LEAST-SQUARES BASED FEATURE EXTRACTION AND SENSOR FUSION FOR EXPLOSIVE DETECTION

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ABSTRACT

The effective and reliable detection of explosive compounds in complex environments is an important problem in many environment and security-related applications. This paper develops an explosive detection approach based on multi-modal sensing and sensor data fusion. Novel feature extraction techniques are designed to isolate explosive signatures in data collected using electrochemical and polymer nanojunction sensors. The information obtained from the two sensors is then efficiently combined using a Bayesian decision fusion scheme. Results are presented for the detection of the explosive compound TNT showing the merit of the proposed approach.

Index Terms— electrochemical and polymer nanojunction sensing, explosive detection, least squares feature extraction, sensor fusion

1. INTRODUCTION

An important problem encountered in many environment, defense, and security-related applications is the reliable real-time detection of traces of explosive chemicals in complex environments. The presence of a large number of interferent chemicals and substances in real scenarios makes the detection problem very challenging. Adequate standoff is of particular importance from safety considerations. Specificity and sensitivity are among the major issues in the design of sensors and data processing algorithms for detecting explosives [1]. Other desirable features of a candidate explosive detection system are speed, low cost, and portability.

Several sensing, analysis, and detection methods have been studied in the past, including those based on fluorescence, electrochemistry [2], ion mobility, and mass spectrometry; see [3] and the references therein for a review. The electrochemical methods rely on the detection of electrochemical reactions of analytes in an electrolyte (which take place at different potentials depending on the analyte) and are attractive due to their selectivity properties.

In this paper, we develop an approach for detection of the explosive compound TNT based on multi-modal sensing and sensor data fusion. Two different sensing platforms are utilized for data collection. The first is an integrated preconcentrator/detection system for electrochemical sensing of TNT which integrates a polymer-coated microfabricated electrochemical sensor with an explosive preconcentrator [4]. The second is a hybrid nanosensor based on the electrochemical reduction of TNT and the interaction of the reduction products with conducting polymer nanojunctions in an ionic liquid. These sensors are capable of detecting ppt-level TNT in the presence of various interferents within a few minutes. We design novel feature extraction techniques based on the method of least-squares to isolate the explosive signatures in data collected using the electrochemical and polymer nanojunction sensors. A Bayesian decision fusion scheme is then implemented to effectively integrate the information obtained from the two sensors for maximizing the performance of the detector. We present results for the detection of TNT and discuss the utility of the proposed approach.

2. FEATURE EXTRACTION BASED ON LEAST-SQUARES

In this section we describe the least-squares based method utilized for extracting features from the measured sensor data. The details of the least-squares principle and optimization can be found in [5, 6].

The purpose of feature extraction is to condense the information contained in the obtained data (measured sensor signals) into a form that is more amenable for further analysis and processing. In the present problem, the measured sensor

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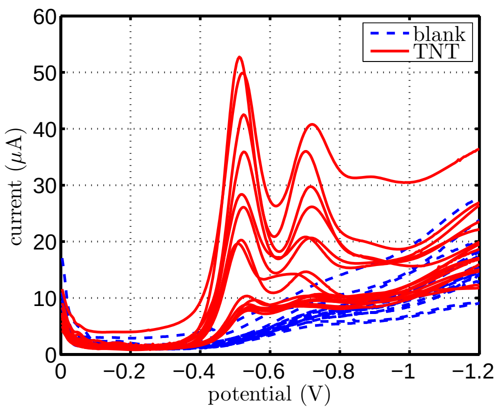
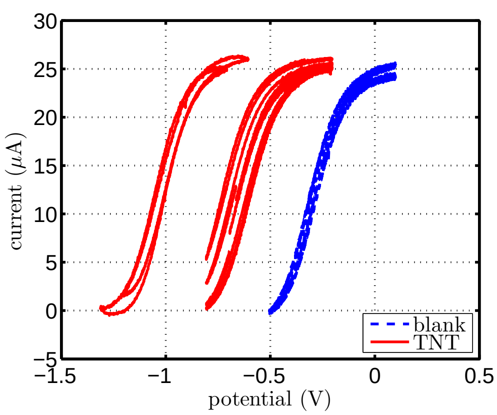
data comprises sampled current vs. voltage signals which contain the indicators about the presence of the explosive compound(s) of interest. Figure 1 shows a few example signals from the electrochemical and polymer nanojunction sensors for the cases when there is no explosive (blank) and when the explosive is present (TNT). From the plots in Figure 1(a) for the electrochemical sensor signals, we see peaks in the current at certain voltage positions for the TNT case as compared to the blank case. From the plots in Figure 1(b) for the polymer nanojunction sensor signals, we see a shift in voltage and/or current in the presence of TNT as compared to the blank case. Since our goal is to detect the presence of TNT, the feature extraction algorithms are designed to isolate these differences between the signals for the blank and TNT cases.



(a) Electrochemical sensor



(b) Polymer nanojunction sensor

Fig. 1. Example signals for the blank and TNT cases.

In this paper, the features used to identify the presence of TNT are the amplitude and curvature of the peaks in the current at known voltage positions (for the electrochemical sensor signals) and the relative magnitude shift in the voltage and/or current (for the polymer nanojunction sensor signals). A simple yet effective tool for extracting these features from the measured sensor signals is provided by the method of least-squares [5, 6].

The least-squares based feature extraction procedure is based on optimizing a suitable parameterized model for the signals in question, with the optimized parameter values then serving as the desired features. Let $\mathbf{i} = [i(V_1), \ldots, i(V_N)]^T$ denote the (discrete) measured sensor signal and $\mathbf{f}(\boldsymbol{\theta}) = [f(V_1, \boldsymbol{\theta}), \ldots, f(V_N, \boldsymbol{\theta})]^T$ the signal model with parameter $\boldsymbol{\theta} = [\theta_1, \ldots, \theta_M]^T$ (the superscript T denotes transpose). The least-squares optimization problem can be written as:

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \|\mathbf{i} - \mathbf{f}(\boldsymbol{\theta})\|^2, \qquad (1)$$

where $\|\cdot\|$ is the 2-norm. Essentially, we seek the parameter $\boldsymbol{\theta}^*$ which minimizes the sum squared error in approximating the signal $\mathbf{i}$ with the model $\mathbf{f}(\boldsymbol{\theta})$. When $\mathbf{f}(\boldsymbol{\theta}) = \mathbf{F}.\boldsymbol{\theta}$ is linear, the least-squares optimization problem (1) is convex and can be solved in a stable and efficient manner using orthogonal matrix factorizations [5, 6] (the analytical solution $\boldsymbol{\theta}^* = (\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\mathbf{i}$ is rarely used due to poor numerical stability). In general, however, iterative techniques must be employed to solve (1).

For the electrochemical sensor signals, in the vicinity of a voltage position V_0 where a peak is expected (defined by a rectangular window of size W), we use a quadratic model:

$$f^{\mathrm{EC}}(V_n, \boldsymbol{\theta}) = \theta_1 + \theta_2 v_n + \theta_3 v_n^2, \;\; n = 1, \ldots, N, \qquad (2)$$

where $v_n = (V_n - V_0)/W$. The derived features are the amplitude θ_1^* and curvature θ_3^* of the optimized quadratic function. For the polymer nanojunction sensor signals, our model is based on a modified logistic function:

$$f^{\mathrm{PNJ}}(V_n, \boldsymbol{\theta}) = \frac{\theta_1}{1 + e^{-(V_n - \theta_2)/\theta_3}}, \;\; n = 1, \ldots, N, \qquad (3)$$

and the derived feature is the shift θ_2^* of the optimized logistic function. Observe that using the model (2) in (1) results in a linear least-squares problem, whereas the least-squares problem resulting from using (3) in (1) is nonlinear.

3. SENSOR FUSION AND DETECTION

We now turn to the framework of sensor fusion and detection. For more details on these methods the reader is referred to the literature [7, 8].

The goal of sensor data fusion is to exploit the information obtained from multiple sensing platforms in order to maximize the detection capability. To that end, we make use of the Bayesian decision fusion approach in which local decisions are first made using data from individual sensors and these are then combined at a decision fusion center to arrive at a global optimal decision. The decision fusion framework has advantages such as flexibility in combining different types of sensing and processing schemes and the availability of local decisions if needed.

The individual detectors which provide the local decisions at the electrochemical and polymer nanojunction sensors are designed as follows. For the electrochemical sensor data, the test statistic for identifying the presence of a peak at voltage position V_0 is defined as the combined amplitude-curvature $x^{\mathrm{EC}}(V_0) = \theta_1^* - w\theta_3^*$ (w is a weighting constant). The local detector uses the presence of a peak at both $V_0^{(1)} = -0.52$ V and $V_0^{(2)} = -0.7$ V (with $W = 0.15$ V) to detect TNT via the decision rule:

$$\text{If } x^{\mathrm{EC}}(V_0^{(1)}) > t \text{ and } x^{\mathrm{EC}}(V_0^{(2)}) > t, \text{ declare TNT present,} \tag{4}$$

where t is a suitable threshold. For the polymer nanojunction sensor data, the test statistic used to identify the presence of TNT is the shift $x^{\mathrm{PNJ}} = (\theta_2^* - \theta_2^{*(\mathrm{ref})})^2$, with $\theta_2^{*(\mathrm{ref})}$ the reference shift feature extracted from a signal for the blank case. The local detector makes use of the decision rule:

$$\text{If } x^{\mathrm{PNJ}} > t, \text{ then declare TNT present.} \tag{5}$$

Note that these decision rules are identical to those of the optimum likelihood-ratio-test (LRT) [7, 8] detector under the assumption that the test statistics have certain Gaussian probability distributions.

Bayesian decision fusion is then implemented as follows. Let z_1 and z_2 denote the decisions from the local detectors at the electrochemical and polymer nanojunction sensors, respectively, and $p(z_1, z_2|H_0)$ and $p(z_1, z_2|H_1)$ their joint probability distributions under the two hypothesis: H_0 (blank) and H_1 (TNT present). The fused detector utilizes the optimum LRT decision rule:

$$\text{If } \frac{p(z_1, z_2|H_1)}{p(z_1, z_2|H_0)} > t, \text{ then declare TNT present.} \tag{6}$$

Figure 2 shows a block diagram of the decision fusion approach. Note that the framework is general and can be easily applied to more number of sensors and/or hypotheses.

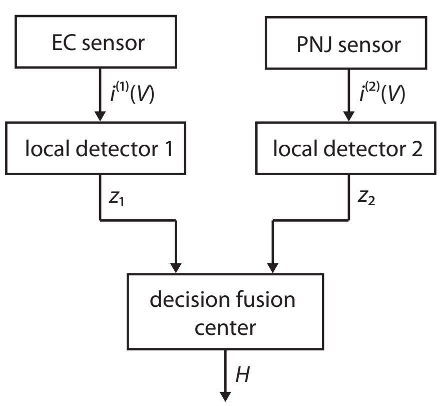


Fig. 2. Block diagram of the sensor fusion approach.

Assuming that the decisions from the two sensors are statistically independent, the joint distributions can be factored into products involving the marginals:

$$p(z_1, z_2|H_j) = p(z_1|H_j)p(z_2|H_j), \ j = 0, 1. \tag{7}$$

Since we have a binary hypothesis problem, the decisions are discrete and boolean. In this work the distributions in (7) are estimated using statistics collected from experimental data.

4. RESULTS

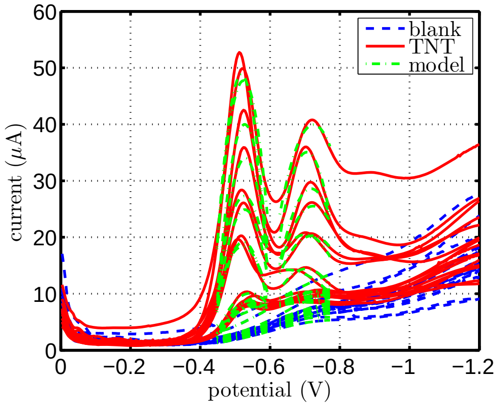
Below we discuss the application of the proposed method to the detection of TNT. Data was collected from the electrochemical and polymer nanojunction sensing platforms in the form of current vs. voltage signals for blank and TNT cases. Sensor data was recorded under various conditions of temperature, flow-rate, and TNT concentration.

Feature extraction is performed using the method of least-squares as described earlier. For the electrochemical sensor, the linear least-squares problem is solved using QR factorizations [5] implemented in the MATLAB backslash operator '\'. For the polymer nanojunction sensor, the nonlinear least-squares problem is solved using the MATLAB `fminsearch` function based on a simplex method.

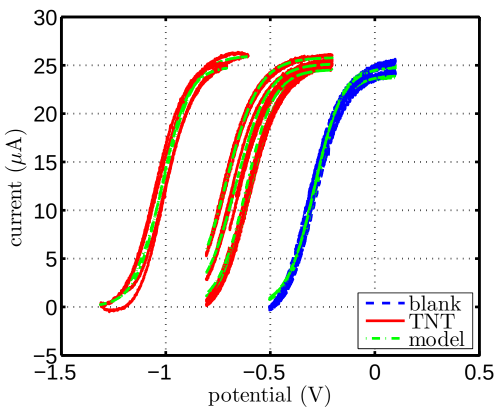
Figure 3 shows the results of the least-squares feature extraction procedure applied to the example sensor signals in Figure 1. For the electrochemical sensor data, features are extracted at two voltage positions: $V_0^{(1)} = -0.52$ V and $V_0^{(2)} = -0.7$ V (with $W = 0.15$ V in both cases). In each case note how the model with the optimized parameters approximates the original signal with small error.

Test statistics are then constructed from the extracted features and thresholded for TNT detection (local detectors). The values of detection and false alarm probabilities are estimated from the data by varying the threshold. Figure 4 shows the receiver operating characteristic (ROC) curves obtained in this manner for the detection for blank vs. TNT using the electrochemical and polymer nanojunction sensors. From the plots, the performance of the polymer nanojunction sensor can be seen to be superior to that of the electrochemical sensor for lower probabilities of false alarm in that it yields higher detection probabilities. At higher false alarm probabilities, the performance is similar for both sensors. Note that the ROC curves are coarse due to the limited amount of data available in our tests.

Finally, Bayesian decision fusion is carried out using the outputs of the local detectors at the electrochemical and polymer nanojunction sensors. The operating points (P_f, P_d) for the local detectors are set to $(0.11, 0.85)$ and $(0.04, 0.95)$, respectively. The required probability distributions on the decisions are estimated using the available data. The ROC curve for the sensor-fused detector is also shown in Figure 4. Compared to the individual detectors, the performance of the fused detector can be seen to be better in general. The slight discrepancy for the lower false alarm rates may be attributed



(a) Electrochemical sensor



(b) Polymer nanojunction sensor

Fig. 3. Least-squares feature extraction procedure applied to example signals for the blank and TNT cases in Figure 1.

to the error in estimating the required probabilities from to a small-sized dataset.

5. CONCLUSION

We have developed an explosive detection approach based on multi-modal sensing and sensor data fusion. Two different sensing modalities are considered: electrochemical and polymer nanojunction. A least-squares based feature extraction technique is used to isolate the signature of the analyte TNT from measured sensor signals. Bayesian decision fusion is then employed to integrate the information obtained from both the sensor platforms. Our results indicate that the sensor-fused detector is capable of achieving high probability of detection (near 90%) at very low false alarm rates. The method is computationally efficient and amenable for field-deployment in a mobile hand-held device.

While these results are encouraging, they are based on a limited amount of data. Further experiments are required to build a statistically significant dataset so that the performance of the explosive detection system can be assessed with greater confidence. Also, in this work we have only considered a binary hypothesis scenario where data is classified either as blank or TNT. This framework needs to be extended to account for the varied chemicals and interferents encountered in real environmental conditions. Perhaps the biggest practical challenge is to be able to detect the analytes in the presence of various interferents in harsh and variable environments. Ongoing research efforts are focused on improving the selectivity, sensitivity, and speed of the sensor systems and the data processing algorithms.

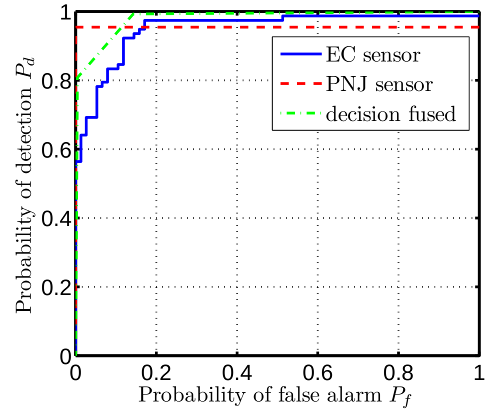


Fig. 4. ROC curves showing detection results for blank vs. TNT using the electrochemical and polymer nanojunction sensors.

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