

Invited: Advances in Active and Adaptive Chemical Sensing

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Abstract. In this presentation, we will review advances at the chemical sensor and data processing levels that may enable the development of adaptive sensors. We will briefly discuss techniques at the sensor and system levels, including modulation of internal parameters (e.g., operating temperatures and absorption wavelengths) and external parameters (e.g., exposure times, preconcentration temperatures). At the signal processing level, we will overview adaptive filtering strategies that may be used to cancel interferences (e.g., environmental variables, drift), adaptive classification techniques for incremental learning in dynamic environments, and active sensing methods for on-line optimization of sensor arrays and individual tunable sensors. We will also present a methodology based on probabilistic graphical models that may be used to model the dynamic response of metal-oxide sensors under temperature modulation and select suitable temperature sequences on-the-fly, as the sensor interacts with its environment.

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METHODS AND RESULTS

Our approach [1] for active sensing consists of modeling the sensor's dynamic response to a sequence of temperature pulses by means of an Input-Output Hidden Markov Model (IOHMM). IOHMMs can be used to learn a dynamic mapping between two data streams, an input (i.e., temperature) and an output (sensor conductance). Given a learned IOHMM model, we approach temperature optimization as a problem of sequential decision making under uncertainty, where we must balance the cost of applying additional temperature steps (i.e., which incur energy costs) against the risk of misclassifying based on limited sensor information. This is solved by casting the problem as a partially observable Markov decision process (POMDP).

We validated the approach using a commercial sensor (TGS 2600; Figaro USA, Inc.) exposed to three analytes (acetone, ammonia, and isopropyl alcohol). To avoid ceiling effects, the analytes were serially diluted in water to a concentration at which the sensor provided similar isothermal responses. We used eight heater voltages (i.e., sensing actions) ranging from 1V to 8V. FIGURE 1 shows the dynamic sensor response to a random temperature sequence and the corresponding predictions from the IOHMMs (one model per chemical). The models explain a significant proportion of the variance in each sensor: 90% for acetone and ISP, 92% for ammonia. FIGURE 2 (a) shows the classification rate and average number of temperature steps selected by

the POMDP as a function of sensing costs: as these costs increase, the POMDP selects fewer temperature steps at the expense of reduced classification performance.

Finally, we analyzed the feature-selection strategy of the POMDP when the relative energy of each action is also considered [2] (results in FIGURE 2 (a) assumed uniform sensing costs). As before, we operated the sensor at eight different voltages, but considered three pulse durations at multiples of the sensor’s time constant $\tau = 5$ sec, or 24 possible actions. Sensing costs were assumed proportional to the product of operating temperature and pulse duration. Results are shown in FIGURE 2 (b). As misclassification costs increase, the POMDP tends to select more expensive actions in order to minimize the risk of misclassification.

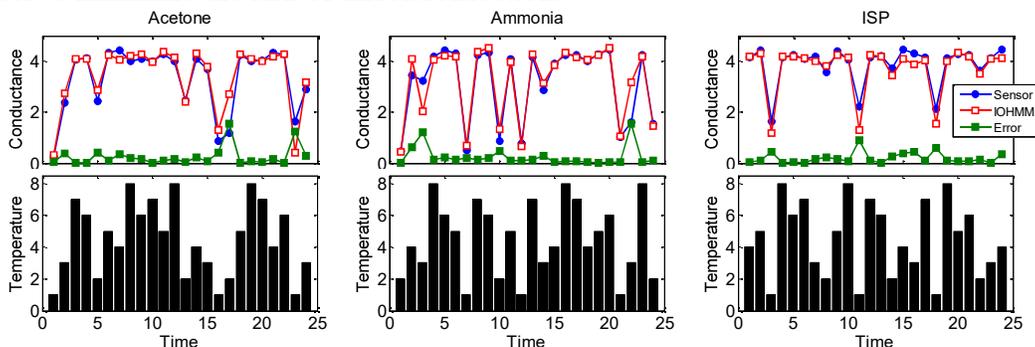


FIGURE 1. Comparison between IOHMM predictions and actual sensor response to a random sequence of heater voltages in the presence of acetone, ammonia, and isopropyl alcohol; information from each transient was reduced to a single observation by computing its integral response.

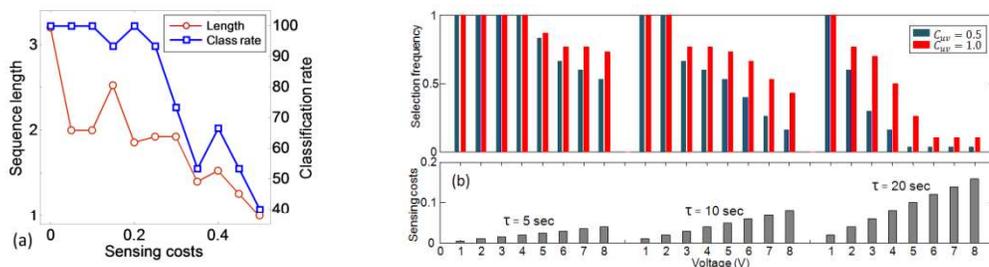


FIGURE 2. (a) Classification rate and average sequence length as a function of sensing costs (assumed independent of temperature). The POMDP attempts to balance sensing costs (shorter sequences) and classification performance (longer sequences). (b) **(top)** Frequency of selecting each action for two misclassification costs and **(bottom)** sensing costs associated with each action. The POMDP tends to select actions with lower energy cost (e.g., lower temperature and duration). As misclassification costs increase, the POMDP selects more expensive actions (higher temperatures and longer pulses)

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REFERENCES

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