Optimal Sensor Control for Fast Target Detection in Hyperspectral Imagery

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Abstract

Real-time, standoff detection of trace chemicals on surfaces in the presence of unknown interferent contaminants using active IR spectroscopy poses significant challenges. The measurement time and computational burden can be prohibitive due to the number of spatial pixels, hundreds of potential wavenumbers, and size of the chemical library containing thousands of signatures. Therefore it is advantageous to optimally sample a small subset of the possible wavenumbers, where optimality is meant in the sense of detection and classification performance. Our approach accomplishes this by selecting wavenumbers which maximize the information about chemical identity. This is done by using submodular optimization, a technique which guarantees near-optimality at vanishingly low computational burden. Therefore, the methods shown here lend themselves to the time and resource constrained problems of data acquisition. This is in contrast to more traditional dimensionality reduction approaches such as lowering spectral resolution, random sparse sampling, and principal component analysis which degrade detection performance. In this work we describe methods for optimal illumination wavenumber selection to address the time constraints while addressing the challenges imposed by hardware and environmental artifacts (e.g., atmospheric effects).
1 Introduction

Standoff detection of chemicals on surfaces is a desirable capability for a wide range of applications such as forensics, defense, border protection and monitoring, and other applications throughout the law-enforcement and intelligence communities. Mid-infrared (MIR) spectroscopy is intrinsically capable of detecting chemicals in all forms (gas, liquid, solid) with high sensitivity and specificity. Active spectroscopy is arguably the only technique capable of rapidly scanning surfaces for chemicals with high sensitivity [1, 2]. Real-time detection reports are needed in many chemical detection applications. The system requirements (e.g., sensitivity at standoff distances, large interrogation area over a surface, and high acquisition and processing speed) pose additional challenges and constraints on the overall system design. One approach to increasing speed is limiting the numbers of wavenumbers used for data collection and/or post-processing. Common methods for dimensionality reduction include lowering the spectral resolution of the system, using random projections in frequency (as in compressed sensing) [3], or limiting the bands used for processing via principal component analysis (PCA) [4]. We focus on information-theoretic approaches for optimal resource allocation under the hardware and detection performance constraints. A notional example of a deployed system including an active IR hyperspectral imaging (HSI) sensor and embedded digital processing platform for real-time detection and estimation is shown in Fig. 1.

Figure 1: Notional depiction of standoff trace chemical detection in a realistic application-relevant environment. Our approach combines active IR illumination to provide high signal-to-noise ratio, a high resolution hyperspectral imaging sensor, and a digital processing platform to implement adaptive algorithms which utilize known chemical spectral signatures.

This paper introduces algorithms for optimal wavelength selection (OWLS) for fast scanning of chemical targets on surfaces. Here, “optimal” is defined with respect to the probability of correctly detecting and identifying the target chemical. This comprises two intertwined problems: the detection problem (determining whether or not any target chemicals are present) and the classification problem (determining which of the target chemicals is present). Specifically, we seek the set of measurements which maximize the mutual information with chemical identity. Optimal wavenumbers may be found using a brute-force, combinatorial search over all possibilities. This approach, however, is prohibitively computationally expensive. Instead, we exploit the fact that mutual information is a submodular set function and use a polynomial time greedy algorithm to obtain a near-optimal set of wavenumbers. Illumination schemes derived from OWLS lead to better target detection performance over the more traditional methods for dimensionality reduction (low resolution over the bandwidth, random wavenumber selection, PCA, etc.) while far surpassing brute-force methods in terms of computational complexity. These methods can be extended to the optimal selection of

\[^1\)Interchangeable with wavenumber 1/λ; the sensors considered here sample linearly in wavenumber space.
spectral bands of operation and look directions, as well as other parameters for configuring the sensor (not discussed in this paper).

Figure 2 depicts the overall algorithm subsystem design. The system is intended to scale to a library of \( \geq 500 \) chemicals, though the present work only considers as many as 54. The complex index of refraction data from the chemical library are fed into physics-based models for predicting reference signatures to be used by the detection and control software. The detection and control software has two main components. The first is the control block which informs the sensor on wavenumbers for sampling (i.e., using OWLS). Before image acquisition, OWLS is used to select an initial set of \textit{a priori} wavenumbers based on the library of known chemical signatures of interest. These \textit{a priori} wavenumbers are used for the initial measurement, which is then fed to the second block: the detection, classification and estimation algorithm. Previous research compares the performance of adaptive subspace approaches, sparse methods, and Bayesian inference techniques [5, 6] for trace chemical detection. In this paper, we use a modified form of the industry-standard adaptive cosine estimator (ACE) [5]. OWLS can be used adaptively in the loop until the detection confidence reaches the stopping criterion.

![Figure 2](image.png)

Figure 2: Image acquisition and detection platform. The digital platform for selecting detector-optimal wavenumbers receives spectral library data. An initial set of wavenumbers is chosen and the corresponding HSI data-cube is measured and processed by the detection algorithm. OWLS then selects the next set of optimal wavenumbers and repeats until the detector-optimal result is found.

## 2 Optimal Wavenumber Selection

OWLS encompasses several approaches to selecting the wavenumbers which optimally distinguish between multiple chemicals. \textit{A priori} OWLS, described in Sec. 2.3, finds the subset of wavenumbers which maximize mutual information with all of the possible chemicals. Adaptive OWLS, described in Sec. 2.4, operates in concert with data collection. Data are taken at the first few wavenumbers selected by \textit{a priori} OWLS, then additional wavenumbers are selected to optimally distinguish between the chemicals which are most likely given the data collected so far. In both cases, we exploit the fact that mutual information is submodular with respect to sets of wavenumbers and use a polynomial-time greedy algorithm to find a near-optimal subset.

### 2.1 Mutual Information and the Submodularity Property

OWLS maximizes detection accuracy for a given number of wavenumbers by finding the set of wavenumbers which have maximal mutual information with chemical identity. Mutual information, \( I(X;Y) \), is an information-theoretic quantity representing how much information random variable \( X \) conveys about random variable \( Y \) (and vice versa, as \( I(Y;X) = I(X;Y) \)) [7]. In this context, \( X \) (the “features” in machine learning parlance) is the reflectance at some set of wavenumbers and \( Y \) (the “labels”) is the chemical identity. The
mutual information of two discrete random variables is defined as

\[ I(X;Y) = \sum_{y \in Y} \sum_{x \in X} p(x,y) \log_2 \left( \frac{p(x,y)}{p(x)p(y)} \right), \]  

(1)

where the base of the logarithm determines the units (bits, in this case). Mutual information is bounded by \( 0 \leq I(X;Y) \leq H(Y) \), where the lower bound corresponds to the case where \( X \) and \( Y \) are independent, and the upper bound (where \( H(Y) = -\sum_{y \in Y} p(y) \log_2 p(y) \) is the entropy in the labels \( Y \); this represents the uncertainty in \( Y \) absent any measurements) corresponds to the case where \( Y \) is completely determined by \( X \). In practice, \( I(X;Y) \) is estimated using the Kozachenko-Leonenko estimator [8] applied to a library consisting of simulated spectra (including simulated noise) at various abundances.

The (weak) Fano inequality sets a lower bound on the probability that a chemical is mis-classified [7]:

\[ P_e \geq \frac{H(Y) - I(X;Y) - 1}{\log_2 |Y|}, \]  

(2)

where \( P_e \) is the probability of mis-classification and \( |Y| \) is the number of possible chemicals. Therefore, to minimize the probability of errors, it is necessary to find the \( X \) which maximizes the mutual information.

Specifically, given the set of possible features \( \Omega \), we would like to pick the \( k \) features \( X \subset \Omega \) which maximize \( I(X;Y) \):

\[ X_{opt} = \underset{|X| \leq k, X \subset \Omega}{\arg \max} I(X;Y). \]  

(3)

In general, this is a combinatorial search problem, requiring exhaustive enumeration of all \( O(2^{|\Omega|}) \) subsets of features with \( |X| \leq k \). Mutual information, however, has the property that it is submodular:

\[ I(X_1;Y) + I(X_2;Y) \geq I(X_1 \cup X_2;Y) + I(X_1 \cap X_2;Y), \]  

for \( X_1, X_2 \subseteq \Omega \).

(4)

A key implication of this property is that an \( O(k|\Omega|) \) greedy algorithm which adds the most informative feature at each step and never removes features will provide a near-optimal solution, within a factor of \( 1 - (k-1)/k \sim (e-1)/e \) of the true maximum [9]. Henceforth, the word “optimal” will be taken to refer to the near-optimal subset obtained in this manner. For submodular set functions, the intractable combinatorial search can be efficiently approximated by a tractable polynomial time greedy search, a substantial time savings illustrated in Fig. 3.

### 2.2 Geometry of Optimal Features

To illustrate the geometry of optimal features (i.e., reflectance at the optimal wavenumbers), consider the simplified problem of distinguishing between isopropanol, triethyl phosphate, and trimethyl phosphate. The
chemical signatures and first three optimal wavenumbers are shown in Fig. 4a. The first three features all correspond to strong absorbance peaks, which makes sense given that these correspond to points of high difference between possible chemicals. Figure 4b shows how an individual feature may not necessarily be sufficient to identify the chemical on its own (as the univariate histograms for the three chemicals overlap) but the pair of features at 959 cm\(^{-1}\) and 1044 cm\(^{-1}\) allow the clusters corresponding to each chemical to be cleanly separated, except at very low abundance where the differences in spectral signatures are below the noise floor.

2.3 A Priori Optimal Wavenumber Selection

A priori OWLS selects the \( k \) optimal wavenumbers which maximize mutual information with chemical identity. This approach is useful when designing a sensor with a limited number of fixed wavenumber bands, as is demonstrated in Sections 3.1, 3.2, and 3.3. Algorithm 1 shows the pseudocode for the greedy algorithm to select \( k \) optimal wavenumbers from a set of candidates \( \Omega \).

<table>
<thead>
<tr>
<th>Algorithm 1 A Priori OWLS Algorithm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1: function APOWLS(( \Omega ), ( k )) ( \epsilon ) ( \Omega ) is the set of candidate wavenumbers ( \epsilon ) ( k \leq</td>
</tr>
<tr>
<td>2: ( \Lambda \leftarrow {} )</td>
</tr>
<tr>
<td>3: while (</td>
</tr>
<tr>
<td>4: ( \lambda_{\text{new}} \leftarrow \arg \max_{\lambda \in \Omega} I(X_{\Lambda \cup {\lambda}}; Y) ) ( \epsilon ) ( I(\cdot; Y) ) is evaluated for each of the (</td>
</tr>
<tr>
<td>5: ( \Lambda \leftarrow \Lambda \cup {\lambda_{\text{new}}} )</td>
</tr>
<tr>
<td>6: ( \Omega \leftarrow \Omega \setminus {\lambda_{\text{new}}} )</td>
</tr>
<tr>
<td>7: return ( \Lambda ) ( \epsilon ) ( \Lambda ) is the set of ( k ) optimal wavenumbers</td>
</tr>
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</table>

2.4 Adaptive Optimal Wavenumber Selection

Adaptive OWLS is used to select, in real time, the next wavenumber(s) to collect with a tunable sensor in response to the data collected so far. The idea is to identify the subset of chemicals \( \hat{Y} \) with the highest detection scores and collect the wavenumbers which, when combined with the data already collected, optimally distinguish between this reduced set of chemicals. As discussed in Sec. 3.4, this approach has the potential to deliver high accuracy with fewer wavenumbers than even a priori OWLS for very large chemical libraries. The pseudocode for the combined detection and wavenumber selection is given in Alg. 2. The initial set of wavenumbers is chosen using a priori OWLS, and then wavenumbers are added adaptively until the required level of confidence is obtained. While the algorithm as-written adds a single wavenumber at a time, it is a simple extension to add batches of wavenumbers at a time. The optimal batch size depends on the tradeoff between the time to measure a set of wavenumbers and the time to compute the detection scores and select the next \( k \) optimal wavenumbers. It is important to note that the high-scoring chemical subset \( \hat{Y} \) is used only to compute the next set of optimal wavenumbers, not to reduce the number of classes the detection algorithm DETECT (e.g., ACE) considers. This has two implications: (1) in the many-wavenumber limit adaptive OWLS should perform at least as well as evenly-spaced wavenumbers (as it does not alter the detection algorithm itself), and (2) the increase in performance delivered by adaptive OWLS is the result of better wavenumber selection and not simply reducing the number of classes considered by the detection algorithm. The computation of \( I(X; Y) \) using the Kozachenko-Leonenko estimator (as in a priori OWLS) can be very time-consuming (multiple hours to obtain 100 optimal wavenumbers), so we use a fast approximate method which will be described in detail in a future publication.
Figure 4: Geometry of optimal features. (a) Chemical signatures and first three optimal wavenumbers. The numbers at the bottom indicate the order in which wavenumbers were selected. In this simple case, the optimal wavenumbers all correspond to strong absorption peaks. (b) Joint distribution of reflectance at the first three optimal wavenumbers. The plots on the diagonal show histograms of the individual features and the plots in the lower half show scatterplots of every pair of features. (c) Accumulation of mutual information as wavenumbers are added to optimally distinguish between the chemicals.
Algorithm 2 Adaptive OWLS Algorithm

1: function AdaptiveOWLSDetection(Λ, Ω, α, q)  
   ▷ Λ is the initial set of wavenumbers  
   ▷ Ω is the set of candidate wavenumbers (Λ ∩ Ω = ∅)  
   ▷ α is the required level of confidence  
   ▷ q is the quantile of chemicals to retain  
2:   D ← Measure(Λ)  
   ▷ D is the measured data at the wavenumbers in Λ  
3:   c, s ← Detect(D)  
   ▷ c is confidence that the chemical with the highest score is correct  
   ▷ s is the detection score for each candidate chemical  
4:   while c < α and |Ω| > 0 do  
5:      ˆY ← {y | s_y ≥ q(s)}  
6:      λ_{new} ← arg max_{λ ∈ Ω} I(X_{Λ ∪ {λ}}; ˆY)  
7:      Λ ← Λ ∪ {λ_{new}}  
8:      Ω ← Ω \ {λ_{new}}  
9:      D ← D ∪ Measure({λ_{new}})  
10:     c, s ← Detect(D)  
11: return arg max s  
   ▷ Return chemical with highest detection score

3 Results and Discussion

3.1 A Priori Selection of Wavenumbers for Low-Cost Sensors

Consider a sensor designed to detect a single chemical, given a library of possible chemicals which may occur in the environment. In order to reduce the complexity and associated cost of the sensor, we would like to use as few wavenumbers as possible. As a specific example, consider the case of designing a sensor to detect triethyl phosphate (TEP) with a library of 54 possible chemicals, including several with fairly similar spectra to TEP. There are 100 wavenumbers to choose from, evenly-spaced between 884 cm\(^{-1}\) and 1350 cm\(^{-1}\).

The mutual information of the spectral signatures \(X\) with the indicator variable

\[ 1_{Y=\text{TEP}} = \begin{cases} 1, & Y = \text{TEP} \\ 0, & Y \neq \text{TEP} \end{cases} \tag{5} \]

sets the bounds on classification performance to distinguish between TEP and the other chemicals. The results of adding the wavenumbers which optimize \(I(X; 1_{Y=\text{TEP}})\) in the order selected using submodular optimization are shown in Fig. 5a. Only the first four optimal wavenumbers are required to capture all of the information available to distinguish TEP from the other 53 chemicals, while an evenly-spaced wavenumber grid does not capture all of the information with ten wavenumbers.

In such a simple classification problem, one might use a wavenumber selection scheme which focuses on the major absorption peaks of TEP. Consider, however, the locations of the first four optimal wavenumbers shown in Fig. 5b: the largest absorption peak is shared with many other chemicals, and hence was only selected fourth when considering mutual information. Furthermore, the second feature is not centered on an absorption peak, but happens to be in a region of the spectrum where TEP has strong absorbance but most of the other chemicals do not. OWLS selects informative bands which other common selection schemes may overlook.

3.2 A Priori Selection of Wavenumbers Accounting for Atmospheric Effects

In the previous section, the chemical signatures used to compute mutual information did not include the effects of environmental interference (e.g., atmospheric attenuation). Bands which are informative for such “vacuum” spectra may not be optimal once the signal degradation from the highly prominent atmospheric attenuation features in the MIR are taken into account. To illustrate this effect, Fig. 6 shows the mutual information of single features with chemical identity for a library of 54 chemicals. The information content of the higher wavenumbers, \(1/\lambda \gtrsim 1100 \text{cm}^{-1}\), is substantially reduced by the strong atmospheric absorption bands. Figure 7 shows the effect of atmospheric effects on the first ten optimal wavenumbers. There are
now fewer points selected in the strongly-attenuated $1/\lambda \gtrsim 1100 \text{cm}^{-1}$ region, and several wavenumbers have moved to avoid narrow atmospheric absorption peaks. Note, however, that the fourth optimal feature for the case with atmospheric attenuation is at a moderate atmospheric absorption peak: the difference between some of the chemicals stays high enough that this feature is useful for distinguishing two of the chemicals from the rest. This illustrates that OWLS can successfully select wavenumbers which are optimal even in the presence of strong atmospheric attenuation, and that the optimal subset is not necessarily one which simply avoids all atmospheric absorption peaks.

3.3 Detection Performance With a Priori OWLS

In order to quantify the increase in detection performance when using OWLS, we generated synthetic images for a variety of abundances of each of the 54 chemicals. We used the modified ACE algorithm [5], and tested on ten images for each condition. Atmospheric attenuation was not included. Figure 8a shows the detection performance for evenly-spaced, a priori optimal, and adaptively-selected wavenumbers (the adaptive OWLS results are discussed in Sec. 3.4). Both adaptive and a priori OWLS perform substantially better than evenly-spaced wavenumbers: the optimal wavenumber selection schemes require half as many wavenumbers to reach 90% accuracy, which represents a substantial savings in both measurement time and power consumption.

3.4 Adaptive Wavenumber Selection

The previous sections described the use of OWLS to select the optimal set of wavenumbers a priori, before any data have been taken. As indicated by the block diagram in Fig. 2 and described in Sec. 2.4, OWLS may also be used adaptively to select wavenumbers in response to the data collected so far: if the detection confidence is low, additional wavenumbers which optimally separate the highest-scoring chemicals are selected and measured. This process continues until the desired detection confidence is reached.

Detection performance for adaptive OWLS is shown in Fig. 8a for the case where there are ten initial wavenumbers and ten wavenumbers are added at each step. For this library size, adaptive OWLS performs slightly worse than a priori OWLS. To understand this result, notice how rapid the accumulation of mutual information shown in Fig. 8b is: the first ten wavenumbers (which are the same for the adaptive and a
Figure 6: From top to bottom: (a) Vacuum spectra for the 54 chemicals to distinguish. (b) MIR atmospheric transmittance, showing many strong absorption peaks for $1/\lambda \gtrsim 1100$ cm$^{-1}$. (c) Mutual information $I(X_i; Y)$ of single features with chemical identity. The mutual information for features with atmospheric attenuation is sometimes greater than that for the same feature without attenuation because of sampling error in the estimator.
Figure 7: Reflectance spectra and first ten optimal wavenumbers computed (a) without and (b) with atmospheric attenuation. The numbers indicate the order in which wavenumbers were selected. Note that the spectra are shown at high resolution (1 cm$^{-1}$ spacing) so that the narrow atmospheric absorption features are visible, but the optimal wavenumbers were selected from a coarser grid of 100 wavenumbers (~4.7 cm$^{-1}$ spacing). The zoomed plot (c) shows the portion of (b) indicated by the green band: even though the fourth optimal feature is in the middle of a (weak) atmospheric absorption band, it can still distinguish the chemicals indicated in orange and yellow from the others. The adjacent, unattenuated region was not used because of the coarse grid of wavenumbers provided to OWLS; the (unselected) candidate wavenumbers are indicated by the dotted black lines. The adjacent feature at 1105 cm$^{-1}$ is not as discriminative as the one at 1100 cm$^{-1}$. 
Figure 8: (a) Contours corresponding to 90% chemical identification accuracy as a function of abundance and number of wavenumbers for evenly-spaced (dashed blue), a priori optimal (dash-dot orange), and adaptive (dotted yellow) selection schemes. Accuracy is greater than 90% above and to the right of these contours. Note the logarithmic mass load scale: performance was assessed on a grid of five points logarithmically spaced between $0.1 \mu g/cm^2$ and $1 \mu g/cm^2$. These contours represent the average performance over all 54 chemicals in the library. Both adaptive and a priori OWLS deliver high accuracy with half the number of wavenumbers as the evenly-spaced scheme. The chemical library is not large enough for adaptive OWLS to make a significant difference when starting with ten initial wavenumbers. (b) Accumulation of mutual information as the first 40 optimal wavenumbers (out of 467 candidates) to distinguish between 54 chemicals are selected. The rise is quite rapid, and most of the information has been captured in the first ten wavenumbers.

Consider instead the specific case where the true target is $10 \mu g/cm^2$ of 2-chloroethyl ethyl sulfide (CEES). As shown in Fig. 9a, CEES has very low absorbance, and hence the peaks are comparable to the noise level for typical concentrations. Figure 9b shows the detection accuracy for this case when a single wavenumber is added at each step. Despite the weak spectral signature, adaptive OWLS rapidly finds the three wavenumbers which successfully identify CEES. Note that this case ends up being somewhat pathological for a priori OWLS, as the first seven optimal wavenumbers contribute to discriminating between chemicals other than CEES while the evenly-spaced wavenumbers happen to end up aligning with the key features with only five wavenumbers.

This example illustrates that the choice between adaptive and a priori OWLS is dictated by the particular application requirements. Adaptive OWLS is best when the application requires detection with the fewest possible wavenumbers (i.e., in the shortest time and with the smallest power consumption), and when the wavenumbers are added in small batches (e.g., one at a time). It is particularly well-suited to the case when the most common and/or important-to-detect chemicals have fairly weak signatures compared to the interferent chemicals, either because of low concentration or intrinsically weak absorbance. Adaptive OWLS is also expected to be well-suited to the case where there are hundreds of potential chemicals, but this was not tested in this paper. A priori OWLS delivers optimal results for moderate numbers of wavenumbers (dozens to hundreds), and has fewer parameters to tune so it delivers reliable performance across a variety of conditions. It is well-suited to the case where all of the chemicals of interest are equally likely and equally important-to-detect (i.e., the ones with weak signatures are not any more likely or important to detect than the others).
Figure 9: (a) Reflectance spectra for all 54 chemicals. Each spectrum is computed for an abundance of 10 µg/cm\(^2\). CEES (thick blue) has a very weak signature: even at high concentration, its peaks are comparable to the noise level. (b) Detection accuracy when the target is 10 µg/cm\(^2\) CEES. Each point represents the result of ten test images.

4 Summary

In this work we described algorithms for optimal wavelength selection (OWLS). Here optimality is defined in terms of chemical detection and classification accuracy rather than proxy metrics such as signal to noise ratio. Exploiting the submodularity property of mutual information allows us to select the optimal wavenumbers while taking into account the noise structure due to the detector and the environment as well as accounting for structured interference due to the presence of other chemicals, atmospheric effects, and/or speckle. Results show that OWLS provides much better accuracy over traditional wavenumber selection methods and may be used adaptively to satisfy detection confidence requirements. Though not discussed in this paper, the approaches described here may be extended to derive optimal scanning patterns in the spatial dimensions.

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