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Gaussian process based modeling and experimental design for sensor calibration in drifting environments

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ABSTRACT

It remains a challenge to accurately calibrate a sensor subject to environmental drift. The calibration task for such a sensor is to quantify the relationship between the sensor's response and its exposure condition, which is specified by not only the analyte concentration but also the environmental factors such as temperature and humidity. This work developed a Gaussian Process (GP)-based procedure for the efficient calibration of sensors in drifting environments. Adopted as the calibration model, GP is not only able to capture the possibly nonlinear relationship between the sensor responses and the various exposure-condition factors, but also able to provide valid statistical inference for uncertainty quantification of the target estimates (e.g., the estimated analyte concentration of an unknown environment). Built on GP's inference ability, an experimental design method was developed to achieve efficient sampling of calibration data in a batch sequential manner. The resulting calibration procedure, which integrates the GP-based modeling and experimental design, was applied on a simulated chemiresistor sensor to demonstrate its effectiveness and its efficiency over the traditional method.

1. Introduction

Chemical sensors have been widely used in indoor and outdoor environment monitoring, vehicle exhaust measurement, human breath detection, etc [1–3]. It has been long recognized that the responses of chemical sensors, especially chemiresistors, are affected by the drift of environmental factors such as temperature and humidity [4–7]. To reduce detection errors and false alarm, it is important to accurately calibrate a sensor in a drifting environment, which primarily motivated this work. The environmental factors are denoted as the vector $\mathbf{x}$, and the task of sensor calibration is to establish the functional dependence of the sensor response r upon the analyte concentration c as well as $\mathbf{x}$.

Quantifying the $c-\mathbf{x}-r$ relationship is challenging due to two main reasons: First, the variables $(c, \mathbf{x})$ may affect the response r in a nonlinear fashion and also interact nonlinearly with each other. The underlying mechanism is complicated [8–11] and difficult to be adequately captured by traditional regression analysis [6]. Second, to estimate a calibration model of high dimension, an extremely large sample size is typically required by the classic design of experiments (DOE) [6,12]. Thus, there is a need to develop new modeling and DOE methods for the efficient calibration of sensors subject to environmental drift.

While focusing on calibrating sensors with environmental drift, this work falls into the research efforts to calibrate sensors with general drifting behaviors, which can be classified into two categories [13,14]: external (i.e. environmental) and internal drifts. The latter is caused by the physical and/or chemical changes of the sensor itself, and examples of such changes include re-organization of the sensing materials and irreversible interaction with analytes. When calibrating drifting sensors, most of the literature used a reference-based linear compensation or linear regression to quantify the drifting effects [15–18]. Recognizing the possible nonlinear nature of sensor drifts, powerful nonlinear models have also been employed, such as neural network [6,19], kernel ridge regression [20] and nonlinear supporting vector machine [21]. However, in this stream of nonlinear modeling work, no effort was ever made to quantify the uncertainty of the target estimates (e.g., the analyte concentration estimated by the calibration model from an observed sensor response). This is at least partly due to the difficulties in deriving valid statistical inference (i.e., quantifying model uncertainty) based on those models [22,23]. It is known that statistical inference lays the basis for optimum DOE: Experiments are designed to minimize the uncertainty on the model estimates of

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interest [24–26]. Thus, optimum DOE is a research issue that has barely been touched in the nonlinear model-based sensor calibration.

In light of the discussions above, our objective is to develop a statistical procedure, which leads to a calibration model of the highest quality by using the least experimental effort. In this work, the calibration model assumes the form of a Gaussian process (GP), which is highly flexible and able to capture practically any continuous functional relationships. GP is chosen over other powerful nonlinear models because of its statistical inference capability [27], which allows for uncertainty quantification and provides the necessary basis for optimum DOE. For sensor calibration, the inference issues are further complicated by the coexistence of forward modeling and inverse estimation (as will become clearer in Section 2.1), and hence a GP-based bootstrap resampling method is developed in this work. The DOE is performed in a batch sequential manner to circumvent the dilemma that the optimum DOE depends on the true $c-\mathbf{x}-r$ relationship, which however, is unknown at the stage of designing experiments [28,25,24]. A learning process is allowed in such a sequential procedure: For the design of a new batch of experiments to be performed, all the information derived from the experimental data already collected is utilized to search for the optimum DOE of that new batch; and the DOE optimization seeks to minimize the calibration model uncertainty with a given batch size.

The remainder of the paper is organized as follows: Section 2 presents the formulation of the calibration model, which takes the form of a GP. The GP-based model fitting and statistical inference issues are discussed in Section 3. The batch sequential procedure for sensor calibration is described in Section 4. Section 5 is devoted to an empirical study to evaluate the effectiveness and efficiency of the calibration procedure. A brief summary is given in Section 6.

2. Formulation of calibration model

2.1. Calibration model

For a sensor exposed to drifting environments, its calibration model needs to functionally relate the sensor response r to the target analyte concentration c as well as the environmental factors $\mathbf{x}$. For notational convenience, all the exposure-condition factors are denoted as the vector $\mathbf{w}=(c,\mathbf{x}^\top)^\top$ of d dimension, with d being a positive integer. The sensor response can be generally written as

$$r(\mathbf{w})=\mathrm{E}[r(\mathbf{w})]+\epsilon=F(\mathbf{w})+\epsilon,\quad \mathbf{w}\in\mathcal{W} \tag{1}$$

where $F(\mathbf{w})$ quantifies the expected sensor response $\mathrm{E}[r(\mathbf{w})]$ as a function of $\mathbf{w}$. The feasible region of interest for exposure conditions is represented by $\mathcal{W}$. The sensor response r is subject to random error ϵ, which arises from instrument noise, variation of sensing materials, etc. The random error ϵ is assumed to be independent and identically distributed (i.i.d.). The exposure condition $\mathbf{w}$ is considered as deterministic, which complies with the actual experimental settings: In calibration experiments, $\mathbf{w}$ can be specified with extremely high accuracy and precision.

The calibration model fitted from experimental data is denoted as $\widehat{F}(\mathbf{w})$, or equivalently $\widehat{F}(c,\mathbf{x})$. In operational use, $\widehat{F}(c,\mathbf{x})$ is coupled with the sensor device to quantify the target analyte. The observed sensor response r_0 and the observed values $\mathbf{x}_0$ for the environmental factors (e.g., temperature and humidity) are used to estimate the underlying analyte concentration c_0 as follows

$$\widehat{c}_0=\widehat{F}^{-1}(r_0,\mathbf{x}_0). \tag{2}$$

In (2), $\widehat{F}^{-1}$ denotes the inverse function of $\widehat{F}$ with respect to (w.r.t.) c at given $\mathbf{x}_0$. This inverse function is assumed to exist in the region $\mathcal{W}$ considered, because otherwise the sensor would not be applicable at all.

Model (1) is also referred to as forward model, since it reflects the forward direction of calibration experiments: For a pre-specified $\mathbf{w}$, the response r is observed. Whereas, when the calibration model is coupled with the sensor device for monitoring, the inverse estimation of analyte concentration from observed r needs to be performed, as shown in (2).

2.2. Gaussian process model

As mentioned in Section 1, a GP is chosen in this work to model the functional dependence of r upon $\mathbf{w}$, and the GP calibration model (1) is represented as

$$r=F(\mathbf{w})+\epsilon=\mu+\mathsf{M}(\mathbf{w})+\epsilon, \tag{3}$$

where μ is the mean parameter, and $\mathsf{M}(\mathbf{w})$ is a realization of a mean-zero stationary GP with constant variance τ^2. The random error ϵ follows a continuous probability distribution (e.g., normal). In this work, it is assumed that the variance of ϵ is a constant σ^2, which is a typical assumption for sensor calibration [29,30]. However, it is worthy of noting that the GP model can be extended to accommodate general variance structures of the errors, as in Ankenman et al. [31].

The GP $\mathsf{M}(\cdot)$ is characterized by its correlation function [32], which is denoted as $\mathrm{Corr}(\mathsf{M}(\mathbf{w}),\mathsf{M}(\mathbf{w}'))$, where $\mathbf{w}=(w_1,w_2,\ldots,w_d)^\top$ and $\mathbf{w}'=(w'_1,w'_2,\ldots,w'_d)^\top$ represent two distinct exposure conditions. In this work, we adopted the widely-used squared exponential form [27] for the correlation function:

$$\mathrm{Corr}(\mathsf{M}(\mathbf{w}),\mathsf{M}(\mathbf{w}'))=K(\mathbf{w},\mathbf{w}')=\exp\left\{\sum_{h=1}^{d}-\theta_h(w_h-w'_h)^2\right\}, \tag{4}$$

where $\boldsymbol{\theta}=(\theta_1,\theta_2,\ldots,\theta_d)$ is a vector of unknown parameters to be estimated from the experimental data. It is required that $\theta_h>0$, and a smaller value of θ_h tends to provide a smoother response surface. Other choices of the correlation forms can be found in the literature [24,27].

For a collection of I distinct exposure conditions $\{\mathbf{w}_i;i=1,2,\ldots,I\}$ with I being a positive integer, an $I\times I$ correlation matrix $\mathbf{R}(\boldsymbol{\theta})$ is defined as:

$$\mathbf{R}(\boldsymbol{\theta})=\begin{pmatrix}1 & K(\mathbf{w}_1,\mathbf{w}_2) & \ldots & K(\mathbf{w}_1,\mathbf{w}_I)\\ K(\mathbf{w}_2,\mathbf{w}_1) & 1 & \ldots & K(\mathbf{w}_2,\mathbf{w}_I)\\ \vdots & \vdots & \ddots & \vdots\\ K(\mathbf{w}_I,\mathbf{w}_1) & K(\mathbf{w}_I,\mathbf{w}_2) & \ldots & 1\end{pmatrix}. \tag{5}$$

Along with an arbitrary condition $\mathbf{w}_0$, we further define the following $I\times 1$ vector

$$\mathbf{v}(\mathbf{w}_0;\boldsymbol{\theta})=\begin{pmatrix}K(\mathbf{w}_0,\mathbf{w}_1)\\ K(\mathbf{w}_0,\mathbf{w}_2)\\ \vdots\\ K(\mathbf{w}_0,\mathbf{w}_I)\end{pmatrix}. \tag{6}$$

3. Model estimation and inferences

3.1. Experimental data for sensor calibration

To calibrate a sensor, experimental data has to be collected at a range of exposure conditions. The calibration sample data can be represented as

$$\{(\mathbf{w}_i,r_j(\mathbf{w}_i));\ i=1,2,\ldots,I,\ j=1,2,\ldots,n\}. \tag{7}$$