PERFORMANCE EVALUATION OF CHEMICAL PLUME DETECTION AND QUANTIFICATION ALGORITHMS

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Abstract

Hyperspectral Imaging sensors provide a wealth of spatial, and more importantly, spectral information, which can be used in a wide variety of applications, including chemical plume detection. In theory, every gaseous chemical has a unique spectrum; by studying, the effect this spectrum has on electromagnetic radiation from the background of a scene, we are able to perform chemical plume detection and quantification. Analysis of the accuracy, strengths, and weaknesses of detection and quantification algorithms is a difficult task, as one typically lacks ground truth data for physical plume parameters such as location, concentration, and temperature. In order to better understand the performance of our algorithms, we developed a tool which allows us to embed synthetic plume into real background data with control of these parameters. In this thesis, we first develop a radiative transfer model for chemical plumes. Using this model, we then build a suite of detection and quantification algorithms, as well as our plume embedding routine. Finally, using our semi-synthetic data, we study the impact of various physical plume parameters, including concentration and thermal contrast, among others, on the results of our algorithms.
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# Contents

Acknowledgments i

1 Introduction 1

2 Background 4

  2.1 At-Sensor Radiance Signal Model ....................... 4
    2.1.1 Plume-Free Model ................................ 5
    2.1.2 Plume Model ...................................... 6
    2.1.3 Approximations .................................... 10
  2.2 Sensor and Data Collection Method ...................... 13
    2.2.1 Michelson Interferometer .......................... 15
    2.2.2 HgCdTe Focal Plane Array ........................ 17
  2.3 Anatomy of Hyperspectral Data ......................... 17

3 Plume Detection and Quantification Theory 21

  3.1 Plume Detection Theory ............................... 21
    3.1.1 Target Detection ................................. 21
    3.1.2 Detection Algorithm Taxonomy .................... 23
    3.1.3 Detection Statistic Analysis ..................... 27
  3.2 Plume Quantification Theory .......................... 32
    3.2.1 Temperature Estimation ........................... 32
    3.2.2 Concentration Pathlength Estimation ............... 34
CONTENTS

4 Plume Embedding Into Background Measurements 35
  4.1 Theory ........................................... 35
  4.2 Implementation .................................. 36
    4.2.1 Spectral Signature ......................... 36
    4.2.2 Plume Concentration Pathlength Mask ........ 38
    4.2.3 Plume Temperature .......................... 43

5 Performance Evaluation of Detection Algorithms 44
  5.1 Implementation .................................. 44
    5.1.1 Detection Pipeline ......................... 45
    5.1.2 I/O Structure ................................. 47
  5.2 Experimental Specifications ..................... 47
  5.3 Results .......................................... 50
    5.3.1 Detectors ...................................... 50
    5.3.2 Data Cubes and CWAs ....................... 51
    5.3.3 Fill Factor and Plume-Free Background Estimation .. 56
    5.3.4 Concentration Pathlength and Plume Mask .... 58
    5.3.5 Temperature and Plume Background ............ 65

6 Performance Evaluation of Quantification Algorithms 71
  6.1 Temperature .......................... 71
    6.1.1 Atmospheric Temperature Estimation Results .... 71
    6.1.2 Background Temperature Estimation Results .... 73
  6.2 Concentration Pathlength .................... 74

7 Conclusions 80
  7.1 Detection ........................................ 80
  7.2 Quantification ................................... 82
  7.3 Future Research ................................. 82

Bibliography 84
## List of Figures

2.1 Pictorial representation of the plume-free radiative transfer radiance signal model for standoff chemical agent detection. .......................... 5  
2.2 Pictorial representation of the on-plume radiative transfer radiance signal model for standoff chemical agent detection. .......................... 7  
2.3 Typical absorption coefficient spectrum. ............................... 8  
2.4 Typical plume transmission functions as a function of \( \gamma \) in ppm-m. .......................... 8  
2.5 Relative error associated with using linear approximation of Beer’s Law. .......................... 11  
2.6 Spectral exitance curves representing plume and LWIR background with a temperature difference of 5 Kelvin. ............................... 13  
2.7 Difference of spectral exitance curves from Figure 2.6 (blue curve). Evaluation of analytical expression equation (2.18) (red curve) for the linear approximation of Planck function. .......................... 14  
2.8 Relative error associated with using linear approximation of Planck function. .......................... 14  
2.9 Michelson interferometer. .................................................. 16  
2.10 LWIR region of atmospheric transmission function. .......................... 18  
2.11 Single detection element in FPA, adapted from [7]. .......................... 18  
2.12 Overview of structure of hyperspectral data. .............................. 20  
3.1 MD, MF, and ACE detector theory. ...................................... 24  
3.2 Sample detection statistics map. .......................................... 28  
3.3 Sample histogram of detection statistics ................................. 29  
3.4 Sample probability of exceedance plot .................................. 30  
3.5 Sample ROC plot and illustration of tradoffs ........................... 30
LIST OF FIGURES

4.1 High level description of plume embedding stage. 37
4.2 Adjustment of high-resolution library spectra for atmospheric transmission, sensor smoothing, and sensor resampling. 38
4.3 Conversion of the $s_4$ high resolution library spectrum (top) to sensor resolution (bottom) including effects of atmospheric absorption. 39
4.4 Conversion of the chemical species studied to sensor resolution. 40
4.5 Sample constant and Gaussian plume masks. Constant mask = 1 inside of white line and 0 outside. 41
4.6 “Realistic” plume mask generation process. 42
4.7 Sample “realistic” plume mask. 42
5.1 Detection pipeline implementation. 46
5.2 Detection pipeline implementation detail. 46
5.3 ROC analysis of MF and ACE detection statistics for datasets A, B and C embedded with $s_2$ at $\gamma = 50$ ppm-m. 51
5.4 Histogram of MF detection statistics dataset C embedded with $s_2$ at $\gamma = 50$ ppm-m. 52
5.5 Histogram of AMF detection statistics dataset C embedded with $s_2$ at $\gamma = 50$ ppm-m. 52
5.6 Histogram of ACE detection statistics dataset C embedded with $s_2$ at $\gamma = 50$ ppm-m. 53
5.7 ROC analysis of ACE detection statistics for datasets A, B and C embedded with $s_2$ at $\gamma = 30$ ppm-m. 54
5.8 $P_y(\eta)$ analysis of ACE detection statistics for datasets A, B and C embedded with $s_2$ at $\gamma = 30$ ppm-m. 54
5.9 ROC analysis of ACE detection statistics for dataset C embedded with $s_1$ through $s_{10}$ at $\gamma = 30$ ppm-m. 55
5.10 Theoretical and empirical SCR and AUROC results of ACE detection statistics for datasets C embedded with $s_1$ through $s_{10}$ at $\gamma = 30$ ppm-m. 57
5.11 ROC analysis of ACE detection statistics for dataset C embedded with $s_2$ at $\gamma = 30$ ppm-m with various fill factors. 58
5.12 Detections statistics of ACE detection statistics for dataset C embedded with $s_2$ at $\gamma = 30$ ppm-m with various fill factors. ........................................ 59
5.13 AUROC and SCR analysis of ACE detection statistics for dataset C embedded with $s_2$ at $\gamma = 30$ ppm-m with various fill factors. ................. 60
5.14 Histogram of ACE detection statistics dataset C embedded with $s_2$ at $\gamma = 30$ ppm-m with PFBGE. .......................................................... 60
5.15 Histogram of ACE detection statistics dataset C embedded with $s_2$ at $\gamma = 30$ ppm-m without PFBGE. .............................................. 61
5.16 ROC analysis of ACE detection statistics dataset A embedded with $s_2$ at a varying $\gamma$. ......................................................... 62
5.17 AUROC and SCR analysis of ACE detection statistics datasets A, B and C embedded with $s_2$ at a varying $\gamma$. .......................... 62
5.18 Detections statistics of ACE detection statistics for dataset A embedded with $s_2$ at various $\gamma$. .............................................. 63
5.19 AUROC and SCR analysis of ACE detection statistics for dataset A embedded with $s_2$ varying $\gamma$ with and without PFBGE. ................. 64
5.20 Relation between AUROC and SCR results for ACE detection statistics for dataset A embedded with $s_2$ varying $\gamma$. ...................... 64
5.21 Detections statistics of ACE detection statistics for dataset A embedded with $s_2$ at $\gamma = 30$ ppm-m with constant, Gaussian and realistic masks. ... 66
5.22 ROC analysis of ACE detection statistics for dataset A embedded with $s_2$ at $\gamma = 30$ ppm-m with constant, Gaussian and realistic masks. ............... 67
5.23 $P_y(\eta)$ analysis of ACE detection statistics for dataset A embedded with $s_2$ at $\gamma = 30$ ppm-m with constant, Gaussian and realistic masks. .......... 67
5.24 Constant plume mask locations for background study. .................... 68
5.25 AUROC and SCR analysis of ACE detection statistics for dataset A embedded with $s_2$ at a $\gamma = 30$ ppm-m varying $\Delta T_p$. ......................... 69
5.26 Mean spectra for each background class. ......................................... 69
5.27 ROC analysis of ACE detection statistics for dataset A embedded with $s_2$ at $\gamma = 30$ ppm-m with varying background. ...................... 70
### LIST OF FIGURES

6.1 $\hat{T}_a$ for Dataset C. ................................................................. 72  
6.2 $\hat{T}_b$ for Dataset C. ................................................................. 73  
6.3 $\hat{SCR}$ sky Dataset C. ................................................................. 75  
6.4 $\hat{\gamma}$ sky Dataset C. ................................................................. 75  
6.5 histogram of $\hat{\gamma}$ sky Dataset C. .............................................. 76  
6.6 $\hat{SCR}$ ground Dataset C. ............................................................... 76  
6.7 $\hat{\gamma}$ ground Dataset C. ................................................................. 77  
6.8 histogram of $\hat{\gamma}$ ground Dataset C. .............................................. 77  
6.9 $\hat{\gamma}$ vs. $\gamma$ for Dataset C. ...................................................... 79  
6.10 $\hat{\gamma}$ vs. $\gamma$ for Dataset C. ...................................................... 79
List of Tables

5.1 Dataset specifications. ................................................. 48
5.2 AUROC and SCR analysis of datasets A, B and C. ............ 53
6.1 Theoretical, estimated SCR and estimated $\gamma$. .............. 78
Chapter 1

Introduction

Why use hyperspectral imaging?

Traditional spatial detectors are often limited by their resolution as well as variations in the morphological properties of many objects; thus, they are far from ideal for many of detection scenarios. Hyperspectral imaging (HSI) sensors provide both spatial and spectral information about a scene; this wealth of information can be combined, making these sensors highly versatile and suitable for many applications in which the capabilities of traditional imaging devices are inadequate. [4]

Hyperspectral imaging takes advantage of the fact that, in theory, every material produces a unique amount of radiance (the amount of radiation it reflects, absorbs and emits), and this radiance varies as a function of wavelength. The output of a hyperspectral imaging sensor, a data cube, is comprised of many pixels, each of which contains a sampled and quantized representation of a segment of the scene, just as in a normal digital image, be it from a digital camera, or any other digital imaging device. The main differences between the output of a normal digital camera and that of a hyperspectral imaging sensor are the number of spectral bands represented in each pixel, and the range of wavelengths which these bands span. A hyperspectral imaging sensor can collect radiance measurements at a large number of contiguous wavelength values (typically anywhere from 50 to a few hundred), spread over a wide range of wavelengths in the visible and infrared range of the electromagnetic spectrum (typically anywhere from 400 nm to 14 μm, depending on the application) [7], while a digital camera collects only three measurements per pixel, at red,
blue and green wavelengths.

Using these radiance measurements, we can design algorithms which are capable of detecting and identifying materials contained within each pixel based on comparisons of an individual pixel’s spectrum with known spectral signatures. The immense increase in dimensionality provided by hyperspectral imaging data typically leads to a great improvement in detector performance when compared with morphological based detectors.

Hyperspectral imaging sensors can be configured in a variety of methods to suite the requirements of a particular detection application. Sensors may be passive or active. Passive sensors capture only radiance reflected off of and emitted from the scene, while active sensors use an infrared source, such as a hot filament or a laser, to illuminate the scene, and then capture the reflected and emitted radiance. Returning to the digital camera analogy, an active sensor is like a camera with a flash, while a passive one is like a camera without one. Hyperspectral imaging sensors may also be deployed in various manners, which can be divided into two classes: downward looking arial sensors, mounted on aircrafts or satellites, and horizontally looking (standoff) sensors, either mounted on a vehicle, or a stationary location such as buildings [7].

Hyperspectral imaging is used in a wide variety of applications including: mineral exploration, characterization of ground cover, target detection, Chemical Warfare Agent (CWA) detection, identification and quantification. This thesis focuses on CWA detection and quantification with HSI in the Long Wave Inferred (LWIR) region of the spectrum using data collected by a passive, stationary horizontal looking sensor [9].

Most detection scenarios allow for validation of algorithm performance via comparison to ground truth data, known targets or observed ground cover, for example; CWA detection algorithms are typically difficult to evaluate because even if a know quantity of a chemical is released, it is difficult to predict how the gas will diffuse throughout the scene as time passes. In order to overcome this obstacle, many researchers have developed tools to create fully synthetic data which can then be used to assess the performance of detection algorithms [2]. The aim of this thesis was to take that idea one step further by simulating CWA plumes in real data taken with HSI sensors in the hopes that they will more closely mimic real detection scenarios. In order to achieve this goal we developed a performance evaluation tool which first embeds a synthetic plume into real data, and then performs
CHAPTER 1. INTRODUCTION

CWA detection and quantification on the resultant semi-synthetic data. The ultimate goal of our research is to produce a modular system which allows the user to easily test different preprocessing, detection and quantification algorithms in a highly controlled setting.

In this thesis we will first discuss the basics of HSI theory and develop the at-sensor radiance signal model in Chapter 2. Chapter 3 presents CWA detection and quantification theory as well as develops the detection and quantification algorithms and the methods used to evaluate their performance. In Chapter 4, we introduce plume embedding theory and its implementation in the performance evaluation tool’s “pipeline.” Next in Chapter 5, we present the detection pipeline and perform various trade studies in order to evaluate the effects of various physical plume parameters on detection performance. Chapter 6 is an evaluation the performance of our temperature and plume concentration pathlength estimation algorithms. Finally, in Chapter 7, we draw conclusions form our work and highlight possible areas of future research motivate by this thesis.
Chapter 2

Background

We begin our study by discussing some of the basics of hyperspectral imaging theory. First, we will discuss the physics of HSI and develop the at-sensor radiance signal model, as it is the foundation for the embedding, detection, and quantification algorithms used throughout this thesis. Next we will address the sensor and data collection methods used to collect our data. Finally, we will study the anatomy of hyperspectral data as its multidimensional nature allows us represent it using various techniques.

2.1 At-Sensor Radiance Signal Model

A hyperspectral imaging (HSI) system is comprised of four basic elements: the radiation source(s), the imaged surface, the atmospheric path, and the sensor [4]. The impact of each component has on the overall system varies based on the specifications of that particular system; however, the general principles remain the same for all systems.

All objects at a temperature above absolute zero (0° K) emit electromagnetic radiation (EMR). Radiance, one of the more commonly used metrics for quantifying this radiation, is defined as the amount of electromagnetic radiation which passes through or is emitted from a particular area per unit time, normalized by both the size of the area and the solid angle from which the light is received. The SI unit of radiance is watts per steradian per square meter, \( \frac{W}{sr \cdot m^2} \). Radiance is a measure of electromagnetic energy over its entire spectrum; however, when we consider the energy at a specific wavelength or frequency, we
are in fact measuring the *spectral radiance*, which has SI units of watts per steradian per cubic meter, \( \frac{\text{W}}{\text{sr} \cdot \text{m}^3} \), or watts per steradian per square meter per hertz, \( \frac{\text{W}}{\text{sr} \cdot \text{m}^2 \cdot \text{Hz}} \), depending on whether the measurement is made per unit wavelength or per unit frequency interval, respectively.

### 2.1.1 Plume-Free Model

The hyperspectral sensor discussed in this thesis operates in the LWIR regime (7 to 14 \( \mu \text{m} \)), and thus, in a plume-free scene, the at-sensor radiance comes from two main sources: radiation emitted from the imaged surface or background, \( L_b(\lambda) \), and radiation emitted by the optical path, in this case, the atmosphere, \( L_a(\lambda) \), see Figure 2.1. One should note that the radiation emitted by the atmosphere (the *path-emitted* component) comes both from the atmospheric path between the sensor and the imaged surface, as well as other parts of the atmosphere which reflect off of the imaged surface into the sensor, \( \tilde{L}_a(\lambda) \). This surface reflected radiance is notably weaker than the other direct radiation sources (due to losses in intensity incurred from the reflection and increased pathlength), so for simplicity, in our model it is considered to be negligible. Contributions to the at-sensor radiance from solar illumination are also negligible in the LWIR region of the electromagnetic spectrum, and thus are left out of the model as well[7].

![Figure 2.1: Pictorial representation of the plume-free radiative transfer radiance signal model for standoff chemical agent detection.](image)

[7]: The reference number is not provided in the text.
The atmospheric path also contributes to the at-sensor radiance by attenuating the background radiance; this effect is what makes chemical warfare agent detection possible. All materials have a unique spectral transmission function, or transmittance, $\tau(\lambda)$, which is defined as the fraction of incident light of a specified wavelength which passes through a medium

$$\tau(\lambda) = \frac{I(\lambda)}{I_0(\lambda)}$$

(2.1)

where $I_0(\lambda)$ is the intensity of the incident light, $I(\lambda)$ is the intensity of the light leaving the medium, and $0 < \tau(\lambda) < 1$. The transmission function of the earth’s atmosphere, $\tau_a(\lambda)$, is known (computed using MODTRAN), and attenuates all background radiance entering the sensor. The plume-free or “off-plume” radiance model is given by

$$L_{off}(\lambda) = \tau_a(\lambda)L_b(\lambda) + L_a(\lambda)$$

(2.2)

2.1.2 Plume Model

The introduction of a plume complicates the model by adding an additional layer through which the background radiance must travel, effectively creating the three-layer model shown in Figure 2.2. The spectral transmission function, $\tau_p(\lambda)$, of a plume with $M$ gaseous elements can be modeled using Beer’s law [11],

$$\tau_p(\lambda) = \exp \left[-\sum_{m=1}^{M} \gamma_m \alpha_m(\lambda)\right]$$

(2.3)

The function $\alpha_m(\lambda)$, which is known as the absorption coefficient spectrum, is unique for each gaseous chemical and can be thought of as a “spectral signature.” The quantity $\gamma_m$ is known as the concentration pathlength, and is the product of two terms: $l$, the length along the sensor boresight that represents the depth of the cloud, and $C_m$, the average concentration of the chemical along the pathlength. $\alpha_m(\lambda)$ is measured in inverse parts-per-million-meters (ppm-m)$^{-1}$, and $\gamma$ is measured in units of parts-per-million-meters (ppm-m). Figures 2.3 and 2.4 show the relationship between a typical absorption coefficient spectrum and the resultant spectral transmission function, respectively. Note that as $\gamma$ grows large, the presence of the plume will tend to block out the majority of the background radiance.
Figure 2.2: Pictorial representation of the on-plume radiative transfer radiance signal model for standoff chemical agent detection.

radiation at the bands where the plume has strong features. The at-sensor radiance model, and in turn, detection and quantification algorithms studied throughout this thesis assume that the plume has not transitioned into this “optically thick” regime.

The plume is part of the optical path, so just as in the plume-free case, it also emits its own radiation, $L_p(\lambda)$ (which is subsequently attenuated by the atmosphere between the plume and the sensor), so our new, “on-plume,” radiance model is given by

$$L_{on}(\lambda) = \tau_a(\lambda)\tau_p(\lambda)L_b(\lambda) + \tau_a(\lambda)L_p(\lambda) + L_a(\lambda)$$

(2.4)

We can further expand our model with the aid of Planck’s Law, which describes the spectral radiance of a blackbody at a given temperature, $T$, and wavelength, $\lambda$.

$$B(\lambda, T) = \frac{C_1}{\lambda^5[e^{C_2/(\lambda T)}−1]}$$

(2.5)

where $T$ is the blackbody’s temperature in Kelvin ($^\circ$K), $C_1 = 3.74151 \times 10^8 \frac{W}{m^2 \mu m}$, and $C_2 = 1.43879 \times 10^4 \mu m \cdot K$. A blackbody is a perfect absorber and emitter of electromagnetic radiation; however, all real-world materials retain some of this incident radiation (the fraction of radiation reflected is considered to be negligible in the LWIR regime [8]), thus Planck’s law must be scaled by the material’s emissivity in order to model its emitted radiation. A material’s emissivity, $\epsilon(\lambda)$, is the ratio at which electromagnetic energy is radiated.
Figure 2.3: Typical absorption coefficient spectrum.

Figure 2.4: Typical plume transmission functions as a function of $\gamma$ in ppm-m.
by that particular material to the energy radiated by a blackbody at the same temperature. Emissivity is a unitless, material dependant quantity, which varies between 0 and 1 with wavelength; however, it is often assumed to be constant for simplicity. Thus, the radiance emitted by a given material or medium, $m$, can be expressed as

$$L_m(\lambda) = \epsilon_m(\lambda)B(\lambda, T_m)$$  \hspace{1cm} (2.6)$$

If we assume that the plume is at thermal equilibrium with the surrounding atmosphere and that the effects of reflectance are negligible, Kirchhoff’s law of thermal radiation permits us to replace emissivity with the following quantity \[7 \],

$$\epsilon_p(\lambda) = 1 - \tau_p(\lambda)$$ \hspace{1cm} (2.7)

This substitution allows us to represent the plume’s radiance as

$$L_p(\lambda) = [1 - \tau_p(\lambda)]B(\lambda, T_p)$$ \hspace{1cm} (2.8)

Most plume detection algorithms exploit the difference between on- and off-plume radiance. We obtain this radiance contrast signal by subtracting (2.2) from (2.4). With the substitution of (2.8) and some algebraic manipulation, we obtain

$$\Delta L(\lambda) \triangleq L_{on}(\lambda) - L_{off}(\lambda)$$

$$= [\tau_a(\lambda)\tau_p(\lambda)L_b(\lambda) + \tau_a(\lambda)L_p(\lambda) + L_a(\lambda)] - [\tau_b(\lambda)L_b(\lambda) + L_a(\lambda)]$$

$$= \tau_a(\lambda) [L_p(\lambda) - (1 - \tau_p(\lambda)) L_b(\lambda)]$$

$$= \tau_a(\lambda) [(1 - \tau_p(\lambda)) B(\lambda, T_p) - (1 - \tau_p(\lambda)) L_b(\lambda)]$$

$$= \tau_a(\lambda)[1 - \tau_p(\lambda)] [B(\lambda, T_p) - L_b(\lambda)]$$ \hspace{1cm} (2.9)

Substitution of (2.3) gives us the at-sensor radiance signal model

$$L_{on}(\lambda) = \tau_a(\lambda) \left\{ 1 - \exp \left[ - \sum_{m=1}^{M} \gamma_m \alpha_m(\lambda) \right] \right\} [B(\lambda, T_p) - L_b(\lambda)] + L_{off}(\lambda)$$ \hspace{1cm} (2.10)
CHAPTER 2. BACKGROUND

Note the exponential relationship between the signals of interest, $\gamma_m \alpha_m(\lambda)$ and the at-sensor radiance $L_{on}(\lambda)$. This nonlinearity is one of the principal factors which makes the detection of gaseous chemicals a difficult problem.

2.1.3 Approximations

Much of the complexity of the above model (2.10) can be reduced through use of the following series of approximations.

Optically-thin plume approximation For weak, optically-thin plumes, where $\gamma_m \ll 1$, we can use the approximation $1 - e^{-x} \approx x$, for small $x$, to linearize Beer’s law (2.3)

$$\exp \left[ - \sum_{m=1}^{M} \gamma_m \alpha_m(\lambda) \right] \approx 1 - \sum_{m=1}^{M} \gamma_m \alpha_m(\lambda) \quad (2.11)$$

Substitution into (2.10) yields

$$L_{on}(\lambda) = \sum_{m=1}^{M} \gamma_m \beta_m(\lambda) + L_{off}(\lambda) \quad (2.12)$$

where

$$\beta_m(\lambda) \triangleq \tau_a(\lambda) \left[ B(\lambda, T_p) - L_b(\lambda) \right] \alpha_m(\lambda) \quad (2.13)$$

is the “in-scene target signature” for optically-thin plumes as measured by the sensor. Figure 2.5 shows that the mean squared error resulting from (2.11) is negligible so long as the plume remains optically thin.

“Flat background emissivity” approximation In order to further simplify (2.13), and in turn our at-sensor radiance signal model (2.12), we use (2.6) to express the radiance emitted from behind the plume as

$$L_b(\lambda) = \epsilon_b(\lambda) B(\lambda, T_b) \quad (2.14)$$
The presence of $\epsilon_b(\lambda)$ in (2.14) complicates the radiance contrast signal of (2.12); however, most background emissivity functions lack the sharp spectral features common of chemical plumes, thus allowing us to adopt a “flat emissivity” approximation, $\epsilon_b(\lambda) \approx 1$. This approximation holds so long as the plume is not comprised of larger molecules having broad, featureless spectra [12]. We can now rewrite (2.9) as

$$\Delta L(\lambda) \equiv \tau_a(\lambda)[1 - \tau_p(\lambda)] [B(\lambda, T_p) - B(\lambda, T_b)]$$  (2.15)

In order to detect a plume, its presence must have some impact on the at-sensor radiance, i.e. at least some spectral channels must contain a nonzero differential spectral radiance, $\Delta L(\lambda)$. Through the inspection of (2.15), we see that a nonzero $\Delta L(\lambda)$ can exist if and only if the following conditions hold for at least some wavelengths: (a) the atmosphere must be transparent ($\tau_a(\lambda) > 0$), (b) the plume must not be entirely transparent ($\tau_p(\lambda) < 1$), and (c) a thermal contrast must exist between the plume and the background ($T_p \neq T_b$).
**Linear Planck function approximation**  Given (2.14), for an optically-thin plume over “flat-emissivity” backgrounds, we can rewrite the “in-scene target signature” (2.13) as

\[
\beta_m(\lambda) = \tau_a(\lambda) [B(\lambda, T_p) - B(\lambda, T_b)] \alpha_m(\lambda)
\]  

(2.16)

While \(|T_p - T_b|\) remains small (typically less than 5° C), the thermal contrast in (2.16) can be approximated, using a local linear approximation of Planck function about \(T_b\), as follows

\[
B(\lambda, T_p) - B(\lambda, T_b) \approx \Delta T_p \frac{\partial B(\lambda, T)}{\partial T} \bigg|_{T=T_b}
\]  

(2.17)

where \(\Delta T_p \triangleq T_p - T_b\). The partial derivative of the Planck function with respect to temperature is given by

\[
\frac{\partial B(\lambda, T)}{\partial T} = B(\lambda, T) \left( \frac{C_2}{\lambda T^2} \right) \left( 1 - e^{-C_2/\lambda T} \right)^{-1}
\]  

(2.18)

The validity of the approximation given in (2.16) can be verified through the following example. First, in Figure 2.6, we show two Planck functions for an arbitrary plume and a LWIR background modeled as black bodies at 300° K and 295° K, respectively. The blue curve in Figure 2.7 shows \(B(\lambda, T_p) - B(\lambda, T_b)\), while the red curve represents \(\Delta T_p \frac{\partial B(\lambda, T)}{\partial T}\), evaluated analytically using (2.18). Figure 2.8 shows the mean squared error incurred as a result of the Planck derivative approximation in this example, which remains negligible for typical thermal contrast values.

The differential Planck function pictured in Figure 2.6 varies smoothly with wavelength; thus, we can further simplify our approximation by ignoring the dependence on \(\lambda\), and replacing with a constant \(B_0\). Using this approximation, the “in-scene target signature” (2.16) can be re-written as

\[
\beta_m(\lambda) = (B_0 \Delta T_p) \tau_a(\lambda) \alpha_m(\lambda)
\]  

(2.19)

where

\[
B_0 = \sum_{\lambda=\lambda_{\text{min}}}^{\lambda_{\text{max}}} \frac{\partial B(\lambda, T)}{\partial T}
\]  

(2.20)
where $\lambda_{min}$ and $\lambda_{max}$ are the minimum and maximum wavelengths imaged by the detector, respectively. Taking into consideration the three previous approximations, the at-sensor radiance signal model (2.12) becomes

$$L_{on}(\lambda) = \sum_{m=1}^{M} (B_0 \Delta T_p \gamma_m) \tau_a(\lambda) \alpha_m(\lambda) + L_{off}(\lambda)$$  \hspace{1cm} (2.21)

This relationship provides the basis for most of the detection, identification, and quantification algorithms used in practical applications and throughout this thesis.

### 2.2 Sensor and Data Collection Method

Fourier transform spectroscopy is widely considered to be the state of the art method for collecting hyperspectral data due to its ability to obtain information from all spectral channels simultaneously; this capability is referred to as the multiplex advantage [3]. The data
CHAPTER 2. BACKGROUND

$$\Delta T = 5 \text{ Kelvin}$$

Figure 2.7: Difference of spectral exitance curves from Figure 2.6 (blue curve). Evaluation of analytical expression equation (2.18) (red curve) for the linear approximation of Planck function.

$$B(\lambda, T_p) - B(\lambda, T_b)$$

$$\Delta T_p \frac{\partial B(\lambda, T)}{\partial \lambda}$$

Figure 2.8: Relative error associated with using linear approximation of Planck function.

$$T_b = 295 \text{ Kelvin}$$
CHAPTER 2. BACKGROUND

referred throughout this thesis was imaged with the Field-Portable Imaging Radiometric Spectrometer Technology (FIRST), a Fourier transform spectrometer manufactured by Telops. FIRST uses a Michelson interferometer and a Mercury(II) Cadmium(II) Telluride (HgCdTe) focal plane array (FPA) to collect hyperspectral data.

2.2.1 Michelson Interferometer

A Michelson interferometer creates an interference pattern by splitting and re-combining an incoming electromagnetic wave with a delayed copy of itself; Figure 2.9 shows a schematic of a typical Michelson interferometer. Light from the imaged scene enters the device and is split into two parts of equal intensity by a beam-splitter. The two beams then reflect off of the mirrors back to the beam-splitter where they are recombined and fed into the detector. They key to the operation of the interferometer is that one of the mirrors is able to move parallel to the propagation of EMR. This movement changes the optical path length which one of the beams must travel, and thus, introduces a delay or optical path difference (OPD). The delay, $\delta$, is equal to

$$\delta = 2 \times d$$  \hspace{1cm} (2.22)

where $d$ is the distance the moveable mirror has traveled from zero path difference (ZPD), the position where both paths of light have an OPD of 0. The delay causes the combination of the two beams of light to create an interference pattern. If the mirror scans at a constant velocity ($v_m$), we can plot the output power of the interferogram as imaged by the detector by ($P(\delta)$) versus $\delta$, where $\delta = 2t \times v_m$; this time-domain representation of the signal is called an interferogram. Finally, by taking the Fourier transform, we are able to convert the interferogram into a radiance spectrum \[10\]

$$L(\lambda) = 2Re\{\int_{-\infty}^{\infty} P(\delta)e^{2\pi\lambda\delta} d\delta\}$$

$$= \int_{-\infty}^{\infty} P(\delta)\cos(2\pi\lambda\delta)d\delta$$  \hspace{1cm} (2.23)
Figure 2.9: Michelson interferometer.
CHAPTER 2. BACKGROUND

2.2.2 HgCdTe Focal Plane Array

The interferograms generated by the Michelson interferometer are projected onto a focal plane array made of Mercury(II) Cadmium(II) Telluride. HgCdTe can be sensitive to wavelengths throughout the infrared spectrum [6]; however, the FPA used in FIRST is tuned specifically to detect EMR in the LWIR range, specifically from 800 cm\(^{-1}\) to 1300 cm\(^{-1}\) (12.5 \(\mu\)m to 7.69 \(\mu\)m) [1]. When using data produced by FIRST, we must take care to note that our at-sensor radiance signal model (2.21) is scaled by \(\tau(\lambda)\), and thus, data recorded near the edges of the atmospheric transmission “window” (see Figure 2.10) tend to be heavily corrupted by noise. In the LWIR region, much of the radiance in the 800 cm\(^{-1}\) to 900 cm\(^{-1}\) range is absorbed by carbon dioxide in the atmosphere while the 1250 cm\(^{-1}\) to 1300 cm\(^{-1}\) range is absorbed by water vapor; as a result, we limit the spectral range of our data from 900 cm\(^{-1}\) to 1250 cm\(^{-1}\).

The FPA is composed of 81920 pixels, arranged into a 320 by 256 array. Each pixel has an instantaneous field of view of 0.35 mrad; thus, the entire sensor can image a scene up to 112 by 89.9 mrad (6.42° by 5.13°). If, for example, the imaged scene is 1 kilometer away, the sensor will produce a ground instantaneous field of view (GIFOV) of 112.12 by 89.66 meters, see Figure 2.11. In order to cut down on processing overhead, FIRST allows the user to window the active portion of the FPA, so smaller IFOVs can be achieved. The detector can image at a spectral resolution, or full-width half-max (FWHM), of 0.25 to 150 cm\(^{-1}\) at a rate of 0.028 to 16 Hz [1].

2.3 Anatomy of Hyperspectral Data

The output of a hyperspectral imaging sensor is a three-dimensional data structure, most commonly known as a data cube. A data cube consists of two spatial dimensions, and one spectral dimension, as shown in Figure 2.12(a). The horizontal spatial dimension is divided into \(l\) lines and is comprised of \(N_l\) pixels and the vertical dimension is divided into \(s\) samples, represented with \(N_s\) pixels. The data cube contains \(N_l \times N_s = N_{pix}\) pixels each of which is divided into \(N_b\) spectral bands. The band locations and full-width half-max (FWHM) values can be quantified in units of wavelength (\(\lambda\)) or wavenumbers (\(\nu\)). The two
Figure 2.10: LWIR region of atmospheric transmission function.

Figure 2.11: Single detection element in FPA, adapted from [7].
metrics are related through the following identity

$$\lambda \triangleq \frac{10^{-4}}{\nu}$$  \hspace{1cm} (2.24)

where $\lambda$ is measured in microns and $\nu$ is given in cm$^{-1}$. Throughout this thesis we use both metrics as convenient.

Individual data cubes are typically transformed into two-dimensional matrices to simplify subsequent processing, as shown in Figure 2.12(b); however, this transformation does nothing to remove the underlying complexity of the data. HSI data is typically collected as a time series of data cubes, so we have to yet one more dimension to deal with; these four-dimensional data structures are called tesseracts. Visualizing three-dimensional data is difficult to do on a computer, and it is impossible to visualize a four-dimensional object, thus, we must limit the number of dimensions we view at a given moment.

Figure (2.12) shows the different methods used to visualize our data throughout this thesis. The simplest representation of the data is obtained by fixing the two spatial dimensions, and keeping the the spectral dimension; the resulting vector $\mathbf{L}(\lambda) = [L(\lambda_1), L(\lambda_2), \ldots, (\lambda_{N_b})]^T$ (plotted in Figure 2.12(c)), exists in an $N_b$ dimensional Euclidian space, and represents the spectrum of a single pixel of the data cube. If we fix the spectral dimension instead, we end up with a two-dimensional grayscale image for a specific wavelength (Figure 2.12(d)), note that the image is often displayed in false-color to increase the contrast. We can also study the distribution of an individual wavelength by plotting a histogram of the spectral radiance value of all the pixels in the cube, as shown in Figure 2.12(e).

The fourth hyperspectral dimension is temporal, by traversing it we can convert our other projections into movies, this technique is particularly useful when considering detection statistics or maps, which are essentially another form of three- to two-dimensional projection.

Using the at-sensor radiance signal model of Section 2.1.3 we can now develop the detection and quantification algorithm algorithms which will be studied throughout the rest of this thesis.
Figure 2.12: Overview of structure of hyperspectral data.
Chapter 3

Plume Detection and Quantification Theory

By applying techniques from the fields of statistical signal processing and detection and estimation theory to the at-sensor radiance signal model of Section 2.1.3, we are able to develop a suite of CWA plume detection algorithms [5]. We will also discuss the temperature and concentration pathlength estimation algorithms developed for our study.

3.1 Plume Detection Theory

We begin the discussion of our detection algorithms with an introducing to detection theory. Next in Section 3.1.2 we provide details of the four detection algorithms used throughout this thesis. Finally, in Section 3.1.3 we present various methods for quantifying the performance of the detection algorithms.

3.1.1 Target Detection

The detection algorithms studied throughout this thesis are based on binary hypothesis testing. We use the likelihood ratio (LR) test to design our detectors, as this approach tends to yield detectors that are optimal for a wide range of performance criteria, such as maximization of the separation between target and background spectra.
The spectrum of each pixel is treated as a random vector with a specific probability distribution, \( x \). Given \( x \), we must decide between the two competing hypotheses

\[ H_0: \text{target absent} \rightarrow x = v(\lambda) \]
\[ H_1: \text{target present} \rightarrow x = S(\lambda)a + v(\lambda) \]

where \( v \) is the background or noise, \( S(\lambda) \triangleq [s_1(\lambda), s_2(\lambda), \ldots, s_M(\lambda)] \) are the spectra contained in the plume, and \( a \triangleq [a_1, a_2, \ldots, a_M]^T \) are the abundances of each spectra, which are subjected to the additivity constraint, \( \sum_{m=1}^{M} a_k = 1 \). Using the notation of the at-sensor radiance model (2.21), we can define the terms of \( x \) as

\[ v(\lambda) = L_{\text{off}}(\lambda) \]  
(3.1)
\[ S(\lambda) = \sum_{m=1}^{M} \tau_a(\lambda)a_m(\lambda) \]  
(3.2)
\[ a = \sum_{m=1}^{M} (B_0 \Delta T_p \gamma_m) \]  
(3.3)

Note that for the remainder of this thesis, we assume that all plumes are composed of only one CWA, and thus, the summation term, \( \sum_{m=1}^{M} \), will be ignored in all further instances of the on-plume radiance model.

Using the conditional probabilities of the two hypotheses, we can express the likelihood ratio as

\[ \Lambda(x) \triangleq \frac{p(x|\text{target present})}{p(x|\text{target absent})} \overset{H_1}{\gtrless} \eta \]  
(3.4)

If \( \Lambda(x) \) exceeds the threshold, \( \eta \), \( H_1 \) is chosen, and the pixel is determined to contain plume, if not, \( H_0 \) is selected; thus, we often refer to the LR test (or any monotonic function of it) as a detection statistic, denoted by \( y \).

When designing a detector, we are mainly concerned with the interplay between two parameters: the probability of detection, \( P_D \), and the probability of a false alarm, \( P_{FA} \). For a given threshold, \( \eta \), we define \( P_D \) as

\[ P_D = p(\Lambda(x) > \eta|H_1) \]  
(3.5)
and $P_{FA}$ as

$$P_{FA} = p(\Lambda(x) > \eta|H_0) \quad (3.6)$$

While we aim to develop detectors capable of achieving high probabilities of detection, it is critical that we hold $P_{FA}$ below a specified value (typically on the order of $10^{-3}$ to $10^{-5}$); this approach is known as the Neyman-Pearson criterion.

In most practical applications, it is impossible to design an optimal detector because the conditional probabilities $p(x|H_0)$ and $p(x|H_1)$ are unknown. The most common technique for avoiding this pitfall is to replace these unknown values with their maximum likelihood estimates, $\hat{p}(x|H_0)$ and $\hat{p}(x|H_1)$. The estimated LR is known as the generalized likelihood ratio test (GLRT), denoted by $\Lambda_G(x)$:

$$\Lambda_G(x) \triangleq \frac{\hat{p}(x|H_1)}{\hat{p}(x|H_0)} \quad (3.7)$$

The detectors used throughout this thesis (also known as adaptive detectors) are derived from the GLRT.

### 3.1.2 Detection Algorithm Taxonomy

Four different detection algorithms were used to detect the presence of CWA plumes in semi-synthetic hyperspectral data in this thesis. Three of the algorithms are based on distance (Mahalanobis distance, the matched filter and the adaptive matched filter), while the adaptive coherence/cosine detector is an angular distance metric. We will first describe how each detector is implemented, then review some commonly used methods for analyzing the results. Figure 3.1 depicts the theory behind the various detectors using a simplified two-dimensional spectral space.

**Mahalanobis Distance**  Strictly speaking, Mahalanobis distance (MD) is not a detection statistic, but rather a distance measure similar to the Euclidean distance; however, unlike its counterpart, the Mahalanobis distance takes into account the correlation of the data and is thus scale invariant. Calculation of the Mahalanobis distance requires that we know the mean vector and covariance matrix of the data. As the probability distribution of the data
is unknown, these quantities must be estimated from the data

\[ \hat{\mu} = \frac{1}{N} \sum_{n=1}^{N} x(n) \]

\[ \triangleq < x(n) > \]  \hspace{1cm} (3.8)

\[ \hat{\Sigma} = \frac{1}{N} \sum_{n=1}^{N} x_{zm}(n)x_{zm}(n)^T \]  \hspace{1cm} (3.9)

where \( x_{zm} \) is the de-meaned data

\[ x_{zm} \triangleq x - \hat{\mu} \]  \hspace{1cm} (3.10)

Note that the subtraction of the mean from the data allows us to convert of measured radiance values \( (L_{on}(\lambda)) \) to differential radiance \( (\Delta L(\lambda)) \). The Mahalanobis distance of a pixel is then calculated as

\[ y_{md}^2 = x_{zm}^T \hat{\Sigma}^{-1} x_{zm} \]  \hspace{1cm} (3.11)

where \( \hat{\Sigma}^{-1} \) is the inverse covariance matrix.

A pixel’s Mahalanobis distance is essentially its distance from the mean in a whitened
spectral space. Pixels with higher Mahalanobis distances deviate more from the “average” data than those with lower scores, thus, we can use that Mahalanobis distance as an anomaly detector. These high-scoring pixels are likely to contain plume, indicate that the FPA could be damaged (particularly if the location of these pixels remains constant from cube to cube), or otherwise indicated that the data is unreliable. If we sort the data by its Mahalanobis distance, we can determine which pixels are likely to be anomalies and exclude them from subsequent mean (3.8) and covariance (3.9) calculations which are used to implement the other detectors. This step is critical because even a few poorly performing pixels can seriously impact the performance of a detector. From this point forward, unless otherwise noted, all instances of $\mu$, $\Sigma^{-1}$, and in turn $x_{zm}$ are assumed to be calculated using uncorrupted background statistics. That is, all the pixels that contain plume (which are known because we embed the plume ourselves) as well as those classified as anomalies (pixels with a Mahalanobis distance in the top percentile) are excluded from these calculations. Referring back to Figure 3.1, the radius of the dotted circle is set such that it contains 99% of the background class data.

**Generalized Likelihood Ratio Test** The basic form of the generalized likelihood ratio test (GLRT) detector used throughout this thesis is

$$y_{GLR} = \frac{(x_{zm}^T \hat{\Sigma}^{-1} s)^2}{(s^T \hat{\Sigma}^{-1} s)(\psi_1 + \psi_2 x_{zm}^T \hat{\Sigma}^{-1} x_{zm})}$$

(3.12)

where $s$ is the target (gas) signature to be detected, $\alpha_m(\lambda)$, and $\psi_1$ and $\psi_2$ are values that vary depending on the specific form of the GLRT detector being implemented (MF, AMF or ACE).

**Matched Filter** The most basic form of the GLRT detector used in this thesis is the matched filter (MF). The MF is obtained by setting $\psi_1 = x_{zm}^T \hat{\Sigma}^{-1} s$ and $\psi_2 = 0$ in 3.12

$$y_{mf} = \frac{x_{zm}^T \hat{\Sigma}^{-1} s}{s^T \hat{\Sigma}^{-1} s}$$

(3.13)
The span of the output of the MF is unbounded; however, inspection of the implementation (3.13) shows that $|y_{mf}|$ will be at a maximum when the input pixel, $x_{zm}^T$, closely matches the target signature, $s$. Conversely, $|y_{mf}|$ will be close to 0 when the two spectra differ greatly. From Figure 3.1, we can see that the $y_{mf}$ is the result of the whitened data projected onto the direction of maximum variance. Ideally, the detection statistics will be separated into two distinct classes (target and background). The projection of (3.13) allows $y_{mf}$ to take both positive and negative values, and thus, we sometimes use two separate thresholds to determine if a plume contains plume, i.e.

$$
\eta_- < y_{mf} < \eta_+ \rightarrow H_0
$$

**Adaptive Matched Filter** Although the opportunity to set two thresholds with the MF can potentially afford us more control over the plume detection process, the potential for negative $y_{mf}$ values tends to make fully automated processing difficult. The adaptive matched filter (AMF) solves this problem by squaring the numerator of the MF. The AMF is generated from the GLRT by setting $\psi_1 = 1$ and $\psi_2 = 0$ in 3.12

$$
y_{amf} = \frac{(x_{zm}^T \hat{\Sigma}^{-1} s)^2}{s^T \hat{\Sigma}^{-1} s}
$$

(3.14)

The result is essentially a squared version of the MF with a different normalization factor. Many implementations of the AMF use $\psi_1 = N_{pix}$ in order to counteract the increase in dynamic range resultant from the quadratic term in the numerator of (3.13). The quadratic term also introduces a nonlinear scaling to $y_{amf}$ which ideally causes the a greater separation between target and background in the detection statistics.

**Adaptive Coherence/Cosine Detector** We obtain the adaptive coherence/cosine detector (ACE) by setting $\psi_1 = 0$ and $\psi_2 = 1$ in 3.12

$$
y_{ace} = \frac{(x_{zm}^T \hat{\Sigma}^{-1} s)^2}{(x_{zm}^T \hat{\Sigma}^{-1} x_{zm})(s^T \hat{\Sigma}^{-1} s)}
$$

(3.15)
Using the adaptive whitening transform, \( z \equiv \hat{\Sigma}^{-1/2}x \), we can express the ACE detector as

\[
y_{ace} = \frac{z^T \tilde{s} (\tilde{s}^T \tilde{s})^{-1} \tilde{s}^T z}{z^T z} = \frac{z^T P_{\tilde{s}}}{z^T z}
\]

(3.16)

where \( \tilde{s} \equiv \hat{\Sigma}^{-1/2} s \) is the whitened plume signature, and \( P_{\tilde{s}} \equiv \tilde{s} (\tilde{s}^T \tilde{s})^{-1} \tilde{s}^T \) is the orthogonal projection operator onto column space of \( \tilde{s} \). Knowing that \( P_{\tilde{s}}^2 = P_{\tilde{s}} \), we can write 3.16 as

\[
y_{ace} = \frac{||P_{\tilde{s}}z||^2}{||z||^2} = \cos^2 \theta
\]

(3.17)

where \( ||\zeta|| \) is the Euclidian norm of vector \( \zeta \)

\[
||\zeta|| = \sqrt{\sum_{k=1}^{K} \zeta(k)^2}
\]

(3.18)

Thus, in the whitened coordinate space, \( y_{ace} \) is equal to the cosine square of the angle between the test pixel and the hyperplane created by connecting the mean of the background class and the target signature. This angular relation tends to make ACE a more robust detector as it is unaffected by changes in illumination because they alter the magnitude of \( x \), but not the angle in relation to the pixel subspace.

### 3.1.3 Detection Statistic Analysis

The output of a detection algorithm, \( y \), is referred to as a detection statistic. After analyzing an entire data cube, we can sort through these detection statistics in search of the pixels with the highest values; a high score indicates that these pixels are more likely to contain plume. Detection statistics are typically viewed as two-dimensional maps which correspond with the data cube’s two spatial dimensions, as shown in Figure 3.2. Although the two-dimensional representation is perhaps the most intuitive manner of displaying the detection statistics, there are several other methods we can use to aid us in our analysis, namely: histograms, probability of exceedance plots, receiver operating characteristic curves, area under the receiver operating characteristic curves, and signal to clutter ratio plots.
Histograms  Perhaps the simplest method for analyzing detection statistics aside from a 2-D map, the histogram offers an “overall picture” of the distribution of the detection statistics of a data cube. As seen in Figure 3.3, in order for detection to be be possible there must be a separation between the target and background classes when the detection statistics are viewed as a histogram. We can then determine where to set the the threshold in order to maximize the probability of detection, while maintaining an acceptable level of false alarms. Note that because we have a known ground truth mask, we know which pixels belong to the target and background classes, and in turn, we can calculate $P_D$ and $P_{FA}$.

Probability of Exceedance  The probability of exceedance, $P_y(\eta)$, is defined as the probability that a random variable, $y$ in our case, will exceed a given threshold, $\eta$.

$$P_y(\eta) = \int_{\eta}^{\infty} f_y(y)dy = 1 - \int_{-\infty}^{\eta} f_y(y)dy = 1 - F_y(\eta)$$ (3.19)

where $f_y(y)$ is the probability density function of the detection statistics, and $F_y(y)$ is the cumulative distribution function. Probability of exceedance plots, as shown in Figure 3.4,
are also useful for analyzing the threshold selection process as they provide an alternate (logarithmic) view of the detection statistics. Probability of exceedance plots are particularly useful when studying the effect of anomaly or plume pixels on a detection statistics, as well as when attempting to model the statistical distribution of a dataset. The statistical modeling of hyperspectral data is a heavily researched topic as has the potential to improve plume-free background estimation.

**Receiver Operating Characteristic** The tradeoff between the probability of detection, $P_D$, and the probability of a false alarm, $P_{FA}$, is described by the receiver operating characteristic (ROC) curve, which plots $P_D(\eta)$ against $P_{FA}(\eta)$ as a function of all possible $\eta$. Figure 3.5 illustrates the tradeoffs in $P_D$ and $P_{FA}$ for a typical ROC curve; progression along the curve from the origin to (1,1) indicates a decrease in $\eta$. Note that because the Neyman-Pearson criterion restricts us to such small $P_{FA}$’s, we often display the ROC curves as a semi-logarithmic plot (with $P_{FA}$ as the logarithmic axis).
CHAPTER 3. PLUME DETECTION AND QUANTIFICATION THEORY

Figure 3.4: Sample probability of exceedance plot

Figure 3.5: Sample ROC plot and illustration of tradeoffs
Area Under the Receiver Operating Characteristic  The area under the ROC curve (AUROC) is another useful indicator of detector performance. By integrating the ROC curve, we are able to represent the two-dimensional metric with a single dimension, this projection allows us to include the fourth hyperspectral dimension in our analysis and compare detection performance as a function of time. In our plume embedding study this increase in dimensionality permits us to track detection performance as we sweep through various physical plume parameters. An AUROC of 1 signifies perfect detection, AUROC $= 0.5$ represents the line of no discrimination, or the “random guess” case, while AUROC $= 0$ would mean that the detector classified every pixel incorrectly.

Signal-to-Clutter Ratio  The signal-to-clutter ratio (SCR) is a similar metric to the AUROC in that it enables us to study the performance of a detector on a series of data cubes. The performance of a detector is innately linked with the estimated background of a data cube. The SCR exploits this association by comparing a target signature with the background in which it is to be detected

$$SCR = a^2 s^T \Sigma^{-1} s$$  \hspace{1cm} (3.20)

where $a = \gamma \Delta T_p$. In practice we do not normally know the value of $a$ so typically use an alternate version of SCR which can be estimated from the detection statistics

$$\hat{SCR} = \frac{\langle y_p \rangle^2}{\text{var}[y_{bg}]}$$  \hspace{1cm} (3.21)

where $y_p$ and $y_{bg}$ are vectors of detection statistics for the pixels containing plume and background, respectively, and $\text{var}[y_{bg}]$ is the variance of the background pixels

$$\text{var}[y_{bg}] = \frac{1}{N_{bg}} \sum_{n=1}^{N_{bg}} [y_{bg}(n) - \langle y_{bg} \rangle]^2$$  \hspace{1cm} (3.22)

SCR can also be used to calculate the expected minimum detectable quantity of a plume in a scene, as well as estimate a plumes concentration, as we will see in the next section.
3.2 Plume Quantification Theory

Using the at-sensor radiance signal model of Section 2.1.3, we develop quantification algorithms in order to estimate temperature and concentration pathlength information from hyperspectral data. The semi-synthetic nature of our data allows us to better evaluate the performance of these algorithms as we have “ground truth” data to compare to our estimates; however, we must consider the fact that our embedding routine is based on the at-sensor radiance signal model, and there is no guarantee that the “ground truth” is 100% accurate. We must also consider that our estimates are developed in a recursive manner, thus, inaccuracies in the first estimate \( T_a \) will propagate through to other estimates, amplifying the associated error.

3.2.1 Temperature Estimation

The basis for our temperature estimation algorithm is Planck’s Law. Our data was recorded with the spectral dimension in wavenumbers, so we use the appropriate form of the law

\[
B(\nu, T) = \frac{C_1 \nu^3}{e^{C_2 \frac{\nu}{T}} - 1}
\]

where \( C_1 = 1.91044 \times 10^{-8}(\text{W m}^2 \text{sr} \text{cm}^{-1}) \) and \( C_2 = 1.438769(\text{cm} \cdot \text{K}) \). Inversion of Planck’s Law along with (2.6) allow us to extract a temperature estimate from our radiance values

\[
T_m = \frac{C_2 \nu}{\ln \left[ \frac{C_1 \nu^3}{B(\nu, T_m)} + 1 \right]}
\]

where \( B(\nu, T_m) \) is derived from the measured radiance - \( m \) may be either the atmosphere, background, or plume, depending on the value of \( \nu \) selected.

**Atmospheric Temperature** In order to estimate the atmospheric temperature we choose a spectral band with the lowest possible transmissivity, ensuring that the majority of the at-sensor radiance comes from the atmosphere and not from the background. Ideally we would use data well into the \( \text{H}_2\text{O} \) absorption band (see Figure 2.10); however, FIRST images in
CHAPTER 3. PLUME DETECTION AND QUANTIFICATION THEORY

the 800 cm\(^{-1}\) to 1300 cm\(^{-1}\) range, so we use the available band closest to \(\nu = 1269 \text{ cm}^{-1}\) to perform the inversion. This spectral band choice allows us to assume that atmospheric transmission and plume emission and transmission effects are negligible in the at-sensor radiance, thus, we are able to reduce (2.4) to

\[
L_{on}(\nu) \approx L_a(\nu) \\
\approx B(\nu, T_a)
\]  

(3.25)

\(B(\nu, T_a)\) is then use to solve for \(T_a\) using (3.24).

**Background Temperature** We calculate background radiance by focusing on a spectral radiance band with relatively high transmittance, such as \(\nu = 990 \text{ cm}^{-1}\). It is clear from Figure 2.10 that even at this relatively strong and flat spectral band approximately 78% of the at-sensor radiance represents emission from the background, the other 22% comes from atmospheric emissions. In order to decouple these two sources we use our atmospheric temperature estimate to estimate \(L_b(\nu)\) from the at-sensor radiance, \(L_{on}(\nu)\)

\[
L_b(\nu) = \frac{L_{on}(\nu) - (1 - \tau_a(\nu))B(\nu, T_a)}{\tau_a(\nu)}
\]  

(3.26)

note that we again ignore the emission and transmission effects of the plume. The “flat background approximation” permits the \(L_b(\nu) \approx B(\nu, T_b)\) approximation and we solve for the background temperature using (3.24)

**Plume Temperature** Plume temperature is the most difficult parameter to estimate. If we attempt to solve in the same manner as atmospheric and background temperature, but choose a spectral radiance band with strong plume emission, we arrive at

\[
B(\nu, T_p) = \frac{L_{on}(\nu) - \tau_a(\nu)\tau_p(\nu)B(\nu, T_b) - (1 - \tau_a(\nu))B(\nu, T_a)}{\tau_a(\nu)(1 - \tau_p(\nu))}
\]  

(3.27)

However, from (2.3) we see that plume transmissivity, and in turn, emissivity, are dependent on the concentration pathlength, thus, we are left with an underdetermined equation. As a result, we are unable to estimate the temperature of the plume directly.
3.2.2 Concentration Pathlength Estimation

Using both the theoretical and calculated values of SCR, (3.20) and (3.21) respectively, along with (3.3), we are able to estimate the concentration pathlength of a CWA plume as

$$\gamma = \frac{a}{\Delta T_p \left. \frac{\partial B(\lambda, T)}{\partial T} \right|_{T=T_b}}$$  \hspace{1cm} (3.28)

where $a$ is derived from the SCR as

$$a = \sqrt{\frac{\text{SCR}}{s^T \Sigma^{-1} s}}$$  \hspace{1cm} (3.29)

Note that (3.28) requires knowledge of $\Delta T_p$, a quantity which we cannot determine from estimation algorithms alone, as we are unable to calculate $T_p$ directly. In order to work around this limitation, we must assume that $T_p = T_a$.

As mentioned in Chapter 1, the lack of ground truth information typically makes analysis of CWA detection and quantification algorithms a difficult task. We will now develop a synthetic CWA plume embedding tool in order to provide a more accurate evaluation of detector performance.
Chapter 4

Plume Embedding Into Background Measurements

To effectively analyze the accuracy, strengths and weaknesses of our detection algorithms, it is useful to know the ground truth for a given data cube. As all of our data is empirical, we lack the ability to perform exhaustive studies of the intricacies of each detection algorithm and how they are affected by variations in such physical plume parameters as, concentration pathlength, temperature, plume size and location, as well as the type of chemical agent released. In order to thoroughly examine these effects, we developed a plume embedding tool that affords us control of the aforementioned physical characteristics. We begin by introducing the some CWA plume embedding theory, and follow with a description of how said this theory is implemented in our performance evaluation tool.

4.1 Theory

The basis of our embedding tool starts with equation (2.9), repeated here for convenience

\[
\Delta L(\lambda) \triangleq L_{on}(\lambda) - L_{off}(\lambda) \\
= \tau_a(\lambda)[1 - \tau_p(\lambda)] [B(\lambda, T_p) - L_b(\lambda)]
\]  

(4.1)
we then use equation (2.2) to create the following identity, which we substitute into (4.1)

\[ \tau_a(\lambda)[B(\lambda, T_p) - L_b(\lambda)] = [L_a(\lambda) - L_{off}(\lambda)] + \tau_a(\lambda)[B(\lambda, T_p) - L_a(\lambda)] \] (4.2)

Note that an extension of the “flat background emissivity” approximation of section 2.1.3 allows us to assume that \( L_a(\lambda) = B(\lambda, T_a) \), as the sharp features of atmospheric transmission function are lost through the downsampling process (discussed in the next section). After simplifying and rearranging terms, (4.1) becomes

\[ L_{on}(\lambda) - L_{off}(\lambda) = (1 - \tau_p(\lambda)) \{ [B(\lambda, T_a) - L_{off}(\lambda)] + \tau_a[B(\lambda, T_p) - B(\lambda, T_a)] \} \] (4.3)

Finally after multiplication, collection of terms, and isolation of \( L_{on}(\lambda) \) on the left hand side, we arrive at

\[ L_{on}(\lambda) = (1 - \tau_p(\lambda))B(\lambda, T_a) + \tau_p(\lambda)L_{off} + \tau_a(\lambda)(1 - \tau_p(\lambda))[B(\lambda, T_p) - B(\lambda, T_a)] \] (4.4)

which is the basis for our plume embedding studies.

## 4.2 Implementation

The plume embedding module takes four inputs in addition to the data cube into which the plume is to be embedded (the pre-release cube). The user must provide a spectral signature from the CWA library, a plume mask, and values for concentration pathlength and plume temperature. A synthetic plume is then embedded into the pre-release cube using using Equation (4.4). The resulting cube, embedded with a synthetic plume, is then passed along to the detection stage of the process. Figure 4.1 shows a block diagram of the embedding process.

### 4.2.1 Spectral Signature

The spectra from the library are sampled at a much higher resolution (~ 700 bands in the LWIR region) than the data cubes, so they must be preprocessed before they can be
 CHAPTER 4. PLUME EMBEDDING INTO BACKGROUND MEASUREMENTS

Figure 4.1: High level description of plume embedding stage.

used by the detection or embedding algorithms. This preprocessing routine includes both compensation for atmospheric and sensor effects. The procedure, which is outlined in Figure 4.2, consists of the following steps:

1. Point-by-point multiplication of the high-resolution library spectra $s_{\text{lib}}(\lambda)$ with the transmission function $\tau_a(\lambda)$ computed by MODTRAN for a specific atmospheric model.

2. Convolution of the resultant spectra with the point spread function $\tau_{\text{sensor}}(\lambda)$ of the FIRST sensor. The point spread function is assumed to have a Gaussian shape with center $\lambda_i$ and full width half maximum (FWHM) $\Delta \lambda_i$, determined by the sensor specifications.

3. Resampling of the reduced resolution spectra at the wavelength locations specified by the center of the sensor bands.

The preprocessing procedure leads to a loss of information which can be detrimental to the performance of our embedding and detection algorithms. Figure 4.3 provides a visual representation of the conversion process. The high-resolution version of $s_4$ is shown
Figure 4.2: Adjustment of high-resolution library spectra for atmospheric transmission, sensor smoothing, and sensor resampling.

in Figure 4.3(a). Figure 4.3(b) is a plot of a typical atmospheric transmission output from MODTRAN over the LWIR spectral regime. The atmosphere adjusted spectrum in Figure 4.3(c) is then calculated by taking the dot product of (a) and (b); we can clearly see the effects of atmospheric absorption (the narrow dips in the plot). Figure 4.3(d) shows the sensor spectral channel response function for FIRST. The band centers ($\lambda_i$) and full-width half-max (FWHM) values ($\Delta \lambda_i$) were obtained from a data file from an experimental release of $s_4$ from Dataset A. Finally, in Figure 4.3(e) we see the result of the convolution and resampling of the atmosphere adjusted spectrum. Note that the atmosphere induced dips and all other high frequency components are filtered by the downsampling process; clearly, gas spectra with sharp peaks suffer more from this process than those with slow trends. Figure 4.4 shows the sensor-atmosphere adjusted CWA threat library used throughout this thesis. Note that $s_4$ has a maximum value of 0.0382 (ppm-m)$^{-1}$ at 946.5 cm$^{-1}$, however, it is truncated in Figure 4.4.

4.2.2 Plume Concentration Pathlength Mask

The user must provide the plume embedding algorithm with a mask to specify where to embed the plume in the data cube and at what concentration pathlength. The dimensions of the mask must be $N_l \times N_s$ pixels and should be normalized so all values are constrained from 0 to 1. Plume is embedded into the cube at locations where the mask value is greater
Figure 4.3: Conversion of the $s_4$ high resolution library spectrum (top) to sensor resolution (bottom) including effects of atmospheric absorption.
than 0 at a concentration of $\gamma \times$ mask value. We evaluated three types of masks throughout this thesis: constant ellipse, Gaussian, and “realistic.” The constant and Gaussian masks are shown in Figure 4.5; the constant mask has a value of 1 inside of the white line and 0 outside of it.

The constant and Gaussian plume masks can be particularly useful when performing trade studies as they are highly controlled situations; however, dynamic atmospheric conditions cause real plumes to diffuse in more complex patterns. While it is possible for the user to manually create more realistic masks, this process can be time consuming, so we developed an automated method of generating such masks. We create these masks using detection results from a post-release cube as well as a contrast image generated using both pre- and post-release cubes as outlined below and shown in Figure 4.6.

1. $y_{mah}$ is calculated for the cube and the pixels which score in the top percentile are excluded from the detector creation process, as outlined in section 3.1.2.
2. A GLRT detector is created and used to process the post-release cube.

3. The detection statistics are displayed as a two-dimensional map and the user creates a conservative plume-free mask with the mouse.

4. A new GLRT detector is created and used to process the post-release data, this time with both the initial anomaly pixels and the user define plume pixels excluded.

5. The new (more accurate due to the lack of background corruption) detection statistics are displayed and the user outlines the plume as accurately as possible. The resultant binary mask will define the spatial extent of the final plume mask.

6. Both the pre- and post-release cubes are band averaged across bands where the plume has strong peaks in its absorption coefficient. All other bands are ignored as they contain little to no information about the strength of the plume.

7. The results of the band averaging process (a two-dimensional representation of the cubes) are subtracted from each other to produce the spectral component of the final plume mask.

8. Finally, the dot-product of the spatial and spectral components of the plume mask is calculated in order to generate the final plume mask. Figure 4.7 shows an example of one such mask.

Figure 4.5: Sample constant and Gaussian plume masks. Constant mask = 1 inside of white line and 0 outside
CHAPTER 4. PLUME EMBEDDING INTO BACKGROUND MEASUREMENTS

Figure 4.6: “Realistic” plume mask generation process.

Figure 4.7: Sample “realistic” plume mask.
4.2.3 Plume Temperature

It has already been shown that a thermal contrast between the plume and the background is necessary if the plume is to be detected (2.15); thus, we aim to further study this relationship by allowing the user to manually adjust the temperature of the plume. Chemical plumes tend to reach thermal equilibrium with the surrounding atmosphere in a matter of seconds, so the default behavior of our embedding algorithm is to embed the plume at this temperature, $T_a$, as discussed in Section 3.2.1.

With the semi-synthetic data generated using the techniques described in this chapter, we can apply the detection and quantification algorithms of Chapter 3 to perform analysis of said techniques.
Chapter 5

Performance Evaluation of Detection Algorithms

The main goals of our research were to: a) validate that the synthetic plume embedding procedure developed in Chapter 4 behaves as the radiance signal model (2.10) predicts, b) evaluate the performance of our detection and quantification algorithms, specifically the limits of the algorithms, and c) demonstrate the utility of our performance evaluation tool. In order to best achieve these goals, we developed a fully automated detection pipeline to analyze our semi-synthetic data. We begin with an overview of how the implementation of CWA plume detection process, followed by details of the experimental specifications used to test the detection algorithms. Finally, we present the our results in the form of several trade studies where effect of each physical plume parameter is isolated.

5.1 Implementation

We begin this section with a description of the method in which our pipeline generates detection statistics. Next, in Section 5.1.2 we detail the input and output structures of the the plume embedding tool.
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

5.1.1 Detection Pipeline

The GLRT detectors described in section 3.1.2 require de-meaned data, $x_{zm}$, the inverse covariance matrix of the background, $\hat{\Sigma}^{-1}$, and a target signature, $s$. Also, note that by transforming the data as shown in Figure 2.12(b), we are able to take advantage of MATLAB’s matrix manipulations capabilities and process the entire data cube in one step, rather than line-by-line. This amounts to replacing the vector $x_{zm}$ with the matrix $X_{zm}$ in the detectors of section 3.1.2, and in turn the scalar $y$, becomes a vector, $\mathbf{y}$. Figures 5.1 and 5.2 detail the implementation of the detection pipeline, outlined below:

1. $s$ is scaled by $\tau_a$, convolved with $\tau_{sensor}$, and resampled to ensure it matches the resolution of the data cube (see section 4.2.1 for details).

2. $y_{mah}$ is calculated for the cube and the pixels which score in the top percentile are flagged as anomalies, as outlined in section 3.1.2.

3. If the user elects to use PFBGE the pixels flagged in step 2 are ored with the pixels from mask which contain plume, the inverse of the result (a list of all “bad” pixels) is then passed to the statistic calculation stage along with $X$. Otherwise, only the flagged outlier and $X$ are passed to the statistic calculation stage.

4. The de-meaned data and inverse covariance matrix of the background are calculated using (3.10) and (3.9), respectively. The results are passed to the detection stage along with $s$.

5. $y_{mf}$, $y_{amf}$, and $y_{ace}$ are calculated as described in section 3.1.2.

6. Finally, the detection statistics are used along with the plume mask to generate histograms, probability of exceedance, ROC, AUROC, and SCR plots.

Note that unlike the detection procedure used to create the “realistic” plume mask in section 4.2.2, the detection pipeline implemented in this stage is a single-pass procedure, as there is no need to estimate the plume-free background from the data.
Figure 5.1: Detection pipeline implementation.

Figure 5.2: Detection pipeline implementation detail.
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

5.1.2 I/O Structure

Our plume embedding tool enables us to control five different parameters: the CWA, plume mask, concentration path length, plume temperature, and use of plume-free background estimation. Each combination of inputs generates four sets of detection statistics (MD and three GLRT), each of which can be viewed using several different methods (see section 3.1.3). Furthermore, in order to study the strengths and weaknesses of our detection algorithms, we typically sweep through a range of values of at least one parameter while keeping the others fixed. These trade studies have the potential to generate a large amount of data, thus it was imperative that we develop a method to organize and analyze it.

Input Structure   The user can provide the plume embedding parameters either as a structure or as a cell array of strings and arrays. Before the performance evaluation tool runs, all the inputs must be checked to ensure that all parameters have been included and are valid, for example, $\gamma \geq 0$ and the plume mask’s dimensions must match those of the data cube. Any parameters that fail this check must be re-entered, or the user can opt to use any of the default values (listed in section 5.2) by simply pressing Enter. The performance evaluation tool then cycles through every possible combination of inputs and saves each result.

Output Structure   The output of the performance evaluation tool is saved as a cell array. Each of the five adjustable parameters is stored in a column, while the detection statistics, detection metrics, and other useful statistics and data used along the way are stored in the sixth column. This configuration allows us to easily sort through the data to generate the plots discussed in section 3.1.3.

5.2 Experimental Specifications

All five of our adjustable plume parameters play a roll in our original at-sensor radiance model in one way or another (2.10); thus, to obtain the highest quality possible analysis for each factor, we must do our best to minimize the impact of the effects of the parameters not under study. This is best done in two ways: (1) by varying only one parameter at a time, and (2) by choosing quantities for the fixed parameters that ensure “reasonable” detection
performance, i.e. neither too difficult nor too easy; these quantities will be termed the “default values” for each plume parameter. Unless otherwise noted, the following default plume parameters were used in all subsequent results.

**Data**  Three different datasets were used throughout this thesis: “A”, “B”, and “C”. As previously mentioned, all three datasets were imaged using the FIRST Fourier transform spectrometer (see section 2.2.2 for details). Figure 5.2 lists some key specifications of the three datasets. Note that the SCR values are provided as a “detection difficulty” metric; the higher the value is, the more a pixel with plume will stand out from the background, and thus, the easier detection should be. The SCR values were calculated using (3.20) assuming $\gamma = 20$ ppm-m, $\Delta T_p = 1^\circ K$, and $s = s_2$. Note that the spectral radiance measurements for the dataset A only extend to 1245 cm$^{-1}$, and thus, we cannot accurately estimate the atmospheric temperature using (3.24) and (3.25).

<table>
<thead>
<tr>
<th>Dataset:</th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCR:</td>
<td>404.47</td>
<td>316.82</td>
<td>267.42</td>
</tr>
<tr>
<td>Range ($cm^{-1}$):</td>
<td>900 - 1245</td>
<td>851 - 1298</td>
<td>800 - 1293</td>
</tr>
<tr>
<td>Bands (good/total):</td>
<td>68/68</td>
<td>53/68</td>
<td>53/75</td>
</tr>
<tr>
<td>Dimensions (pixels):</td>
<td>128 x 320</td>
<td>256 x 256</td>
<td>200 x 200</td>
</tr>
<tr>
<td>FWHM ($cm^{-1}$):</td>
<td>5.14</td>
<td>6.65</td>
<td>8.00</td>
</tr>
</tbody>
</table>

Table 5.1: Dataset specifications.

**CWAs**  Figure 4.4 shows the wide variety of spectral signatures used throughout this thesis. Note the differences in peak height, width and location. Spectra with high or wide peaks will impact the at-sensor radiance (2.10) more than those lacking such distinct features. For this reason, we chose to use $s_2$ as the default CWA as it has one relatively strong peak and one weaker peak, neither of which is excessively wide.

**Plume Masks**  Three main factors must be considered when selecting a plume mask: shape, size or fill factor (FF), and location. We ran our performance evaluation tool using constant ellipse, Gaussian, and “realistic” shaped masks. When performing trade studies we must consider the fact that the Gaussian and “realistic” masks introduce unwanted
variations in $\gamma$, for this reason, we use the constant ellipse mask as our default mask type. A plume mask’s fill factor is defined as the ratio of the area which the plume subtends to the total area of the data cube.

$$\text{FF} \triangleq \frac{N_{\text{plume}}}{N_{\text{pix}}} \times 100$$ (5.1)

where $N_{\text{plume}}$ is the number of pixels which contain plume. This value is important to consider as it limits the number of pixels available to construct a the background statistics necessary to great the detectors. The default plume mask used throughout this thesis filled 6.8% of the cube. The plume location comes into play when considering $\Delta T_p$, as background and atmospheric temperatures typically vary as a function of location throughout a data cube.

**Concentration Pathlength**  We vary $\gamma$ from 0 to $10^5$ ppm-m. Reasonable detection performance can be achieved with $5 < \gamma < 100$ ppm-m, where the value chosen for $\gamma$ depends on the other plume embedding parameters; we found that $\gamma = 30$ ppm-m works well in conjunction with our other default values.

**Plume Temperature**  Chemical plumes tend to reach thermal equilibrium with the surrounding atmosphere in a matter of seconds, so the default behavior of our embedding algorithm is to embed the plume at this temperature, i.e. $T_p = T_a$. For the trade study, plume temperature is constrained to the range $|\Delta T_p| < 10^5$ K in order to preserve the linear planck function approximation (2.17).

**Plume-Free Background Estimation**  The GLRT detectors of section 3.1.2 assume uncorrupted background statistics, thus, unless otherwise noted these statistics are always calculated without the pixels containing plume and those flagged as anomalies.
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

5.3 Results

Our investigation of the effects of various physical plume parameters is organized into five sections. We begin with a survey of the performance of the three different GLRT detectors in order to provide a basis to better understand all subsequent detection results. Next, in Section 5.3.2, we study what is perhaps the most fundamental factors when considering the performance of HSI CWA detectors, the relationship between the dataset and the chemical to be detected. Section 5.3.3 is an investigation of how plume-free background estimation and fill factor affects detection performance. Next, in Section 5.3.4, we study how concentration pathlength and plume mask impact detection performance. Finally, Section 5.3.5, we examine the effects of plume-background temperature in relationship.

5.3.1 Detectors

In order to evaluate the performance of our the GLRT detectors, we compare the detection statistics of each algorithm for a single semi synthetic cube. Figure 5.3 shows ROC curves for both the MF and ACE for all three datasets with \( s_2 \) embedded at thermal equilibrium at a concentration of 50 ppm-m. In all three datasets, ACE tend to outperform the MF at the low false alarm rates that we are concerned with (\( 10^{-5} \) to \( 10^{-3} \)). Note that the AMF has been omitted from the plot because it produces ROC curves identical to the MF, as the detection statistics are simply a scaled versions of one another.

The disparity in performance is relatively low in datasets A and C; however, dataset B exhibits an extremely large variation in detector performance, particularly at low false alarm rates. The poor performance of the (A)MF detectors can be better understood through examination of Figures 5.4, 5.5 and 5.6, which show histograms of MF, AMF and ACE detection statistics for dataset C, respectively. Figure 5.4 shows a large overlapping area common of both the target and background classes of the MF, while there is significantly less overlap in the distribution of the ACE. One should also note that as the MF can take both positive and negative values; while the background class distribution is typically centered about 0 (assuming reliable PFBGE), the target class can have either a positive or negative mean. This fact makes setting a threshold in a fully automated detection environment a difficult task; one common solution to this problem is to square the MF output, essentially
converting the MF to an AMF. As a result, from this point forward, all detection statistics and results will be generated using the ACE detector.

### 5.3.2 Data Cubes and CWAs

The interplay between the background data and the CWA spectrum is the most fundamental factor when considering the performance of a particular detector. The statistical distribution of the data is unknown in most practical detection scenarios, and thus must be estimated as detailed in section 3.1.2. In turn, detection performance is clearly linked with the accuracy of the estimates of the background statistics (3.8) and (3.9). A perfectly homogenous background, in which every pixel had an identical spectrum, for example, or any data with a known statistical distribution, would yield optimal detectors, and thus, the best possible detection results. Such a scenario is physically unrealizable, so we must consider what happens when our estimates contain error. As the accuracy of these estimates deteriorate, detection performance will decline as well; thus, as the complexity of a dataset increases,
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

Figure 5.4: Histogram of MF detection statistics dataset C embedded with $s_2$ at $\gamma = 50$ ppm-m.

Figure 5.5: Histogram of AMF detection statistics dataset C embedded with $s_2$ at $\gamma = 50$ ppm-m.
the quality of the estimated statistics, and in turn, detection performance will decrease.

Figure 5.7 shows the ROC curves generated from detection of a 30 ppm-m plume embedded with $S_2$ in each dataset at $T_p = T_a$. Note that as indicated by probability of exceedance plot of Figure 5.8, dataset A yields the strongest detection statistics, closely followed by C, while dataset B performs markedly worse. This trend is also clearly visible when noting the area under the ROC and signal-to-clutter ratio values of Table 5.2. The link between the quality of the estimated background statistics and detection performance motivates need for the widely studied topic of statistical background modeling.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>AUROC</td>
<td>0.91</td>
<td>0.69</td>
<td>0.89</td>
</tr>
<tr>
<td>SCR</td>
<td>49.99</td>
<td>4.66</td>
<td>41.51</td>
</tr>
</tbody>
</table>

Table 5.2: AUROC and SCR analysis of datasets A, B and C.
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

Figure 5.7: ROC analysis of ACE detection statistics for datasets A, B and C embedded with \( s_2 \) at \( \gamma = 30 \text{ ppm-m} \).

Figure 5.8: \( P_y(\eta) \) analysis of ACE detection statistics for datasets A, B and C embedded with \( s_2 \) at \( \gamma = 30 \text{ ppm-m} \).
various CWAs on detection performance. The background radiance in our basic on-plume at-sensor radiance model (2.4), is scaled by the transmittance of the plume, which is a function of the absorption coefficient spectrum of the CWA present in the cube; therefore, we should be able to predict which predict which CWAs will perform well through analysis of their spectra, given in Figure 4.4. Figure 5.9 shows the ROC curves of these CWA spectra.

As expected, the spectra with larger peaks perform better, than those without distinguishable features. The performance of six of the spectra can be classified from “good” to “fair” (listed in order of decreasing AUROC) as: 1) $s_1$, 2) $s_2$, 3) $s_9$, 4) $s_7$, 5) $s_{10}$, 6) $s_5$. These spectra all contain strong peaks which enable the plume to stand out from the background radiance values. The other four CWAs performed poorly: 7) $s_4$, 8) $s_3$, 9) $s_6$, 10) $s_8$. Note that the spectra $s_3$, $s_6$, and $s_8$ all lack the strong and/or wide features necessary to cause the plume to stand out; however, the spectra of $s_4$ is very similar in size and shape to that of $s_{10}$, yet we see a vast difference in performance. This disparity is a result of

Figure 5.9: ROC analysis of ACE detection statistics for dataset C embedded with $s_1$ through $s_{10}$ at $\gamma = 30$ ppm-m.
the fact that spectral peak of $s_4$ lies near the end of LWIR atmospheric transmission ”window” ($\sim 1190 \text{ cm}^{-1}$), and is thus heavily corrupted by noise caused by the $H_2O$ absorption band. Figure 5.10 summarizes detection performance for the different CWAs as a function of AUROC and both theoretical (3.20) and estimated (3.21) SCR.

### 5.3.3 Fill Factor and Plume-Free Background Estimation

The quality of the background statistics, and in turn, the that of the detection statistics, are clearly functions of the data used to create the estimates. When assessing the quality we must consider both the amount of data used to generate these statistics, and whether the pixels used are truly representative of the background, or if they are corrupted by plume. It is clear from (5.1) that as the FF increases, the quality of $\hat{\mu}$ and $\hat{\Sigma}^{-1}$ will deteriorate, as a smaller portion of the data is used to form these estimates, thus causing a degradation of the detection statistics. This trend is visible in the ROC curves, detection statistics, AUROC and SCR plots of Figures 5.11, 5.12, and 5.13, respectively. Note that the gradient effect in detection strength in the maps of Figure 5.12, this trend is a result of variations in $\Delta T_p$ and will be discussed further in section 5.3.5.

Accurate plume-free background (PFBG) estimation is also critical for the maximization of detector performance. As the number of plume pixels which are included in the calculation of the background statistics increases, it stands to reason that the detector will be less sensitive to the effects that a plume’s spectrum will have on the background data. This effect is visible in Figure 5.13 as plume-free background estimation case outperforms the corrupted background case in both AUROC and SCR at all measured fill factors; this trend holds as we vary other plume parameters as well. Furthermore, as the impact of the plume on the scene (its fill factor, for example) increases, so to will difference in performance between the two cases, until the “random guess” case (AUROC = 0.5) is reached. We can get a better picture of the effect of PFBG estimation by considering the distributions of the target and background classes of each case. Note how the separation between the two classes seen in the plume-free case (Figure 5.14) is absent in the corrupted case (Figure 5.15). Without this separation it becomes difficult to set a threshold for detection.
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

Figure 5.10: Theoretical and empirical SCR and AUROC results of ACE detection statistics for datasets C embedded with $s_1$ through $s_{10}$ at $\gamma = 30$ ppm-m.
5.3.4 Concentration Pathlength and Plume Mask

Examination of our on-plume at-sensor radiance model (2.10) suggests that an increase of a plumes concentration pathlength will result in a corresponding increase in the strength of the detection statistics. Although the relationship between the $L_{on}(\lambda)$ and $\gamma$ is exponential, in section 2.1.3, we showed that it can be approximated as linear, so long as the plume remains “optically thin.” Figure 5.16 shows this trend as observed in cube A; as the plume’s concentration increases, the ROC curves shift upwards. Once the plume becomes “optically thick,” the detection performance begins to peak, as shown in the AUROC plots of Figure 5.17(a). The transition to optical thickness at $\gamma \approx 100$ ppm-m in cubes A and C, and at $\gamma \approx 250$ ppm-m in cube B.

As $\gamma$ continues to increase the plume eventually becomes “optically opaque,” detection performance begins to decrease, as indicated by the decline in the AUROC plots at $\gamma \approx 1000$ ppm-m for cubes A and C, and $\gamma \approx 5000$ ppm-m for cube B. This phenomenon occurs in the limit of $\tau_p(\lambda) \approx 0$. Once the transmissivity get low enough, the radiance from
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

Figure 5.12: Detections statistics of ACE detection statistics for dataset C embedded with $s_2$ at $\gamma = 30$ ppm-m with various fill factors.
Figure 5.13: AUROC and SCR analysis of ACE detection statistics for dataset C embedded with $s_2$ at $\gamma = 30$ ppm-m with various fill factors.

Figure 5.14: Histogram of ACE detection statistics dataset C embedded with $s_2$ at $\gamma = 30$ ppm-m with PFBGE.
Layer 1 in Figure 2.2, $L_b(\lambda)$ is prevented from passing through the plume. At this point, the plume replaces the background, and acts as blackbody, and the on-plume at-sensor radiance model becomes

$$L_{oa}(\lambda) = \tau_a(\lambda)L_p(\lambda) + L_a(\lambda)$$

and thus, our detectors which are based on (2.4), become ineffective. Figure 5.18 illustrates the optically thin to thick to opaque transition with a Gaussian plume mask embedded into cube A at various values of $\gamma$.

The estimated signal-to-clutter ratioo (3.21), shown in Figure 5.17(b) serves as a reasonable indicator of plume performance until the plume transitions to the “optically thick” regime. Figure 5.20 shows the relationship between the two metrics for cube A. The line begins to wrap back around on itself at $\gamma = 100$ ppm-m, when the SCR begins to fail to represent the plume concentration. The metric begins to break down due to the lack of proportionality between $y_p$ and $\gamma$ for thick plumes.

The type of plume mask selected, constant or varying (whether it be gaussian, realistic,
Figure 5.16: ROC analysis of ACE detection statistics dataset A embedded with $s_2$ at a varying $\gamma$.

Figure 5.17: AUROC and SCR analysis of ACE detection statistics datasets A, B and C embedded with $s_2$ at a varying $\gamma$. 
Chapter 5. Performance Evaluation of Detection Algorithms

\[ \gamma = 30 \text{ ppm-m} \]

\[ \gamma = 100 \text{ ppm-m} \]

\[ \gamma = 2500 \text{ ppm-m} \]

Figure 5.18: Detections statistics of ACE detection statistics for dataset A embedded with \( s_2 \) at various \( \gamma \).
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

Figure 5.19: AUROC and SCR analysis of ACE detection statistics for dataset A embedded with $s_2$ varying $\gamma$ with and without PFBGE.

Figure 5.20: Relation between AUROC and SCR results for ACE detection statistics for dataset A embedded with $s_2$ varying $\gamma$.
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

or any other user defined shape) impacts detection performance by changing the concentration pathlength of the embedded plume. Figure 5.21 shows the detection statistics of a $\gamma = 30$ ppm-m plume embedded into dataset A, using the three masks shown in Figure 4.5 and 4.7.

5.3.5 Temperature and Plume Background

The effects of plume temperature and background are perhaps the most complicated of the variable parameters to study as they are intrinsically coupled. The original on-plume radiance model (2.4) indicates that the at-sensor radiance includes both background- and plume-generated terms, and in turn from (2.6), $T_b$ and $T_p$. Furthermore, as mentioned in the previous section, CWA plumes tend to come to a thermal equilibrium with the surrounding atmosphere, and thus, $T_a$ also plays a role in the interaction.

We begin by simulating this transition towards thermal equilibrium ($T_p - T_a = 0$) where $T_a$ is estimated over the region into which the plume is to be embedded, as described in Section 3.2.1. Figure 5.25 assesses detection performance as a function of plume temperature relative to atmospheric temperature using the AUROC and SCR. The plume was embedded at three locations - with the ground, mountains and sky as background - as shown in Figure 5.24. All three cases display a similar trend: detection performance reaches a minimum value at a certain $T_p - T_a$ differential, and increases rapidly as $T_p$ shifts away from this point; however, the location of this point varies depending on the background. This inconsistency is a result of the fact that the differential radiance signal is proportional to the difference between the plume and background temperature, as described by (2.15). Figure 5.26 shows the mean radiation produced by each background, as defined by the spatial extent of the embedded plume. The clear separation between the three classes indicates a difference in background temperature.

Further complicating the temperature-background relationship is the fact that neither $T_b$ nor $T_a$ (and in turn $T_p$) need be constant, but rather tend to follow a gradient, and thus, a plume which subtends a large area will often produce inconsistent detection statistics, as seen in Figure 5.12. Note that the inability of our algorithm to embed plumes with varying $T_p$ values exaggerates this effect, as we lose the natural smooth variations in temperature.
Figure 5.21: Detections statistics of ACE detection statistics for dataset A embedded with $s_2$ at $\gamma = 30$ ppm-m with constant, Gaussian and realistic masks.
CHAPTER 5. PERFORMANCE EVALUATION OF DETECTION ALGORITHMS

Figure 5.22: ROC analysis of ACE detection statistics for dataset A embedded with $s_2$ at $\gamma = 30$ ppm-m with constant, Gaussian and realistic masks.

Figure 5.23: $P_y(\eta)$ analysis of ACE detection statistics for dataset A embedded with $s_2$ at $\gamma = 30$ ppm-m with constant, Gaussian and realistic masks.
that real CWA plumes exhibit; however, atmospheric and background temperatures will generally vary independently, so as long as the synthetic plume is not too large, the largest source of variation in detection performance will be changes in background, as shown in Figure 5.27.

Figure 5.24: Constant plume mask locations for background study.

In this chapter we studied how the performance of CWA plume detection algorithms is impacted by variation in various physical plume parameters, and in turn, validated that the plume embedding procedure functions as predicted by the at-sensor radiance signal model of Section 2.1.3. Indeed, any one of the trade studies presented could be expanded into a more thorough analysis, and the modular nature of the performance evaluation tool would easily permit such an expansion; however, one of the primary aims of this thesis was to motivate these simply to motivate and identify possible areas for further study. It is not only important that we can detect potential instances of CWA plumes, but also quantify their strength; in the next chapter we present results for the basic quantification algorithms developed in Section 3.2.
Figure 5.25: AUROC and SCR analysis of ACE detection statistics for dataset A embedded with $s_2$ at a $\gamma = 30$ ppm-m varying $\Delta T_p$.

Figure 5.26: Mean spectra for each background class.
Figure 5.27: ROC analysis of ACE detection statistics for dataset A embedded with $s_2$ at $\gamma = 30$ ppm-m with varying background.
Chapter 6

Performance Evaluation of Quantification Algorithms

The ultimate goal of CWA plume detection research is not only to detect instances of chemical plumes, but also quantify the strength of a detected plume in terms of its concentration pathlength. This task is a difficult one, and as seen in Section 3.2, it requires that we solve an underdetermined system of equations; in order to do so we must make a few assumptions and estimate several parameters. In the following chapter we detail our results, including the intermediary estimates needed to extract concentration pathlength estimates from our data.

6.1 Temperature

In this section we summarize the results of our temperature estimation algorithm for both the atmospheric and background cases.

6.1.1 Atmospheric Temperature Estimation Results

We begin the plume quantification process by estimating the atmospheric temperature as discussed in Section 3.2.1. We used Dataset C to test the quantifications algorithms because the atmospheric temperature at the location of the sensor was known to have a value of 306.0 K. The results of the process are displayed in Figure 6.1; with the outlier pixels excluded, \( \hat{T}_a \)
ranges from 297.8 to 311.4 K. Note the clear difference in estimated temperature between the ground and sky pixels. This separation is indicative of the fact that our assumption that the at-sensor radiance at \( \nu = 1269 \text{ cm}^{-1} \) is just that, an assumption. The actual radiance data band used is centered at \( \nu = 1266.9 \text{ cm}^{-1} \) and has a FWHM of 8 cm\(^{-1}\); from Figure 2.10, we can see that the atmospheric transmission function is not uniformly equal to 0 in this region, and thus, a minimal amount of background radiation is included in the estimate, which causes the variations in \( \hat{T}_a \) seen in Figure 6.1.

The area directly above the horizon line yields a mean estimated temperature of \( \hat{T}_a = 299.6 \text{ K} \) (2.16 \% error) while the area of the datacube with a ground background produces, \( \hat{T}_a = 306.3 \text{ K} \) (0.09 \% error). The wide range in variation in \( \hat{T}_a \) of the ground pixels is largely a result of the variation in background spectra of these pixels when compared to the sky pixels. In the next section we will see that the brightness temperature of the ground is much closer to measured atmospheric temperature than that of the sky; the cooler temperature of the sky causes the \( \hat{T}_a \) to be a few degrees colder in this region of the cube. We conclude that our atmospheric temperature algorithm is reasonably accurate, and the accuracy increases for cases where the atmosphere-background temperature remains small.

Figure 6.1: \( \hat{T}_a \) for Dataset C.
6.1.2 Background Temperature Estimation Results

Figure 6.2 shows the estimated background temperature as calculated from (3.24) and (3.26). The temperature of the ground pixels span from 295.9 to 311.6 K with a mean value of 303.6 K. Unfortunately, we have no ground truth temperature data with which to validate our estimated; however, a nearly 16 °K variation in ground temperature is not likely over such a small area. This fluctuation is mostly likely a result of both the variation in the estimated atmospheric temperature, as well as the individual pixel spectra. Perhaps our estimates could be improved by averaging the spectral radiance values from a few different spectra.

The brightness temperature of the sky portion of the data cube varies over a much larger range, from 119.7 to 274.2 K; however, the estimates vary smoothly as a function of altitude as expected. This behavior explains why detection performance is closely correlated with altitude for a plume embedded at a constant temperature, as shown in Figure (5.12).

Figure 6.2: $\hat{T}_b$ for Dataset C.
6.2 Concentration Pathlength

The final step of the quantification algorithm is estimation of the concentration pathlength as described in Section 3.2.2. From (3.28) and (3.29), we see that $\hat{\gamma}$ is dependent on the detection statistics (through $\hat{SCR}$) as well as $\hat{T}_a$ and $\hat{T}_b$. From Figures 6.1 and 6.2, we see that our $\hat{T}_a$ and $\hat{T}_b$ estimates are much less reliable for the ground pixels than for the sky pixels, thus, we validate our $\gamma$ estimation algorithm using plumes in both locations.

Figure 6.3 shows the $\hat{SCR}$ for a 60 ppm-m plume embedded into Dataset C over the ground while Figure 6.4 is a map of the resulting estimated concentration pathlength. The $\hat{\gamma}$ values of the on-plume pixels tend to be off by roughly one order of magnitude with mean and median values of 779.6 and 803.0 ppm-m, respectively. From Figure 6.5 we see that the estimated concentration pathlength values fall between 0 and 1040 ppm-m with a standard deviation of 128.6 ppm-m. Table 6.2 summarizes the results of the estimated concentration pathlength, as well as the theoretical and estimated SCR, where the theoretical SCR values were calculated using (3.20) with $\Delta T_p = \hat{T}_a - \hat{T}_b$. The large discrepancy between the theoretical and estimated SCR values is to blame for high degree of inaccuracy of the $\hat{\gamma}$ values.

Figures 6.6 and 6.7 show the $\hat{SCR}$ and $\hat{\gamma}$ for the ground case, respectively. This case produces mean and median $\hat{\gamma}$ values off by over two orders of magnitude, 16144.2 and 6385.4 ppm-m, respectively. From Figures 6.7 and 6.8 we can see that these values must be taken with a grain of salt as the standard deviation of $\hat{\gamma}$ is 411793.7 is over an order of magnitude greater than both the mean and median. In fact, the estimated $\hat{\gamma}$ spans from $-9.03 \times 10^7$ to $1.53 \times 10^7$, with 5.9% of the estimations falling below -1000 ppm-m and 2.2% above $10^5$. This extremely large range is primarily a result of the inaccuracies in $\hat{SCR}$, $\hat{T}_a$ and $\hat{T}_b$ for the ground pixels.

Figures 6.9 and 6.10 show the relationship between the actual and estimated values of concentration pathlength for the sky and ground cases, respectively. Despite the inaccuracies in the estimation of $\gamma$, both cases exhibit the expected relationship, namely, for low concentration pathlength values, $\hat{\gamma}$ increases in a roughly linear manner as the embedded plume $\gamma$ increases. This relationship breaks down as the plume begins to reach “optical thickness”, at which point the SCR measurement ceases to accurately represent the plume.
CHAPTER 6. PERFORMANCE EVALUATION OF QUANTIFICATION ALGORITHMS

Figure 6.3: $\hat{SCR}$ sky Dataset C.

Figure 6.4: $\hat{\gamma}$ sky Dataset C.
Figure 6.5: histogram of $\hat{\gamma}$ sky Dataset C.

Figure 6.6: $\hat{SCR}$ ground Dataset C.
CHAPTER 6. PERFORMANCE EVALUATION OF QUANTIFICATION ALGORITHMS

Figure 6.7: $\hat{\gamma}$ ground Dataset C.

Figure 6.8: histogram of $\hat{\gamma}$ ground Dataset C.
Table 6.1: Theoretical, estimated SCR and estimated $\gamma$.

<table>
<thead>
<tr>
<th>Dataset:</th>
<th>Sky Pixels</th>
<th>Ground Pixels</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean ther. SCR:</td>
<td>707033.4</td>
<td>7314.2</td>
</tr>
<tr>
<td>Median ther. SCR:</td>
<td>684669.9</td>
<td>1182.2</td>
</tr>
<tr>
<td>Std. dev. ther. SCR:</td>
<td>313852.3</td>
<td>78483.5</td>
</tr>
<tr>
<td>Mean est. SCR:</td>
<td>154.7</td>
<td>136.9</td>
</tr>
<tr>
<td>Median est. SCR:</td>
<td>164.9</td>
<td>95.6</td>
</tr>
<tr>
<td>Std. dev. est. SCR:</td>
<td>61.1</td>
<td>144.7</td>
</tr>
<tr>
<td>Mean est. $\gamma$:</td>
<td>779.6</td>
<td>16144.2</td>
</tr>
<tr>
<td>Median est. $\gamma$:</td>
<td>803.0</td>
<td>6385.4</td>
</tr>
<tr>
<td>Std. dev. est. $\gamma$:</td>
<td>128.6</td>
<td>411793.7</td>
</tr>
</tbody>
</table>

concentration (see Section 5.3.4). Again, note that the mean and median values for the ground pixel case are not necessarily accurate representations of the actual “average” of data due to the large number of outliers; however, the relative strength of $\hat{\gamma}$ tends to maintain a distribution similar to Figure 6.7.

Although the preceding results lack the desired precision and accuracy to reliably determine temperature and concentration pathlength information from the semi-synthetic data, they do provide us with a basis that can be used to further develop these algorithms in the future.
CHAPTER 6. PERFORMANCE EVALUATION OF QUANTIFICATION ALGORITHMS

Figure 6.9: \( \hat{\gamma} \) vs. \( \gamma \) for Dataset C.

Figure 6.10: \( \hat{\gamma} \) vs. \( \gamma \) for Dataset C.
Chapter 7

Conclusions

The main strength of our performance evaluation tool is perhaps its highly modular nature; the user can add his or her own pre-processing, detection or quantification algorithm to the detection pipeline, and easily evaluate the results. Our research focused on the evaluation of a few simple detection and quantification routines in order to: a) verify that the embedding routine functions as predicted by the at-sensor radiance signal model, b) study the effects of various plume parameters, and c) motivate further study in appropriate areas. We will summarize possible future work motivated by this thesis.

7.1 Detection

The performance evaluation of the detection algorithms used throughout this thesis provides insight on how these algorithms responded to CWA plumes under ideal conditions, and more importantly, the limits of these detection algorithms, namely, when can we expect this breakdown to occur, and what sort of response should we expect to see in these situations. This knowledge enables the designer of HSI algorithms for CWA detection to better understand how his or her algorithm responds to plumes with various physical characteristics, and in turn, modify their design to produce more meaningful results.

Although we only focused on a few basic detection algorithms, we were able to determine that of the three studied, the ACE detector regularly out performed the MF and AMF both in terms of strength and consistency of detections statistics. The ACE detector
outperformed the others due to its angular nature, which tends to make it more robust.

Of all the characteristics studied, the relationship between the dataset and the CWA seemed to be the most important. In many ways this relationship is an intuitive one. For example, all the detectors used throughout this thesis take the mean and covariance matrix of the background into account, thus, the estimation of this statistic is critical. A dataset for which these estimated statistics poorly represent the actual distribution will tend to yield poor detection results. Anomaly pixels, those which are broken, or contain materials which drastically vary from the “average” background, are detrimental to detector performance, so it is critical that we can identify these pixels, and any pixels which contain plume before generating background statistics. The characteristics of the CWA spectra to be detected is also of critical performance. If the features of the spectra are weak, or located in areas where the data are noisy, detection performance will suffer.

In general, we saw that the physical plume parameters studied effected detection performance as expected. As the Fill Factor of a plume in a dataset increased, detection performance deteriorated because less data was available to form an accurate representation of the background statistics. If reliable plume-free background estimation is not employed, this effect will be magnified as an increasingly large portion of the background will include the signature which is to be detected.

When we consider optically thin plumes, detection performance increases as we increase the concentration pathlength. As the plume begins to reach optical thickness and eventually opacity, detection performance plateaus, and eventually declines because the background radiance becomes eclipsed by the plume, causing our at-sensor radiative transfer model to break down. Again, this effect is further magnified without accurate plume-free background estimation.

Finally, the variation of plume temperature also produces the expected trends when considering detection statistics, although, this parameter is difficult to effectively analyze because the radiance model predicts that the temperature differential between the plume and the background determines how well the detector will perform. As the temperature of the plume-background temperature differential increased, detector performance decreased. This portion of the performance evaluation too could be improved by allowing for the embedding of more natural varying temperature plumes.
7.2 Quantification

Although our parameter estimation algorithms showed some promise, they did not produce accurate results. In general, our estimation routines fail due to the need to make overly simple assumptions because we are trying to solve an underdetermined system of equations.

The temperature estimation algorithms (both atmospheric and background) worked best for simple homogeneous backgrounds such as the sky, however displayed highly erratic results for more complex backgrounds like the ground. These inaccuracies are a result of the fact that the atmospheric estimation assumes that the effect of background radiance is negligible, a claim that would perhaps be valid if data from further into the $H_2O$ absorption band were available. The background temperature estimation is formed using results from the atmospheric temperature, so the inaccuracies of the first step are amplified in the second. Perhaps these estimates could be improved if multiple spectral radiance values were used to generate the estimates?

The concentration pathlength estimates were much less accurate and precise for a variety of reasons. First and foremost, the estimate is based on the atmospheric and background temperature estimates, which have already been determined to be inaccurate. Secondly, due to the underdetermined nature of the problem, the plume was assumed to be at thermal equilibrium, and although real plumes tend towards this value, it is not always an accurate assumption to make. Finally, our estimate is based on the SCR. This method is problematic because the estimated SCR values have been shown to be erratic, and it assumes that the theoretical and estimated SCR values agree, when in fact, the two tend to be off by at least an order of magnitude. All in all, despite picking up on the general trends of CWA data, our estimation algorithms require further development if they are to yield reliable results.

7.3 Future Research

The modular nature of our performance evaluation tool allows for the future expansion of our work in various areas. As previously mentioned, any one of the trade studies of Section 5.3 could easily be expanded upon. Ultimately, detection performance is directly correlated with the accuracy of the background statistics used to generate the various filters,
thus, future research will focus on plume-free background statistic estimation techniques such as: principal component analysis, independent component analysis, dominant mode rejection filtering, and the use of clustering techniques to generate weighted background statistics. The temperature and concentration pathlength estimation techniques of Section 3.2 will also be revisited and improved in future work. Advancements in temperature estimation algorithms will lead to improvements in the embedding routine, as it depends on these values to embed CWA plumes at thermal equilibrium. Finally, the embedding routine will also be modified to allow the user to embed a plume at varying temperature throughout a single dataset, using either temperature estimation results, or a user defined temperature mask.

We have demonstrated the functionality and utility of our performance evaluation tool, as well as surveyed the impact of various physical plume parameters on the resultant detection statistics. As hyperspectral imaging is such a new and ever expanding field of study, there is no doubt that new and improved CWA detection and quantification algorithms will continue to be developed in the future. The modular nature of our performance evaluation tool will allow for the detailed study and testing of these algorithms as they emerge.
Bibliography


