques have been identified that allow efficient on-line filtering of sensor response. One direct technique, which can be applied in real time, is simple average of the previous n measurements. The advantages of Kalman filtering technique over simple averaging have been presented in [5]. First, the Kalman filter incorporates all available measurements, regardless of their precision, and is not limited to a narrow window of n measurements to estimate the actual gas concentration. Second, the Kalman filter is computationally efficient although the equations are more complex than averaging technique, because it is recursive and only requires two sets of information instead of n to be transferred from measurement to measurement for filter calculations. Finally, the Kalman filter is adaptive and can adjust to changes in signal statistics and dynamic range during operation. In multivariate systems, feature selection methods have been fully studied [6, 7] and Kalman fiter has been used for drift correction [8, 9].

2 Theory

2.1 Multilayer perceptron (MLP)

With knowledge of the strong nonlinear relationship between the responses of the sensor array and the concentrations of an odor, MLP uses the back-propagation algorithm to adjust its weights and biases to perform the response-concentration approximation. The back-propagation algorithm is a gradient descent algorithm in which the MLP network weights are moved along the negative of the gradient of the performance function. We refer the reader to [10] for detailed description of the learning process in MLP. Suppose an array is made up of m sensors, let $x_p = (x_{p1}, x_{p2}, \cdots, x_{pi}, \cdots, x_{pm})^T$ be the preprocessed response of a sensor array for sample p, which is taken as the real input of the MLP, and x_{pi} is the response of the ith sensor. The real output of the MLP is the concentration from a known odor. Let the structure of MLP be $m - s_1 - s_2 - 1 (m = 6, s_1 = 10, s_2 = 10)$, which works for many-to-one approximation. Here, s1 and s2 are the number of hidden neurons of the two hidden layers. In this paper, the activation functions in the two hidden layers and the output layer are log-sigmoid, log-sigmoid and pure linear function, respectively. The diagram of the multilayer perceptron network used in this paper is illustrated as Fig.1.

2.2 Adaptive kalman filter model

Kalman filter is based on two models, rather than a single model. The system model is expressed as

$$x(k|k-1) = x(k-1|k-1) + \omega(k) \tag{1}$$

The measurement model is expressed as

$$z(k) = x(k|k-1) + \nu(k) \tag{2}$$

where $x(k)$, $z(k)$, $\omega(k)$ and $v\nu(k)$ are the state, measurement output, input noise and measurement noise of electronic nose system, respectively. Here, the expected value $E[\omega(k)] = E[\nu(k)] = 0$, and $\omega(k)$ and $\nu(k)$ are uncorrelated random variables with white noise variance of σ_ω^2 and σ_ν^2, respectively.

$$E[\omega(k)\omega^T(k)] = \sigma_\omega^2 \tag{3}$$

$$E[\nu(k)\nu^T(k)] = \sigma_\nu^2 \tag{4}$$

$$E[\omega(k)\nu^T(k)] = 0 \tag{5}$$

The two variances will have different meaning for different applications. In Kalman filter pre-processing step for sensor responses, the variance σ_ω^2 respesents the true environment variability while σ_ν^2 represents measurement noise introduced by the sensor circuit. At post-processing step for gas concentration, σ_ω^2 represents the true concentration variability and σ_ν^2 represents the noise of concentration prediction system. $\hat{x}_k^-$ can be defined to be the a priori estimation for a step k and $\hat{x}_k^-$ to be a posteriori estimate for step k after the measurement value z_k is incorporated. The a priori and a posteriori estimate errors can be defined as

$$e_k^- = x_k - \hat{x}_k^- \tag{6}$$

And

$$e_k = x_k - \hat{x}_k \tag{7}$$

The a priori estimate error variance is then given by the expected value

$$P_k^- = E[e_k^- e_k^-] \tag{8}$$

And the a posteriori estimate error variance is given by the expected value

$$P_k = E[e_k e_k] \tag{9}$$

The a posteriori estimate $\hat{x}_k$ can be recognized as a linear combination of the a priori estimate $\hat{x}_k^-$ and a weighted innovation $(z_k - \hat{x}_k)$ which can be shown as

$$\hat{x}_k = \hat{x}_k^- + K_k(z_k - \hat{x}_k) \tag{10}$$

Where K_k is called the Kalman filter gain and is used to minimize the a posteriori error variance. Solving for K_k yields the definition of the Kalman filter gain, given by

$$K_k = P_k^-(P_k^- + \sigma_v^2)^{-1} \tag{11}$$

We can find that as the measurement error variance σ_v^2 approaches zero, K_k approaches '1', and the actual measurement z_k becomes more trusted. However, as the measurement error variance σ_ν^2 increases to infinity, K_k approaches zero, and the predicted measurement is trusted more.

The solution provides the a posteriori estimate error variance as

$$p_k = (1 - K_k) - p_k^- \tag{12}$$

2.3 Kalman filter parameters self-tuning

Generally, determination of the value σ_ν^2 through operating the sensor at a constant environment is possible. However, obtain the system noise variance σ_ω^2 is extremely difficult. Though it can be estimated in practice, it is impossible to obtain the accurate values. Since sensor variability scales roughly linearly as environmental factors, the error variance ratio can be defined as [5, 11]

$$\lambda = \sigma_\nu^2/\sigma_\omega^2 \tag{13}$$

where λ is a constant. σ_ω^2 can be calculated by dividing σ_ν^2 by λ. Note that the ratio λ is determined in experiment for each gas sensor, and it depends on the specific circumstances including the sensor and the system that is being measured. Thus,λ is not an intrinsic property of the gas sensor.

2.4 Adaptive kalman filter algorithm

The time update equations act as predictor equations while measurement update equations act as corrector equations. The measurement update equations are responsible for the feedback or for incorporating a new measurement into the a priori estimate to obtain an improved a posteriori estimate.

The time updating equations from time step k to step k+1 can be given by

$$\hat{x}_{k+1}^- = \hat{x}_k \tag{14}$$

$$p_{k+1}^- = P_k + \sigma_\omega^2 \tag{15}$$

The measurement updating equations are shown as

$$K_k = P_k^-(P_k^- + \sigma_\nu^2)^{-1} \tag{16}$$

$$P_k = (1 - K_k)P_k^- \tag{17}$$

$$\hat{x}_k = \hat{x}_k^- + K_k(z_k - \hat{x}_k^-) \tag{18}$$

$$\sigma_\omega^2 = \sigma_\nu^2/\lambda \tag{19}$$

3 Experiments

3.1 Experimental setup

The sensor array consists of seven sensors: temperature, humidity, TGS2602, TGS2620, T-GS2201A and TGS2201B sensor. Measurements were carried out on formaldehyde by an electronic nose in a Constant Temperature and Humidity chamber. The chamber can accurately simulate indoor environments with common temperature and humidity. For all the measurements, target temperature value (degree Celsius) of 15, 20, 25, 30, and 35 were considered; whereas the target humidity values were 40%, 60%, and 80%. Thus, there are 15 different environments of temperature and humidity considered for kinds of experienced concentrations indoor. As for the gas sampling, high precision chromatography syringes were used to inject the volume of formaldehyde needed to create a concentration in the chamber, within the desired range. The experimental concentration range of formaldehyde is set within 0.1 10 ppm. The exact concentration value for each measurement is obtained from the spectrophotometer by analyzing the sampling formaldehyde for 10mins during each experiment. Totally, 142 measurements are employed. Therein, 126 samples are used to learn the hyper-parameters of the MLP for concentration estimation; the left 16 samples are used for validation in real time. For the purpose of clarity, the 126 samples used for training were collected in the controlled temperature and humidity, that is, the temperature and humidity remain constant and have little fluctuations. However, the 16 samples used for validation were collected without controlling the temperature and humidity, namely, the sensor responses will have large fluctuations because of the variable temperature and humidity. Note that each sample contains 370 points collected in one measurement.

The diagram of the concentration predictor in this paper is shown as **Fig.2**.

3.2 Experimental results

3.2.1 Data preprocessing

In this work, the measurement noise σ_ν^2 is determined as constant $1 \times 10_{-5}$, according to our experience. Fig.3(a)-(d) denote the preprocessed results of TGS2602, TGS2201B, TGS2620 and TGS2201A, respectively. Total, 5940 sampling points of 16 validation samples are collected for each sensor. From these three figures, we can find that with larger ratio λ value, the curve would become smoother compared with the curve of raw data. That's mean the small fluctuations are reduced through the adaptive Kalman filter. However, the true information of concentration variations are not removed, and the features of sensor response variations are still reflected in the filtered data. The effect of Kalman filter can be expressed better from the 2600^{th} points that have significantly sawtooth (fluctuations).

3.2.2 Post-processing of gas concentration

For comparison, we present two figures illustrated the predicted concentrations using the MLP trained on the measured 126 samples with controlled temperature and humidity. The training iterations (epochs) are set as 2000, and the converging goal is set as 0.05. The well trained MLP was directly tested on the 16 validation samples. **Fig.4(e)** illustrated the concentrations without Kalman filter preprocessing of sensor responses; **Fig.4(f)** denoted the predicted concentrations in which the inputs (sensor responses) of MLP have been first preprocessed by Kalman filter. From **Fig.4(e)**, we can find that the dashed line (raw MLP) is fluctuated significantly. This is because of the non-preprocessed sensor response with small variations result from the background noise (see the dashed lines in **Fig.3**). After Kalman filtering on the raw predicted concentrations with $\lambda = 500$ and 5000 separately, the concentrations have become stable. From **Fig.4(f)**, we can find the dashed line (raw predicted concentrations) is smooth when the sensor responses have been preprocessed by Kalman filter. The dashed line is almost the same as the curve ($\lambda = 500$) in **Fig.4(e)**. This fully demonstrates the effect of the filter. And also, $\lambda = 500$ can be recognized as the accepted level of filtering in our system.

4 Conclusions

This paper proposes a hybrid algorithm of adaptive Kalman filter and multilayer perceptron neural network to estimate gas concentration by an electronic nose. We introduce the tuning ratio λ to adaptively control the Kalman filter. Experimental results demonstrate that the proposed hybrid method can more accurately estimate gas concentration in real time, and also prove the extensive application of Kalman filter in multivariate nonlinear systems.

5 Figure Section

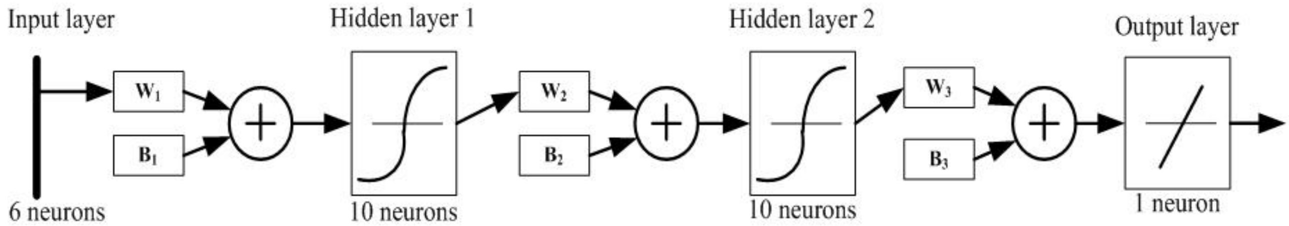

Fig. 1: Structure of multilayer perceptron neural network

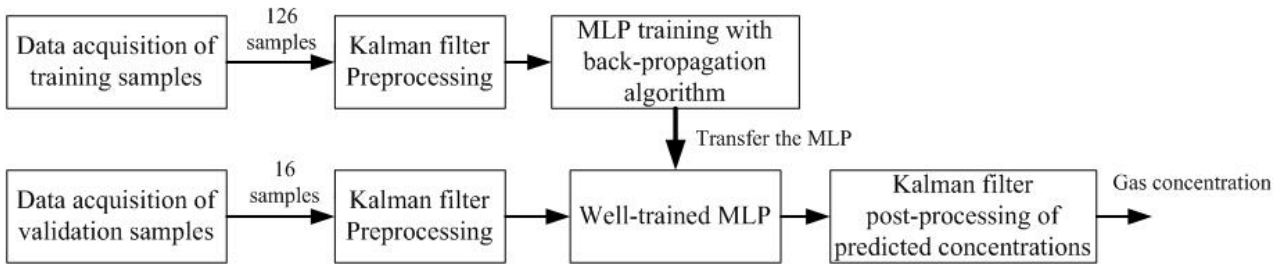

Fig. 2: Algorithm structure of the concentration predictor

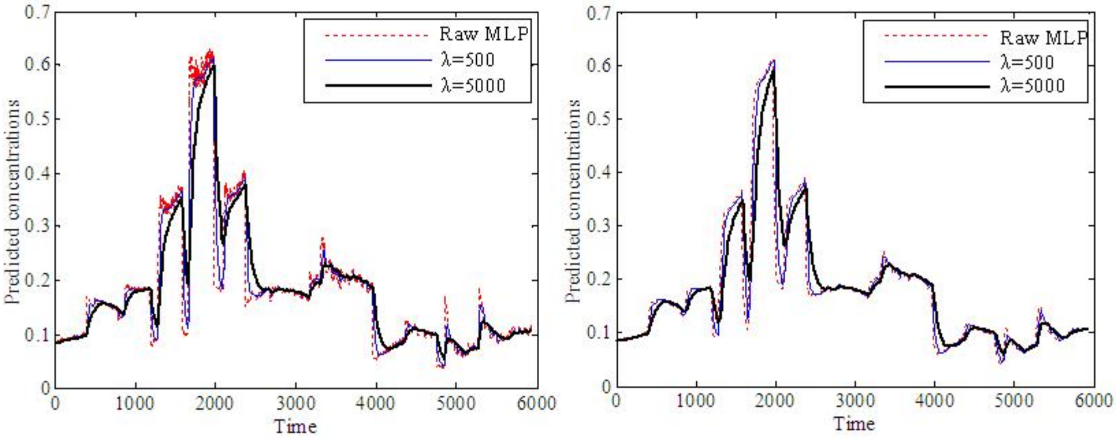

Fig. 4: Gas concentration post-processing after MLP using the adaptive Kalman filter

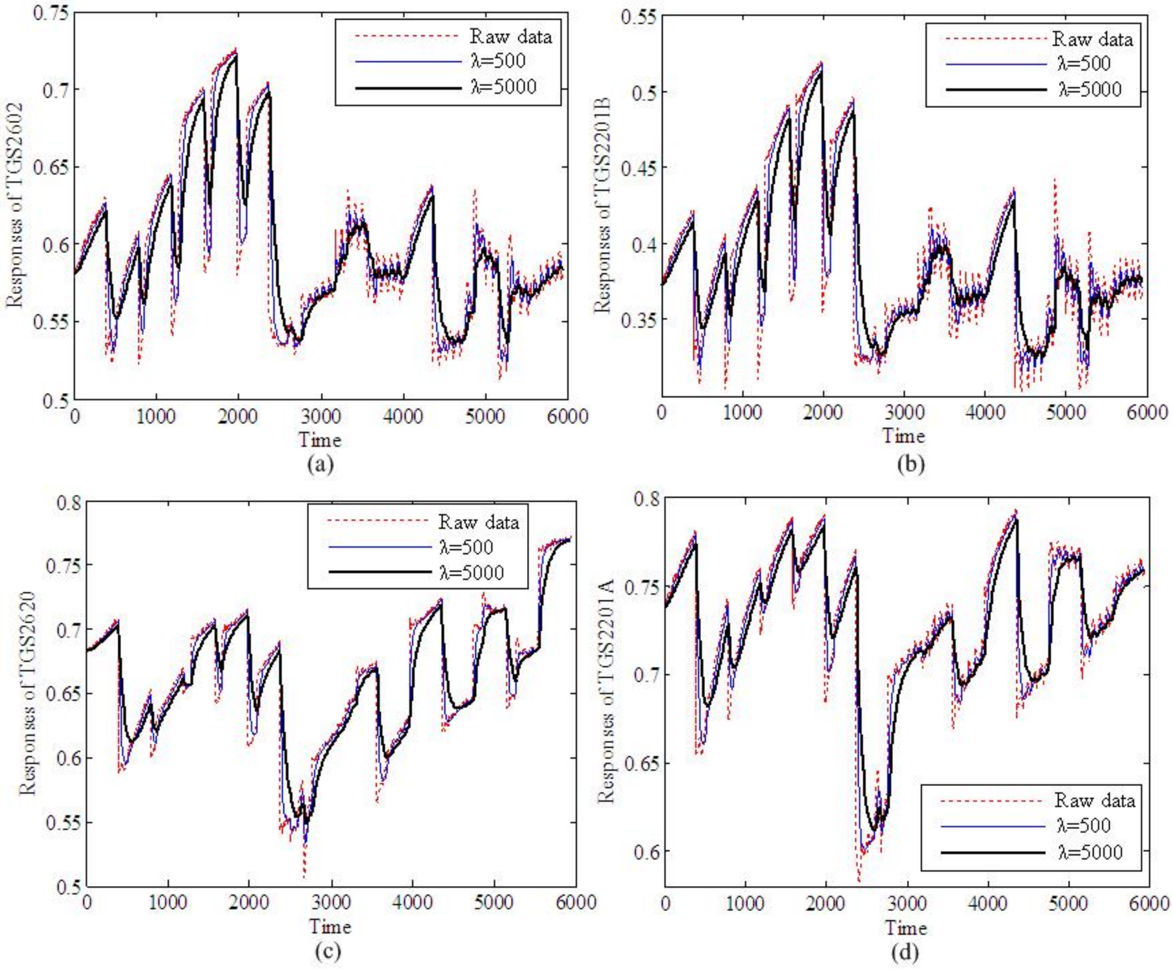

Fig. 3: Gas sensor transient responses preprocessing using the adaptive Kalman filter

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