Quantification of Gas Mixtures with Active Recursive Estimation

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Abstract. We present an active-sensing strategy to estimate the concentrations in a gas mixture using temperature modulation of metal-oxide (MOX) sensors. The approach is based on recursive Bayesian estimation and uses an information-theoretic criterion to select operating temperatures on-the-fly. Recursive estimation has been widely used in mobile robotics, e.g., for localization purposes. Here, we employ a similar approach to estimate the concentrations of the constituents in a gas mixture. In this formulation, we represent a concentration profile as a discrete state and maintain a 'belief' distribution that represents the probability of each state. We employ a Bayes filter to update the belief distribution whenever new sensor measurements arrive, and a mutual-information criterion to select the next operating temperature. This allows us to optimize the temperature program in real time, as the sensor interacts with its environment. We validate our approach on a simulated dataset generated from temperature modulated responses of a MOX sensor exposed to a mixture of three analytes. The results presented here provide a preliminary proof of concept for an agile approach to quantifying gas mixtures.

Keywords: Metal-oxide sensors, Active sensing, Recursive estimation.
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METHODS AND RESULTS

We used a sensor model based on [1] to generate data for ternary gas mixtures. We model the sensor's steady-state response $G(T)$ when exposed to a mixture of non-interacting gases as eq.(1), where T denotes temperature, $G_0\ (T)$ is the static sensor response to air, $S_i\ (T)$ is the sensitivity of the sensor to gas i, c_i is the concentration of gas i, β_i is a gas-dependent parameter, and r_0 is random noise. Using this dataset, we trained a Bayesian network to model the joint distribution of responses, concentrations and temperatures $p(G, T, \theta)$, where $\theta = (c_1, c_2, c_3)$.

$$G(T) = G_0\left(1 + \sum_i S_i(T) c_i{}^{\beta_i}\right) + r_0 \tag{1}$$

Given a sequence of t temperatures $\{T_1, T_2, \ldots, T_t\}$ and their corresponding sensor responses $\{o_1, o_2, \ldots, o_t\}$, the recursive estimation algorithm updates the posterior density $p(\theta_t)$ using eq.(2). The updated posterior $p(\theta_t)$ and the sensor model are then used to determine the 'best' temperature for time $t + 1$. This is performed by estimating the mutual information $I(\theta; T^a) = H(\theta) - H(\theta | T^a)$ associated with each temperature T^a and selecting the temperature that maximizes this measure.

$$p(\theta_t | o_{1\ldots t}, T_{1\ldots t}) = \frac{p(o_t|\theta_t)\, p(\theta_t | o_{1\ldots t-1}, T_{1\ldots t-1})}{p(o_t|\theta_{t-1})} \tag{2}$$

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To validate the approach, we created a scenario with a simulated MOX sensor operating at 20 different temperatures. FIGURE 1 (b) shows the sensitivity of the MOX sensor to three hypothetical gases as a function of temperature. To discretize the state space $\theta = (c_1, c_2, c_3)$, we assumed that each gas could have 5 concentrations (200, 400 … 1000); thus, θ can take 125 discrete values (5×5×5). FIGURE 2 (a) shows the simulated sensor response to three sample concentration profiles. Results from the method are illustrated through a test case. In the example, the concentration profile is set to θ^F= (400,800,400) and the sensor responses were obtained with eq.(1). The recursive estimation method required three temperature steps to identify the concentration profile. FIGURE 2 (b) shows how the probability $p(\theta = \theta^F)$ increases as new sensor measurements are obtained, and also shows how the uncertainty in the concentration profile θ reduces over time.

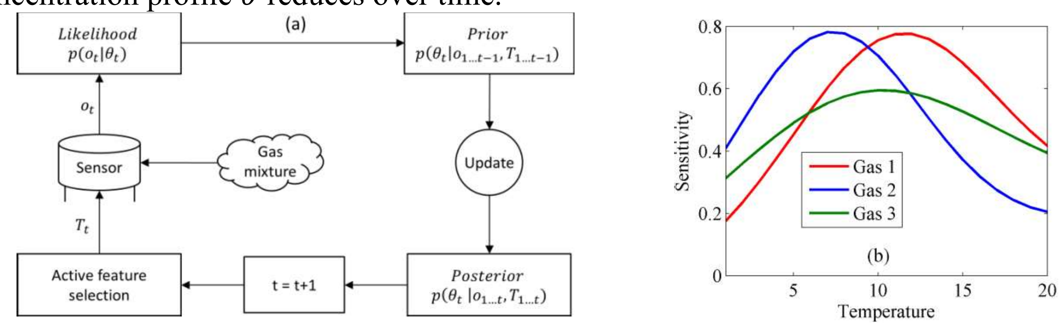

FIGURE 1. (a) Recursive Bayesian estimation combined with an active feature selection strategy to estimate the concentrations of a gas mixture. **(b)** Sensitivity of the MOX sensor to three hypothetical chemicals as a function of temperature.

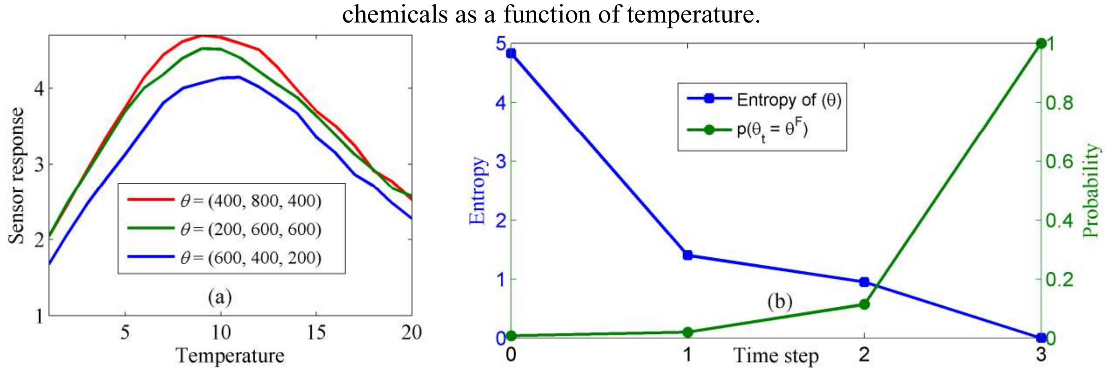

FIGURE 2. (a) Steady-state responses of the MOX sensor to a ternary mixture of gases at different concentrations. **(b)** Entropy $\boldsymbol{H(\theta_t)}$ and probability $\boldsymbol{p(\theta = \theta^F)}$ as a function of time. At time $\boldsymbol{t = 0}$, no sensor measurements have been made, so all profiles are equally likely $\boldsymbol{p(\theta_0 = \theta^F) = 1/125}$ and the entropy $\boldsymbol{H(\theta_0) = \log_e(125) = 4.82}$. The recursive filter selects three temperatures $\boldsymbol{\{T_1 = 4, T_2 = 2, T_3 = 20\}}$, after which the probability $\boldsymbol{p(\theta_3 = \theta^F) = 1.0}$ and the uncertainty reduces to $\boldsymbol{H(\theta_3) = 0}$.

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