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# Hyperspectral unmixing: a theoretical aspect and applications to CRISM data processing 

Yuki Itoh<br>University of Massachusetts Amherst

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# HYPERSPECTRAL UNMIXING: A THEORETICAL ASPECT AND APPLICATIONS TO CRISM DATA PROCESSING 

A Dissertation Presented
by

## YUKI ITOH

Submitted to the Graduate School of the University of Massachusetts Amherst in partial fulfillment of the requirements for the degree of

## DOCTOR OF PHILOSOPHY

September 2022

Department of Electrical and Computer Engineering
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# ABSTRACT <br> HYPERSPECTRAL UNMIXING: A THEORETICAL ASPECT AND APPLICATIONS TO CRISM DATA PROCESSING 

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Hyperspectral imaging has been deployed in earth and planetary remote sensing, and has contributed the development of new methods for monitoring the earth environment and new discoveries in planetary science. It has given scientists and engineers a new way to observe the surface of earth and planetary bodies by measuring the spectroscopic spectrum at a pixel scale.

Hyperspectal images require complex processing before practical use. One of the important goals of hyperspectral imaging is to obtain the images of reflectance spectrum. A raw image obtained by hyperspectral remote sensing usually undergoes conversion to a physical quantity representing the intensity of light energy, called radiance. In order to obtain the reflectance spectrum of surface, the contribution of atmosphere needs to be addressed and then divided by a spectrum of "white reference." Furthermore, the obtained reflectance spectra of image pixels are likely to be the mixtures of multiple species due to limited spatial resolution from orbits around planets.

Hyperspectral unmixing is an attempt to unmix those pixels - to identify substantial components and estimate their fractional abundances. Hyperspectral unmixing has been
widely explored in the literature, but there are still many aspects yet to be studied. The majority of research focuses on the development of methods to retrieve correct substantial components and accurate fractional abundances. Their theoretical aspects are rarely investigated. Chapter 2 will pursue a theoretical aspect of sparse unmixing, one of the hyperspectral unmixing problems and derive its theoretical conditions that guarantee the correct identification of substantial components.

Hyperspectral unmixing can also be used for other stages of hyperspectral data processing. Chapter 3 explores the application of hyperspectral unmixing to the processing of hyperspectral image acquired by the Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) onboard the Mars Reconnaissance Orbiter (MRO). In particular, new atmospheric correction and de-noising methods for the CRISM data that use a hyperspectral unmixing to model surface spectra, are introduced. The new methods remove most of the problematic systematic artifacts present in CRISM images and significantly improve signal quality.

Chapter 4 investigates how hyperspectral images acquired from orbits can be combined with ground exploration. In the recent rush of the launch of many Martian ground rover missions, it is important to effectively integrate knowledge obtained by hyperspectral remote sensing from orbits into ground exploration for facilitating Martian exploration. In specific, this dissertation solves the problem of matching hyperspectral image pixels obtained by the CRISM with ground mega-pixel images acquired by the Mast Camera (Mastcam) installed on the Curiosity rover on Mars. A new systematic methodology to map the CRISM and Mastcam images onto high resolution surface topography is developed.

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## CHAPTER1

## INTRODUCTION

Hyperspectral imaging splits incoming light of each pixel into continuous wavelength components, allowing scientists and engineers to observe the electromagnetic spectrum that is reflected/scattered at, emitted from, or passed through targets. The acquired spectrum provides the abundant information of the targets, and it has been leveraged in remote sensing from airplanes and satellites for detecting and mapping surface species of the earth and planetary bodies.

Hyperspectral imagers collect and focus the incoming electromagnetic wave, and then disperse it into hundreds of narrowly consecutive wavelength components by a spectrograph. The acquired image is considered as an image cube where the first two dimensions represent the horizontal and vertical spatial coordinates, and the third represents the wavelength of the spectrum of each image pixel. Fig. 1.1 shows an example of a hyperspectral image cube. The depth direction represents the wavelength direction. Pixels are characterized by their spectra, which are interpreted as feature vectors and utilized by machine learning and applied mathematical methods to further analyze.

One of the important missions in hyperspectral remote sensing is the acquisition of the reflectance image cube of earth or planetary surface. Reflectance is the ratio of the intensity of light reflected on the surface with respect to that of its incident light energy. Different species show distinct reflectance spectra characterized by their shape and absorption features. In addition, the reflectance spectrum is ideally a property invariant to sensors and environmental conditions; therefore, it can be directly used for


Figure 1.1. Hyperspectral image cube.
the identification of species by comparing it with the reflectance spectrum of known species either measured in the laboratory or in the field.

The retrieval of the reflectance spectrum in the laboratory setting may be simple. Hyperspectral imagers sense and record the intensity of light energy in a digitized integer format. The retrieval of the reflectance spectrum in the laboratory can be performed by the division of the raw integer values with the measurement of a "white reference," a material with a known refelectance spectrum that has mostly flat features over a targeted wavelength region. On the other hand, the retrieval of the surface reflectance spectrum in remote sensing from airplanes and spacecrafts involves complex processing steps. The raw integer values are first converted to a physical quantity representing the intensity of light energy per wavelength, called radiance. This procedure is called calibration. Then, surface reflectance is retrieved by addressing interactions through atmosphere and on the surface. These processing steps are necessary since it is challenging to obtain a white reference measurement at the scale of remotely sensed image pixels and the atmospheric interaction is unavoidable.

Furthermore, the obtained reflectance spectra of image pixels are likely to be the mixtures of multiple species due to the limited spatial resolution of orbital measure-
ments. Hyperspectral unmixing is an attempt to unmix these mixed pixels - to retrieve substantial components (also called endmembers) and their fractional abundances. In general, hyperspectral unmixing models surface mixing with a mathematical model that integrates endmember spectra and their fractional abundances, and performs model inversion. The simplest mixing model is the linear mixture model (LMM) that models the observed spectrum with a non-negative linear combination of endmember spectra weighted by their fractional abundances.

Hyperspectral unmixing has been widely explored in the literature to make the most of acquired images [1]. The majority of research in the field of hyperspectral unmixing focuses on the development of methods to retrieve correct endmembers and their accurate fractional abundances. Their theoretical aspects are rarely investigated. Chapter 2 pursues a theoretical aspect of sparse unmixing. Sparse unmixing [2] is a semi-supervised unmixing method that identifies endmembers present in the observation from the large collection of spectra in the spectral database. Inspired by Tropp's approach [3], we derive the theoretical conditions of sparse unmixing formulated as non-negative lasso (Nlasso) that guarantee the correct identification of substantial components. The chapter further introduces approximately perfect recovery condition (APMRC) that practically performs as good as a necessary and sufficient condition of Nlasso. A rigorous mathematical proof of the necessity and sufficiency of the APMRC is also provided.

Hyperspectral unmixing can also be used for other stages of hyperspectral data processing. Chapter 3 explores the application of hyperspectral unmixing to the processing of hyperspectral image acquired by Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) [4] onboard the Mars Reconnaissance Orbiter (MRO). The traditional atmospheric correction method "volcano scan correction," successfully removes a large part of the contribution of atmospheric gaseous absorption on the CRISM spectra, but is known to cause several artifacts large enough to mask underlying surface spectral features $[5,6]$. The chapter first introduces simultaneous atmospheric correction and
de-noising for CRISM (SABCOND). SABCOND models light transmission through the Martian atmosphere by the Beer-Lambert's law and surface interaction using an unmixing model. An optimal atmospheric transmission spectrum is estimated by the inversion of the model via a minimization problem that also takes noise into account. SABCOND turns out to remove most of the problematic systematic artifacts present in the CRISM images that would have been caused by the volcano scan correction and significantly improve signal quality. The chapter also provides the algorithmic details of SABCOND.

The chapter further introduces the two-step SABCOND, aiming for more accurate atmospheric correction. SABCOND sometimes suffers from artifacts due to its poor initialization of the transmission spectrum. The two-step SABCOND addresses this issue by using a more optimized initial transmission spectrum obtained by performing the SABCOND on a spectrally unremarkable image that has atmospheric transmission similar to that of the image of interest. Although the spectrally unremarkable image needs to be manually selected, this methodology leads to more accurate atmospheric correction with higher fidelity.

Chapter 4 then investigates how hyperspectral images acquired from orbits can be effectively and precisely combined with ground observation. In the recent rush of the launch of many Martian ground rover missions, it is important to effectively integrate knowledge obtained by hyperspectral remote sensing from orbits into ground exploration for facilitating Martian ground rover exploration. In specific, this dissertation solves the problem of matching hyperspectral image pixels obtained by the CRISM with ground mega-pixel images acquired by the Mast Camera (Mastcam) installed on the Curiosity rover on Mars. In order to accurately map the image pixels of CRISM observation onto Mastcam images, both images are projected onto surface topography based on a high resolution digital elevation model. It is necessary to recognize visible and invisible surface for the Mastcam image projection onto the surface topography as many occlusions are observed from the Mastcam viewpoint on the ground. A new rigid and fast algorithms
to solve this visiblity problem are presented. In order to accurately map CRISM image pixels, each CRISM pixel is directly mapped onto the high resolution surface topography using the MRO trajectory and CRISM orientation data. We propose an algorithm to precisely project each of the pixel footprints onto the surface. Finally, these two projections are combined, and the map projection of the CRISM image pixels onto the Mastcam images is implemented.

## CHAPTER 2

## A THEORETICAL ASPECT OF HYPERSPECTRAL UNMIXING

This chapter will pursue the theoretical aspect of sparse unmixing [2] - the formulation of hyperspectral unmixing as non-negative sparse modeling. ${ }^{1}$

### 2.1 Introduction

Sparse modeling has achieved significant recognition in a variety of research areas such as signal processing, machine learning, computer vision, and pattern recognition. Sparse models refer to the formulation of a signal of interest (or an approximation of it) as the linear combination of a small number of elements (known as atoms) drawn from a so-called sparsity dictionary (or dictionary for short). The sparse recovery problem refers to the identification of the relevant dictionary atoms for a particular signal of interest. Sparse modeling and recovery has a rich history in signal processing, and has received significant attention recently due to the emergence of compressed sensing $[9,10]$, a framework for compressed signal acquisition that leverages sparse modeling.

We can further restrict the coefficients of the atoms to be non-negative. In general, non-negativity is advantageous as it makes the model parameters more interpretable. For instance, Lee and Seung present non-negative matrix factorization [11], which can learn a part-based representation of faces or documents. Just adding non-negativity constraints

[^1]on a linear model to decompose spectral data gives the model coefficients the meaning of fractional abundances [12]. Non-negative constraints have been applied to independent component analysis in face recognition tasks [13].

Many approaches have combined non-negativity and sparse modeling. By adding nonnegative constraints, several researchers $[14,15]$ refined the performance of applying sparse modeling on a face recognition task obtained by Wright et al. [16]. Non-negative least squares (NNLS) has been traditionally used, sometimes accompanied with abundance sum-to-one constraints, to extract the spectral components from hyperspectral pixels (e.g., [12]), a process called spectral unmixing. Recently, NNLS has been combined with sparsity with improvements in the unmixing performance [2,17]. Other examples of combining non-negativity and sparse modeling can be found in astronomical imaging [18], proteomics [19], and economics [20]. It has been noted that sparse solutions can be obtained by NNLS with subsequent thresholding [21-23].

Several contributions on theoretical analysis of non-negative sparse modeling approaches exist in the literature. Many of them [24-31] are devoted to modeling in the absence of noise, focusing on questions such as the performance of convex optimizationbased approaches for sparse recovery and the uniqueness of the sparse solution. Other works studied the theoretical performance of non-negative sparse modeling in the presence of noise [19-21]; however, those analyses focus on the specific case of either Gaussian or sub Gaussian noise.

In contrast to the statistical noise modeling used in previous analyses [19-21], this chapter considers the performance of non-negative sparse modeling under a more general scenario, where the observed signals have an unknown arbitrary distortion. Although analysis proposed here can be applied to the additive random noise to obtain existing results, it is also immediately applicable to many other types of distortion, e.g., distortion present due to nonlinear mixing of the individual components. In the case of spectral unmixing, nonlinear mixing may come from nonlinear mixing of atoms [32,33] or spectral
mismatches between the spectra of the minerals in the library and those involved in the observation [34].

Under this general scenario, I will investigate the conditions for successful reconstruction - or regression - of a signal using non-negative lasso by expanding previous analyses on the general lasso. Some of these studies consider dictionaries drawn according to a random distribution [35]. Others assume an arbitrary dictionary and pose conditions for successful regression that require a combinatorial amount of computation: examples include the spark, restricted isometry property, the restricted eigenvalue property, and the irrepresentable condition [10,36-39]. It is possible to relax the computational complexity of the verification process, using tools such as coherence [3,36, 40-42]; however, all the aforementioned frameworks consider all possible combinations of atoms simultaneously, and therefore are found to often give very conservative assessments of regression performance.

Derivation follows the line of Tropp's work [3]. In contrast to the references above, Tropp has performed an analysis based on the so-called exact recovery condition (ERC), which provides conditions on successful reconstruction for all combinations of a fixed subset of atoms. The ERC can be easily computed and is compatible with well-known optimization-based and iterative greedy algorithms for sparse signal recovery and regression, and so it appears suitable for the analysis of non-negative versions. Furthermore, because the ERC is focused on sparse signals featuring a specific support (i.e., a set of indices for the signal's nonzero entries), its guarantees are less pessimistic than those provided by alternative approaches, which consider success for all sparse signals simultaneously, regardless of their support. Nonetheless, one could conceivably argue that restricting the set of signals of interest to a fixed support with non-negative entries may provide guarantees that are even closer to the actual performance of non-negative sparse recovery. While the proposed conditions require a specific set of atoms as an input, they are motivated by applications, such as hyperspectral unmixing, in which it is more useful
to determine whether a specific set of atoms can be identified via sparsity-based methods, rather than provide guarantees on the recovery for all subsets, since many combinations of atoms might never materialize.

This chapter is organized as follows. Section 2.2 describes background of this research including mathematical notation throughout this chapter. Section 2.4 clarifies the contribution of this chapter and Section 2.4 describes my contribution. Section 2.5 illustrates an application of the MRCs to a hyperspectral unmixing task and Section 2.6 concludes this paper.

### 2.2 Background

### 2.2.1 Mathematical notation

I specify the mathematical notation used in this chapter. The support of $\boldsymbol{x} \in \mathbb{R}^{N}$ is the set of the indices associated with the non-zero elements of $\boldsymbol{x}$, denoted by $\operatorname{supp}(\boldsymbol{x})$. $\mathcal{R}(\mathbf{X})$ is the range of the matrix $\mathbf{X} . \mathbf{M}^{\top}, \mathbf{M}^{-1}$, and $\mathbf{M}^{\dagger}$ denote the transpose, inverse, and pseudoinverse of the matrix $\mathbf{M}$, respectively. $\|\mathbf{M}\|_{\infty, \infty}$ is an $(\infty, \infty)$ matrix operator norm and gives the maximum $\ell_{1}$-norm of the row vectors of $\mathbf{M}$.

I denote a subset of the column indices of $\mathbf{A} \in \mathbb{R}^{L \times N}$ by $\Lambda \subseteq\{1,2, \ldots, N\}$, and the subdictionary that is composed of atoms associated with indices in $\Lambda$ by $\mathbf{A}_{\Lambda}$. Note that all of the theorems are discussed on a subset $\Lambda$ of the column indices as Tropp [3] did. For any coefficient vector $\boldsymbol{x} \in \mathbb{R}^{N}$, I denote the vector composed of the elements of $\boldsymbol{x}$ indexed by $\Lambda$ by $\boldsymbol{x}_{\Lambda}$. I also denote the whole column index set $\Omega=\{1,2, \ldots, N\}$, and the complement of $\Lambda$ by $\Lambda^{\mathrm{c}}=\Omega \backslash \Lambda$ where $\backslash$ is the difference of two sets.

### 2.2.2 Lasso and its model recovery condition

The lasso is an unconstrained optimization algorithm that regularizes a least-square fit penalty with a sparsity-inducing cost on the coefficient vector. Lasso assumes the
following linear model:

$$
\begin{equation*}
\boldsymbol{y}=\mathbf{A} \boldsymbol{x}+\boldsymbol{e} \tag{2.1}
\end{equation*}
$$

where $\boldsymbol{y} \in \mathbb{R}^{L}$ is an observation vector, $\mathbf{A} \in \mathbb{R}^{L \times N}$ is a dictionary matrix where the components $\boldsymbol{a}_{j}(j=1, \ldots, N)$, called atoms, are stored in its columns, $\boldsymbol{x} \in \mathbb{R}^{N}$ is a coefficient vector, $\boldsymbol{e} \in \mathbb{R}^{L}$ is an error vector, and $\succeq$ (and its variants) denotes elementwise inequality. Lasso searches for the atoms that best describe the input signal as a linear combination in a least square sense while reducing the number of contributing atoms. The lasso is written as:

$$
\begin{equation*}
\underset{\boldsymbol{x}}{\operatorname{minimize}} \frac{1}{2}\|\boldsymbol{y}-\mathbf{A} \boldsymbol{x}\|_{2}^{2}+\gamma\|\boldsymbol{x}\|_{1} \tag{2.2}
\end{equation*}
$$

where $\gamma$ is a positive constant that controls the degree of sparsity. The weight $\gamma$ could be adaptively tuned for each element, e.g., as done in adaptive lasso [43]. An analysis of the lasso was provided by Tropp [3] and hinges on the exact recovery coefficient (ERC), defined as

$$
\begin{equation*}
\operatorname{ERC}(\Lambda):=1-\max _{n \notin \Lambda}\left\|\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{a}_{n}\right\|_{1} \tag{2.3}
\end{equation*}
$$

where $\Lambda \subseteq\{1, \ldots, N\}$ are indices for a subset of the columns of $\mathbf{A}$ and $\boldsymbol{a}_{n}$ denotes the $n$th column of $\mathbf{A}$. Note that it is implicitly assumed that the columns of $\mathbf{A}_{\Lambda}$ are linearly independent so that the pseudoinverse exists. Broadly speaking, the ERC evaluates how far the atoms outside of $\Lambda$ are from the subspace determined by the atoms in $\Lambda$. When the columns of $\mathbf{A}$ have unit $\ell_{2}$-norm, the condition considers the minimum angle between atoms outside of $\Lambda$ and the subspace spanned by $\mathbf{A}_{\Lambda}$. Intuitively, a larger ERC is preferred because it reduces correlation between $\mathbf{A}_{\Lambda}$ and atoms outside the set. The following theorem provides performance guarantees for the lasso that are specific to a particular support $\Lambda$.

Theorem 2.1 [3, Theorem 8] Let $\Lambda$ index a linearly independent collection of columns of A for which $\operatorname{ERC}(\Lambda) \geq 0$. Suppose that $\boldsymbol{y}$ is an input signal whose $\ell_{2}$ best approximation
$\boldsymbol{y}_{\Lambda}=\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}$ over $\mathbf{A}_{\Lambda}$ satisfies the correlation condition

$$
\begin{equation*}
\left\|\mathbf{A}^{\top}\left(\boldsymbol{y}-\boldsymbol{y}_{\Lambda}\right)\right\|_{\infty} \leq \gamma \operatorname{ERC}(\Lambda) \tag{2.4}
\end{equation*}
$$

Let $\boldsymbol{x}^{\star}$ be the solution of the lasso (2.2) with parameter $\gamma$. We may conclude the following.

- $\operatorname{supp}\left(\boldsymbol{x}^{\star}\right)$, is contained in $\Lambda$;
- the distance between $\boldsymbol{x}^{\star}$ and the optimal coefficient vector $\boldsymbol{c}_{\Lambda}=\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}$ (appropriately zero-padded) satisfies

$$
\begin{equation*}
\left\|\boldsymbol{x}_{\Lambda}^{\star}-\boldsymbol{c}_{\Lambda}\right\|_{\infty} \leq \gamma\left\|\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1}\right\|_{\infty, \infty} ; \tag{2.5}
\end{equation*}
$$

- and $\operatorname{supp}\left(\boldsymbol{x}^{\star}\right)$ contains the indices $\lambda \in \Lambda$ for which

$$
\begin{equation*}
\left|\boldsymbol{c}_{\Lambda}(\lambda)\right|>\gamma\left\|\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1}\right\|_{\infty, \infty} \tag{2.6}
\end{equation*}
$$

In words, the theorem states that if the approximation error of the input over the group $\Lambda$ of columns of $\mathbf{A}$ is sufficiently uncorrelated with all other columns of $\mathbf{A}$, then the solution of the lasso does not pick any columns outside $\Lambda$, while picking columns corresponding to all sufficiently large entries of the approximation coefficients for $\boldsymbol{y}$ in $\mathbf{A}_{\Lambda}$.

### 2.2.3 Non-negative lasso

Non-negative lasso assumes a linear model with non-negative coefficients,

$$
\begin{equation*}
\boldsymbol{y}=\mathbf{A} \boldsymbol{x}+e \quad(\boldsymbol{x} \succeq \mathbf{0}) \tag{2.7}
\end{equation*}
$$

Hereinafter, this chapter assumes this model. Based on this model, the problem of inferring atoms contributing the observation is considered. In particular, I focus on the non-negative lasso (NLasso, also known as the non-negative Garrote in the statistics literature [44]):

$$
\begin{array}{ll}
\underset{\boldsymbol{x}}{\operatorname{minimize}} & \frac{1}{2}\|\boldsymbol{y}-\mathbf{A} \boldsymbol{x}\|_{2}^{2}+\gamma\|\boldsymbol{x}\|_{1}  \tag{2.8}\\
\text { subject to } & \boldsymbol{x} \succeq \mathbf{0} .
\end{array}
$$

NLasso has been used as a regression method in hyperspectral unmixing [2, 45], as a variable selection method in economics [20], and as a sparse recovery algorithm for face recognition $[14,15,46]$ and hyperspectral classification [47]. Many methods have been proposed for solving (2.8) such as non-negativity constrained least angle regression and selection [48], full regularization path [49], alternating direction algorithms [45], iterative reweighted shrinkage [2], split Bregman [17], interior point [50], and multiplicative updates [20].

### 2.3 Contribution of this chapter

Model recovery conditions (MRCs) for NLasso (2.8) are derived. The MRCs allow us to predict if the correct atoms are identifiable via NLasso given a signal model for a specific set of atoms with noise or nonlinearity. The MRCs are reminiscent of [23, Theorem 6] due the fact that both results are based on the Karush-Kuhn-Tucker (KKT) conditions for convex optimization solutions. The contribution of this chapter includes

1. the development of MRCs in geometrically interpretable forms that are directly adopted to performance analysis of NLasso on any observation,
2. the development of an approximately perfect MRC which not only guarantees correct signal recovery but also provides a "practical converse" that guarantees the failure of recovery in a practical sense.

The MRCs indicate whether a certain distortion to a linear observation is tolerable by NLasso while succeeding in identifying the components of the dictionary being observed; for the specific case of nonlinear mixing, my result predicts accurately whether NLasso succeeds in component identification under nonlinear distortion, depending on its specific direction and magnitude. The approximately perfect MRC practically meets both necessity and sufficiency. Although the approximately perfect MRC is imperfect in a
rigorous mathematical sense, it is quite powerful and in the experiments provides perfect prediction of the performance of NLasso. I also present some simplified variants of the approximately perfect MRC, which can be considered as customizations of Tropp's conditions [3] and are rigorously proved mathematically. A criterion for perfect identification is that the atoms present in the observation are exactly identified by the algorithm (i.e., no missed atoms and no false alarms), without consideration for accuracy of the coefficient estimate values involved.

This chapter also showcases how the theorem can be used in real applications. More specifically, it can predict whether NLasso will succeed in selecting the correct materials from a hyperspectral unmixing dictionary in the presence of deviations from the noiseless linear model, including measurement nonlinearities, bias, mismatch, and noise. Experiments show that the approximately perfect MRC practically gives perfect assessment of the performance of NLasso.

### 2.4 Main results

### 2.4.1 ERC-based MRC

The first MRC I will introduce is from my earlier work [7]. Using Theorem 2.1, the following theorem to guarantee the performance of NLasso is derived:

Theorem 2.2 (ERC-based MRC) Assume a signal model $\boldsymbol{y}=\mathbf{A} \boldsymbol{x}^{\text {true }}+\boldsymbol{e}$, where the abundance vector $\boldsymbol{x}^{\text {true }} \succeq \mathbf{0}, \Lambda=\operatorname{supp}\left(\boldsymbol{x}^{\text {true }}\right)$ indexes a linearly independent collection of columns of $\mathbf{A}$, and $\boldsymbol{e}$ represents the effect of noise or nonlinear distortion during acquisition. Let $\widehat{\boldsymbol{x}}$ be the solution of NLasso with parameter $\gamma$. If the noise $\boldsymbol{e}$ obeys

$$
\begin{equation*}
\left\|\mathbf{A}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{e}\right\|_{\infty} \leq \gamma \operatorname{ERC}(\Lambda) \tag{2.9}
\end{equation*}
$$

where $\mathbf{P}_{\Lambda}^{\perp}$ is the projector onto the orthogonal complement of $\mathcal{R}\left(\mathbf{A}_{\Lambda}\right)$, and

$$
\begin{equation*}
\boldsymbol{x}_{\Lambda}^{\text {true }} \succ \gamma\left\|\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1}\right\|_{\infty, \infty}-\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{e}, \tag{2.10}
\end{equation*}
$$

then we have that $\operatorname{supp}(\widehat{\boldsymbol{x}})=\Lambda$.

Proof: We begin by considering the solution $\boldsymbol{x}^{\star}$ to the lasso with parameter $\gamma$ for the input $\boldsymbol{y}$. By applying Theorem 2.1 and seeing that

$$
\begin{align*}
\left\|\mathbf{A}^{\top}\left(\boldsymbol{y}-\boldsymbol{y}_{\Lambda}\right)\right\|_{\infty} & =\left\|\mathbf{A}^{\top}\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}\right)\right\|_{\infty} \\
& =\left\|\mathbf{A}^{\top}\left(\mathbf{A} \boldsymbol{x}^{\text {true }}+\boldsymbol{e}-\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger}\left(\mathbf{A} \boldsymbol{x}^{\text {true }}+\boldsymbol{e}\right)\right)\right\|_{\infty} \\
& =\left\|\mathbf{A}^{\top}\left(\mathbf{A}_{\Lambda} \boldsymbol{x}_{\Lambda}^{\text {true }}+\boldsymbol{e}-\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger}\left(\mathbf{A}_{\Lambda} \boldsymbol{x}_{\Lambda}^{\text {true }}+\boldsymbol{e}\right)\right)\right\|_{\infty} \\
& =\left\|\mathbf{A}^{\top}\left(\mathbf{A}_{\Lambda} \boldsymbol{x}_{\Lambda}^{\text {true }}+\boldsymbol{e}-\mathbf{A}_{\Lambda} \boldsymbol{x}_{\Lambda}^{\text {true }}-\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{e}\right)\right\|_{\infty} \\
& =\left\|\mathbf{A}^{\top}\left(\boldsymbol{e}-\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{e}\right)\right\|_{\infty}=\left\|\mathbf{A}^{\top}\left(\mathbf{I}-\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger}\right) \boldsymbol{e}\right\|_{\infty} \\
& =\left\|\mathbf{A}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{e}\right\|_{\infty} . \tag{2.11}
\end{align*}
$$

We have that (2.11) and (2.9) imply (2.4). Thus, we obtain the following results:

- The support of $\boldsymbol{x}^{\star}, \operatorname{supp}\left(\boldsymbol{x}^{\star}\right)$, is contained in $\Lambda$, and
- the distance between $\boldsymbol{x}^{\star}$ and the optimal coefficient vector

$$
\begin{aligned}
\boldsymbol{c}_{\Lambda} & =\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}=\mathbf{A}_{\Lambda}^{\dagger}\left(\mathbf{A} \boldsymbol{x}^{\text {true }}+\boldsymbol{e}\right)=\mathbf{A}_{\Lambda}^{\dagger}\left(\mathbf{A}_{\Lambda} \boldsymbol{x}_{\Lambda}^{\text {true }}+\boldsymbol{e}\right) \\
& =\boldsymbol{x}_{\Lambda}^{\text {true }}+\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{e}
\end{aligned}
$$

(appropriately zero-padded) satisfies

$$
\begin{equation*}
\left\|\boldsymbol{x}^{\star}-\boldsymbol{x}_{\Lambda}^{\text {true }}-\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{e}\right\|_{\infty} \leq \gamma\left\|\left(\mathbf{A}_{\Lambda}^{T} \mathbf{A}_{\Lambda}\right)^{-1}\right\|_{\infty, \infty} \tag{2.12}
\end{equation*}
$$

The result (2.12) implies that for each $n \in \Lambda$ we have

$$
\begin{aligned}
& \mid \boldsymbol{x}^{\star}(n)-\left(\boldsymbol{x}^{\text {true }}(n)+\boldsymbol{w}(n)\right) \mid \leq \gamma\left\|\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1}\right\|_{\infty, \infty}, \\
&-\gamma\left\|\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1}\right\|_{\infty, \infty} \leq \boldsymbol{x}^{\star}(n)-\boldsymbol{x}^{\text {true }}(n)-\boldsymbol{w}(n), \\
& \boldsymbol{x}^{\text {true }}(n)+\boldsymbol{w}(n)-\gamma\left\|\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1}\right\|_{\infty, \infty} \leq \boldsymbol{x}^{\star}(n),
\end{aligned}
$$

where $\boldsymbol{w}=\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{e}$. Thus, from the condition (2.10), we have that $\boldsymbol{x}^{\star}(n)>0$ for all $n \in \Lambda$, which implies that $\Lambda \subseteq \operatorname{supp}\left(\boldsymbol{x}^{\star}\right)$. Furthermore, $\operatorname{since} \operatorname{supp}\left(\boldsymbol{x}^{\star}\right) \subseteq \Lambda$, then we have that
$\operatorname{supp}\left(\boldsymbol{x}^{\star}\right)=\Lambda$ and so it follows that $\boldsymbol{x}^{\star} \succ 0$, i.e., the solution of the lasso is non-negative. This implies that the solution of NLasso for the same input and parameter value obeys $\widehat{\boldsymbol{x}}=\boldsymbol{x}^{\star}$ (i.e., the solution of NLasso matches the solution of the unconstrained lasso), and so $\operatorname{supp}(\widehat{\boldsymbol{x}})=\operatorname{supp}\left(\boldsymbol{x}^{\star}\right)=\Lambda=\operatorname{supp}\left(\boldsymbol{x}^{\text {true }}\right)$.

The sufficient condition is composed of two inequalities; the first one (2.9) explains how much deviation from linearity is allowed, and the second one (2.10) shows the minimum value of the coefficient to be detected. This condition is a demanding sufficient MRC. More specifically, there are still many observations on which NLasso is successful, but for which the condition is not met.

### 2.4.2 Fundamental results for NLasso

NLasso is equivalent to

$$
\begin{array}{ll}
\underset{\boldsymbol{x}}{\operatorname{minimize}} & \frac{1}{2}\|\boldsymbol{y}-\mathbf{A} \boldsymbol{x}\|_{2}^{2}+\gamma \mathbf{1}_{N}^{\top} \boldsymbol{x}  \tag{2.13}\\
\text { subject to } & \boldsymbol{x} \succeq \mathbf{0}
\end{array}
$$

where $\mathbf{1}_{N}$ is the $N$ length vector with all elements being one. This minimization problem becomes NNLS when $\gamma=0$. First, I provide MRCs for which the subset of atoms $\Lambda$ contains the support of minimizers of NLasso. In particular, I will give a condition for which a solution to the restricted NLasso

$$
\begin{array}{ll}
\underset{\boldsymbol{v}_{\Lambda}}{\operatorname{minimize}} & \frac{1}{2}\left\|\boldsymbol{y}-\mathbf{A}_{\Lambda} \boldsymbol{v}_{\Lambda}\right\|_{2}^{2}+\gamma \mathbf{1}_{J}^{\top} \boldsymbol{v}_{\Lambda}  \tag{2.14}\\
\text { subject to } & \boldsymbol{v}_{\Lambda} \succeq \mathbf{0}
\end{array}
$$

also becomes a solution to the original NLasso (2.8). The condition is given by the following theorem.

Theorem 2.3 Let $\Lambda$ be a subset of column indices of the dictionary matrix $\mathbf{A}$ such that $|\Lambda|=J \leq N$. If the inequalities

$$
\begin{equation*}
\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)^{\top} \boldsymbol{a}_{j}<\gamma \quad \text { for all } j \in \Lambda^{\mathrm{c}} \tag{2.15}
\end{equation*}
$$

hold for all solutions $\widehat{\boldsymbol{v}}_{\Lambda} \in \mathbb{R}^{J}$ of the restricted NLasso (2.14) over the column subset $\Lambda$, then all solutions to the general NLasso (2.8) have their supports contained in $\Lambda$.

A proof of this theorem is found in Section 2.4.3. This theorem states a condition for which the restricted NLasso (2.14) yields a global solution of the original problem (2.8). Although this condition requires knowledge of the solutions of the restricted NLasso, the theorem considers quite general cases:

1. the subdictionary $\mathbf{A}_{\Lambda}$ can have linearly dependent columns,
2. the restricted NLasso over columns in $\Lambda$ can have multiple minimizers,
3. the columns of $\mathbf{A}$ are not restricted to be normalized.

Thus, the theorem serves as a fundamental result to derive other practical MRCs in subsequent sections. When atoms associated with indices in $\Lambda$ are linearly independent to each other, we can further assume the uniqueness of the solution because the restricted problem has the unique solution.

The condition (2.15) is a sufficient but not necessary condition for the event $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq$ 1. However, (2.15) is quite close to a necessary condition, as shown in the following theorem.

Theorem 2.4 Under the assumption of Theorem 2.3, if the support $\operatorname{supp}(\widehat{\boldsymbol{x}})$ of each solution $\widehat{\boldsymbol{x}}$ to the general NLasso (2.8) is contained in $\Lambda$, then the following condition holds for all solutions $\widehat{\boldsymbol{v}}_{\Lambda} \in \mathbb{R}^{J}$ of the restricted NLasso (2.14) over the column subset $\Lambda$ :

$$
\begin{equation*}
\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)^{\top} \boldsymbol{a}_{j} \leq \gamma \quad \text { for all } j \in \Lambda^{\mathrm{c}} \tag{2.16}
\end{equation*}
$$

The proof of this theorem is found in Section 2.4.3. This theorem indicates that the condition (2.16) is a necessary condition for $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda$. Hence, a necessary and sufficient condition for the event $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda$ lies somewhere between (2.15) and (2.16). More specifically, equalities need to be added to (2.15) only for some indices $j$ to obtain a necessary and sufficient condition. Nonetheless, it is worth noting that the cases in which (2.16) holds with equality will be rare in practice. Therefore, the conditions (2.15)
and (2.16) are practically identical, implying that (2.15) is a practically valid necessary and sufficient condition for the event $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda$.

Remark 2.5 Just like NLasso becomes NNLS when $\gamma=0$, a restricted NNLS problem is given by the minimization problem (2.14) when $\gamma=0$. As a special case of Theorem 2.3, we can define an optimal condition for $N N L S$ specific to an index set $\Lambda$ :

Corollary 2.6 Let $\Lambda$ be a subset of column indices of the dictionary matrix $\mathbf{A}$ such that $|\Lambda|=J \leq N$. If the inequalities

$$
\begin{equation*}
\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)^{\top} \boldsymbol{a}_{j}<0 \quad \text { for all } j \in \Lambda^{\text {c }} \tag{2.17}
\end{equation*}
$$

hold for the solution $\widehat{\boldsymbol{v}}_{\Lambda} \in \mathbb{R}^{J}$ of the restricted NNLS problem over the column subset $\Lambda$, then all solutions to the general NNLS have their supports contained in $\Lambda$.

I note in passing that the set of inequalities (2.17) is identical to one of the stopping criteria introduced for non-negative orthogonal matching pursuit [51, 52], an alternative algorithm for non-negative sparse signal recovery.

### 2.4.3 Proof of Theorems 2.3 and 2.4

Theorems 2.3 and 2.4 are proved together because they share assumptions. The next two statements are proved:

$$
\begin{array}{ll}
(\text { Theorem 2.3) } & (2.15) \Rightarrow \operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda \\
(\text { Theorem 2.4) } & \operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda \Rightarrow(2.16) \tag{2.19}
\end{array}
$$

where $\widehat{\boldsymbol{x}}$ is a solution to NLasso.
Before proceeding with the proof, we first transform the event $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda$ into an equivalent form. More specifically, $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda$ means that the solution of NLasso is equivalent to a solution of the restricted problem (2.14), $\widehat{\boldsymbol{v}}_{\Lambda}$, with appropriate zeropadding; this can be written as $\mathbf{A} \widehat{\boldsymbol{x}}=\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}$, where $\widehat{\boldsymbol{v}}_{\Lambda}$ is an optimal solution of the
restricted NLasso. The problem is first rewritten as

$$
\begin{align*}
\underset{\boldsymbol{v}_{\Lambda}}{\operatorname{minimize}} & \frac{1}{2}\left\|\boldsymbol{y}-\mathbf{A}_{\Lambda} \boldsymbol{v}_{\Lambda}\right\|_{2}^{2}+\gamma \mathbf{1}_{J}^{\top} \boldsymbol{v}_{\Lambda}  \tag{2.20}\\
\text { subject to } & \boldsymbol{v}_{\Lambda} \succeq \mathbf{0} .
\end{align*}
$$

Thus, we have $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda$ if and only if the following inequality holds:

$$
\begin{equation*}
\frac{1}{2}\|\boldsymbol{y}-\mathbf{A} \widehat{\boldsymbol{x}}\|_{2}^{2}+\gamma \mathbf{1}_{N}^{\top} \widehat{\boldsymbol{x}}<\frac{1}{2}\|\boldsymbol{y}-\mathbf{A}(\widehat{\boldsymbol{x}}+\Delta \boldsymbol{x})\|_{2}^{2}+\gamma \mathbf{1}_{N}^{\top}(\widehat{\boldsymbol{x}}+\Delta \boldsymbol{x}) \tag{2.21}
\end{equation*}
$$

for every $\Delta \boldsymbol{x}$ such that $0<\Delta x_{j}$ for any $j \in \Lambda^{c}$ and $\boldsymbol{x}+\Delta \boldsymbol{x} \succeq \mathbf{0}$ where $\Delta x_{j}$ is the $j^{\text {th }}$ element of $\boldsymbol{x}$. In other words, the minimum cost achieved by the solution of the restricted problem is less than any cost achieved by another $\boldsymbol{x}$ that involves an atom outside $\Lambda$. Let the exact support of $\widehat{\boldsymbol{x}}_{\Lambda}$ be $\Gamma \subseteq \Lambda(|\Gamma|=M \leq J)$. Then the inequality $\boldsymbol{x}+\Delta \boldsymbol{x} \succeq \mathbf{0}$ is expressed as:

$$
\begin{align*}
& \text { 1) } \quad-x_{j} \leq \Delta x_{j} \text { for all } j \in \Gamma  \tag{2.22}\\
& \text { 2) } 0 \leq \Delta x_{j} \text { for all } j \in \Gamma^{c},
\end{align*}
$$

which defines a region of interest for the vector $\Delta \boldsymbol{x}$. By canceling terms common to both sides, the inequality (2.21) is transformed into

$$
\begin{align*}
& \frac{1}{2}\|\mathbf{A}(\Delta \boldsymbol{x})\|_{2}^{2}+\gamma \mathbf{1}_{N}^{\top}(\Delta \boldsymbol{x})-\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)^{\top} \mathbf{A}(\Delta \boldsymbol{x})>0 \\
& \Leftrightarrow \frac{1}{2}\|\mathbf{A}(\Delta \boldsymbol{x})\|_{2}^{2}+\sum_{j \in \Omega} \Delta x_{j}\left(\gamma-\boldsymbol{a}_{j}^{\top}\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)\right)>0 \tag{2.23}
\end{align*}
$$

where $\Omega=\{1,2, \ldots, N\}$ is the whole column index set as defined in Section 2.2.1. Next, let us explore a property of $\widehat{\boldsymbol{v}}_{\Lambda}$. The Lagrangian of the restricted NLasso (2.20) above is given by

$$
L_{\Lambda}\left(\boldsymbol{v}_{\Lambda}, \boldsymbol{\lambda}_{\Lambda}\right)=\frac{1}{2}\left\|\boldsymbol{y}-\mathbf{A}_{\Lambda} \boldsymbol{v}_{\Lambda}\right\|_{2}^{2}+\gamma \mathbf{1}_{J}^{\top} \boldsymbol{v}_{\Lambda}-\boldsymbol{\lambda}_{\Lambda}^{\top} \boldsymbol{v}_{\Lambda}
$$

where $\boldsymbol{\lambda}_{\Lambda}$ is a vector of Lagrangian multipliers. From the KKT condition in Theorem 28.3 [53, p. 281], $\boldsymbol{v}_{\Lambda}=\widehat{\boldsymbol{v}}_{\Lambda}$ and $\boldsymbol{\lambda}=\widehat{\boldsymbol{\lambda}}$ become a minimizer and a Kuhn-Tucker vector, respectively, if and only if the following three conditions hold:

1) $\widehat{\boldsymbol{v}}_{\Lambda}, \widehat{\boldsymbol{\lambda}}_{\Lambda} \succeq \mathbf{0}$
2) $\quad \widehat{\boldsymbol{\lambda}}_{\Lambda}(n) \widehat{\boldsymbol{v}}_{\Lambda}(n)=0$ for all $n$
3) $\mathbf{0}=\partial L_{\Lambda}\left(\widehat{\boldsymbol{v}}_{\Lambda}, \widehat{\boldsymbol{\lambda}}_{\Lambda}\right) /\left.\partial \boldsymbol{v}_{\Lambda}\right|_{\boldsymbol{v}_{\Lambda}=\widehat{\boldsymbol{v}}_{\Lambda}}$.

The third KKT condition (2.24c) is equivalently expressed as:

$$
\begin{aligned}
& \mathbf{A}_{\Lambda}^{\top}\left(\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}-\boldsymbol{y}\right)+\gamma \mathbf{1}_{J}-\widehat{\boldsymbol{\lambda}}_{\Lambda}=\mathbf{0} \\
\Leftrightarrow & \gamma-\boldsymbol{a}_{j}^{\top}\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)=\widehat{\boldsymbol{\lambda}}_{\Lambda}(j) \quad \text { for all } j \in \Lambda
\end{aligned}
$$

For $j \in \Gamma$, we have $\widehat{\boldsymbol{v}}_{\Lambda}(j)>0$, leading to $\widehat{\boldsymbol{\lambda}}_{\Lambda}(j)=0$ because of the second KKT condition (2.24b). For $j \in \Lambda \backslash \Gamma$, we have $\widehat{\boldsymbol{v}}_{\Lambda}(j)=0$, leading to $\widehat{\boldsymbol{\lambda}}_{\Lambda}(j) \geq 0$. Thus we have

$$
\left\{\begin{array}{l}
\gamma-\boldsymbol{a}_{j}^{\top}\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)=0 \text { for } j \in \Gamma  \tag{2.25}\\
\gamma-\boldsymbol{a}_{j}^{\top}\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right) \geq 0 \text { for } j \in \Lambda \backslash \Gamma .
\end{array}\right.
$$

Considering the conditions above for $\widehat{\boldsymbol{v}}_{\Lambda}$, the inequality (2.23) is equivalently transformed into
$\frac{1}{2}\|\mathbf{A}(\Delta \boldsymbol{x})\|_{2}^{2}+\sum_{j \in \Lambda \backslash \Gamma} \Delta x_{j}\left(\gamma-\boldsymbol{a}_{j}^{\top}\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)\right)+\sum_{j \in \Lambda^{c}} \Delta x_{j}\left(\gamma-\boldsymbol{a}_{j}^{\boldsymbol{\top}}\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)\right)>0 .(2.26)$
where the second term is always non-negative because of the non-negativity of the two factors $((2.22)$ and $(2.25))$. Summarizing this discussion, $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda$ if and only if the inequality (2.26) holds for all $\Delta \boldsymbol{x}$ in the defined region (2.22).

We now prove the statement (2.18) for Theorem 2.3. Given the condition (2.15) is true, then the summation of the third term on the left side in (2.26) becomes always non-negative. Furthermore, because we are considering $\Delta \boldsymbol{x}$ with a non-zero $j^{\text {th }}$ element for any $j \in \Lambda^{\mathrm{c}}$, the third term is always strictly positive. Therefore, (2.26) holds for every $\Delta \boldsymbol{x}$ in the defined region (2.22). Because that condition is equivalent to $\operatorname{supp}(\widehat{\boldsymbol{x}}) \subseteq \Lambda$, the statement (2.18) is proven.

Next, we prove the statement (2.19) for Theorem 2.4. We can prove this by the principle of contradiction. Assume the inequality (2.26) is true for every $\Delta \boldsymbol{x}$ in the defined region and every solution $\widehat{\boldsymbol{v}}_{\Lambda}$. Suppose there exists a solution $\widehat{\boldsymbol{v}}_{\Lambda}$ and an index $j^{\prime} \in \Lambda^{\mathrm{c}}$ such that

$$
\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)^{\top} \boldsymbol{a}_{j^{\prime}}>\gamma,
$$

which is the opposite of (2.16). The inequality (2.26) is true for $\Delta x^{\prime}$ such that only the $j^{\prime \text { th }}$ element is greater than zero and the others are zero. Let such a $\Delta \boldsymbol{x}^{\prime}$ be

$$
\begin{equation*}
\Delta \boldsymbol{x}^{\prime}=\left[0, \ldots 0, \Delta x_{j^{\prime}}, 0, \ldots 0\right]^{\top} \quad\left(\Delta x_{j^{\prime}}>0\right) \tag{2.27}
\end{equation*}
$$

The inequality (2.26) then becomes

$$
\begin{equation*}
\frac{1}{2}\left\|\boldsymbol{a}_{j^{\prime}}\right\|_{2}^{2}\left(\Delta x_{j^{\prime}}\right)^{2}-\left(\left(\boldsymbol{y}-\boldsymbol{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)^{\top} \boldsymbol{a}_{j^{\prime}}-\gamma\right) \Delta x_{j^{\prime}}>0 \tag{2.28}
\end{equation*}
$$

The left hand side is a quadratic function with regard to a scalar variable $\Delta x_{j^{\prime}}$. By defining the quadratic equation's coefficients as

$$
\begin{align*}
& b_{j^{\prime}}=\frac{1}{2}\left\|\boldsymbol{a}_{j^{\prime}}\right\|_{2}^{2}>0  \tag{2.29}\\
& c_{j^{\prime}}=\left(\boldsymbol{y}-\boldsymbol{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)^{\top} \boldsymbol{a}_{j^{\prime}}-\gamma>0 \tag{2.30}
\end{align*}
$$

the quadratic inequality (2.28) becomes

$$
\begin{equation*}
\Delta x_{j^{\prime}}\left(b_{j^{\prime}} \Delta x_{j^{\prime}}-c_{j^{\prime}}\right)>0 \tag{2.31}
\end{equation*}
$$

Because both the coefficients $b_{j^{\prime}}$ and $c_{j^{\prime}}$ are positive, the left hand side becomes negative for sufficiently small $\Delta x_{j^{\prime}}$ such that $0<\Delta x_{j^{\prime}}<c_{j^{\prime}} / b_{j^{\prime}}$. Since $\Delta x_{j^{\prime}}$ can take any positive value, we can say that there exists a $\Delta x_{j^{\prime}}$ that breaks the inequality (2.26). This contradicts to the starting assumption. Thus, by the principle of contradiction, the statement (2.19) is proven.

### 2.4.4 Approximately Perfect MRC for NLasso

This section provides MRCs for which the subset of atoms $\Lambda$ exactly matches the support of the minimizers of NLasso. We again assume that the atoms associated with indices in $\Lambda$ are linearly independent. First, I define a metric, positive subset coherence (PSC):

$$
\begin{equation*}
\operatorname{PSC}(\Lambda ; j):=1-\mathbf{1}_{J}^{\top} \mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{a}_{j} . \tag{2.32}
\end{equation*}
$$



Figure 2.1. Illustration of geometric interpretation of PSC.
The PSC measures how positively aligned the $j^{\text {th }}$ atom $\boldsymbol{a}_{j}$ in the library is to the convex cone determined by the columns of $\mathbf{A}_{\Lambda}$. The index $j$ is usually selected from outside $\Lambda$. Figure 2.1 illustrates a geometric interpretation of PSC focusing on when the sign of PSC changes. The PSC becomes positive when the orthogonal projection of $\boldsymbol{a}_{j}$ onto the subspace spanned by the column vectors of $\mathbf{A}_{\Lambda}$ falls on the same side of the hyperplane passing through the column vectors of $\mathbf{A}_{\Lambda}$ as the origin; negative when the origin and the column $\boldsymbol{a}_{j}$ are on opposite sides of the aforementioned hyperplane; and zero when $\boldsymbol{a}_{j}$ is contained in this hyperplane. This PSC plays an important role in the next approximately perfect MRC.

Theorem 2.7 (Approximately Perfect MRC for NLasso) Let $\Lambda$ be a subset of the column indices of the dictionary matrix $\mathbf{A}$ such that $|\Lambda|=J \leq \min (L, N)$ and the atoms associated with indices in $\Lambda$ are linearly independent. Let $\widehat{\boldsymbol{x}}$ be a solution to NLasso. The support of $\widehat{\boldsymbol{x}}, \operatorname{supp}(\widehat{\boldsymbol{x}})$, is equal to $\Lambda$ if the following two conditions hold:

1) Minimum coefficient condition (MCC):

$$
\begin{equation*}
\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y} \succ \gamma\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1} \mathbf{1}_{J} \tag{2.33}
\end{equation*}
$$

2) Non-linearity vs. Subset Coherence Condition (NSCC):

$$
\begin{equation*}
\boldsymbol{y}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{a}_{j}<\gamma \operatorname{PSC}(\Lambda ; j) \quad \text { for all } j \in \Lambda^{c} . \tag{2.34}
\end{equation*}
$$

Furthermore, the minimizer $\widehat{\boldsymbol{x}}$ is equal to the appropriate zero-padding of the solution to the restricted NLasso

$$
\widehat{\boldsymbol{v}}_{\Lambda}=\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}-\gamma\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1} \mathbf{1}_{J} .
$$

The proof of this theorem is found in Section 2.4.5. The MCC measures whether the entries of the least squares solution $\left(\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}\right)$ are sufficiently large. The NSCC specifies the degree of nonlinear distortion that can be tolerated with respect to each PSC and dictionary atom $\boldsymbol{a}_{j}$. The left hand side of (2.34) is the inner product between $\boldsymbol{a}_{j}$ and the orthogonal projection of $\boldsymbol{y}$ onto the orthogonal complement of $\mathcal{R}\left(\mathbf{A}_{\Lambda}\right)$. The latter projection can be interpreted as nonlinear noise because it is considered as the deviation of the observation $\boldsymbol{y}$ from the span of $\mathbf{A}_{\Lambda}$. Figure 2.2 shows a geometric interpretation of the NSCC. As explained, the right hand side of (2.34) quantifies the alignment of $\boldsymbol{a}_{j}$ with the convex cone obtained from $\mathbf{A}_{\Lambda}$. Because $\gamma$ is usually positive, a larger PSC relaxes the upper bound of $\boldsymbol{y}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{a}_{j}$. Thus, it is preferable for $\boldsymbol{a}_{j}$ to be less aligned to the columns of $\mathbf{A}_{\Lambda}$.

The inequality (2.33) needs to strictly hold for mathematical rigor because of the definition of the support (the set of indices that have non-zero entries). If we instead allowed for equality in (2.33), we would not be able to guarantee that $\Lambda$ exactly matches the support of $\widehat{\boldsymbol{x}}$ since some of the entries in $\widehat{\boldsymbol{v}}_{\Lambda}$ might be zero-valued, cf. eq. (2.35), although the solution $\widehat{\boldsymbol{x}}$ would be still expressed in the same way, i.e., as the appropriate zero-padding of the solution $\widehat{\boldsymbol{v}}_{\Lambda}$ to the restricted NLasso. Nonetheless, equality can be added in practice since the event for which the equations hold with equality is quite rare, as described in the discussion of Section 2.4.2. This discussion is also true for the


Figure 2.2. Illustration of geometric interpretation of NSCC.
inequality (2.34); equality could be added to the inequality in practical settings.
Interestingly, Conditions (2.9) and (2.10) in Theorem 2.2 are similar to the NSCC and MCC, but the former are not specific to particular indices $j$. This structure of the condition is shared with the simplified sufficient conditions derived in Section 2.4.6.

Remark 2.8 Theorem 2.7 can be specialized to specific noise models. In the case of random noise (e.g., Gaussian or subgaussian), it is possible to obtain the likelihood of the NSCC being met in terms of the noise variance; such a result matches [23, Theorem 6]. Under a linear noise model (e.g., the distortion corresponds to a linear combination of the atoms in lies in $\mathbf{A}_{\Lambda}$ ), the left hand side of (2.34) always becomes equal to zero, and it suffices to require a non-negative PSC for each of the atoms indexed in $\Lambda^{c}$. In all other cases, the NSCC allows us to distinguish between tolerable and intolerable distortions. If the nonlinear distortion (i.e., the portion of the distortion in the space orthogonal to $\mathcal{R}\left(\mathbf{A}_{\Lambda}\right)$ ) forms obtuse angles with the atoms indexed by $\Lambda^{c}$, the NSCC will be satisfied regardless of the magnitude of the nonlinearity. Conversely, for atoms for which these angles are acute, the value of the PSC for the specific atom will dictate the tolerable
magnitude of the projection of the nonlinear distortion onto the atom.

Remark 2.9 I note that meeting the $M C C$ and NSCC will also depend on the value of the trade-off parameter $\gamma$. Intuitively, the chance for false alarm increases as $\gamma$ decreases (promoting denser solutions) and missed detection is more likely to occur as $\gamma$ increases (promoting sparser solutions). The MCC provides an upper bound on $\gamma$ needed to avoid missed detections, while the NSCC provides a lower bound needed to prevent false alarms. The bounds will depend on the observation $\boldsymbol{y}$ and support $\Lambda$, which indicates that the performance of NLasso can be improved by adaptively optimizing $\gamma$. It is also easy to see that one can formulate configurations $(\boldsymbol{y}, \Lambda)$ for which no value of $\gamma$ meets both the $M C C$ and NSCC.

Remark 2.10 Theorem 2.7 can also be specialized to NNLS (e.g., $\gamma=0$ ), providing the following corollary.

Corollary 2.11 (Approximately Perfect MRC for $\boldsymbol{N N L S}$ ) Let $\Lambda$ be a subset of column indices of the dictionary matrix $\mathbf{A}$ such that $|\Lambda|=J \leq \min (L, N)$ and the atoms associated with indices in $\Lambda$ are linearly independent. Let $\widehat{\boldsymbol{x}}$ be the solution of NNLS. The support of $\widehat{\boldsymbol{x}}, \operatorname{supp}(\widehat{\boldsymbol{x}})$, is equal to $\Lambda$ if $\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y} \succ 0$ and $\max _{j} \boldsymbol{y}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{a}_{j}<0$.

In this case, the MCC requires for the restricted least squares solution to be non-negative, while the NSCC requires all angles between the atoms indexed in $\Lambda^{c}$ and the nonlinear distortion in the orthogonal space of $\mathcal{R}\left(\mathbf{A}_{\Lambda}\right)$ to be obtuse.

### 2.4.5 Proof of Theorem 2.7

Recall that the atoms associated with the index set $\Lambda$ are linearly independent to each other and the two conditions (2.33) and (2.34) hold. First let us consider the restricted NLasso defined by (2.14). The problem (2.14) has the unique minimizer because the objective function is strictly convex and the domain is a convex region. The Lagrangian
of (2.14) is given by

$$
L\left(\boldsymbol{v}_{\Lambda}, \boldsymbol{\lambda}\right)=\frac{1}{2}\left\|\boldsymbol{y}-\mathbf{A}_{\Lambda} \boldsymbol{v}_{\Lambda}\right\|_{2}^{2}+\gamma \mathbf{1}_{J}^{\top} \boldsymbol{v}_{\Lambda}-\boldsymbol{\lambda}^{\top} \boldsymbol{v}_{\Lambda},
$$

where $\boldsymbol{\lambda} \in \mathbb{R}^{J}$ is a Lagrange multiplier with $\boldsymbol{\lambda} \succeq \mathbf{0}$. According to [53, Theorem 28.3, p. 281], $\widehat{\boldsymbol{v}}_{\Lambda}$ and $\widehat{\boldsymbol{\lambda}}$ are optimal if and only if they satisfy the KKT conditions

1) $\widehat{\boldsymbol{v}}_{\Lambda}, \widehat{\boldsymbol{\lambda}} \succeq \mathbf{0}$ and $\widehat{\boldsymbol{\lambda}}(n) \widehat{\boldsymbol{v}}_{\Lambda}(n)=0$ for all $n=1, \ldots, J$
2) $\mathbf{0}=\partial L\left(\boldsymbol{v}_{\Lambda}, \widehat{\boldsymbol{\lambda}}\right) /\left.\partial \boldsymbol{v}_{\Lambda}\right|_{\boldsymbol{v}_{\Lambda}=\widehat{\boldsymbol{v}}_{\Lambda}}$.

Those conditions are true for $\widehat{\boldsymbol{v}}_{\Lambda}=\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}-\gamma\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1} \mathbf{1}_{J}$ and $\widehat{\boldsymbol{\lambda}}=\mathbf{0}$. Taking the uniqueness of the solution into consideration, we can conclude that the unique minimizer of (2.14) is given by

$$
\begin{equation*}
\widehat{\boldsymbol{v}}_{\Lambda}=\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}-\gamma\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1} \mathbf{1}_{J} \succ \mathbf{0} . \tag{2.35}
\end{equation*}
$$

By manipulating the inequality (2.34) and substituting (2.35), we have

$$
\begin{array}{ll} 
& \left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}\right)^{\top} \boldsymbol{a}_{j}<\gamma\left(1-\mathbf{1}_{J}^{\top} \mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{a}_{j}\right) \\
\Leftrightarrow & \left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}+\gamma\left(\mathbf{A}_{\Lambda}^{\dagger}\right)^{\top} \mathbf{1}_{J}\right)^{\top} \boldsymbol{a}_{j}<\gamma \\
\Leftrightarrow\left\{\boldsymbol{y}-\mathbf{A}_{\Lambda}\left(\mathbf{A}_{\Lambda}^{\dagger} \boldsymbol{y}-\gamma\left(\mathbf{A}_{\Lambda}^{\top} \mathbf{A}_{\Lambda}\right)^{-1} \mathbf{1}_{J}\right)\right\}^{\top} \boldsymbol{a}_{j}<\gamma \\
\Leftrightarrow \quad\left(\boldsymbol{y}-\mathbf{A}_{\Lambda} \widehat{\boldsymbol{v}}_{\Lambda}\right)^{\top} \boldsymbol{a}_{j}<\gamma \quad(\because(2.35))
\end{array}
$$

for all $j \in \Lambda^{c}$. Directly applying Theorem 2.3, we can assert that $\Lambda$ contains the support of $\widehat{\boldsymbol{x}}$. Furthermore, since all the elements of the minimizer (2.35) are greater than zero, $\Lambda$ is the support of $\widehat{\boldsymbol{x}}$. This completes the proof.

### 2.4.6 Simplified sufficient conditions for NLasso

Although these conditions are quite simple, they are still more elaborate than those provided by Tropp [3] for general lasso. We can further simplify and introduce two
sufficient conditions in this section. To start with, let us define the positive exact recovery coefficient (PERC) by

$$
\operatorname{PERC}(\Lambda):=\min _{j \in \Lambda^{c}} \operatorname{PSC}(\Lambda ; j) .
$$

PERC is considered as the positive counterpart of the ERC, and PERC is interpreted as the minimum of the right hand side in the NSCC (2.34). Note that ( $1-\mathrm{PERC}$ ) is equivalent to non-negative irrepresentable constant of [23]. We can also take the maximum on the left hand side of the inequality (2.34) after concatenating all $\boldsymbol{a}_{j}$, and then a modified sufficient condition for the multiple NSCCs is written as

$$
\begin{equation*}
\max _{j \in \Lambda^{c}} \boldsymbol{a}_{j}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{y}<\gamma \operatorname{PERC}(\Lambda), \tag{2.36}
\end{equation*}
$$

and is referred to as PERC-Max, leading to the next corollary.

Corollary 2.12 (PERC-Max MRC for NLasso) Under the assumptions of Theorem 2.7, the support of $\widehat{\boldsymbol{x}}, \operatorname{supp}(\widehat{\boldsymbol{x}})$, is equal to $\Lambda$ if the two conditions, MCC (2.33) and PERC-Max (2.36), hold. Furthermore, the minimizer $\widehat{\boldsymbol{x}}$ is also given as in Theorem 2.7.

We can still introduce another NSCC condition that is more strict than Corollary 2.12 but more relaxed than Theorem 2.2 by taking the absolute maximum value on the left side of (2.36),

$$
\begin{equation*}
\left\|\mathbf{A}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{y}\right\|_{\infty}<\gamma \operatorname{PERC}(\Lambda) . \tag{2.37}
\end{equation*}
$$

We refer this condition as PERC-absolute Max (PERC-AMax), leading to the next corollary.

Corollary 2.13 (PERC-AMax MRC for NLasso) Under the assumptions of Theorem 2.7, the support of $\widehat{\boldsymbol{x}}, \operatorname{supp}(\widehat{\boldsymbol{x}})$, is equal to $\Lambda$ if the two conditions, MCC (2.33) and PERC-AMax (2.37), hold. Furthermore, the minimizer $\widehat{\boldsymbol{x}}$ is also given as in Theorem 2.7.

PERC-AMax is more demanding than PERC-Max. Additionally, it provides a broader guarantee than Theorem 2.2, which assumes the linear model (3.7) and requires not only the support of the true coefficient vector $\boldsymbol{x}^{\text {true }}$ but also its values and the error term in advance, while Corollary 2.13 can be applied to arbitrary vectors $\boldsymbol{y}$ and index sets $\Lambda$.

### 2.5 Application to hyperspectral unmixing

Hyperspectral imagers collect electromagnetic radiation over the Visible and Near Infrared (VNIR) to Short Wave Infrared (SWIR) region (300-2600nm) with hundreds of narrow contiguous bands. Each pixel position of a hyperspectral image (HSI) is associated with a spectrum or spectral signature, an array of dimension equal to the number of bands, which is used by practitioners to reveal the compositional characteristics of targets in a variety of applications.

One of the tasks routinely performed in hyperspectral imaging is spectral unmixing. Unmixing is a process to decompose an observed spectrum into pure constituent signatures, which are usually called endmembers, associated with their fractional abundances [1], [54]. The linear model (3.7) has been widely used in unmixing, where $\boldsymbol{y}$ represents the observed spectrum, $\mathbf{A}$ is the dictionary matrix with atoms corresponding to endmember spectra, and the coefficient vector $\boldsymbol{x}$ is interpreted as a fractional abundance vector.

Recently, sparse unmixing [2] has been proposed for hyperspectral unmixing tasks where one is given a large collection - the spectral library - of pure spectral signatures to be used as candidate endmembers. The first goal for unmixing is to correctly identify the library spectra that are combined to form the observed spectrum. One typically expects that only a few endmembers in the collection are involved in the observation, as the number of materials occupying the region subtended by a pixel is small in most scenarios. Motivated by this observation, sparse unmixing [2] employs NLasso to detect
endmembers and estimate abundances for hyperspectral images using a large library of laboratory spectra.

Nonetheless, sparse unmixing faces several limitations in practical applications. An observed spectrum could be composed by a nonlinear mixture of endmembers. The atoms in the library might not match exactly the image endmembers (typical examples are spectra of the same material acquired at different conditions). Moreover, the library spectra are usually highly correlated, which intuitively seems undesirable for the nonnegative sparse modeling.

Given such complications, the theorems derived in this paper serve as a way to assess the performance of NLasso in hyperspectral unmixing. Since we have not restricted the definition of the "error" term $\boldsymbol{e}$ in the linear model equation (2.7), it could accommodate any deviation from linearity, such as nonlinear mixing or spectral distortions.

I test the performance of NLasso in unmixing a real hyperspectral image of an oil painting. In particular, I am interested in assessing the performance of the sparse modeling approach in identifying the endmembers involved in each pixel of the HSI. This example presents the typical complications of unmixing problems: the artist creates the colors in the painting by mechanically mixing the paints (nonlinear mixing) and adding water (nonlinear distortion of all pixel spectra). Further nonlinearities stem from the different density and thickness of the paint in different regions. I first describe the creation of training data including endmembers and their true abundance maps. I then assess the ability of the MRCs to predict the outcome of numerical computations using NLasso.

### 2.5.1 Data set

The data set used for this experiment is a hyperspectral image (HSI) of an oil painting acquired by a Micro-Hyperspec ${ }^{\circledR}$ VNIR imaging sensor (E-Series). ${ }^{2}$ The imager captures spectral information in the $400-1000 \mathrm{~nm}$ wavelength region with 370 bands at 1.6 nm inter-

[^2]

Figure 2.3. $500 \times 308$ pseudo RGB color image of a hyperspectral image of the oil painting. R: band 125 ( 601 nm ), G: band 86 ( 536 nm ), B: band 49 ( 471 nm ).
vals. The image was acquired on Hyperspec Starter Kit manufactured by Headwall Inc. Since the painting was larger than the field of view of the camera, I first separated the whole area into three strip regions, acquired the images of them separately, and stitched them together. The size of the resulting hyperspectral image is $3347 \times 1233 \times 370$, where the first two dimensions are the number of pixels in the spatial directions and the last dimension records the number of spectral bands. The image was converted to reflectance using a Spectralon ${ }^{\circledR}$ reference. ${ }^{3}$ The image was then spatially downsampled to $500 \times 308$ by averaging $4 \times 4$ neighboring pixels in order to improve its signal-to-noise ratio. Figure 2.3 shows a pseudo RGB rendition of the HSI.

The artist used acrylic paint in five distinct colors: red, blue, yellow, white, and green. An HSI of the pure colors, which is shown on the lower right side in Figure 2.4, were then acquired. The averaged spectra of the five colored areas can be considered as the endmembers of the pixels depicting the painting: they are shown in Figure 2.4 and used to construct a spectral library.

The artist did not provide in advance the information about true distribution of the endmembers for each pixel. I will use the term "ground truth", borrowed from hyperspectral remote sensing, for such map. This information is required in order to

[^3]

Figure 2.4. Averaged endmember spectra. The image on the lower right is a pseudo RGB color image of a hyperspectral image of endmembers.
assess the performance of the unmixing algorithm. Since the artist used 2 or 3 colors at each location (single-endmember pixels are not present) we could generate the ground truth by solving the following minimization problem for each pixel

$$
\begin{array}{ll}
\underset{\boldsymbol{x}}{\operatorname{minimize}} & \frac{1}{2}\|\boldsymbol{y}-\mathbf{A} \boldsymbol{x}\|_{2}^{2}  \tag{2.38}\\
\text { subject to } & \boldsymbol{x} \succeq \mathbf{0},\|\boldsymbol{x}\|_{0} \leq 3
\end{array}
$$

where $\boldsymbol{y} \in \mathbb{R}^{370}$ is the spectral signal of each pixel, $\mathbf{A} \in \mathbb{R}^{370 \times 5}$ is the matrix of the spectral library of five colors, and $\boldsymbol{x} \in \mathbb{R}^{5}$ is the fractional abundance vector. In practice, the solution by conducting least square minimizations for all possible combinations of less than or equal to three endmembers and it is reasonable to select as the ground truth the combination with the smallest number of endmembers among the ones that achieved the least error. Figure 2.5 shows the ground truth at each pixel. The distribution map in Figure 2.5 shows that not all the pixels are assigned to mixtures of three endmembers; some pixels are to mixtures of only two endmembers, which means that any other third endmember cannot help reduce the residual for these pixels. We could also interpret this fact from the proposed theorems. The minimization problem (2.38) can be converted to NLasso (2.8) with an appropriate trade-off parameter $\gamma$. I conjecture that a combination of only two endmembers suffices to meet the APMRC in Theorem 2.7.


Figure 2.5. The true distribution of the mixtures. The letters R, B, Y, W, and G are the first letters of the pure colors.

Although the minimization problem above also produces abundance values for each endmember at each pixel location, such information is discarded as the performance evaluated here is the correct recovery of endmembers. Furthermore, while the artist agrees that the retrieved distribution is largely accurate, a similar assessment would not be possible for the abundances. I nevertheless report the abundances for all colors in Figure 2.6 for the sake of completeness and to show that they show reasonable effects. From Figure 2.6, one can see that the white color is dominant around the clouds in Figure 2.3, the sky is mainly painted in white and blue, and the grass that can be found around the bottom in Figure 2.3 consists of mainly green.

### 2.5.2 Theorem validation

This section evaluates the predictive power of the MRCs. The performance of NLasso is predicted by four MRCs: Theorem 2.2 (ERC-based MRC), Theorem 2.7 (APMRC), Corollary 2.12 (PERC-Max MRC), and Corollary 2.13 (PERC-AMax MRC). The algorithm employed to produce numerical solutions for NLasso is the sparse unmixing by variable splitting and augmented Lagrangian (SUnSAL) [45]. Then it is evaluated how well the predictions of the MRCs match the result obtained by SUnSAL.

Table 2.1 shows the number of pixels that satisfy each of MRCs hold for a different value of $\gamma=0.2,0.1,0.05$. For each value of $\gamma$ the table displays the confusion matrix


Figure 2.6. The true abundance maps in the painting image: (a) red, (b) blue, (c) yellow, (d) white, and (e) green.
between the prediction by each MRC and the SUnSAL result. In each row, the label "True" refers to the points fulfilling the specific condition and "False" the ones violating it. Similarly, in each column, the label "Correct" ("Incorrect") refers to points for which

SUnSAL correctly identifies (fails to identify) the endmembers.
For all the MRCs, the values in the True-Incorrect cells are all zeros, indicating that if the MRCs hold, the SUnSAL always succeeds. This is a confirmation for the sufficiency of all the MRCs in all the theorems.

One remarkable fact is that the "False-Correct" cell of the APMRC is always zero, which means the APMRC is always true when SUnSAL succeeds in detecting the correct endmembers, confirming the necessity of the APMRC condition in practical settings. In contrast, there are non-zero values in the False-Correct cells for the other MRCs, and the values increase as the conditions become increasingly strict.

None of the pixels satisfy the strict conditions required by the ERC-based MRC. It is worth noting that this application tests the limits of the theory of sparse recovery in at least two ways. First, hyperspectral mixing processes can deviate significantly from the linear model; second, spectra of different endmembers are very correlated. This observation supports the utility of the APMRC, PERC-Max MRC and PERC-AMax MRC as prediction tools for signal spaces in which previously proposed metrics would not be applicable.

Figure 2.7 shows an interesting behavior in the performance of NLasso. In Figure 2.7 (a), the pixels where NLasso succeeds at identifying endmembers are shown in red, while failures are shown in blue. Figure 2.7 (b) shows the distribution of the residual given by the optimum value of (2.38). This residual is interpreted as the deviation from linearity; therefore, one may expect that a large deviation is linked to failure of NLasso, but this intuition does not bear out in practice. Deviations seem to be relatively high in the horizontal belt near the bottom of the painting, but NLasso is able to detect the correct endmembers in that area. The reason for this phenomenon is explained in Figure 2.8. This figure focuses only on the region classified as the mixture of blue and green that mostly overlaps with the horizontally belted region. Figure 2.8 shows the distribution of the values $\boldsymbol{y}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{a}_{j}$ where $j$ indexes the red, yellow, and white colors, which are

Table 2.1. Performance of MRCs on the painting data

|  |  | $\gamma=0.2$ |  | $\gamma=0.1$ |  | $\gamma=0.05$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | SUnSAL retrieval |  | SUnSAL retrieval |  | SUnSAL retrieval |  |
|  |  | Correct | Incorrect | Correct | Incorrect | Correct | Incorrect |
| Thm. 2.7 <br> (APMRC) | True | $\begin{gathered} 56718 \\ {[\mathrm{pts}]} \end{gathered}$ | 0 | 70256 | 0 | 64459 | 0 |
|  | False | 0 | 97282 | 0 | 83744 | 0 | 89541 |
| Cor. 2.12 <br> (PERC-Max <br> MRC) | True | 56053 | 0 | 67252 | 0 | 62547 | 0 |
|  | False | 665 | 97282 | 3004 | 83744 | 1912 | 89541 |
| $\begin{aligned} & \text { Cor. 2.13 } \\ & \text { (PERC-AMax } \\ & \text { MRC) } \end{aligned}$ | True | 46349 | 0 | 53122 | 0 | 32361 | 0 |
|  | False | 10369 | 97282 | 17134 | 83744 | 32098 | 89541 |
| Thm. 2.2 <br> (ERC-based <br> MRC) | True | 0 | 0 | 0 | 0 | 0 | 0 |
|  | False | 56718 | 97282 | 70256 | 83744 | 64459 | 89541 |

associated with the subscripts $r$, $y$, and $w$, respectively. The values in the region of interest in Figures 2.8 are always negative, while their corresponding $\operatorname{PSC}(\Lambda ; j)$ are always positive $(\operatorname{PSC}(\Lambda ; r)=0.141, \operatorname{PSC}(\Lambda ; y)=0.151$, and $\operatorname{PSC}(\Lambda ; w)=0.061)$, meaning the NSCC conditions for the APMRC, PERC-Max MRC, PERC-AMax MRC are always true. Even when the deviation is large, NLasso is successful if the residual is negatively correlated with the signatures of all the other endmembers and PSC is positive and vice versa. Although this does not always happen, this specific example demonstrates that the direction of the deviation affects the performance of NLasso.

One final observation about Figure $2.7(\mathrm{~b})$ is that the region of maximum deviation from nonlinearity (green to yellow) corresponds with a region to which the artist confirmed having applied more than one layer of paint (this is called pentimento in art jargon). This is consistent with our understanding of the radiative transfer aspects of unmixing, e.g [54] and suggests the potential utility of unmixing techniques to aspects of the artist painting style in addition to identifying the different pigments.


Figure 2.7. (a) The distribution of correct model recovery of NLasso and (b) the distribution of the deviation from the linear model.

(a) $\boldsymbol{y}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{a}_{\mathrm{r}}$

(b) $\boldsymbol{y}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{a}_{\mathrm{y}}$

(c) $\boldsymbol{y}^{\top} \mathbf{P}_{\Lambda}^{\perp} \boldsymbol{a}_{\mathrm{w}}$

Figure 2.8. Mappings of the values of the left hand side of the NSCC for each atom in $\Lambda^{c}$. The letters, $r, y$, and $w$, means the first letter of the three colors: red, yellow, and white.

### 2.6 Summary

This chapter explored several recovery conditions that guarantee the correct identification of endmembers by the non-negative sparse modeling for mixed signals exhibiting deviations from linearity. Those conditions reveal an interesting property of NLasso, which is expressed by two conditions: minimum coefficient condition and nonlinearity vs subset coherence condition. In particular, the approximately perfect recovery condition (APMRC) can exactly predict the performance of NLasso in a practical sense. The exactness was inferred from mathematical inspection and further verified through experiments. These conditions are proven to be useful for analyzing the performance of numerical solutions of NLasso.

## CHAPTER 3

## ATMOSPHERIC CORRECTION AND DE-NOISING OF CRISM DATA

This chapter presents an application of hyperspectral unmixing to atmospheric correction and de-noising of CRISM data. ${ }^{1}$

### 3.1 Introduction

Since the beginning of its operations, the Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) [4] onboard the Mars Reconnaissance Orbiter (MRO) has made signicant contributions towards understanding many detailed aspects of the surface mineralogy of Mars thanks to its high spectral and spatial resolution. CRISM has reinforced and detailed previous findings made by OMEGA (Observatoire pour la Mineralogie, L'Eau, les Glaces et l'Activitié), such as the identification of phyllosilicates including kaolinite, montmorillonite, muscovite, illite, chlorite, saponite, nontronite, and hydrated silica [58-60]. Moreover, CRISM has confirmed the existence of opaline silica [61] and $\mathrm{Fe}-\mathrm{Mg}$ carbonate [62-65], two minerals that were not previously discovered. Many other minerals have been identified [66]. Mineral detections are compiled and summarized in [67] and [68]. More recently, mineral detections and mapping derived from CRISM images for Jezero crater [62,63,65,69-75] are supporting the Perseverance rover

[^4]mission [76] launched in 2020.
Raw image cubes acquired by CRISM require complex processing protocols before they can be used for mineral identification [4, 77, 78]. In the current pipeline for CRISM products, a raw image cube recorded in a 12-bit integer format undergoes calibration and corrections to be converted to an apparent reflectance, I/F image cube [78]. I/F (I-overF) represents the ratio of light energy observed by CRISM instrument (radiance) by that incident at the top of the atmosphere (irradiance). The I/F image is then processed to the TRR3 I/F product (TRR: Targeted Reduced Data Record), with TRR3 filtering using iterative kernel filter (IKF) and ratio shift correction (RSC) applied in order to remediate outstanding noise and spatial stripes. Some data are further processed with photometric correction, atmospheric correction, repetitive filtering using RSC for de-spiking and de-striping, smile correction, and empirical geometric normalization. Finally, visible and near infrared (VNIR) and infrared (IR) images, are map projected and spectrally combined, producing the TER/MTRDR data, currently the most advanced products available for CRISM (TER:Targeted Empirical Data Record, non-map projected version and MTRDR: Map Projected Targeted Reduced Data Record) [78-80].

Despite of the development of such complex and sophisticated processing, artifacts still persist in the corrected I/F spectra as residuals of the atmospheric correction process. The so-called "volcano scan" correction, the atmospheric compensation method currently used in the pipeline for CRISM IR images [77,80-82], is known to create some artifacts [6]. Several amendments $[5,83]$ are insufficient to remove them.

Other artifacts due to calibration errors are also observed. The current calibration and correction pipeline for IR cubes was designed to operate at a range of IR detector temperatures much smaller than the ones recorded in a large set of scenes. As a result, CRISM IR images acquired at elevated IR detector temperatures, which already suffer from more severe noise and higher frequency of bad pixels, can exhibit problematic artifacts after calibration. In some cases, the current processing pipeline also causes the
emergence of spurious absorptions occasionally in small outcrops due to TRR3 filtering on spike clusters regardless of IR detector temperature [84]. Leask et al. [84] showed that the detection of perchlorate [85] is likely to be a false positive brought by such spurious absorption features.

Practitioners successfully abate systematic, column-dependent distortions by spectral ratioing $[60-63,86]$, i.e., by dividing the spectral signature of interest with a hopefully unremarkable spectrum in the same column. The division carries, however, the risk of changing the shape of the continuum of the spectrum that may cause the misinterpretation of spectral absorption features. Furthermore, spectral ratioing requires spatial averaging as the division always amplifies random noise. This complicates the identification of species in small deposits. Finally, the selection of unremarkable spectral denominators relies on a manual and subjective inspection by the individual user.

This chapter investigates and proposes new methods for simultaneous atmospheric correction and de-noising of CRISM IR images, particularly on the wavelength region over $1.0-2.6 \mu \mathrm{~m}$, where many mineral diagnostic features are present while observed spectra are strongly affected by significant atmospheric gaseous absorption. The proposed methods remove most of the residuals of the atmospheric correction endemic in the volcano scan method and mitigates the outstanding noise even in images acquired at elevated IR detector temperatures. The removal of systematic column-dependent artifacts, makes spectral ratioing unnecessary in most cases, which will expedite the analysis of images.

I first propose simultaneous atmospheric correction and de-noising method using the adaptive background (SABCOND) for CRISM published in [55]. SABCOND extracts an atmospheric transmission spectrum directly from each image rather than estimating it from the atmospheric parameters using radiative transfer models. The underlying idea is that information regarding small static errors and time-varying and spatiallyvarying atmospheric gaseous absorption detected at a certain instrument temperature is
encoded in the spectra of each CRISM image column. On the other hand, the extraction of the underlying atmospheric transmission spectrum from the image requires isolating the atmospheric contribution from surface contributions, which are unknown a priori. I address this issue by accurately modeling the surface reflectance using a modified version of the hyperspectral unmixing with adaptive background [56]. I believe that the unmixing model is suitable since it is specifically designed for geological exploration where observed reflectance is expected to be mixed with smooth unremarkable spectra caused by dust and aerosols. SABCOND estimates the surface mixing model and the transmission spectrum in an iterative way. A de-noising stage is also integrated, where large noise spikes are flagged and removed.

Second, I introduce a methodology, which I call two-step SABCOND, that utilizes SABCOND twice, aiming for retrieving spectral signals with higher fidelity. The two-step SABCOND can address some problems and concerns in the SABCOND, while it involves additional manual and engaging procedures and applicability may be limited.

This chapter is organized as follows. Section 3.2 describes the background of this work. Section 3.3 derives optimization algorithms internally used in the SABCOND. Section 3.4 introduces the formulation of SABCOND, and Section 3.5 introduces the formulation of the two-setp SABCOND. Finally, Section 3.6 concludes this chapter.

### 3.2 Background

### 3.2.1 CRISM

CRISM is a hyperspectral imager, observing the Martian surface at hundreds of narrow wavelength bands over the visible to infrared region. The instrument has two sets of spectrographs and detector focal planes, for the VNIR wavelength region ( $0.362-1.053 \mu \mathrm{~m}$ ) and the IR wavelength region ( $1.002-3.920 \mu \mathrm{~m}$ ), with their slit shared. The VNIR and IR image cubes are simultaneously recorded during acquisition. The pitch of the spectral
channels is as good as 6.5 nm to achieve fine mineral identifications and a total of 107 bands for the VNIR and 438 bands for the IR are measured. CRISM has several observation modes with different spatial resolutions and spectral samplings to achieve multiple research objectives.

This study focuses on image cubes acquired in the Full Targeted Resolution (FRT), the Half Resolution Long (HRL), the Half Resolution Short (HRS), the Full Resolution Short (FRS), or Along Track Oversampled (ATO) modes, where the imager operates with the highest spectral resolution. I focus on IR image cubes over $1.0-2.6 \mu \mathrm{~m}$ wavelength region. This wavelength region has been used for many mineral identifications in the literature, but it is significantly affected by artifacts caused by the volcano scan method and occasionally by severe noise and other calibration errors. The proposed methods here cannot be directly expanded into other wavelength regions. For instance, applying the proposed method to the longer wavelength region $(2.8-4.0 \mu \mathrm{~m})$ of CRISM IR images would require complementing it with the compensation of the thermal emission component. For the VNIR wavelength region, artifacts and noise corrected by the proposed method are scarcely present, because of little atmospheric gaseous absorption over this range and a much lower noise level of the VNIR detector.

### 3.2.2 Volcano Scan Correction

The so-called volcano scan correction, is the atmospheric compensation method currently used in the pipeline for CRISM IR images [77, 80-82]. The technique was first proposed for atmospheric correction by the OMEGA team $[86,87]$ and has been used to produce the CRISM TER and MTRDR data products. It assumes a Beer-Lambert model for the light interaction through the atmosphere and uses empirical transmission spectra derived from the ratio of I/F spectra at the the summit and the base of Olympus Mons. The atmospheric contribution is removed by dividing each of the I/F spectra in the image by the empirically derived transmission spectra scaled appropriately by a
factor estimated for each I/F spectrum.
Let us denote the observed signal (I/F) at one pixel by $\boldsymbol{y} \in \mathbb{R}^{L \times 1}$ where $L$ is the number of wavelength channels, its associated surface reflectance by $\boldsymbol{r} \in \mathbb{R}^{L \times 1}$, and its atmospheric transmission spectrum by $t \in \mathbb{R}^{L \times 1}$. The Beer-Lambert law models the transmission spectrum by:

$$
\begin{equation*}
t_{i}=\exp \left(-k_{i} \cdot l\right) \tag{3.1}
\end{equation*}
$$

where $t_{i}$ is the $i$ th elements of $\boldsymbol{t}, k_{i}$ is the absorption coefficient at the spectral band $i$, and $l$ is the path length. The absorption coefficient is assumed to be constant along the path. Then the observed I/F spectrum is expressed as:

$$
\begin{equation*}
y_{i}=\exp \left(-k_{i} \cdot l\right) \cdot r_{i} \tag{3.2}
\end{equation*}
$$

for all $i=1, \ldots, L$, where $y_{i}$ and $r_{i}$ are the $i$ th elements of $\boldsymbol{y}$ and $\boldsymbol{r}$.
The observed I/F spectra at the top and bottom of Olympus Mons $\boldsymbol{y}^{\text {top }}$ and $\boldsymbol{y}^{\mathrm{btm}} \in$ $\mathbb{R}^{L \times 1}$ are expressed as:

$$
y_{i}^{\mathrm{top}}=\exp \left(-k_{i} \cdot l^{\mathrm{top}}\right) \cdot r_{i}^{\mathrm{top}} \quad \text { and } \quad y_{i}^{\mathrm{btm}}=\exp \left(-k_{i} \cdot l^{\mathrm{btm}}\right) \cdot r_{i}^{\mathrm{btm}}
$$

for all $i=1, \ldots, L$, where $y_{i}^{\text {top }}$ and $y_{i}^{\text {btm }}$ are the $i$ th elements of $\boldsymbol{y}^{\text {top }}$ and $\boldsymbol{y}^{\mathrm{btm}}, l^{\mathrm{top}}$ and $l^{\mathrm{btm}}$ are the path length associated with the two measurements, $r_{i}^{\mathrm{top}}$ and $r_{i}^{\mathrm{btm}}$ are the $i$ th spectral band of the surface reflectance spectra at top and bottom of the Olympus Mons. The empirical transmission spectrum $\boldsymbol{t}^{\text {emp }} \in \mathbb{R}^{L \times 1}$ is obtained by the following simple division:

$$
t_{i}^{\mathrm{emp}}=\frac{y_{i}^{\mathrm{btm}}}{y_{i}^{\mathrm{top}}}=\exp \left(-k_{i} \cdot\left(l^{\mathrm{btm}}-l^{\mathrm{top}}\right)\right)
$$

for all $i=1, \ldots, L$, where $t_{i}^{\text {emp }}$ is the $i$ th elements of $\boldsymbol{t}^{\mathrm{emp}}$. It is assumed that $r_{i}^{\text {top }}$ and $r_{i}^{\mathrm{btm}}$ are identical and they are canceled out by the division. Practically, their spectral slopes are different and slope correction is additionally performed after the simple division to compensate it.

The atmospheric transmission component of the observation I/F spectrum $\boldsymbol{y}$ is obtained by the appropriate exponential scaling of $\boldsymbol{t}^{\mathrm{emp}}$ :

$$
\begin{equation*}
t_{i}=\left(t_{i}^{\mathrm{emp}}\right)^{\beta}(i=1, \ldots, L) \tag{3.3}
\end{equation*}
$$

with

$$
\beta=\frac{l}{l^{\mathrm{btm}}-l^{\mathrm{top}}},
$$

where $l$ is the path length parameter for the observation $\boldsymbol{y}$ introduced in equation (3.1).
The volcano scan correction can be performed using the publicly available software, CRISM Analysis Toolkit (CAT). CAT estimates the the scaling exponent $\beta$ by taking the difference between two reference spectral bands $i_{1}$ and $i_{2}$ to match the magnitude of $\boldsymbol{t}^{\mathrm{emp}}$ and the transmission component of $\boldsymbol{y}$ :

$$
\beta=\frac{\log \left(y_{i_{1}} / y_{i_{2}}\right)}{\log \left(t_{i_{1}}^{\text {ep }} / t_{i_{2}}^{\text {epp }}\right)} .
$$

Here, the numerator $\log \left(y_{i_{1}} / y_{i_{2}}\right)$ should only represent the difference in transmission to measure the scale of the transmission component in the observation, and other components such as its surface reflectance and emission should have the same value. In addition, larger difference in transmission is preferred to minimize the impact of noise. Therefore, a best practice is to select two close bands that have sufficiently large difference in transmission. Since reflectance and emission spectra are, in general, continuous and slowly varying functions for CRISM wavelength samples, proximal bands are likely to have close reflectance and emission values, and would minimize the risk of having large difference in them. Such two bands can be found around $2.0 \mu \mathrm{~m}$ wavelength region, where the CRISM I/F spectrum shows a sufficiently large, sharp triplet-like absorption feature of carbon dioxide gas dominant in the Martian atmosphere. The sharpness of the absorption allows the selection of two close bands that have sufficiently large difference in transmission. In the first version of the volcano scan of the CRISM data, a spectral band associated with $\left(i_{1}=1.890 \mu \mathrm{~m}\right)$ outside of the $\mathrm{CO}_{2}$ absorption and one $\left(i_{2}=2.011 \mu \mathrm{~m}\right)$


Figure 3.1. Triplet coupled with hump-shape artifacts. Dashed line segments on the fourth and fifth spectra from the bottom show their inferred continuum level.
corresponding to a deep $\mathrm{CO}_{2}$ absorption are used. Later, McGuire et al. [5] proposed to use $i_{1}=1.980 \mu \mathrm{~m}$ and $i_{2}=2.007 \mu \mathrm{~m}$ to avoid complication with surface spectral features of hydrated phases, which is currently set as the default band set in the latest version (currently 7.4) of CAT.

Under the assumption that the atmosphere is uniform and Beer's law is sufficiently valid at the wavelength sampling of CRISM, the empirical derivation would produce sufficiently accurate transmission spectra. However, they are known to cause a number of artifacts, such as the bowl-shape artifact over $2.0 \mu \mathrm{~m}$ wavelength region, the zig-zag artifacts over the $1.1-1.7 \mu \mathrm{~m}$ wavelength region and under-correction over $2.6 \mu \mathrm{~m}$ [6]. While the bowl-shape artifact is partially addressed by the artifact correction present in the current CRISM correction software [83], it now leaves triplet-over-hump like artifacts (see Fig. 3.1) caused by the mismatch of the artifact patch in the ADR VS data and the actual bowl-shape artifacts.

The latest version of CAT also includes the optimal selection of a transmission spec-
trum for each scene among multiple empirically derived transmission spectra in the Ancillary Data Records (ADR) created for supporting different seasons and times. However, the set of available transmission spectra, which are all derived from the region around the Olympus Mons, only partially models temporal and spatial variations of atmospheric conditions and thermally-induced random shifts of the central wavelength of the detectors.

While these modifications led to significant improvements in the quality of the signal, a considerable amount of distortions remains due to atmospheric absorptions and instrument artifacts. Furthermore, you cannot theoretically scale the empirical transmission spectrum for obtaining the transmission component of an observed spectrum, as performed in Eq. (3.3). Also, multiplicative calibration errors cannot be corrected by the ADR transmission spectra since the errors are canceled out in the production of the transmission spectra by division operation.

### 3.2.2.1 Theoretical limitation of the empirical volcano scan

This section describes a theoretical limitation of the empirical volcano scan method the violation of the log-linearity of the transmission spectrum empirically obtained from the CRISM instrument:

$$
\begin{equation*}
\log y=\log t+\log r \tag{3.4}
\end{equation*}
$$

where $\boldsymbol{y} \in \mathbb{R}^{L}$ is an observed I/F spectrum vector, $\boldsymbol{r} \in \mathbb{R}^{L}$ is a surface reflectance spectrum vector, $\boldsymbol{t} \in \mathbb{R}^{L}$ is a transmission spectrum vector, and the operator log. represents the element-wise logarithmic operation of a vector. Even in the uniform atmosphere, the discretized atmospheric transmission spectrum sensed by the CRISM instrument does not decay log-linearly with respect to path length since the CRISM sensing process involves the convolution of gaseous absorption bands much narrower than the instrument's spectral response functions.

The violation of the log-linearity of the transmission was also discussed in [6] under
the simulated Martian atmospheric condition. It may occur even under much simpler conditions - the Beer-Lambert model with constant pressure and temperature without scattering. The decomposition (3.4) is the basic principle that supports the empirical volcano scan method. At a first look, the principle seems to be justified by assuming the uniformity of the atmospheric transmission spectrum and the Beer-Lambert law for radiative propagation. Even under this ideal condition, the principle itself does not hold for the implementation using the CRISM measurements because of its insufficient wavelength resolution.

The actual sensing process is expressed by the convolution of a continuous I/F spectrum with a spectral bandpass function. The spectral bandpass function models how each detector element reacts to an input radiation spectrum. An ideal spectrometer could perfectly split the light into wavelength components and its spectral response function would be a rectangle centered at the designed center wavelength of the channel. Practically such perfect spectroscope is unattainable and a spectral bandpass function is modeled as a function that peaks at the designed center wavelength of the channel, drops toward both of the wings, and converging to zero. The measured I/F at the $i$ th wavelength channel, namely the $i$ th element of $\boldsymbol{y}$, is modeled as

$$
\begin{equation*}
y_{i}=\int_{\mathcal{C}_{i}} r(w) e^{-k(w) \cdot l} f_{i}(w) d w, \tag{3.5}
\end{equation*}
$$

where $y_{i}$ is the $i$ th element of the measured I/F spectrum vector $\boldsymbol{y}, r(w)$ and $k(w)$ are a continuous reflectance spectrum and a continuous absorption coefficient spectrum as a function of wavelength $w$, respectively, $f_{i}(w)$ is the spectral bandpass function of the $i$ th channel $(i=1, \ldots, L)$ satisfying $\int f_{i}(x) d x=1$, and $\mathcal{C}_{i}$ is the effective range of $f_{i}(w)$ outside of which $f_{i}(w)$ sufficiently rolls off to zero and is thus negligible, namely $\int_{\mathcal{C}_{i}} f_{i}(x) d x \approx 1$. In case of CRISM imager, the band pass function is modeled as the summation of three Gaussian functions [4].

The right hand side of (3.5) is, in general, not log-linear with respect to $l$. The decoupling shown in (3.4) requires an additional assumption: $r(w)$ and $k(w)$ are approximately
constant over the effective range. If this assumption should be true, $r(w)$ and $k(w)$ would be reasonably taken out of the integration, making decoupling possible:

$$
y_{i} \approx \bar{r}_{i} \cdot e^{-\bar{k}_{i} \cdot l} \int_{\mathcal{C}_{i}} f_{i}(w) d w \approx \bar{r}_{i} e^{-\bar{k}_{i} \cdot l} \cdot 1
$$

where $\bar{r}_{i}$ and $\bar{k}_{i}$ are the approximated mean values of $r(w)$ and $k(w)$ over the range $\mathcal{C}_{i}$, respectively. Then, the transmission spectrum is empirically estimated by

$$
\begin{equation*}
t_{i}^{\mathrm{emp}}=\frac{\int_{\mathcal{C}_{i}} e^{-k(w) \cdot l^{\mathrm{btm}}} f_{i}(w) d w}{\int_{\mathcal{C}_{i}} e^{-k(w) \cdot l^{\mathrm{top}}} f_{i}(w) d w} \approx e^{-\bar{k}_{i} \cdot\left(l^{\mathrm{btm}}-l^{\mathrm{top})}\right.}, \tag{3.6}
\end{equation*}
$$

for $i=1, \ldots, L$, where $l^{b t m}$ and $l^{\text {top }}$ are the path lengths associated with the CRISM measurements at the bottom and top of Olympus Mons, respectively. Finally, the transmission spectrum for each pixel the scene is simply obtained by scaling with a single scaling parameter $\beta: t_{i}=\left(t_{i}^{\mathrm{emp}}\right)^{\beta}(i=1, \ldots, L)$.

The assumption that $r(\lambda)$ and $k(\lambda)$ are approximately constant over $\mathcal{C}_{i}$ indicates that their variation is sufficiently broader than the width of the effective range. Put another way, the width of the effective range, which is roughly represented by the full-width-halfmaximum (FWHM) of the spectral response function, needs to be sufficiently smaller than the scale of the variation of $r(\lambda)$ and $k(\lambda)$. While this may be valid for the surface reflectance, this assumption is hardly true for the absorption coefficient spectrum of the atmosphere. The absorption coefficient spectrum of $\mathrm{CO}_{2}$, which could be simulated using the absorption line parameters in the HITRAN database [88], exhibits many much narrower bands than the full-width-half-maximums of the CRISM wavelength channels. Thus, the empirically derived transmission spectrum vector $t_{i}^{\text {emp }}$ cannot be scaled to the transmission spectrum vector with arbitrary path length. It will cause a static error when the path length $l$ is same over pixels.

The bowl-shape artifact around the $2.0 \mu \mathrm{~m}$ wavelength region might be explained by this static error. Many isotopes of gaseous carbon dioxide have many narrow strong absorption bands around this region. The absorption coefficient spectrum varies a lot within one wavelength channel of CRISM. The approximated transmission spectrum (3.6)
is not guaranteed to accurately model the transmission spectrum with arbitrary path length. The similar pattern of the residual seen over the $1.0-2.0 \mu \mathrm{~m}$ region could be also explained by this error. Further investigation is necessary on this aspect.

### 3.2.3 CRISM noise and artifacts

This section investigates four major issues observed in the current CRISM products: 1) a systematic effect caused either by atmospheric distortions or within the calibration pipeline, 2) random noise, 3) interpolation bias, namely systematic spike trains created in the calibration pipeline, which is informally known as bed-of-nails, and 4) the spectral effect of water-ice aerosols. Here, I define an image frame as the image captured at the detector array at a time, spanning the cross-track and wavelength directions, and a pixel as an image cell in one image frame spanning the cross-track and wavelength dimensions. If the image is binned in the cross-track dimension, the pixel refers to the binned cell, not the detector element.

### 3.2.3.1 Atmospheric residuals

The residuals caused by atmospheric correction are large enough to obscure some absorption features, such as the water absorption around $1.4 \mu \mathrm{~m}$. Also, they appear to be consistent not only in the along-track direction but also in the cross-track direction over several pixels. Fig. 3.2 shows representative examples. Fig. 3.2 (a) and (b) show some atmospherically corrected I/F spectra from the same column in the image FRT00009312_07_IF166L_TRR3, compared with the transmission spectrum used for their correction by the volcano scan method. The transmission spectrum that minimizes artifacts is selected with an empirical optimization method implemented in the CAT software. Triplet-like spikes around $2.0 \mu \mathrm{~m}$, a relatively small spike around $1.44 \mu \mathrm{~m}$, and small dual spikes around $1.6 \mu \mathrm{~m}$ are likely to be residuals caused by atmospheric correction because they coincide with absorption features shown in the atmospheric transmission spectrum


Figure 3.2. I/F spectra atmospherically corrected using CAT 7.4 on TRR3 data - (a) spectra in column 156 at line 170 and every 50 lines starting 50 to 450 from top to bottom, compared with the transmission spectrum (green) used for correcting these spectra (column 156 in ADR10000000000_1B815_VS00L_9); (b) zoomed version of (a) into the $1.0-1.8 \mu \mathrm{~m}$ wavelength region; (c) spectra in the image frame (200) over neighboring columns from 153 to 159 from top to bottom; (d) the zoomed version of (c) into the $1.0-1.8 \mu \mathrm{~m}$ wavelength region. ( $\mathrm{s}, \mathrm{l}$ ) in the legends represents image coordinate (sample (column), line). All I/F spectra are offset for clarity.


Figure 3.3. Same comparison as in Fig. 3.2 of the I/F spectra from the TER product of the observation FRT00009312. Refer to Fig. 3.2 for an explanation of each panel.
(green). Overall, the current atmospheric correction exhibits a similar fluctuation pattern in the $1.0-1.7 \mu \mathrm{~m}$ and $2.0 \mu \mathrm{~m}$ regions of the corrected spectra along the cross-track column. Furthermore, Fig. 3.2 (c) and (d) indicate that the similar pattern of fluctuations is also consistently observed across the cross-track direction over several pixels. This suggests that the systematic pattern is likely to be the residual of atmospheric correction rather than a calibration error, under the assumption of the uniformity of atmospheric transmission.

These artifacts are not fully removed even in the most advanced TER products. Fig. 3.3 shows the same analysis on the corresponding TER I/F product, as performed in Fig. 3.2. One can still observe a similar fluctuation pattern on the spectra both along the column and across several neighboring columns, although the shape of such a pattern changes on the spectra in Fig. 3.2 due to additional processing made for the TER product.

Such artifacts are also observed in the simulation of the volcano scan correction using radiative transfer modeling [6]. As discussed in [6] and Section 3.2.2, some are related to the violation of the assumptions made in the empirical volcano scan method. The empirical method requires that the atmospheric transmission spectrum at the Olympus Mons be exponentially scaled to the one in the image to be corrected by a single exponential factor. Differences in atmospheric conditions, such as the amounts of dust and ice aerosols, the amount of water vapor, and temperature and pressure, from those at Olympus Mons break this assumption, causing the artifacts. This problem is partly addressed by the optimal selection of transmission spectrum from the several empirically derived transmission spectra measured in different seasons and different atmospheric conditions, although the small collection of the empirically derived spectra is unlikely to be sufficient to fully consider temporal and spatial variations. Their inverted version, hump-shape artifacts are also observed. Fig. 3.1 highlights that the continua around $2.0 \mu \mathrm{~m}$ is above the continua of the whole spectra, a hump-shape artifact exists underneath the triplets. While any triplet-like shapes would be easily recognized as artifacts, the hump/bowl-
shape artifacts are more difficult to assess, as it only affects the continuum level of the spectra. In addition, Wiseman et al. [6] showed that the absorption coefficient of carbon dioxide for each wavelength channel is not constant along the optical path due to the vertical variation of the Martian atmosphere.

### 3.2.3.2 Random noise

There are several sources of random noise in CRISM images. The behavior of noise at each detector element over time can be observed within the profile in the along track direction because the along-track direction is equivalent to the "time" direction as CRISM is a pushbroom scanner. Fig. 3.4 shows representative examples of four different aspects of the along-track dynamics of the noise - an example of a "good" detector and three different kinds of "bad" detectors, together with a spectrum that intersects those profiles. The residual ${ }^{2}$ profiles in the along-track direction of bad detectors are shown in black and that of a good detector is in red in Fig. 3.4 (b)-(d). Each of the bad detectors shows different time dependent behaviors: autoregressive random noise, random spikes, and a telegraph pattern. The residual profile shown in black in Fig. 3.4 (b) is always larger than zero and seems to be highly related to its previous residual, indicating a strong autoregressive property. The black profile in Fig. 3.4 (c) shows mostly small variance (but slightly larger than that of the good detector shown in red) and often corrupted with spiky noise of various magnitudes. The occurrence of spikes seems to be random. Finally, the black profile in Fig. 3.4 (d) shows a clear telegraph noise, exhibiting occasional sudden step-like transitions between two levels. These different sources of noise, which confirm and expand previous observations by [89], make holistic statistical modeling difficult. Fortunately when we observe a spectral profile, as shown in Fig. 3.4 (a), these various kinds of noise manifest themselves as spikes with varying magnitudes.

[^5]

Figure 3.4. (a) an I/F spectrum atmospherically corrected by the proposed method and (b)-(d) the residual profiles in the along-track direction of some wavelength channels used for the acquisition of the spectrum (a). The spectrum (a) is obtained at the image coordinate (sample, line) of $(117,275)$ in the scene image FRT00024C1A. Black profiles in (b), (c), and (d) are associated with the bands $369(1459.5 \mathrm{~nm}), 300(1913.7 \mathrm{~nm})$, and $369(2098.5 \mathrm{~nm})$ of the cross-track pixel number 117, respectively, which are supposed to be "bad." The red profiles in (b)-(d) are all from the band $342(1637 \mathrm{~nm})$, which is supposed to be "good." The black and red circles in (a) are associated with the wavelength channels of the residual profiles. The blue vertical lines in (b)-(d) shows the image frame number where the spectrum (a) is acquired.


| $\square$ | ATM-corr I/F (w/ filter) |
| :--- | :--- |
| $\square$ | ATM-corr I/F (w/o filter) |
| Bad pixels |  |
| $\square$ | Left and right neighbors |
| $\square$ | Mean of the neighbors |




Figure 3.5. Comparison of non-Filtered I/F spectra atmospherically corrected by CAT (red) with their column neighbors (gray), the mean of column neighbors (yellow), and filtered I/F spectra atmospherically corrected by CAT (blue). The image coordinates (sample, line) of these spectra are (a) $(403,172)$ in FRT0000A546, (b) $(386,166)$ in FRT000174F4, and (c) $(90,318)$ in HRL0000C0BA. Spurious features caused by the filtering over BPs are highlighted in yellow.

### 3.2.3.3 Interpolation bias

Some pixels are corrupted with elevated noise. In some pixels, only the value indicating saturation (4095 in the 12-bit format) is recorded in the raw image cube and therefore, no information relevant to radiative energy is measured. Those pixels are marked as "bad pixels" (BP), discarded, and replaced in the calibration by linear interpolation in the same wavelength channel of the spatial neighbors in the cross-track direction in each image frame [4,78]. If both sides of the neighboring pixels are not "bad", then linear interpolation is simply the mean of the neighbors.

The linear spatial interpolation of BPs sometimes causes small spikes, which we can
call interpolation bias. In a CRISM image, the continuum shapes of spatially neighboring spectra tend to be similar but their magnitudes do not completely align. In particular, the magnitude of the continuum of the spectrum does not correspond to the average of the continua of its two spatial neighbors. Every bad pixel (channel) that is replaced by the average of the spatial neighbors will exhibit a spike whose peak is exactly equal to that average. The overall effect of the interpolation is a "train" of spikes of similar magnitude. Fig. 3.5 shows three representative examples of the interpolation bias. The red spectrum has BPs marked with purple dots. These BPs are replaced with the interpolation of crosstrack spatial neighbors, namely the mean (in yellow) of the two gray spectra, if the same bands of both of the neighbors are not marked as BPs themselves. I note that not all the BPs (purple dots) are aligned exactly at their spatial average with neighbors because volcano scan correction is further applied to these spectra, or one of the neighbors could also be BPs.

The interpolation bias can be alleviated by the filtering stage in the TRR3 processing pipeline. The comparison of atmospherically corrected I/F spectra with (blue) or without (red) filtering in Fig. 3.5 (a) shows that filtering largely removes isolated spikes over $1.6-2.6 \mu \mathrm{~m}$. However, the filter is sensitive to the occurrence of many spectrally adjacent BPs. A spurious artifact is created around $1.37 \mu \mathrm{~m}$ where there is a concentration of BPs (highlighted in yellow). Fig. 3.5 (b) shows spike clusters are left over 1.4-2.0 and $2.2-2.6 \mu \mathrm{~m}$ after filtering (highlighted in yellow). Fig. 3.5 (c) shows a spurious absorption created by the filter over $2.0-2.2 \mu \mathrm{~m}$ by many adjacent BP's (highlighted in yellow). This phenomenon also explains the emergence of spike clusters and spurious absorptions investigated by [84].

The interpolation bias often occurs when the spectral continuum or shape changes rapidly in the spatial domain. In particular, it tends to happen in small areas that are spectrally distinctive from its surroundings. The BPs and interpolation bias occur more frequently on spatially binned images (HRL and HRS).


Figure 3.6. Atmospherically corrected I/F spectra by CAT that exhibit the absorption features of water ice aerosols. Their image coordinates (sample, line) are (a) $(597,220)$ in FRT0000B573 and (b) $(247,230)$ in HRL0002422E.

### 3.2.3.4 Water ice aerosols

Depending on seasons and locations, the Martian atmosphere may contain water ice aerosols, which may significantly affect acquired spectra [6]. It is reported that a significant amount of water ice aerosols is observed at low latitudes near Mars aphelion [90], which corresponds to observation IDs $\mathrm{A}^{* * *}, \mathrm{~B}^{* * *}, \mathrm{C}^{* * *}, 18^{* * *}$, or $24^{* * *}$. Water ice aerosol spectra are characterized by significant absorption features at 1.5 and $2.0 \mu \mathrm{~m}$, a shallow wide absorption over $2.3 \mu \mathrm{~m}$, and a downward slope over $2.6 \mu \mathrm{~m}$ wavelength region toward longer wavelengths. The presence of water ice aerosols in CRISM I/F spectra could be visually confirmed by the observation of both an absorption at $1.5 \mu \mathrm{~m}$ that may look like a downward continuum shift and a depression around $2.0 \mu \mathrm{~m}$ (e.g., Fig. 3.6). The depression around $2.0 \mu \mathrm{~m}$ may not be sufficient by itself to confirm the presence of water ice aerosols because it could be a bowl-shape artifact $[6,83]$. The feature at $2.0 \mu \mathrm{~m}$ can mask a mineral hydration feature at $1.9 \mu \mathrm{~m}$. While some atmospheric transmission spectra stored as "VS" in the ancillary data records (ADR) consider the presence of the water ice aerosol, the set is not extensive.

### 3.2.4 Linear mixture model with concave background

Linear mixing model (LMM) represents a single measured hyperspectral spectrum $\boldsymbol{y} \in \mathbb{R}^{L \times 1}$ ( $L$ is the number of spectral bands) as the linearly weighted sum of pure endmember spectra according to their fractional abundances:

$$
\begin{equation*}
\boldsymbol{y}=\mathbf{A} \boldsymbol{x}+\boldsymbol{n} \quad(\boldsymbol{x} \succeq \mathbf{0}), \tag{3.7}
\end{equation*}
$$

where $\mathbf{A} \in \mathbb{R}^{L \times N_{A}}$ ( $N_{A}$ is the number of endmembers) is a matrix storing endmember spectra in its columns, $\boldsymbol{x} \in \mathbb{R}^{N_{A} \times 1}$ is the vector of the abundances of the endmembers, $\boldsymbol{n} \in \mathbb{R}^{L \times 1}$ is the vector of noise, and succeq represents element-wise inequality operation. LMM is the most basic and traditional model for unmixing and has been widely used for hyperspectral unmixing $[1,91,92]$. The LMM can be easily extended to a matrix form to express the LMM for multiple observation spectra together:

$$
\begin{equation*}
\mathbf{Y}=\mathbf{A X}+\mathbf{N} \quad(\mathbf{X} \succeq \mathbf{0}), \tag{3.8}
\end{equation*}
$$

where $\mathbf{Y} \in \mathbb{R}^{L \times N}$ ( $N$ is the number of observed spectra) is the matrix whose columns stores observed spectra, $\mathbf{X} \in \mathbb{R}^{N_{A} \times N}$ is a matrix whose columns store abundances of endmembers for the observed spectra, and $\mathbf{N} \in \mathbb{R}^{L \times N}$ is a noise matrix.

The observation spectrum may have distortion from the linear combination of endmembers. Natural surfaces are easily covered with dust, which obscures observed signals. In addition, inaccurate estimation of aerosols could cause difference in the continuum of the spectra. Those effects could behave like additional endmembers in spectral mixture and result in a distortion to spectral signals [93, 94]. Furthermore, unknown (spectrally unremarkable) endmembers may be present in the library. LMM with concave background (LMM-CB) addresses these problems by augmenting the LMM with a concave "background":

$$
y=\mathbf{A} x+b+n \quad(x \succeq \mathbf{0}, \mathbf{C} b \succeq \mathbf{0})
$$

where $\boldsymbol{b} \in \mathbb{R}^{L \times 1}$ is the vector of a concave spectrum and $\mathbf{C} \in \mathbb{R}^{(L-2) \times L}$ is a concavity
operator matrix the $i$ th row of which is defined as:

$$
C_{i, j}=\left\{\begin{array}{ll}
w_{i+1}-w_{i+2} & \text { if } j=i  \tag{3.9}\\
w_{i+2}-w_{i} & \text { if } j=i+1 \\
w_{i}-w_{i+1} & \text { if } j=i+2 \\
0 & \text { otherwise }
\end{array} \quad(j=1, \ldots, L)\right.
$$

for $i=1, \ldots, L-2$, where $w_{i}$ is the center wavelength position of the $i$ th wavelength channel. It is assumed that the wavelength samples $w_{1}, w_{2}, \ldots, w_{L}$ strictly monotonically increase with respect to the spectral band indices. The $i$ th row of the inequalities $\mathbf{C B} \succeq \mathbf{0}$ represents the window of three consecutive channels $i, i+1$, and $i+2$, and can be expressed as:

$$
\begin{aligned}
& b_{i}\left(w_{i+1}-w_{i+2}\right)+b_{i+1}\left(w_{i+2}-w_{i}\right)+b_{i+2}\left(w_{i}-w_{i+1}\right) \geq 0 \\
\Leftrightarrow \quad & b_{i+1} \geq \frac{b_{i}\left(w_{i+2}-w_{i+1}\right)+b_{i+2}\left(w_{i+1}-w_{i}\right)}{w_{i+2}-w_{i}},
\end{aligned}
$$

where $b_{i}$ is the $i$ th elements of $\boldsymbol{b}$. This inequality restricts the middle point $\left(w_{i+1}, b_{i+1}\right)$ to be above the internal division at $w_{i+1}$ obtained by both neighbors $\left(w_{i}, b_{i}\right)$ and $\left(w_{i+2}, b_{i+2}\right)$, ensuring the concavity of the curvature over the three channels $i, i+1$, and $i+2$, i.e., the middle point of the three channels is above the line segment determined by the other two adjacent points. The collection of these inequalities for all $i=1, \ldots, L-2$ constrains the whole curvature of $\boldsymbol{b}$ to be concave. Note that, if spectral sampling is uniform, the matrix $\mathbf{C}$ becomes much simpler, but the definition of $\mathbf{C}$ is more general and applicable to non-uniform sampling, which you may encounter when you manually exclude some badly behaving spectral bands, e.g., BP bands of CRISM.

The concave background spectra are interpreted as continuum components, which are conventionally considered to be generally spectrally unremarkable and insignificant for the presence of scientifically meaningful species in geological applications [95-97]. In addition, the concave background spectra fit the contribution of unknown dust aerosols prevalent on Mars that may give negative slopes in this wavelength region [6, 93, 98]. Although the dust aerosols residing in the atmosphere cannot be considered as a part of surface, it improves the fit to the observed I/F spectra.

Next, I convert the expression (3.9) into another format that can be easily handled in optimization problems. Let us create a square matrix $\overline{\mathbf{C}} \in \mathbb{R}^{L \times L}$ by augmenting the first and last rows of $\mathbf{C}$ with cardinal vectors $\boldsymbol{e}_{1}=[1,0, \ldots, 0]^{\top} \in \mathbb{R}^{L}$ and $\boldsymbol{e}_{L}=[0, \ldots, 0,1]^{\boldsymbol{\top}} \in$ $\mathbb{R}^{L}$, respectively:

$$
\overline{\mathbf{C}}=\left[\begin{array}{ll}
e_{1} & \mathbf{C}^{\top} \\
e_{L}
\end{array}\right]^{\top} .
$$

Since $\overline{\mathbf{C}}$ is a tri-diagonal matrix whose diagonal elements are nonzero, it is invertible. Let $\boldsymbol{z}=\overline{\mathbf{C}} \boldsymbol{b}$, namely, we have $\boldsymbol{b}=\overline{\mathbf{C}}^{-1} \boldsymbol{z}$. Let

$$
\gamma=\left[\begin{array}{c}
-\infty \\
\mathbf{0}_{L-2} \\
-\infty
\end{array}\right]
$$

where $\mathbf{0}_{L-2}$ is an $(L-2) \times 1$ vector whose elements are all zeros. The constraint $\mathbf{C} \boldsymbol{b} \succeq \mathbf{0}$ is equivalently expressed as $\boldsymbol{z} \succeq \gamma$. Then LMM-CB can also be formulated as:

$$
\boldsymbol{y}=\mathbf{A} \boldsymbol{x}+\overline{\mathbf{C}}^{-1} \boldsymbol{z}+\boldsymbol{n} \quad(\boldsymbol{x} \succeq \mathbf{0}, \boldsymbol{z} \succeq \gamma) .
$$

This format is useful as the term $\overline{\mathbf{C}}^{-1} \boldsymbol{z}$ is easy to stack with the LMM term $\mathbf{A} \boldsymbol{x} \cdot \overline{\mathbf{C}}^{-1}$ has also an interesting geometric property. The $i$ th column of $\overline{\mathbf{C}}^{-1}$ is a triangular spectrum that is based at the both edge (namely, the first and last elements of the $i$ th column $\boldsymbol{c}_{i}$, $\left(\boldsymbol{c}_{i}\right)_{1}$ and $\left(\boldsymbol{c}_{i}\right)_{L}$, are equal to zero) and topped at the $i$ th element $\left(\left(\boldsymbol{c}_{i}\right)_{i}\right.$ is the top of the triangle). It controls the strict local concavity at the $i$ th element over three successive channels centered at $i$. This matrix $\overline{\mathbf{C}}^{-1}$ can interpreted as a concave base matrix, as it stacks all the substantial components (concave bases) for representing arbitrary concave curvatures.

As performed for the LMM (3.8), LMM-CB can also be expressed in a matrix form:

$$
\begin{equation*}
\mathbf{Y}=\mathbf{A} \mathbf{X}+\overline{\mathbf{C}}^{-1} \mathbf{Z}+\mathbf{N} \quad(\mathbf{X} \succeq \mathbf{0}, \mathbf{Z} \succeq \boldsymbol{\Gamma}) \tag{3.10}
\end{equation*}
$$

where $\mathbf{Z} \in \mathbb{R}^{L \times N}$ is a matrix whose columns stores the coefficients of the concave bases and $\boldsymbol{\Gamma} \in \mathbb{R}^{L \times N}$ is the $N$ replication of $\gamma$ in the column dimension: $\boldsymbol{\Gamma}=\gamma \cdot \mathbf{1}_{1 \times N}$, where $\mathbf{1}_{1 \times N}$ is a $1 \times N$ vector whose elements are all ones.

### 3.2.5 Related work

To improve upon the traditional volcano-scan technique, atmospheric-correction approaches based on forward modeling of radiative transfer using discrete ordinate radiative transfer code (DISORT) have been proposed [99-103]. Input atmospheric parameters are initialized/estimated from Martian climatological data measured by other instruments. This method also considers scattering and absorption by dust and water ice aerosols.

The presence of noise and artifacts in CRISM products have compelled the development of several de-noising approaches. For the previous iteration of CRISM targeted observations (TRR2), the CRISM Iterative Recognition and Removal of Unwanted Spiking (CIRRUS) [104] and a filtering based approach implemented within the mapping method proposed by [105] were implemented. The major update of the CRISM targeted products to version 3 (TRR3) provided an improvement in calibration with the addition of TRR3 filtering [78,106]. In this new era, a denoising method [107] and a Complement to CRISM Analysis Toolkit (CoTCAT) [108] were proposed to complement the TRR3 filtering. More recently, Kreisch et al. [103] implemented a simultaneous de-noising and map-projecting method using a maximum likelihood for single scattering albedo obtained by DISORT under that assumption that noise follows a Poisson distribution, combining with prior processing using a median filter. He et al. [109] advanced this idea by injecting hypothesis testing into maximum likelihood based de-noising method, which allows the automatic evaluation of noise distribution.

### 3.3 Convex optimization algorithms for SABCOND

This section describes algorithms for efficiently solving convex optimization problems encountered in SABCOND. I starts with a brief introduction of alternating direction method of multipliers (ADMM), which has been widely used to solve minimization problems in hyperspectral unmixing [45, 110-122]. I also review a technique called
residual balancing, that balances the magnitude of a penalty term commonly used for ADMM to practically achieve faster convergence. Then, I propose ADMM with generalized augmented terms (ADMM-GAT) and a modified residual balance technique tailored for ADMM-GAT, which are subsequently applied to two convex optimization problems: least absolute deviation (LAD) and constrained basis pursuit (CBP) problems that are internally employed in SABCOND. Finally, it is shown that how convex optimization problems in SABCOND can be equivalently transformed into CBP formats to enable the utilization ADMM-GAT algorithms for CBP.

This section is organized as follows. Section 3.3 .1 briefly reviews ADMM and its residual balancing technique. Section 3.3.2 describes the theory of ADMM-GAT, including the new residual balancing technique (Section 3.3.2.1), the application of ADMM-GAT to LAD and CBP (Section 3.3.2.2), a compromised version of the residual balancing for batch processing of these two applications (Section 3.3.2.3), and then their pseudo codes (Section 3.3.2.4). Finally, Section 3.3.3 shows the equivalent transformation of the several convex optimization problems into the CBP formats.

### 3.3.1 ADMM

ADMM is an algorithm for solving convex optimization problems that combines the dual ascent method and the augmented Lagrangian method [123]. ADMM solves problems expressed in the following format:

$$
\begin{array}{ll}
\underset{\boldsymbol{x}, \boldsymbol{y}}{\operatorname{minimize}} & f(\boldsymbol{x})+g(\boldsymbol{z})  \tag{3.11}\\
\text { subject to } & \mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}=\boldsymbol{c}
\end{array}
$$

where $\boldsymbol{x} \in \mathbb{R}^{m}, \boldsymbol{z} \in \mathbb{R}^{n} \boldsymbol{c} \in \mathbb{R}^{p}, \mathbf{A} \in \mathbb{R}^{p \times m}, \mathbf{B} \in \mathbb{R}^{p \times n}$, and $f$ and $g$ are convex functions with respect to $\boldsymbol{x}$ and $\boldsymbol{z}$, respectively. ADMM considers a Lagrangian with an augmentation term:

$$
\begin{equation*}
\mathcal{L}_{\rho}(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{y})=f(\boldsymbol{x})+g(\boldsymbol{z})+\boldsymbol{y}^{\boldsymbol{\top}}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c})+\frac{\rho}{2}\|\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c}\|_{2}^{2} \tag{3.12}
\end{equation*}
$$

where $\boldsymbol{y} \in \mathbb{R}^{p}$ is a vector of Lagrangian multipliers and $\rho(>0)$ is a scalar spectral penalty parameter. ADMM iterates the following procedure until convergence:

$$
\begin{align*}
& \boldsymbol{x}^{(k+1)} \underset{\boldsymbol{x}}{\arg \min } \mathcal{L}_{\rho}\left(\boldsymbol{x}, \boldsymbol{z}^{(k)}, \boldsymbol{y}^{(k)}\right)  \tag{3.13a}\\
& \boldsymbol{z}^{(k+1)} \leftarrow \underset{\boldsymbol{z}}{\arg \min } \mathcal{L}_{\rho}\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{z}, \boldsymbol{y}^{(k)}\right)  \tag{3.13b}\\
& \boldsymbol{y}^{(k+1)} \leftarrow \boldsymbol{y}^{(k)}+\rho\left(\mathbf{A} \boldsymbol{x}^{(k+1)}-\mathbf{B} \boldsymbol{z}^{(k+1)}-\boldsymbol{c}\right), \tag{3.13c}
\end{align*}
$$

where the superscript ( $k$ ) indicates the number of iteration. The first two update equations (3.13a) and (3.13b) are the minimization of the augmented Lagrangian with respect to primal variables. The equation (3.13c) is a dual ascent step. Similarly, the scaled form of the augmented Lagrangian is

$$
\mathcal{L}_{\rho d}(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{d})=f(\boldsymbol{x})+g(\boldsymbol{z})+\rho \boldsymbol{d}^{\top}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c})+\frac{\rho}{2}\|\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c}\|_{2}^{2}
$$

where $\boldsymbol{d}=\boldsymbol{y} / \rho$ is the vector of a scaled Lagrangian multipliers and its update scheme is

$$
\begin{align*}
& \boldsymbol{x}^{(k+1)} \leftarrow \underset{\boldsymbol{x}}{\arg \min } \mathcal{L}_{\rho d}\left(\boldsymbol{x}, \boldsymbol{z}^{(k)}, \boldsymbol{d}^{(k)}\right)  \tag{3.14a}\\
& \boldsymbol{z}^{(k+1)} \leftarrow \underset{\boldsymbol{z}}{\arg \min } \mathcal{L}_{\rho d}\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{z}, \boldsymbol{d}^{(k)}\right)  \tag{3.14b}\\
& \boldsymbol{d}^{(k+1)} \leftarrow \boldsymbol{d}^{(k)}+\left(\mathbf{A} \boldsymbol{x}^{(k+1)}-\mathbf{B} \boldsymbol{z}^{(k+1)}-\boldsymbol{c}\right) . \tag{3.14c}
\end{align*}
$$

The convergence of the ADMM algorithm can be assessed by the residual of primal and dual feasibility conditions [123,124]:

$$
\begin{aligned}
& \boldsymbol{r}^{(k+1)}=\mathbf{A} \boldsymbol{x}^{(k+1)}+\mathbf{B} \boldsymbol{z}^{(k+1)}-\boldsymbol{c} \\
& \boldsymbol{s}^{(k+1)}=\rho \mathbf{A}^{\top} \mathbf{B}\left(\boldsymbol{z}^{(k+1)}-\boldsymbol{z}^{(k)}\right) .
\end{aligned}
$$

The primary residual evaluates how much the equality constraint in the primal problem (3.11) is violated. The dual residual is associated the amount of the violation of the stationary condition of the Lagrangian without the augmented term. At the very optima, both of the residual must be equal to zero and their magnitudes indicate the degree of convergence of the minimization problem. Boyd et al. [123] show that the magnitude of these primal and dual residuals can bound the difference between the current cost and
the optimal cost. Therefore, if both $\left\|\boldsymbol{r}^{(k+1)}\right\|_{2}$ and $\left\|\boldsymbol{s}^{(k+1)}\right\|_{2}$ become smaller than the pre-defined tolerance, the current cost is considered to be sufficiently close to the optimal cost, and the iteration of the algorithm is stopped.

While the convergence of the algorithm can be theoretically verified for any $\rho$, the rate of convergence is affected by $\rho$. Residual balancing $[123,124]$ is a common heuristic to automatically adjust $\rho$ to practically achieve faster convergence, although convergence is not guaranteed in general unless $\rho$ is fixed after a finite number of iterations. Residual balancing keeps the primal and dual residuals within the same order of magnitude. If the primal residual becomes excessively larger than the dual residual, the residual balancing increases $\rho$. If the dual residual becomes excessively larger than the primal residual, it decreases $\rho$. Practically, the following operation is performed:

$$
\rho \leftarrow \begin{cases}\tau \rho & \text { if }\left\|\boldsymbol{r}^{(k+1)}\right\|_{2} \geq \mu\left\|\boldsymbol{s}^{(k+1)}\right\|_{2}  \tag{3.15}\\ \rho / \tau & \text { if }\left\|\boldsymbol{s}^{(k+1)}\right\|_{2} \geq \mu\left\|\boldsymbol{r}^{(k+1)}\right\|_{2} \\ \rho & \text { otherwise }\end{cases}
$$

where $\tau$ and $\mu$ are normally predefined hyper parameters. Typical values are $\tau=10$ and $\mu=2$. This operation is intuitively interpreted as follows. $\rho$ controls the balance between the Lagrangian and the augmented term. If the primal residual $\mathbf{A} \boldsymbol{x}^{(k+1)}+\mathbf{B} \boldsymbol{z}^{(k+1)}-\boldsymbol{c}$ is too large, then $\rho$ is increased to strengthen the impact of the augmented term in the augmented Lagrangian (3.12). Large dual residual indicates the augmented term is weighted too much and it is reasonable to reduce its weight by decreasing the value of $\rho$.

### 3.3.2 ADMM-GAT

ADMM-GAT generalizes ADMM by introducing a different spectral penalty parameter for each constraint. ADMM-GAT is briefly mentioned in Section 3.4.2 in [123], where they only comment that you can allow a different spectral penalty parameter for each constraint. They also mention that you can generalize it even more by replacing $\rho$ with a symmetric positive definite matrix $\mathbf{P}$ that allows a decomposition $\mathbf{P}=\mathbf{F}^{\top} \mathbf{F}$, and re-
place the equality constraint $\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{x}-\boldsymbol{c}=\mathbf{0}$ by $\mathbf{F}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{x}-\boldsymbol{c})=\mathbf{0}$, to cast it as a standard ADMM. However, there is no further investigation on the benefits of the generalizations and how $\mathbf{F}$ should be determined. In addition, it is not clear how residual balancing, which turned out to practically speed up the convergence of ADMM, can be implemented for ADMM-GAT. This section will investigate ADMM-GAT, which allows a spectral penalty parameter for each constraint, and further provides a residual balancing technique tailored to the ADMM-GAT.

ADMM-GAT considers the same minimization problem (3.11) as ADMM and defines the augmented Lagrangian with a diagonal spectral penalty parameter matrix $\mathbf{P} \in \mathbb{R}^{p \times p}$, instead of the scalar penalty parameter $\rho$ :

$$
\begin{align*}
\mathcal{L}_{P}(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{y})= & f(\boldsymbol{x})+g(\boldsymbol{z})+\boldsymbol{y}^{\top}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c}) \\
& +\frac{1}{2}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c})^{\top} \mathbf{P}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c}) \tag{3.16}
\end{align*}
$$

Letting $\boldsymbol{r}=\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c}$, the augmented term is also expressed as:

$$
\begin{equation*}
\frac{1}{2} \boldsymbol{r}^{\top} \mathbf{P} \boldsymbol{r}=\frac{1}{2} \sum_{i=1}^{p} P_{i} r_{i}^{2} \tag{3.17}
\end{equation*}
$$

where $P_{i}$ is the $(i, i)$ element of $\mathbf{P}$, and $r_{i}$ is the $i$ th element of $\boldsymbol{r}$. This indicates that $P_{i}$ only penalizes the $i$ th element of the equality constraint $\boldsymbol{r}=\mathbf{0}$, and therefore it is the spectral penalty parameter dedicated to the $i$ th constraint. I also note that $\mathcal{L}_{P}$ can be expressed using a square diagonal matrix $\mathbf{F} \in \mathbb{R}^{\times p}$ whose $(i, i)$ element $\mathrm{F}_{i i}$ is equal to $\sqrt{P_{i}}\left(\right.$ therefore, $\left.\mathbf{F}^{\boldsymbol{\top}} \mathbf{F}=\mathbf{P}\right)$ as:

$$
\begin{equation*}
\mathcal{L}_{P}(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{y})=f(\boldsymbol{x})+g(\boldsymbol{z})+\boldsymbol{y}^{\boldsymbol{\top}}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c})+\frac{1}{2}\|\mathbf{F}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c})\|_{2}^{2} . \tag{3.18}
\end{equation*}
$$

This formulation does not replace the equality constraint $\boldsymbol{r}=\mathbf{0}$ with $\mathbf{F r}=\mathbf{0}$, but it does not make any difference in any case, especially when you consider its scaled form.

The scheme of the ADMM-GAT is same as that of ADMM in equations (3.13a),
(3.13b), and (3.13c), which is the iteration of the following problems:

$$
\begin{align*}
& \boldsymbol{x}^{(k+1)} \leftarrow \underset{\boldsymbol{x}}{\arg \min } \mathcal{L}_{P}\left(\boldsymbol{x}, \boldsymbol{z}^{(k)}, \boldsymbol{y}^{(k)}\right)  \tag{3.19a}\\
& \boldsymbol{z}^{(k+1)} \leftarrow \underset{\boldsymbol{z}}{\arg \min } \mathcal{L}_{P}\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{z}, \boldsymbol{y}^{(k)}\right)  \tag{3.19b}\\
& \boldsymbol{y}^{(k+1)} \leftarrow \boldsymbol{y}^{(k)}+\mathbf{P}\left(\mathbf{A} \boldsymbol{x}^{(k+1)}-\mathbf{B} \boldsymbol{z}^{(k+1)}-\boldsymbol{c}\right) \tag{3.19c}
\end{align*}
$$

Similarly, the scaled form of the augmented Lagrangian is $\mathcal{L}_{P d}(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{d})=f(\boldsymbol{x})+g(\boldsymbol{z})+\boldsymbol{d}^{\top} \mathbf{P}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c})+\frac{1}{2}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c})^{\top} \mathbf{P}(\mathbf{A} \boldsymbol{x}+\mathbf{B} \boldsymbol{z}-\boldsymbol{c})$, where $\boldsymbol{d}=\mathbf{P}^{-1} \boldsymbol{y}$ is the vector of a scaled Lagrangian multipliers and its update scheme is

$$
\begin{align*}
& \boldsymbol{x}^{(k+1)} \leftarrow \underset{\boldsymbol{x}}{\arg \min } \mathcal{L}_{P d}\left(\boldsymbol{x}, \boldsymbol{z}^{(k)}, \boldsymbol{d}^{(k)}\right)  \tag{3.20a}\\
& \boldsymbol{z}^{(k+1)} \leftarrow \underset{\boldsymbol{z}}{\arg \min } \mathcal{L}_{P d}\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{z}, \boldsymbol{d}^{(k)}\right)  \tag{3.20b}\\
& \boldsymbol{d}^{(k+1)} \leftarrow \boldsymbol{d}^{(k)}+\left(\mathbf{A} \boldsymbol{x}^{(k+1)}-\mathbf{B} \boldsymbol{z}^{(k+1)}-\boldsymbol{c}\right) . \tag{3.20c}
\end{align*}
$$

Similar to ADMM, the convergence of ADMM-GAT can be verified by the primal and dual residuals:

$$
\begin{align*}
\boldsymbol{r}^{(k+1)} & =\mathbf{A} \boldsymbol{x}^{(k+1)}+\mathbf{B} \boldsymbol{z}^{(k+1)}-\boldsymbol{c}  \tag{3.21a}\\
\boldsymbol{s}_{P}^{(k+1)} & =\mathbf{A}^{\top} \mathbf{P B}\left(\boldsymbol{z}^{(k+1)}-\boldsymbol{z}^{(k)}\right) . \tag{3.21b}
\end{align*}
$$

The dual residual is obtained by taking the stationary condition of the problem (3.20a), as shown in Section 3.3 in [123] for ADMM:

$$
\begin{aligned}
0 & \in \boldsymbol{\partial}_{\boldsymbol{x}} \mathcal{L}_{P}\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{z}^{(k)}, \boldsymbol{y}^{(k)}\right) \\
& =\boldsymbol{\partial}_{\boldsymbol{x}} f\left(\boldsymbol{x}^{(k+1)}\right)+\mathbf{A}^{\top} \boldsymbol{y}^{(k)}+\mathbf{A}^{\top} \mathbf{P}\left(\mathbf{A} \boldsymbol{x}^{(k+1)}+\mathbf{B} \boldsymbol{z}^{(k)}-\boldsymbol{c}\right) \\
& =\boldsymbol{\partial}_{\boldsymbol{x}} f\left(\boldsymbol{x}^{(k+1)}\right)+\mathbf{A}^{\top}\left(\boldsymbol{y}^{(k)}+\mathbf{P}\left(\mathbf{A} \boldsymbol{x}^{(k+1)}+\mathbf{B} \boldsymbol{z}^{(k+1)}-\boldsymbol{c}\right)\right)+\mathbf{A}^{\top} \mathbf{P B}\left(\boldsymbol{z}^{(k)}-\boldsymbol{z}^{(k+1)}\right) \\
& =\boldsymbol{\partial}_{\boldsymbol{x}} f\left(\boldsymbol{x}^{(k+1)}\right)+\mathbf{A}^{\top} \boldsymbol{y}^{(k+1)}+\mathbf{A}^{\top} \mathbf{P B}\left(\boldsymbol{z}^{(k)}-\boldsymbol{z}^{(k+1)}\right),
\end{aligned}
$$

where $\boldsymbol{\partial}_{\boldsymbol{x}}$ represents the subgradient operator for a function with respect to $\boldsymbol{x}$ and $\boldsymbol{\partial}_{\boldsymbol{x}} \mathcal{L}_{P}\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{z}^{(k)}, \boldsymbol{y}^{(k)}\right)$ and $\boldsymbol{\partial}_{\boldsymbol{x}} f\left(\boldsymbol{x}^{(k+1)}\right)$ are the subgradients of $\mathcal{L}_{P}$ and $f$ with respect
to $\boldsymbol{x}$ at $\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{z}^{(k)}, \boldsymbol{y}^{(k)}\right)$ and $\boldsymbol{x}^{(k+1)}$, respectively. Namely we have

$$
\mathbf{A}^{\top} \mathbf{P B}\left(\boldsymbol{z}^{(k+1)}-\boldsymbol{z}^{(k)}\right) \in \boldsymbol{\partial}_{\boldsymbol{x}} f\left(\boldsymbol{x}^{(k+1)}\right)+\mathbf{A}^{\top} \boldsymbol{y}^{(k+1)},
$$

where the right hand side is identical to the stationary condition of the Lagrangian without the augmented term with respect to $\boldsymbol{x}$. Therefore, the left hand side is considered to be the residual for the stationary condition.

ADMM-GAT is potentially beneficial over ADMM. If the elements of primal residual $r$ have large variation, it is likely that an optimal spectral parameter is different for each element. ADMM-GAT allows the adjustment of the spectral penalty parameters for each element, and could further speed up the convergence. In addition, a benefit is observed for the optimization of the dual variable. As we can see from the update of the dual variable, Eq. (3.13c) (or Eq. (3.19c)), $\rho$ (or $\mathbf{P}$ ) controls the learning rate of the dual variable. If you have large diversity among the elements of the dual variable, a different learning rate for each element of the dual variable would accelerate the algorithm toward convergence.

### 3.3.2.1 Residual-balancing for ADMM-GAT

Since, in general, we do not know the optimal spectral penalty parameters in advance, automatic adjustment methods, such as residual balancing, would be necessary to take advantage of the generalization. Although residual balancing supports only ADMM with a single spectral penalty parameter, its idea can be extended to ADMM-GAT to further increase its convergence rate.

Residual balancing controls the balance of the primal residual and the dual residual. A single scalar $\rho$ is the only spectral penalty parameter affects both of them, and their total magnitudes are evaluated. In ADMM-GAT, you could still think about balancing the primal and dual residuals. We can evaluate the balance of the primal and dual residuals for each spectral penalty parameter $P_{i}$. This can be realized by decomposing the primal and dual variables with respect to $P_{i}$ and then, assessing the balance of each
pair of the primal and dual components associated with $P_{i}$.
The component of the primal residual associated with $P_{i}$ can be directly observed from the decomposition (3.17) of the augmented term of $\mathcal{L}_{P}$. Each $P_{i}$ only penalizes the $i$ th element $r_{i}$ of $\boldsymbol{r}$, Therefore, the component of $\boldsymbol{r}^{(k+1)}$ associated with $P_{i}$ is determined to $r_{i}^{(k+1)}$. To obtain its counterpart in the dual residual, let us start with an expansion of each element of the dual residual $(3.21 \mathrm{~b}) \boldsymbol{s}_{P}^{(k+1)}$ with respect to $P_{i}$ :

$$
\left(s_{P}^{(k+1)}\right)_{j}=\sum_{i=1}^{p} P_{i} \cdot \mathrm{~A}_{i j} \cdot \boldsymbol{b}^{i} \cdot\left(\boldsymbol{z}^{(k+1)}-\boldsymbol{z}^{(k)}\right) \quad(j=1, \ldots, m),
$$

where $\left(s_{P}^{(k+1)}\right)_{j}$ is the $j$ th element of $\boldsymbol{s}_{P}^{(k+1)}, \mathrm{A}_{i j}$ is the $(i, j)$ element of $\mathbf{A}$ and $\boldsymbol{b}^{i}$ is the $i$ th row of $\mathbf{B}$. Therefore, we can expand $\boldsymbol{s}^{(k+1)}$ with respect to $P_{i}$ by stacking $\left(s_{P}^{(k+1)}\right)_{j}$ for $j=1, \ldots, m$ in a column:

$$
\boldsymbol{s}_{P}^{(k+1)}=\sum_{i=1}^{p} P_{i} \cdot\left[\begin{array}{c}
\mathrm{A}_{i 1} \\
\mathrm{~A}_{i 2} \\
\vdots \\
\mathrm{~A}_{i m}
\end{array}\right] \cdot \boldsymbol{b}^{i} \cdot\left(\boldsymbol{z}^{(k+1)}-\boldsymbol{z}^{(k)}\right)=\sum_{i=1}^{p} P_{i} \cdot \boldsymbol{a}^{i \boldsymbol{\top}} \cdot \boldsymbol{b}^{i} \cdot\left(\boldsymbol{z}^{(k+1)}-\boldsymbol{z}^{(k)}\right),
$$

where $\boldsymbol{a}^{i}=\left[\begin{array}{llll}\mathrm{A}_{i 1} & \mathrm{~A}_{i 2} & \ldots & \mathrm{~A}_{i m}\end{array}\right] \in \mathbb{R}^{1 \times m}$ is the $i$ th row of $\mathbf{A}$. The $i$ th component in the summation is considered as the dual residual associated with $P_{i}$ and denote it by $\boldsymbol{\sigma}_{P_{i}}^{(k+1)}=P_{i} \cdot \boldsymbol{a}^{i^{\top}} \cdot \boldsymbol{b}^{i} \cdot\left(\boldsymbol{z}^{(k+1)}-\boldsymbol{z}^{(k)}\right)$. Then, in a similar way to the operation (3.15) for ADMM, residual balancing for ADMM-GAT can be performed for each element $P_{i}$ by comparing the magnitudes of its associated primal and dual residuals:

$$
P_{i} \leftarrow \begin{cases}\tau P_{i} & \text { if }\left|r_{i}^{(k+1)}\right| \geq \mu\left\|\boldsymbol{\sigma}_{P_{i}}^{(k+1)}\right\|_{2} \\ P_{i} / \tau & \text { if }\left\|\boldsymbol{\sigma}_{P_{i}}^{(k+1)}\right\|_{2} \geq \mu\left|r_{i}^{(k+1)}\right| \\ P_{i} & \text { otherwise }\end{cases}
$$

for $i=1, \ldots, p$. Again, $\tau$ and $\mu$ are predefined hyper parameters. Typical values are $\tau=10$ and $\mu=2$.

### 3.3.2.2 Examples of ADMM-GAT realizations

This section shows the two examples of the ADMM-GAT algorithm for LAD and CBP. In these examples, the spectral penalty parameter matrix $\mathbf{P}$ is further replaced
with $\rho \mathbf{P}$. This redundant generalization is beneficial when solving the collection of the same problem with partially independent input parameters. With $\rho=1$, it is easy to go back to the original ADMM-GAT formulation.

### 3.3.2.2.1 ADMM-GAT for LAD

Least absolute deviation (LAD) is defined as:

$$
\text { LAD : } \underset{\boldsymbol{x}}{\operatorname{minimize}}\|\boldsymbol{h}-\mathbf{A} \boldsymbol{x}\|_{1},
$$

where $\boldsymbol{x} \in \mathbb{R}^{n}, \mathbf{A} \in \mathbb{R}^{m \times n}$, and $\boldsymbol{h} \in \mathbb{R}^{m}$. Letting $\boldsymbol{z}=\mathbf{A} \boldsymbol{x}-\boldsymbol{h}$, the above problem is reformulated as

$$
\begin{array}{ll}
\underset{\boldsymbol{x}, \boldsymbol{z}}{\operatorname{minimize}} & \|\boldsymbol{z}\|_{1} \\
\text { subject to } & \mathbf{A} \boldsymbol{x}-\boldsymbol{z}=\boldsymbol{h}
\end{array}
$$

The scaled version of the generalized augmented Lagrangian of this problem is

$$
\begin{aligned}
\mathcal{L}_{P d}(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{d}) & =\|\boldsymbol{z}\|_{1}+\rho \boldsymbol{d}^{\top} \mathbf{F}^{\top} \mathbf{F}(\mathbf{A} \boldsymbol{x}-\boldsymbol{z}-\boldsymbol{h})+\frac{\rho}{2}\|\mathbf{F}(\mathbf{A} \boldsymbol{x}-\boldsymbol{z}-\boldsymbol{h})\|_{2}^{2} \\
& =\|\boldsymbol{z}\|_{1}+\frac{\rho}{2}\|\mathbf{F}(\mathbf{A} \boldsymbol{x}-\boldsymbol{z}-\boldsymbol{h}+\boldsymbol{d})\|_{2}^{2}-\frac{\rho}{2}\|\mathbf{F} \boldsymbol{d}\|_{2}^{2}
\end{aligned}
$$

where $\rho$ is a scalar spectral penalty parameter, $\mathbf{F} \in \mathbb{R}^{m \times m}$ is a diagonal spectral penalty parameter matrix such that $\mathbf{F}^{\top} \mathbf{F}=\mathbf{P}$, and $\boldsymbol{d} \in \mathbb{R}^{n}$ is a vector of Lagrangian multipliers. The ADMM-GAT algorithm solves the minimization problem by the alternating optimization of the following

$$
\begin{align*}
& \boldsymbol{x}^{(k+1)} \leftarrow \underset{\boldsymbol{x}}{\arg \min } \frac{\rho}{2}\left\|\mathbf{F}\left(\mathbf{A} \boldsymbol{x}-\boldsymbol{z}^{(k)}-\boldsymbol{h}+\boldsymbol{d}^{(k)}\right)\right\|_{2}^{2} \\
& \boldsymbol{z}^{(k+1)} \leftarrow \underset{\boldsymbol{z}}{\arg \min }\|\boldsymbol{z}\|_{1}+\frac{\rho}{2}\left\|\mathbf{F}\left(\mathbf{A} \boldsymbol{x}^{(k+1)}-\boldsymbol{z}-\boldsymbol{h}+\boldsymbol{d}^{(k)}\right)\right\|_{2}^{2} \\
& \boldsymbol{d}^{(k+1)} \leftarrow \boldsymbol{d}^{(k)}+\left(\mathbf{A} \boldsymbol{x}^{(k+1)}-\boldsymbol{z}^{(k+1)}\right), \tag{3.22}
\end{align*}
$$

where $k$ indicates the number of iteration. The update of $\boldsymbol{x}$ is an unconstrained last square problem.

$$
\begin{equation*}
\boldsymbol{x}^{(k+1)} \leftarrow\left(\mathbf{A}^{\top} \mathbf{P A}\right)^{-1} \mathbf{A}^{\top} \mathbf{P}\left(\boldsymbol{h}+\boldsymbol{z}^{(k)}-\boldsymbol{d}^{(k)}\right) . \tag{3.23}
\end{equation*}
$$

Since $\mathbf{P}$ is a diagonal matrix, the minimization with regard to $\boldsymbol{z}$ becomes separable for each element:

$$
\begin{equation*}
\boldsymbol{z}^{(k+1)} \leftarrow \operatorname{soft}\left(\mathbf{A} \boldsymbol{x}^{(k+1)}-\boldsymbol{h}+\boldsymbol{d}^{(k)}, \frac{1}{\rho} \cdot \operatorname{diag}\left(\mathbf{P}^{-1}\right)\right) \tag{3.24}
\end{equation*}
$$

where $\operatorname{diag}\left(\mathbf{P}^{-1}\right)=\left[\begin{array}{llll}1 / P_{1} & 1 / P_{2} \ldots 1 / P_{m}\end{array}\right]^{\top} \in R^{m}$ and $\operatorname{soft}(\cdot)$ is a function for performing element-wise soft-thresholding of the vector of the first input (or matrix):

$$
\begin{gathered}
\operatorname{soft}(\boldsymbol{x}, \boldsymbol{\kappa})=\boldsymbol{x}_{\boldsymbol{\kappa}}, \\
\text { where } \quad \boldsymbol{x}_{\boldsymbol{\kappa}}[i]= \begin{cases}0 & \text { if }|\boldsymbol{x}[i]| \leq \kappa \\
\operatorname{sign}(\boldsymbol{x}[i]) \cdot(|\boldsymbol{x}[i]|-\kappa) & \text { otherwise. }\end{cases}
\end{gathered}
$$

This algorithm converges much faster than the original ADMM especially when the solution of the unconstrained problem is much differ from its constraint version. The drawback is that the matrix inversion in the equation (3.23) needs updating whenever $\mathbf{P}$ is updated.

### 3.3.2.2.2 ADMM-GAT for CBP

Constrained basis pursuit (CBP) de-nosing problem is defined as:

$$
\begin{array}{ll}
\underset{\boldsymbol{x}}{\operatorname{minimize}} & \left\|\boldsymbol{c}_{1} \odot \boldsymbol{x}\right\|_{1}  \tag{3.25}\\
\text { subject to } & \boldsymbol{G} \boldsymbol{x}=\boldsymbol{h} \text { and } \boldsymbol{x} \succeq \boldsymbol{c}_{2},
\end{array}
$$

where $\boldsymbol{x} \in \mathbb{R}^{n}, \mathbf{G} \in \mathbb{R}^{m \times n}, \boldsymbol{h} \in \mathbb{R}^{m}, \boldsymbol{c}_{1} \in \mathbb{R}^{n}, \boldsymbol{c}_{2} \in \mathbb{R}^{n}$, and $\odot$ represents the element-wise multiplication of the two operands. The problem is equivalent to its variable augmented version:

$$
\begin{array}{ll}
\underset{\boldsymbol{x}, \boldsymbol{z}}{\operatorname{minimize}} & \left\|\boldsymbol{c}_{1} \odot \boldsymbol{z}\right\|_{1}  \tag{3.26}\\
\text { subject to } & \boldsymbol{G} \boldsymbol{x}=\boldsymbol{h}, \boldsymbol{z} \succeq \boldsymbol{c}_{2}, \text { and } \boldsymbol{x}-\boldsymbol{z}=\mathbf{0}
\end{array}
$$

which could be solved via alternating minimization. The scaled form of its generalized augmented Lagrangian is defined as

$$
\begin{aligned}
\mathcal{L}_{P d}(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{d}) & =\left\|\boldsymbol{c}_{1} \odot \boldsymbol{z}\right\|_{1}+\mathcal{I}_{\boldsymbol{z} \succeq \boldsymbol{c}_{2}}(\boldsymbol{z})+\mathcal{I}_{\mathbf{G} \boldsymbol{x}=\boldsymbol{h}}(\boldsymbol{x})+\rho \boldsymbol{d}^{\top} \mathbf{F}^{\top} \mathbf{F}(\boldsymbol{x}-\boldsymbol{z})+\frac{\rho}{2}\|\mathbf{F}(\boldsymbol{x}-\boldsymbol{z})\|_{2}^{2} \\
& =\left\|\boldsymbol{c}_{1} \odot \boldsymbol{z}\right\|_{1}+\mathcal{I}_{\boldsymbol{z} \succeq \boldsymbol{c}_{2}}(\boldsymbol{z})+\mathcal{I}_{\mathbf{G} \boldsymbol{x}=\boldsymbol{h}}(\boldsymbol{x})+\frac{\rho}{2}\|\mathbf{F}(\boldsymbol{x}-\boldsymbol{z}+\boldsymbol{d})\|_{2}^{2}-\frac{\rho}{2}\|\mathbf{F} \boldsymbol{d}\|_{2}^{2},
\end{aligned}
$$

where $\mathcal{I}_{\boldsymbol{z} \succeq \boldsymbol{c}_{2}}(\boldsymbol{z})$ is an indicator function of $\boldsymbol{z}$ that outputs zero if $\boldsymbol{z} \succeq \boldsymbol{c}_{2}$ and $\infty$ otherwise, $\mathcal{I}_{\mathbf{G} \boldsymbol{x}=\boldsymbol{h}}(\boldsymbol{x})$ is also an indicator one that outputs zero if $\mathbf{G} \boldsymbol{x}=\boldsymbol{h}$ and $\infty$ otherwise, $\rho$ is a scalar spectral penalty parameter, $\mathbf{F} \in \mathbb{R}^{n \times n}$ is a diagonal matrix (such that $\mathbf{F}^{\top} \mathbf{F}=\mathbf{P}$ ) and $\boldsymbol{d} \in \mathbb{R}^{n}$ is a vector of scaled Lagrangian multipliers. Likewise, the minimization is performed via the repetition of three simplified problems:

$$
\begin{align*}
& \boldsymbol{x}^{(k+1)} \leftarrow \underset{\boldsymbol{x}}{\arg \min } L\left(\boldsymbol{x}, \boldsymbol{z}^{(k)}, \boldsymbol{d}^{(k)}\right)  \tag{3.27a}\\
& \boldsymbol{z}^{(k+1)} \leftarrow \underset{\boldsymbol{z}}{\arg \min } L\left(\boldsymbol{x}^{(k+1)}, \boldsymbol{z}, \boldsymbol{d}^{(k)}\right)  \tag{3.27b}\\
& \boldsymbol{d}^{(k+1)} \leftarrow \boldsymbol{d}^{(k)}+\boldsymbol{x}^{(k+1)}-\boldsymbol{z}^{(k+1)}, \tag{3.27c}
\end{align*}
$$

where superscripts $(k)$ and $(k+1)$ represent the number of iteration. The last equation $(3.27 \mathrm{c})$ is a dual-ascent step. Considering the top two problems are formulated as

$$
\begin{aligned}
& \boldsymbol{x}^{(k+1)} \leftarrow \underset{\boldsymbol{x}}{\arg \min } \frac{\rho}{2}\left\|\mathbf{F}\left(\boldsymbol{x}-\boldsymbol{z}^{(k)}+\boldsymbol{d}^{(k)}\right)\right\|_{2}^{2} \text { subject to } \mathbf{G} \boldsymbol{x}=\boldsymbol{h} \\
& \boldsymbol{z}^{(k+1)} \leftarrow \underset{\boldsymbol{z}}{\arg \min }\left\|\boldsymbol{c}_{1} \odot \boldsymbol{z}\right\|_{1}+\mathcal{I}_{\boldsymbol{z} \succeq \boldsymbol{c}_{2}}(\boldsymbol{z})+\frac{\rho}{2}\left\|\mathbf{F}\left(\boldsymbol{x}^{(k+1)}-\boldsymbol{z}+\boldsymbol{d}^{(k)}\right)\right\|_{2}^{2},
\end{aligned}
$$

the first equation (3.27a) is analytically solved by

$$
\begin{equation*}
\boldsymbol{x}^{(k+1)} \leftarrow\left(\mathbf{I}-\mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\right)^{-1} \mathbf{G}\right)\left(\boldsymbol{z}^{(k)}-\boldsymbol{d}^{(k)}\right)+\mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\right)^{-1} \boldsymbol{h} \tag{3.28}
\end{equation*}
$$

and the equation (3.27b) can be also analytically solved by

$$
\begin{equation*}
\boldsymbol{z}^{(k+1)} \leftarrow \operatorname{soft}\left(\max \left(\boldsymbol{x}^{(k+1)}+\boldsymbol{d}^{(k)}, \boldsymbol{c}_{2}\right), \frac{\boldsymbol{c}_{1}}{\rho} \odot \operatorname{diag}\left(\mathbf{P}^{-1}\right)\right), \tag{3.29}
\end{equation*}
$$

where $\max (\cdot)$ is a function for taking element-wise maximum of two vectors (or matrices).

### 3.3.2.2.3 Matrix form of CBP and LAD and their ADMM-GAT algorithms

Let us consider solving a collection of the problem in the same form. In case of CBP you may have a set $\{\boldsymbol{h}\}=\left\{\boldsymbol{h}_{1}, \boldsymbol{h}_{2}, \ldots \boldsymbol{h}_{N}\right\}$ with the other parameters, $\mathbf{G}, \boldsymbol{c}_{1}$, and $\boldsymbol{c}_{2}$, fixed. In case of LAD you may have a set $\{\boldsymbol{h}\}$ with the other parameters $\mathbf{A}$ fixed. In this scenario, the LAD problem can be then expressed with a matrix form:

$$
\underset{\mathbf{X}}{\operatorname{minimize}}\|\mathbf{H}-\mathbf{A} \mathbf{X}\|_{1,1}
$$

where $\mathbf{H}=\left[\boldsymbol{h}_{1} \boldsymbol{h}_{2} \ldots \boldsymbol{h}_{N}\right] \in \mathbb{R}^{m \times N}$ and $\|\cdot\|_{1,1}$ takes the sum of absolute values of all the elements of a matrix. Similarly, CBP is also expressed with a matrix form:

$$
\begin{array}{ll}
\underset{\mathbf{X}}{\operatorname{minimize}} & \left\|\mathbf{C}_{1} \odot \mathbf{X}\right\|_{1,1}  \tag{3.30}\\
\text { subject to } & \mathbf{G X}=\mathbf{H} \text { and } \mathbf{X} \succeq \mathbf{C}_{2}
\end{array}
$$

where $\mathbf{C}_{1}=[\underbrace{\boldsymbol{c}_{1}}_{N} \boldsymbol{c}_{1} \ldots \boldsymbol{c}_{1}]$ and $\mathbf{C}_{2}=[\underbrace{\boldsymbol{c}_{2}}_{N} \boldsymbol{c}_{2} \ldots \boldsymbol{c}_{2}$, .
It is possible to separate this problem into each column of $\mathbf{H}$ and $\mathbf{X}$, but it would be more efficient to solve this as one problem to avoid redundantly performing matrix inversion whenever the spectral penalty parameters are updated. The redundant formulation of $\mathbf{P}$ with $\rho \mathbf{P}$ is a compromised solution for this. $\mathbf{P}$ takes the variation over different row dimensions and $\rho$ does over different columns. The previous sections 3.3.2.2.1 and 3.3.2.2.2 saw that with the redundant formulation, $\rho$ is taken outside of the matrix inversion. By defining $\rho$ for each column, ADMM-GAT can be efficiently performed. Let $\rho_{i}(i=1,2, \ldots, N)$ as $\rho$ for the $i$ th column and $\rho^{-1}=\left[\rho_{1}^{-1} \rho_{2}^{-1} \ldots \rho_{N}^{-1}\right] \in \mathbb{R}^{1 \times N}$ (and $\boldsymbol{\rho}=\left[\rho_{1} \rho_{2} \ldots \rho_{N}\right] \in \mathbb{R}^{1 \times N}$.). Then the update equations are straightforwardly obtained. For the CBP problem, the update equations (3.28), (3.29), and (3.27c) become

$$
\begin{align*}
& \mathbf{X}^{(k+1)} \leftarrow\left(\mathbf{I}-\mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\right)^{-1} \mathbf{G}\right)\left(\mathbf{Z}^{(k)}-\mathbf{D}^{(k)}\right)+\mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\right)^{-1} \mathbf{H}  \tag{3.31a}\\
& \mathbf{Z}^{(k+1)} \leftarrow \operatorname{soft}\left(\max \left(\mathbf{X}^{(k+1)}+\mathbf{D}^{(k)}, \mathbf{C}_{2}\right), \mathbf{C}_{1} \odot\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \boldsymbol{\rho}^{-1}\right)\right)  \tag{3.31b}\\
& \mathbf{D}^{(k+1)} \leftarrow \mathbf{D}^{(k)}+\mathbf{X}^{(k+1)}-\mathbf{Z}^{(k+1)} \tag{3.31c}
\end{align*}
$$

where $\mathbf{D}$ is a matrix form of scaled Lagrangian multipliers. The update equations are straightforwardly obtained. For the LAD problem, the update equations (3.23), (3.24), and (3.22) becomes

$$
\begin{align*}
\mathbf{X}^{(k+1)} & \leftarrow\left(\mathbf{A}^{\top} \mathbf{P A}\right)^{-1} \mathbf{A}^{\top} \mathbf{P}\left(\mathbf{H}+\mathbf{Z}^{(k)}-\mathbf{D}^{(k)}\right),  \tag{3.32a}\\
\mathbf{Z}^{(k+1)} & \leftarrow \operatorname{soft}\left(\mathbf{A} \mathbf{X}^{(k+1)}-\mathbf{H}+\mathbf{D}^{(k)},\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \boldsymbol{\rho}^{-1}\right)\right),  \tag{3.32b}\\
\mathbf{D}^{(k+1)} & \leftarrow \mathbf{D}^{(k)}+\left(\mathbf{A} \mathbf{X}^{(k+1)}-\mathbf{Z}^{(k+1)}\right) \tag{3.32c}
\end{align*}
$$

### 3.3.2.3 Residual balancing for $\rho \mathbf{P}$ in a matrix form

The last section introduces the matrix forms of the two convex optimization problems, LAD and CBP. This section discusses residual balancing for them. First, the matrix form of ADMM is redefined. A general form of the matrix forms discussed in the last section is the batch processing of the collection of the minimization problem (3.11):

$$
\begin{array}{ll}
\underset{\substack{\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{N} \\
z_{1}, z_{2}, \ldots, \boldsymbol{z}_{N}}}{\operatorname{minimize}} & \sum_{l=1}^{N}\left(f\left(\boldsymbol{x}_{l}\right)+g\left(\boldsymbol{z}_{l}\right)\right)  \tag{3.33}\\
\text { subject to } & \mathbf{A} \boldsymbol{x}_{l}+\mathbf{B} \boldsymbol{z}_{l}=\boldsymbol{c} \quad \text { for } l=1, \ldots, N,
\end{array}
$$

where $\boldsymbol{x}_{l} \in \mathbb{R}^{m}, \boldsymbol{z}_{l} \in \mathbb{R}^{n}$ for $l=1, \ldots, N, \boldsymbol{c} \in \mathbb{R}^{p}, \mathbf{A} \in \mathbb{R}^{p \times m}, \mathbf{B} \in \mathbb{R}^{p \times n}$, and $f$ and $g$ are convex functions with respect to $\boldsymbol{x}$ and $\boldsymbol{z}$, respectively. Let $\mathbf{X} \in \mathbb{R}^{m \times N}$ and $\mathbf{Z} \in \mathbb{R}^{n \times N}$ be the concatenation of $\boldsymbol{x}_{l}$ and $\boldsymbol{z}_{l}$ for $l=1, \ldots, N$, respectively as: $\mathbf{X}=\left[\begin{array}{llll}\boldsymbol{x}_{1} & \boldsymbol{x}_{2} & \ldots & \boldsymbol{x}_{\boldsymbol{N}}\end{array}\right]$ and $\mathbf{Z}=\left[\begin{array}{llll}\boldsymbol{z}_{1} & \boldsymbol{z}_{2} & \ldots & \boldsymbol{z}_{\boldsymbol{N}}\end{array}\right]$. The equality constraint in the problem (3.33) is expressed as:

$$
\mathbf{A X}+\mathbf{B Z}=\mathbf{C}
$$

where $\mathbf{C} \in \mathbb{R}^{p \times N}$ is $\mathbf{C}=\underbrace{[\boldsymbol{c} \boldsymbol{c} \ldots \boldsymbol{c}]}_{N}$. Redefining the terms of the cost function with respect to $\mathbf{X}$ and $\mathbf{Z}$ by:

$$
\mathcal{F}(\mathbf{X})=\sum_{l=1}^{N} f\left(\boldsymbol{x}_{l}\right) \quad \text { and } \quad \mathcal{G}(\mathbf{Z})=\sum_{l=1}^{N} g\left(\boldsymbol{z}_{l}\right),
$$

and the minimization problem (3.33) can be expressed in a matrix form:

$$
\begin{array}{ll}
\underset{\mathbf{X}, \mathbf{Z}}{\operatorname{minimize}} & \mathcal{F}(\mathbf{X})+\mathcal{G}(\mathbf{Z})  \tag{3.34}\\
\text { subject to } & \mathbf{A X}+\mathbf{B Z}=\mathbf{C}
\end{array}
$$

This transformation (3.34) using matrix variables is still separable across the column and equivalent to the binding of the collection of the standard form of ADMM, as shown in (3.33). As we saw in the last section, we can formulate its augmented Lagrangian with a spectral parameter matrix $\rho_{l} \mathbf{P}$ for each column $l=1, \ldots N$ :

$$
\begin{align*}
\mathcal{L}_{\rho P F \mathcal{G}}(\mathbf{X}, \mathbf{Z}, \mathbf{Y})= & \mathcal{F}(\mathbf{X})+\mathcal{G}(\mathbf{Z})+\operatorname{Tr}\left(\mathbf{Y}^{\top}(\mathbf{A X}+\mathbf{B Z}-\mathbf{C})\right) \\
& +\frac{1}{2} \operatorname{Tr}\left((\mathbf{A X}+\mathbf{B Z}-\mathbf{C})^{\top} \mathbf{P}(\mathbf{A X}+\mathbf{B Z}-\mathbf{C}) \boldsymbol{\Omega}\right), \tag{3.35}
\end{align*}
$$

where $\Omega \in \mathbb{R}^{N \times N}$ is a diagonal matrix such that its $(l, l)$ element $\Omega_{l, l}$ is equal to $\rho_{l}$ for $l=1, \ldots, N$. The primal and dual residuals of this problem are obtained as:

$$
\begin{align*}
\mathbf{R}^{(k+1)} & =\mathbf{A} \mathbf{X}^{(k+1)}+\mathbf{B} \mathbf{Z}^{(k+1)}-\mathbf{C}  \tag{3.36}\\
\mathbf{S}^{(k+1)} & =\sum_{l=1}^{N} \rho_{l} \mathbf{A}^{\top} \mathbf{P B}\left(\boldsymbol{z}_{l}^{(k+1)}-\boldsymbol{z}_{l}^{(k)}\right)=\mathbf{A}^{\top} \mathbf{P B}\left(\mathbf{Z}^{(k+1)}-\mathbf{Z}^{(k)}\right) \boldsymbol{\Omega}, \tag{3.37}
\end{align*}
$$

which are also the binding of the residuals over columns. Residual balancing is performed for both $\rho_{l}(l=1, \ldots, N)$ and $P_{i}(i=1, \ldots, p)$ by decomposing the primal and dual residuals into their corresponding components. Since $\rho_{l}$ and $\mathbf{P}$ cannot be separable, two decompositions, one with respect to $\rho_{l}(l=1, \ldots, N)$ and the other with respect to $P_{i}$ ( $i=1, \ldots, p$ ) are considered to assess the balance of their assoicated primal and dual residuals associated. To update $\rho_{l}$, the primal and dual residuals are decomposed with respect to $\rho_{l}$ and their corresponding components are compared.

The component of the primal residual associated with $\rho_{l}$ can be observed by the transformation of the augmented term in (3.35):

$$
\begin{equation*}
\frac{1}{2} \operatorname{Tr}\left((\mathbf{A X}+\mathbf{B Z}-\mathbf{C})^{\top} \mathbf{P}(\mathbf{A X}+\mathbf{B Z}-\mathbf{C}) \boldsymbol{\Omega}\right)=\frac{1}{2}\left\|\mathbf{F}(\mathbf{A X}+\mathbf{B Z}-\mathbf{C}) \boldsymbol{\Omega}^{1 / 2}\right\|_{F}^{2}, \tag{3.38}
\end{equation*}
$$

where $\|\cdot\|_{F}$ is the Frobenius norm of a matrix inside and $\boldsymbol{\Omega}^{1 / 2} \in \mathbb{R}^{N \times N}$ is a diagonal matrix such that its $(l, l)$ element is equal to $\sqrt{\rho_{l}}$ for $l=1, \ldots, N$ (therefore, $\boldsymbol{\Omega}^{1 / 2} \boldsymbol{\Omega}^{1 / 2}=$ $\boldsymbol{\Omega}$. This shows that $\rho_{l}$ only contributes to the $l$ th column $\boldsymbol{r}_{l}^{(k+1)}$ of $\mathbf{R}^{(k+1)}$ and therefore, $\boldsymbol{r}_{l}^{(k+1)}$ is the primal residual associated with $\rho_{l}$.

The dual residual (3.37) shows that $\rho_{l}$ only affects the $l$ th column $s_{l}^{(k+1)}$ of $\mathbf{S}^{(k+1)}$ and the component of dual residual associated with $\rho_{l}$ is

$$
\begin{aligned}
\boldsymbol{s}_{l}^{(k+1)} & =\rho_{l} \mathbf{A}^{\top} \mathbf{P B}\left(\boldsymbol{z}_{l}^{(k+1)}-\boldsymbol{z}_{l}^{(k)}\right) \\
& =\rho_{l} \sum_{i=1}^{p} P_{i} \cdot \boldsymbol{a}^{i^{\top}} \cdot \boldsymbol{b}^{i} \cdot\left(\boldsymbol{z}_{l}^{(k+1)}-\mathbf{z}_{l}^{(k)}\right),
\end{aligned}
$$

for $l=1, \ldots, N$. Thus, residual balancing operation for $\rho_{l}$ can be performed as follows:

$$
\rho_{l} \leftarrow \begin{cases}\tau \rho_{l} & \text { if }\left\|\boldsymbol{r}_{l}^{(k+1)}\right\|_{2} \geq \mu\left\|s_{l}^{(k+1)}\right\|_{2}  \tag{3.39}\\ \rho_{l} / \tau & \text { if }\left\|s_{l}^{(k+1)}\right\|_{2} \geq \mu\left\|\boldsymbol{r}_{l}^{(k+1)}\right\|_{2} \\ \rho_{l} & \text { otherwise }\end{cases}
$$

for $(l=1, \ldots, N)$.
Next, the update of $P_{i}$ for $i=1, \ldots, p$ is discussed. Similarly to $\rho_{l}$, the decomposition (3.38) of the augmented term shows that $P_{i}$ only affects the $i$ th row $\boldsymbol{r}^{i(k+1)}$ of $\mathbf{R}^{(k+1)}$. Thus, the primal residual assoicated with $P_{i}$ is $\boldsymbol{r}^{i^{(k+1)}}$. In a similar way shown in Section 3.3.1, the component of the dual residual associated with $P_{i}$ can be obtained by the expansion of the dual residual matrix with respect to $P_{i}$ :

$$
\mathbf{S}^{(k+1)}=\sum_{i=1}^{p} P_{i} \cdot \boldsymbol{a}^{i^{\top}} \cdot \boldsymbol{b}^{i} \cdot\left(\mathbf{Z}^{(k+1)}-\mathbf{Z}^{(k)}\right) \boldsymbol{\Omega}
$$

where $\boldsymbol{a}^{i}$ and $\boldsymbol{b}^{i}$ is the $i$ th row of $\mathbf{A}$ and $\mathbf{B}$, respectively. The $i$ th component in the summation is the dual residual associated with $P_{i}$, and denoted by $\boldsymbol{\Sigma}_{P_{i}}^{(k+1)}$ :

$$
\boldsymbol{\Sigma}_{P_{i}}^{(k+1)}=P_{i} \cdot \boldsymbol{a}^{i \boldsymbol{\top}} \cdot \boldsymbol{b}^{i} \cdot\left(\mathbf{Z}^{(k+1)}-\mathbf{Z}^{(k)}\right) \boldsymbol{\Omega}
$$

The residual balancing for $P_{i}$ can be performed by evaluating the magnitudes of the associated primal and dual residuals:

$$
P_{i} \leftarrow \begin{cases}\tau P_{i} & \text { if }\left\|\boldsymbol{r}^{i(k+1)}\right\|_{2} \geq \mu\left\|\boldsymbol{\Sigma}_{P_{i}}^{(k+1)}\right\|_{F}  \tag{3.40}\\ P_{i} / \tau & \text { if }\left\|\boldsymbol{\Sigma}_{P_{i}}^{(k+1)}\right\|_{F} \geq \mu\left\|\boldsymbol{r}^{(k+1)}\right\|_{2} \\ P_{i} & \text { otherwise }\end{cases}
$$

for $i=1, \ldots, p$. Note that we could use different parameters $\tau$ and $\mu$ for the two update rules above. It is recommended that the update of the second one uses the updated spectral parameter of the first one. For example, if you perform the update of $\rho_{l}$ first and $P_{i}$ second, the updated $\rho_{l}^{(k+1)}$ will be used for the update of $P_{i}$.

### 3.3.2.4 Pseudo codes of ADMM-GAT algorithms using the residual balancing for CBP and LAD

Below are the pseudo codes of CBP and LAD. Practically, the update of the spectral penalty parameters $\rho_{i}$ and $\mathbf{P}$ is not performed every iteration. Some of the parameters in the update equations are pre-computed and updated only when $\rho_{i}$ or $\mathbf{P}$ is changed. In addition, tolerance is scaled in accordance with the size of the problem.

```
Algorithm 3.1 CBP ADMM-GAT(G,H, \(\left.\mathbf{C}_{1}, \mathbf{C}_{2}, \epsilon_{\text {tol }}, k_{\text {maxiter }}\right)\)
Input: \(\mathbf{G} \in \mathbb{R}^{m \times n}, \mathbf{H} \in \mathbb{R}^{m \times N}, \mathbf{C}_{1} \in \mathbb{R}^{n \times N}, \mathbf{C}_{2} \in \mathbb{R}^{n \times N}\)
Output: \(\mathbf{X}^{\star} \in \mathbb{R}^{n \times N}\)
    Set \(\rho_{i}=1(i=1, \ldots, N)\) and \(\mathbf{P}=\mathbf{I}\)
    Pre-compute \(\left(\mathbf{I}-\mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{T}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{T}}\right)^{-1} \mathbf{G}\right), \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{T}}\right)^{-1} \mathbf{H}\), and \(\mathbf{C}_{1} \odot\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \boldsymbol{\rho}^{-1}\right)\)
    3: Set \(R, S \leftarrow \infty\) ( \(R\) and \(S\) are the magnitude of primal and dual residuals, respectively.)
    4: Initializations (if not given):
\[
\begin{aligned}
\mathbf{X}^{(0)} & \leftarrow \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\left(\mathbf{G P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\right)^{-1} \mathbf{H} \\
\mathbf{Z}^{(0)} & \leftarrow \operatorname{soft}\left(\max \left(\mathbf{X}^{(0)}, \mathbf{C}_{2}\right), \mathbf{C}_{1} \odot\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \boldsymbol{\rho}^{-1}\right)\right) \\
\mathbf{D}^{(0)} & \leftarrow \mathbf{X}^{(0)}-\mathbf{Z}^{(0)} .
\end{aligned}
\]
Set \(k=0\) and \(\epsilon \leftarrow N \cdot m \cdot \epsilon_{\text {tol }}\)
while \(\left(k<k_{\text {maxiter }}\right)\) and \(((R>\epsilon)\) or \((S>\epsilon))\) do
Minimize the augmented Lagrangian w.r.t. \(\mathbf{X}\) (Eq. (3.31a)) :
\[
\mathbf{X}^{(k+1)} \leftarrow\left(\mathbf{I}-\mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\right)^{-1} \mathbf{G}\right)\left(\mathbf{Z}^{(k)}-\mathbf{D}^{(k)}\right)+\mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{\top}}\right)^{-1} \mathbf{H}
\]
Minimize the augmented Lagrangian w.r.t. Z (Eq. (3.31b)) :
\[
\mathbf{Z}^{(k+1)} \leftarrow \operatorname{soft}\left(\max \left(\mathbf{X}^{(k+1)}+\mathbf{D}^{(k)}, \mathbf{C}_{2}\right), \mathbf{C}_{1} \odot\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \boldsymbol{\rho}^{-1}\right)\right)
\]
Dual ascent step (Eq. (3.31c))
\[
\mathbf{D}^{(k+1)} \leftarrow \mathbf{D}^{(k)}+\left(\mathbf{X}^{(k+1)}-\mathbf{Z}^{(k+1)}\right)
\]
Update primal residual: \(\mathbf{R}^{(k+1)} \leftarrow \mathbf{X}^{(k+1)}-\mathbf{Z}^{(k+1)}\)
Update dual residual: \(\mathbf{S}^{(k+1)} \leftarrow(\operatorname{diagP} \cdot \boldsymbol{\rho}) \odot\left(\mathbf{Z}^{(k+1)}-\mathbf{Z}^{(k)}\right)\)
if \(\bmod (k, 10)=0\) or \(k=1\) then
for \(l \leftarrow 1\) to \(N\) do
\(\boldsymbol{s}_{\rho_{l}}^{(k+1)} \leftarrow \rho_{l} \cdot \operatorname{diag} \mathbf{P} \odot\left(\boldsymbol{z}_{l}^{(k+1)}-\mathbf{z}_{l}^{(k)}\right)\)
Update \(\rho_{l}\) by (3.39)
end for
for \(i \leftarrow 1\) to \(n\) do
\(\boldsymbol{\Sigma}_{P_{i}}^{(k+1)} \leftarrow P_{i} \cdot \boldsymbol{\rho} \odot\left(\boldsymbol{z}^{i(k+1)}-\boldsymbol{z}^{i(k)}\right)\) (updated \(\boldsymbol{\rho}\) is used)
Update \(P_{i}\) by (3.40)
```


## end for

```
if any change in \(\boldsymbol{\rho}\) or \(\mathbf{P}\) then
Update \(\left(\mathbf{I}-\mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{T}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{T}}\right)^{-1} \mathbf{G}\right), \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{T}}\left(\mathbf{G} \mathbf{P}^{-1} \mathbf{G}^{\boldsymbol{T}}\right)^{-1} \mathbf{H}\), or \(\mathbf{C}_{1} \odot\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \boldsymbol{\rho}^{-1}\right)\) end if
end if
\(k \leftarrow k+1\)
end while
\(\mathbf{X}^{\star} \leftarrow \mathbf{Z}^{(k)}\)
```

```
Algorithm 3.2 LAD ADMM-GAT \(\left(\mathbf{A}, \mathbf{H}, \epsilon_{\text {tol }}, k_{\text {maxiter }}\right)\)
Input: \(\mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{H} \in \mathbb{R}^{m \times N}\)
Output: \(\mathbf{X}^{\star} \in \mathbb{R}^{n \times N}\)
    1: Set \(\rho_{i}=1(i=1, \ldots, N)\) and \(\mathbf{P}=\mathbf{I}\)
    2: Pre-compute \(\left(\mathbf{A}^{\top} \mathbf{P A}\right)^{-1} \mathbf{A}^{\top} \mathbf{P},\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \boldsymbol{\rho}^{-1}\right)\)
    3: Set \(R, S \leftarrow \infty\) ( \(R\) and \(S\) are the magnitude of primal and dual residuals, respectively.)
    4: Initializations (if not given):
\[
\begin{aligned}
& \mathbf{X}^{(0)} \leftarrow\left(\mathbf{A}^{\top} \mathbf{P A}\right)^{-1} \mathbf{A}^{\top} \mathbf{P H} \\
& \mathbf{Z}^{(0)} \leftarrow \operatorname{soft}\left(\mathbf{A X} \mathbf{X}^{(0)}-\mathbf{H},\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \rho^{-1}\right)\right) \\
& \mathbf{D}^{(0)} \leftarrow \mathbf{A X} \mathbf{X}^{(0)}-\mathbf{Z}^{(0)} .
\end{aligned}
\]
5: Set \(k=0\) and \(\epsilon \leftarrow N \cdot n \cdot \epsilon_{\text {tol }}\)
6: while \(\left(k<k_{\text {maxiter }}\right)\) and \(((R>\epsilon)\) or \((S>\epsilon))\) do
7: \(\quad\) Minimize the augmented Lagrangian w.r.t. X (Eq. (3.31a)) :
\[
\mathbf{X}^{(k+1)} \leftarrow\left(\mathbf{A}^{\top} \mathbf{P A}\right)^{-1} \mathbf{A}^{\top} \mathbf{P}\left(\mathbf{H}+\mathbf{Z}^{(k)}-\mathbf{D}^{(k)}\right)
\]
Minimize the augmented Lagrangian w.r.t. Z (Eq. (3.31b)) :
\[
\mathbf{Z}^{(k+1)} \leftarrow \operatorname{soft}\left(\mathbf{A X} \mathbf{X}^{(k+1)}-\mathbf{H}+\mathbf{D}^{(k)},\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \rho^{-1}\right)\right)
\]
9: Dual ascent step (Eq. (3.31c))
\[
\mathbf{D}^{(k+1)} \leftarrow \mathbf{D}^{(k)}+\left(\mathbf{A X}^{(k+1)}-\mathbf{Z}^{(k+1)}\right)
\]
Update primal residual: \(\mathbf{R}^{(k+1)} \leftarrow \mathbf{A} \mathbf{X}^{(k+1)}-\mathbf{Z}^{(k+1)}\)
Update dual residual: \(\mathbf{S}^{(k+1)} \leftarrow \mathbf{A}^{\top}\left((\operatorname{diagP} \cdot \boldsymbol{\rho}) \odot\left(\boldsymbol{Z}^{(k+1)}-\boldsymbol{Z}^{(k)}\right)\right)\)
if \(\bmod (k, 10)=0\) or \(k=1\) then
for \(l \leftarrow 1\) to \(N\) do \(\boldsymbol{s}_{\rho_{l}}^{(k+1)} \leftarrow \rho_{l} \cdot \mathbf{A}^{\boldsymbol{T}} \cdot\left(\operatorname{diagP} \odot\left(\boldsymbol{z}_{l}^{(k+1)}-\boldsymbol{z}_{l}^{(k)}\right)\right)\) Update \(\rho_{l}\) by (3.39)
end for
for \(i \leftarrow 1\) to \(m\) do \(\boldsymbol{\Sigma}_{P_{i}}^{(k+1)} \leftarrow P_{i} \cdot \boldsymbol{a}^{\boldsymbol{i} \top} \cdot\left(\boldsymbol{\rho} \odot\left(\boldsymbol{z}^{i(k+1)}-\boldsymbol{z}^{i(k)}\right)\right)\) (updated \(\boldsymbol{\rho}\) is used) Update \(P_{i}\) by (3.40)
end for
if any change in \(\boldsymbol{\rho}\) or \(\mathbf{P}\) then
Update \(\left(\mathbf{A}^{\top} \mathbf{P A}\right)^{-1} \mathbf{A}^{\top} \mathbf{P}\) or \(\left(\operatorname{diag}\left(\mathbf{P}^{-1}\right) \cdot \boldsymbol{\rho}^{-1}\right)\)
end if
end if
\(k \leftarrow k+1\)
end while \(\mathbf{X}^{\star} \leftarrow \mathbf{Z}^{(k)}\)
```


### 3.3.3 Transformation of convex optimization into CBP

This section provides the equivalent transformation of three minimization problems: constrained sparse LAD (CSLAD), constrained sparse weighted LAD, (CS-WLAD), and weighted LAD (WLAD).

### 3.3.3.1 Transformation of CSLAD into CBP

CSLAD is a convex minimization problem such that

$$
\begin{array}{ll}
\underset{\boldsymbol{x}}{\operatorname{minimize}} & \|\boldsymbol{h}-\mathbf{G} \boldsymbol{x}\|_{1}+\|\boldsymbol{\lambda} \odot \boldsymbol{x}\|_{1} \\
\text { subject to } & \boldsymbol{x} \succeq \boldsymbol{\gamma},
\end{array}
$$

where $\boldsymbol{x} \in \mathbb{R}^{n}, \boldsymbol{h} \in \mathbb{R}^{m}, \mathbf{G} \in \mathbb{R}^{m \times n}, \boldsymbol{\lambda} \in \mathbb{R}^{n}$, and $\boldsymbol{\gamma} \in \mathbb{R}^{n}$. CSLAD comes down to CBP with a variable conversion as follows. First, letting $\boldsymbol{r}=\boldsymbol{h}-\mathbf{G} \boldsymbol{x}$, CSLAD is equivalently transformed into:

$$
\begin{array}{ll}
\underset{\boldsymbol{x}, \boldsymbol{r}}{\operatorname{minimize}} & \|\boldsymbol{r}\|_{1}+\|\boldsymbol{\lambda} \odot \boldsymbol{x}\|_{1} \\
\text { subject to } & \boldsymbol{x} \succeq \boldsymbol{\gamma} \text { and } \boldsymbol{r}=\boldsymbol{h}-\mathbf{G} \boldsymbol{x}
\end{array}
$$

Then CSLAD is further equivalently converted to a general CBP form:

$$
\begin{array}{ll}
\underset{\boldsymbol{u}}{\operatorname{minimize}} & \|\hat{\boldsymbol{\lambda}} \odot \boldsymbol{u}\|_{1} \\
\text { subject to } & \boldsymbol{u} \succeq \hat{\boldsymbol{\gamma}} \text { and } \boldsymbol{h}=\hat{\mathbf{G}} \boldsymbol{u},
\end{array}
$$

$$
\text { where } \quad \boldsymbol{u}=\left[\begin{array}{l}
\boldsymbol{x} \\
\boldsymbol{r}
\end{array}\right], \quad \hat{\mathbf{G}}=\left[\begin{array}{ll}
\mathbf{G} & \mathbf{I}_{L}
\end{array}\right], \quad \hat{\boldsymbol{\lambda}}=\left[\begin{array}{c}
\boldsymbol{\lambda} \\
\mathbf{1}_{m}
\end{array}\right], \quad \text { and } \quad \hat{\boldsymbol{\gamma}}=\left[\begin{array}{c}
\boldsymbol{\gamma} \\
-\inf \cdot \mathbf{1}_{m}
\end{array}\right] .
$$

This way the solver of CBP can be used for CSLAD.
In case of a matrix form:

$$
\begin{array}{ll}
\underset{\mathbf{X}}{\operatorname{minimize}} & \|\mathbf{H}-\mathbf{G X}\|_{1,1}+\|\boldsymbol{\Lambda} \odot \mathbf{X}\|_{1,1} \\
\text { subject to } & \mathbf{X} \succeq \mathbf{\Gamma}
\end{array}
$$

where $\mathbf{X} \in \mathbb{R}^{n \times N}, \mathbf{H} \in \mathbb{R}^{m \times N}, \boldsymbol{\Lambda} \in \mathbb{R}^{n \times N}$, and $\boldsymbol{\Gamma} \in \mathbb{R}^{n \times N}$. Letting $\mathbf{R}=\mathbf{H}-\mathbf{G X}$, we have

$$
\begin{array}{ll}
\underset{\mathbf{X}, \mathbf{R}}{\operatorname{minimize}} & \|\mathbf{R}\|_{1,1}+\|\boldsymbol{\Lambda} \odot \mathbf{X}\|_{1,1} \\
\text { subject to } & \mathbf{X} \succeq \boldsymbol{\Gamma} \text { and } \mathbf{R}=\mathbf{H}-\mathbf{G X}
\end{array}
$$

Then CSLAD is further equivalently converted to a matrix form of CBP:

### 3.3.3.2 Transformation of CS-WLAD to CBP

This section analyzes the reformulation o constrained sparse weighted LAD (CSWLAD) to a constrained basis pursuit (CBP) problem. CS-WLAD is:

$$
\begin{array}{ll}
\underset{\boldsymbol{x}}{\operatorname{minimize}} & \left\|\boldsymbol{\lambda}_{r} \odot(\boldsymbol{h}-\mathbf{G} \boldsymbol{x})\right\|_{1}+\|\boldsymbol{\lambda} \odot \boldsymbol{x}\|_{1}  \tag{3.41}\\
\text { subject to } & \boldsymbol{x} \succeq \boldsymbol{\gamma}
\end{array}
$$

where $\boldsymbol{x} \in \mathbb{R}^{n}, \boldsymbol{h} \in \mathbb{R}^{m}, \mathbf{G} \in \mathbb{R}^{m \times n}, \boldsymbol{\lambda} \in \mathbb{R}^{n}$, and $\boldsymbol{\gamma} \in \mathbb{R}^{n}$, and $\boldsymbol{\lambda}_{r} \in \mathbb{R}^{m}$. The difference of CS-WLAD from CSLAD is the weighted vector $\boldsymbol{\lambda}_{r}$ is multiplied to the $\ell_{1}$-error. Letting $\boldsymbol{r}=\boldsymbol{h}-\mathbf{G} \boldsymbol{x}$,

$$
\begin{array}{ll}
\underset{\boldsymbol{x}, \boldsymbol{r}}{\operatorname{minimize}} & \left\|\boldsymbol{\lambda}_{r} \odot \boldsymbol{r}\right\|_{1}+\|\boldsymbol{\lambda} \odot \boldsymbol{x}\|_{1} \\
\text { subject to } & \boldsymbol{x} \succeq \boldsymbol{\gamma} \text { and } \boldsymbol{r}=\boldsymbol{h}-\mathbf{G} \boldsymbol{x}
\end{array}
$$

and this is further converted to

$$
\begin{array}{ll}
\underset{\boldsymbol{u}}{\operatorname{minimize}} & \|\hat{\boldsymbol{\lambda}} \odot \boldsymbol{u}\|_{1} \\
\text { subject to } & \boldsymbol{u} \succeq \hat{\boldsymbol{\gamma}} \text { and } \boldsymbol{h}=\hat{\mathbf{G}} \boldsymbol{u},
\end{array}
$$

$$
\text { where } \quad \boldsymbol{u}=\left[\begin{array}{l}
\boldsymbol{x} \\
\boldsymbol{r}
\end{array}\right], \quad \hat{\mathbf{G}}=\left[\begin{array}{ll}
\mathbf{G} & \mathbf{I}_{m}
\end{array}\right], \quad \hat{\boldsymbol{\lambda}}=\left[\begin{array}{c}
\boldsymbol{\lambda} \\
\boldsymbol{\lambda}_{r}
\end{array}\right], \quad \text { and } \hat{\boldsymbol{\gamma}}=\left[\begin{array}{c}
\boldsymbol{\gamma} \\
-\inf \cdot \mathbf{1}_{m}
\end{array}\right] .
$$

In case of a matrix form:

$$
\begin{aligned}
& \underset{\mathbf{U}}{\operatorname{minimize}} \quad\|\hat{\boldsymbol{\Lambda}} \odot \mathbf{U}\|_{1,1} \\
& \text { subject to } \mathbf{U} \succeq \hat{\boldsymbol{\Gamma}} \text { and } \mathbf{H}=\hat{\mathbf{G}} \mathbf{U}, \\
& \text { where } \quad \mathbf{U}=\left[\begin{array}{l}
\mathbf{X} \\
\mathbf{R}
\end{array}\right], \quad \hat{\mathbf{G}}=\left[\begin{array}{ll}
\mathbf{G} & \mathbf{I}_{L}
\end{array}\right], \quad \hat{\boldsymbol{\Lambda}}=\left[\begin{array}{c}
\boldsymbol{\Lambda} \\
\mathbf{1}_{m \times N}
\end{array}\right], \quad \text { and } \quad \hat{\boldsymbol{\Gamma}}=\left[\begin{array}{c}
\boldsymbol{\Gamma} \\
-\inf \cdot \mathbf{1}_{m \times N}
\end{array}\right] \text {. }
\end{aligned}
$$

$$
\begin{array}{ll}
\underset{\mathbf{X}}{\operatorname{minimize}} & \left\|\boldsymbol{\Lambda}_{r} \odot(\mathbf{H}-\mathbf{G X})\right\|_{1,1}+\|\boldsymbol{\Lambda} \odot \mathbf{X}\|_{1,1} \\
\text { subject to } & \mathbf{X} \succeq \boldsymbol{\Gamma}
\end{array}
$$

where $\mathbf{X} \in \mathbb{R}^{n \times N}, \mathbf{H} \in \mathbb{R}^{m \times N}, \boldsymbol{\Lambda} \in \mathbb{R}^{n \times N}, \boldsymbol{\Gamma} \in \mathbb{R}^{n \times N}$, and $\boldsymbol{\Lambda}_{r} \in \mathbb{R}^{m \times N}$. Letting $\mathbf{R}=\mathbf{H}-\mathbf{G X}$, we have

$$
\begin{array}{ll}
\underset{\mathbf{X}, \mathbf{R}}{\operatorname{minimize}} & \left\|\boldsymbol{\Lambda}_{r} \odot \mathbf{R}\right\|_{1,1}+\|\boldsymbol{\Lambda} \odot \mathbf{X}\|_{1,1} \\
\text { subject to } & \mathbf{X} \succeq \boldsymbol{\Gamma} \text { and } \mathbf{R}=\mathbf{H}-\mathbf{G X}
\end{array}
$$

Then CSLAD is further equivalently converted a matrix form of CBP:

$$
\begin{aligned}
& \underset{\mathbf{U}}{\operatorname{minimize}} \quad\|\hat{\boldsymbol{\Lambda}} \odot \mathbf{U}\|_{1,1} \\
& \text { subject to } \mathbf{U} \succeq \hat{\boldsymbol{\Gamma}} \text { and } \mathbf{H}=\hat{\mathbf{G}} \mathbf{U} \text {, } \\
& \text { where } \quad \mathbf{U}=\left[\begin{array}{l}
\mathbf{X} \\
\mathbf{R}
\end{array}\right], \quad \hat{\mathbf{G}}=\left[\begin{array}{ll}
\mathbf{G} & \mathbf{I}_{m}
\end{array}\right], \quad \hat{\boldsymbol{\Lambda}}=\left[\begin{array}{c}
\boldsymbol{\Lambda} \\
\boldsymbol{\Lambda}_{r}
\end{array}\right], \quad \text { and } \quad \hat{\boldsymbol{\Gamma}}=\left[\begin{array}{c}
\boldsymbol{\Gamma} \\
-\inf \cdot \mathbf{1}_{m \times N}
\end{array}\right] .
\end{aligned}
$$

The difference from CSLAD is very simple; just the lower block of $\hat{\boldsymbol{\Lambda}}$ is the only change. You could use the original solver just changing the variable.

### 3.3.3.3 Transformation of WLAD to CBP

WLAD can be transformed into a CBP format using variable conversion. WLAD is defined as:

$$
\text { WLAD : } \underset{\boldsymbol{x}}{\operatorname{minimize}} \quad\left\|\boldsymbol{\lambda}_{r} \odot(\boldsymbol{h}-\mathbf{A} \boldsymbol{x})\right\|_{1},
$$

where $\boldsymbol{x} \in \mathbb{R}^{n}, \mathbf{A} \in \mathbb{R}^{m \times n}, \boldsymbol{h} \in \mathbb{R}^{m}$, and $\boldsymbol{\lambda}_{r} \in \mathbb{R}^{m}$ is a weighted vector. With $\boldsymbol{r}=\boldsymbol{h}-\mathbf{A} \boldsymbol{x}$, the above problem is reformulated as a CBP problem:

$$
\begin{array}{ll}
\underset{\boldsymbol{s}}{\operatorname{minimize}} & \left\|\boldsymbol{c}_{1} \odot \boldsymbol{s}\right\|_{1} \\
\text { subject to } & \boldsymbol{K} \boldsymbol{s}=\boldsymbol{h}
\end{array}
$$

where

$$
\boldsymbol{s}=\left[\begin{array}{l}
\boldsymbol{x} \\
\boldsymbol{r}
\end{array}\right], \boldsymbol{c}_{1}=\left[\begin{array}{l}
\mathbf{0}_{n} \\
\boldsymbol{\lambda}_{r}
\end{array}\right], \text { and } \mathbf{K}=\left[\begin{array}{ll}
\mathbf{A} & \mathbf{I}_{m}
\end{array}\right] .
$$

In case of a matrix form:

$$
\underset{\mathbf{X}}{\operatorname{minimize}}\left\|\boldsymbol{\Lambda}_{r} \odot(\mathbf{H}-\mathbf{A X})\right\|_{1,1},
$$

where $\mathbf{X} \in \mathbb{R}^{n \times N}, \mathbf{H} \in \mathbb{R}^{m \times N}$, and $\boldsymbol{\Lambda}_{r} \in \mathbb{R}^{m \times N}$. Letting $\mathbf{R}=\mathbf{H}-\mathbf{A X}$, we have

$$
\begin{array}{ll}
\underset{s}{\operatorname{minimize}} & \left\|\mathbf{C}_{1} \odot \mathbf{S}\right\|_{1} \\
\text { subject to } & \mathbf{K} \boldsymbol{s}=\mathbf{H},
\end{array}
$$

where

$$
\mathbf{S}=\left[\begin{array}{l}
\mathbf{S} \\
\mathbf{R}
\end{array}\right], \mathbf{C}_{1}=\left[\begin{array}{c}
\mathbf{0}_{n \times N} \\
\boldsymbol{\Lambda}_{r}
\end{array}\right] \text {, and } \mathbf{K}=\left[\begin{array}{ll}
\mathbf{A} & \mathbf{I}_{m}
\end{array}\right] .
$$

The difference from LAD is very simple; just the lower block of $\mathbf{C}_{1}$ is the only change. You could use the original solver just changing the variable.

### 3.4 Simultaneous Atmospheric Correction and De-noising (SABCOND)

The proposed combined atmospheric correction and de-noising method aims to derive a refined atmospheric transmission spectrum from the observed I/F spectra within the image, while simultaneously detecting large noise. The computed transmission spectrum is then used for atmospheric correction. The surface contribution and the transmission spectrum and its scaling parameters are simultaneously determined through a minimization process. In order to avoid interpolation bias and subsequent artifacts, the proposed method is performed on I/F spectra produced by my own implementation of the calibration pipeline [78] without applying TRR3 filtering or interpolating BPs. First, I describe the signal model adopted in the proposed method, including a spectral mixing model for the surface and a model for atmospheric transmission, and then discuss the adopted methodology to perform the estimation of the atmospheric transmission spectrum and atmospheric compensation.

### 3.4.1 Signal model

Let us denote the observed signal (I/F) at one pixel by $\boldsymbol{y} \in \mathbb{R}^{L \times 1}$ where $L$ is the number of wavelength channels, its associated surface reflectance by $r \in \mathbb{R}^{L \times 1}$, and its atmospheric transmission spectrum by $t \in \mathbb{R}^{L \times 1}$. Assuming that the spectral contribution of the atmosphere is uniform along the optical path, the signal model under the BeerLambert law is:

$$
\begin{equation*}
y_{i}=t_{i}^{\beta} r_{i} \tag{3.42}
\end{equation*}
$$

for all $i=1, \ldots, L$, where $y_{i}, t_{i}$, and $r_{i}$ are the $i$ th elements of $\boldsymbol{y}, \boldsymbol{t}$, and $\boldsymbol{r}$, respectively, and $\beta$ is a scaling parameter that depends on the optical path length. Since $\mathrm{I} / \mathrm{F}$, transmission, and surface reflectance are all assumed to be positive, the observed signal $\boldsymbol{y}$ is readily converted to the logarithmic domain:

$$
\begin{equation*}
\log \left(y_{i}\right)=\beta \log \left(t_{i}\right)+\log \left(r_{i}\right) \tag{3.43}
\end{equation*}
$$

for all $i=1, \ldots, L$. In this domain, the transmission spectrum present in all pixels is interpreted as an additive component to the surface reflectance. For the sake of simplicity, let us express the element-wise logarithmic operation on a vector $\boldsymbol{x}$ (on a matrix $\mathbf{X}$ ) as $\log x(\log \mathbf{X})$. Then the vector form of equation (3.43) will be

$$
\begin{equation*}
\log y=\beta \log t+\log r \tag{3.44}
\end{equation*}
$$

Let us collect the spectra in the same cross-track column and denote the lateral stacks of the observed I/F and the surface reflectance spectra by $\mathbf{Y} \in \mathbb{R}^{L \times N}$ and $\mathbf{R} \in \mathbb{R}^{L \times N}$ respectively, where $N$ is the number of lines in the along-track direction. If we assume that the atmospheric transmission spectrum is constant in the along-track direction, we have

$$
\begin{equation*}
\log Y=\log t \cdot \beta^{\top}+\log R \tag{3.45}
\end{equation*}
$$

where $\boldsymbol{\beta} \in \mathbb{R}^{N \times 1}$ is the concatenation of the $\beta$ coefficients for all measurements in the column. The whole image cube is not stacked together because measured atmospheric
spectra are different depending on cross-track columns due to smile effects of the CRISM instrument.

Next, I introduce a model for the surface reflectance. I transfer the LMM-CB (3.10) to the logarithm of reflectance, and propose the logarithmic LMM-CB (LogLMM-CB):

$$
\begin{equation*}
\log \mathbf{R}=\log \mathbf{A} \cdot \mathbf{X}+\overline{\mathbf{C}}^{-1} \mathbf{Z} \quad(\mathbf{X} \succeq \mathbf{0}, \mathbf{Z} \succeq \mathbf{\Gamma}) \tag{3.46}
\end{equation*}
$$

where $\log \mathbf{A} \in \mathbb{R}^{L \times N_{A}}$ is the spectral library matrix whose columns correspond to the logarithm of endmember spectra ( $N_{A}$ is the number of endmembers), $\mathbf{X} \in \mathbb{R}^{N_{A} \times N}$ is a matrix whose elements stores their associated coefficients that would be related to abundances of the endmembers, $\overline{\mathbf{C}}^{-1} \mathbf{Z}$ is the background concave components as also in LMM-CB. Although the LogLMM-CB is not straightforwardly justified from the LMM-CB, the goal is not to accurately model mineral abundances but rather to accurately model the shape of the surface spectrum to isolate the effect of the atmosphere. LogLMM-CB is proposed because it is easier to handle in optimization. Whether or not it is physically validated, the model would be acceptable as long as it can sufficiently accurately model the variation of the logarithmic reflectance of surface. I experimentally verified that the model sufficiently fits the surface.

Combining the equations (3.45) and (3.46), the I/F signals can be modeled as

$$
\begin{equation*}
\log \mathbf{Y}=\log t \cdot \boldsymbol{\beta}^{\top}+\log \mathbf{A} \cdot \mathbf{X}+\overline{\mathbf{C}}^{-1} \mathbf{Z} \quad(\mathbf{X} \succeq \mathbf{0}, \mathbf{Z} \succeq \boldsymbol{\Gamma}) \tag{3.47}
\end{equation*}
$$

### 3.4.1.1 Library

I construct a "global" spectral library rather than a small spectral library for each image, aiming for wide applicability of the proposed method with little customization. The spectral library A must be as large as possible to represent as many known endmembers so that it can accurately model all the possible mixed surface spectra encountered in the CRISM observations. This can be accomplished by using all the spectra of potential mineral phases in publicly available spectral databases, such as CRISM spectral
library [4], U.S. Geological Survey (USGS) spectral library [125], Reflectance Experiment Laboratory (RELAB) spectral database [126], and the Minerals Identified through CRISM Analysis (MICA) Library [67]. I select 686 spectra from the mineral group of the CRISM spectral library, splib06, and all the spectra from the MICA library.

The library endmember spectra are convolved with CRISM spectral channels using the ground calibrated band pass functions whose parameters are stored in the data labeled as "SB" in the CRISM calibration data records (CDR) [4]. The convolved endmember spectra are converted to logarithmic scale and normalized with respect to their $\ell_{2}$-norm in the log-domain, where the $\ell_{2}$-norm of a vector is the square root of the mean of the square of its elements. In my implementation, I further apply continuum removal to the normalized logarithmic endmember spectra. The continuum of each spectrum here is defined as the concave hull that minimally envelops it. An 1d convex hull computation algorithm [127] is used. Now the term AX represents the continuum-removed absorption features of the surface reflectance spectra. The removed continua are interpreted as a part of the background term since they are concave. The continuum removal increases the dissimilarity of the spectra in the library, also making computation faster. In addition, the continuum removal can be performed beforehand and cached for all WA files and therefore, the computational burden accompanied with this pre-processing is small. Although this continuum removal results in a different optimization problem and it may have a different optimal solution, I confirmed that almost identical solutions are obtained while reducing computational time.

The method operates in two modes depending on whether or not water ice aerosol contributions are taken into account. In the mode with water ice aerosols, the absorption efficiency of water ice is included into the library. Absorption efficiency of water ice aerosol is computed using miepython ${ }^{3}$ based on a solution [128] of Mie scattering theory. The input imaginary part of refractive index is obtained from the absorption coefficient data

[^6]reported in [129] with the relationship $k_{a}=4 \pi n_{k} / \lambda$ where $k_{a}$ is the absorption coefficient, $n_{k}$ is the imaginary part of the refractive index, and $\lambda$ is the wavelength. The real part of it is obtained from the Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics (GhoSST) database ${ }^{4}$ that was originally reported by [130] and linearly interpolated to the wavelength samples of the absorption coefficients. Spherical shapes are assumed for the particles and in total, 27 absorption efficiency spectra with several different temperatures and nine different particle radii $(0.5,0.8,1,1.2,1.5,1.8,2,3$, and $4 \mu \mathrm{~m})$ are created. These spectra are convolved to CRISM wavelength channels as done on the mineral spectra using CDR SB data and added to the library A.

### 3.4.2 Atmospheric correction and de-noising

Based on this model, we will estimate the true transmission spectrum given the observation $\mathbf{Y}$ and the library matrix $\mathbf{A}$. It is reasonable to assume that the true $\log t$ could fit the model sufficiently well. A straightforward way to assess the quality of fit is a loss function defined by a norm of the error. In order to achieve robustness to various random noise sources described in Section 3.2.3.2, I opt for the $\ell_{1}$-norm of the error, equivalent to the absolute sum of the errors (ASE):

$$
\begin{equation*}
L_{\mathrm{ASE}}(\log \mathbf{Y}, \log t, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z})=\left\|\log \mathbf{Y}-\log t \cdot \boldsymbol{\beta}^{\top}-\log \mathbf{A} \cdot \mathbf{X}-\overline{\mathbf{C}}^{-1} \mathbf{Z}\right\|_{1,1} \tag{3.48}
\end{equation*}
$$

where $\|\mathbf{M}\|_{1,1}$ represents the sum of absolute values of all the elements in $\mathbf{M}$. The $\ell_{1}$ norm of a vector is the sum of absolute values of its elements and $\|\cdot\|_{1,1}$ is the equivalent operator for matrices. Model inversion based on $\ell_{1}$-errors is known to be robust to corruptions such as dense large random spikes, while the more commonly used $\ell_{2}$-errors assume that the noise follows a Gaussian distribution and perform poorly in the presence of such noise [131, 132].

It is reasonable to assume that the number of endmembers composing each mixed surface spectrum is small. Then, given a large global library matrix A, The goal is to

[^7]find a combination of a small number of endmembers, in other words, a sparse $\mathbf{X}$, the transmission spectrum, and its scaling parameter that fit the model well enough in terms of the ASE (3.48). Such a solution is approximately obtained by adding a $\ell_{1}$-norm penalty on $\mathbf{X}$, known as a sparsity promoting regularizer, to the minimizing function [2]. I define a cost function:
$$
f(\log \mathbf{Y}, \log \boldsymbol{t}, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z})=L_{\mathrm{ASE}}(\log \mathbf{Y}, \log \boldsymbol{t}, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z})+\left\|\boldsymbol{\Lambda}_{\mathrm{A}} \odot \mathbf{X}\right\|_{1,1},
$$
where $\boldsymbol{\Lambda}_{\mathrm{A}} \in \mathbb{R}^{N_{A} \times N}$ is a matrix of trade-off parameters controlling the sparsity of $\mathbf{X}$. Consider the minimization problem:
\[

$$
\begin{array}{ll}
\underset{\log t, \mathbf{X}, \boldsymbol{\beta}, \mathbf{Z}}{ } & f_{Z}(\log \boldsymbol{t}, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z})  \tag{3.49}\\
\text { subject to } & \mathbf{X} \succeq \mathbf{0} \text { and } \mathbf{Z} \succeq \boldsymbol{\Gamma} .
\end{array}
$$
\]

I note that sparsity constrained unmixing on CRISM images has been proposed for the purpose of mineral mapping in the literature [133-135]. The proposed method differs from them in a sense that the main goal is the removal of atmospheric residuals together with large noise, and the sparsity constrained unmixing model is only internally used. Furthermore, the formulation is novel in three aspects - 1) the effect of the atmosphere is integrated and the method is combined with atmospheric correction, 2) the logarithmic domain is considered, and 3) the $\ell_{1}$-norm is considered as a loss function.

The function to be optimized in Eq. (3.49) is non-convex, making it difficult to find an optimal solution. I propose a variable splitting alternating optimization algorithm. The variables are separated into two groups, $(\boldsymbol{\beta}, \mathbf{X}, \mathbf{Z})$, which represents continuum and surface contributions, and $(\log t)$, which represents the atmospheric transmission, so that the minimization with regard to each group becomes easier to handle.

The algorithm alternates between three operations. First, surface and continuum parameters for all the spectra in the column are estimated using the current atmospheric transmission spectrum. Then channels of $\log \mathbf{Y}$ exhibiting unusually high values in the residual of the model (Eq. (3.48)) are flagged and approximated by the corresponding
model estimate $\log \boldsymbol{t} \cdot \boldsymbol{\beta}^{\boldsymbol{\top}}+\log \mathbf{A} \cdot \mathbf{X}+\overline{\mathbf{C}}^{-1} \mathbf{Z}$, the right hand side of Eq. (3.47) substituted by the current estimated parameters. ${ }^{5}$ Finally, a single atmospheric spectrum is estimated from the surface and continuum spectra in the column. It is also important to properly initialize the atmospheric transmission spectrum for this non-convex optimization problem. I use the collection of the empirically derived transmission spectra in the ADR distributed with the CAT software. The detailed description of the algorithm to solve this minimization problem including the initialization of $\log t$ is presented in Section 3.4.3.

After the minimization problem is solved, atmospherically corrected $\log \mathrm{I} / \mathrm{F}, \log \mathbf{Y}_{\text {corr }}$ is finally obtained by

$$
\begin{equation*}
\log Y_{\text {corr }}=\log Y-\log t^{\star} \cdot \beta^{\star \top} \tag{3.50}
\end{equation*}
$$

where $\log \boldsymbol{t}^{\star}$ and $\boldsymbol{\beta}^{\star}$ are the optimal solutions of the minimization problem (3.49). One might be tempted to use the learned surface contribution, $\log \mathbf{A} \cdot \mathbf{X}^{\star}+\overline{\mathbf{C}}^{-1} \mathbf{Z}^{\star}$ where $\mathbf{X}^{\star}$ and $\mathbf{Z}^{\star}$ are the optimal solutions of the problem (3.49), as the best candidate outputs for the atmospheric compensation algorithm. Indeed, they are smoother because they are the linear combination of a smooth background and the endmember spectra in the library $\mathbf{A}$; however, they are likely to underestimate uncertainty present in the signal. The proposed method models the surface spectra with moderate accuracy to achieve the precise estimation of the transmission spectrum. Since the estimation of surface model inside the algorithm is performed independently for each spectrum, it is possible that some minor variations due to noise would be fit by the surface model, potentially leading to the false detection of mineral species. On the other hand, the transmission spectrum is less likely to experience such problems because it is collectively estimated by using all the spectra in the column. In other words, the estimate of the surface need only be accurate enough to contribute to the model of the transmission spectrum and

[^8]I am not interested in accurate estimation of surface mineral abundances at this stage. The correction (Eq. (3.50)) retains small random noise fluctuations in the observation, representing the uncertainty in the signal. In addition, I do not recommend to directly interpret the estimated abundances $\mathbf{X}^{\star}$ since multiple sets of abundance values could model a spectral curve equally well enough in the presence of noise [136]. The surface unmixing result would need careful validation but this effort is beyond the scope of this contribution.

In case of the method with water ice, water ice components are also removed from I/F:

$$
\begin{equation*}
\log Y_{\text {corr }}=\log Y-\log t^{\star} \cdot \beta^{\star \top}-\log A_{\text {ice }} \cdot \mathbf{X}_{\text {ice }}, \tag{3.51}
\end{equation*}
$$

where $\log \mathbf{A}_{\text {ice }}$ and $\mathbf{X}_{\text {ice }}$ are the part of $\log \mathbf{A}$ and $\mathbf{X}$ that correspond to water ice absorption efficiencies, respectively.

### 3.4.2.1 Prior exclusion and post substitution of BPs

Some of the pixels in the image frames are severely corrupted by noise to an extent that would negatively affect the performance of the proposed method. In my implementation, the significantly corrupted BPs detected at the early stage in the calibration are still excluded from all the image frames ahead of processing, although it is possible to apply the proposed method without any prior exclusion of BPs. The BP information is extracted from CDR BP data derived from dark frame measurements prior (and post, if it exists) scene measurements. These BPs are substituted with the model estimate after the atmospheric correction and de-noising method is performed.

### 3.4.3 Algorithm for minimization

This section details the algorithm to solve the minimization problem (3.49). The minimization (3.49) is split into two easily solvable subproblems:

$$
\left(\begin{array}{l}
\boldsymbol{\beta}^{(k+1)}  \tag{3.52}\\
\mathbf{X}^{(k+1)} \\
\mathbf{Z}^{(k+1)}
\end{array}\right)=\underset{\underset{\boldsymbol{\beta}, \mathbf{X}, \mathbf{B}}{\mathbf{X} \succeq \mathbf{0} \succeq \boldsymbol{Z}}}{\arg \min } f\left(\log \boldsymbol{t}^{(k)}, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z}\right),
$$

and

$$
\begin{equation*}
\log \boldsymbol{t}^{(k+1)}=\underset{\log t}{\arg \min } f\left(\log \boldsymbol{t}, \boldsymbol{\beta}^{(k+1)}, \mathbf{X}^{(k+1)}, \mathbf{Z}^{(k+1)}\right), \tag{3.53}
\end{equation*}
$$

where $k$ indicates an iteration number. De-noising is performed between those two operations in the algorithm. The separation of the variable $\log t$ from the other ones makes both of the problems solvable. Both of the subproblems (3.52) and (3.53) are convex optimization problems [137] and have unique solutions, but their analytical solutions cannot be calculated, and their numerical ones need to be computed. It is possible to use any solver (CVX [138, 139], CPLEX ${ }^{6}$, etc.) to solve them. I implemented solvers for the subproblems that employ ADMM-GAT (see Section 3.3 for details) for achieving fast convergence to reasonably precise solutions. In order to achieve the smaller computational time for the subproblems (3.52) and (3.53), the variables of the problems, including their dual variables, are initialized with their output variables in the last iteration (or the current values). Algorithm 3.3 summarizes a general methodology in the pseudo code format. The total number $k_{\text {maxiter }}$ of iteration is currently fixed to 5 .

### 3.4.3.1 Subproblem (3.52)

The problem (3.52) is cast into a matrix form of constrained sparse least absolute deviation (CSLAD):

$$
\begin{array}{ll}
\underset{\mathbf{S}}{\operatorname{minimize}} & \left\|\log \mathbf{Y}-\mathbf{G}^{(k)} \mathbf{S}\right\|_{1,1}+\|\hat{\boldsymbol{\Lambda}} \odot \mathbf{S}\|_{1,1}  \tag{3.54}\\
\text { subject to } & \mathbf{S} \succeq \hat{\boldsymbol{\Gamma}}
\end{array}
$$

[^9]```
Algorithm 3.3
    Construct the concave preserving operator \(\mathbf{C}\) using (3.9)
    Initialize atmospheric transmission spectrum (See Section 3.4.3.4)
    for \(k \leftarrow 1\) to \(k_{\text {maxiter }}\) do
        Solve the subproblem (3.52) (See Section 3.4.3.1)
        Denoising (See Section3.4.3.3)
        Solve the subproblem (3.53) (See Section 3.4.3.2)
        Update \(\boldsymbol{\Lambda}_{\mathrm{A}}\) using (3.58) (See Section 3.4.3.5)
        \(k \leftarrow k+1\)
    end for
    Solve the subproblem (3.52) for final estimation
```

where

$$
\begin{aligned}
\mathbf{G}^{(k)} & =\left[\begin{array}{ll}
\log \boldsymbol{t}^{(k)} & \log \mathbf{A} \\
\overline{\mathbf{C}}^{-1}
\end{array}\right], \\
\mathbf{S}=\left[\begin{array}{c}
\boldsymbol{\beta}^{\boldsymbol{\top}} \\
\mathbf{X} \\
\mathbf{Z}
\end{array}\right], \quad \hat{\boldsymbol{\Lambda}} & =\left[\begin{array}{c}
\mathbf{0}_{1 \times N} \\
\boldsymbol{\Lambda}_{\mathbf{A}} \\
\mathbf{0}_{L \times N}
\end{array}\right], \quad \text { and } \quad \hat{\boldsymbol{\Gamma}}=\left[\begin{array}{c}
\mathbf{0}_{1 \times N} \\
\mathbf{0}_{N_{A} \times N} \\
\boldsymbol{\Gamma}
\end{array}\right],
\end{aligned}
$$

where $\mathbf{0}_{1 \times N}, \mathbf{0}_{L \times N}$, and $\mathbf{0}_{N_{A} \times N}$ are $1 \times N, L \times N$, and $N_{A} \times N$ matrices whose elements are all zeros. This optimization problem is readily solved via any convex optimization solvers such as CVX $[138,139]$ or CPLEX. My implementation utilizes alternating direction method of multipliers (ADMM). Refer Section 3.3 for further details on my implementation.

### 3.4.3.2 Subproblem (3.53)

The subproblem (3.53) is cast as a matrix form of least absolute deviation (LAD) problem. The problem (3.53) is expressed as

$$
\underset{\log t}{\operatorname{minimize}}\left\|\log \mathbf{Y}-\log t \cdot\left(\boldsymbol{\beta}^{(k+1)}\right)^{\top}-\log \mathbf{A} \cdot \mathbf{X}^{(k+1)}-\overline{\mathbf{C}}^{-1} \mathbf{Z}^{(k+1)}\right\|_{1,1} .
$$

This problem is interpreted as a matrix form of least absolute deviation:

$$
\begin{equation*}
\underset{\log t}{\operatorname{minimize}}\left\|\left(\mathbf{R}_{\log t}^{(k+1)}\right)^{\top}-\boldsymbol{\beta} \cdot(\log t)^{\top}\right\|_{1,1} \tag{3.55}
\end{equation*}
$$

where

$$
\mathbf{R}_{\log t}^{(k+1)}=\log \mathbf{Y}-\log \mathbf{A} \cdot \mathbf{X}^{(k+1)}-\overline{\mathbf{C}}^{-1} \mathbf{Z}^{(k+1)} .
$$

As with CSLAD, LAD can be solved via any convex optimization solvers. Again, refer Section 3.3 for further details on my implementation.

### 3.4.3.3 De-noising step

The main purpose of the de-noising step is to flag large spikes as seen in Fig. 3.5, and replace them with their estimated values. Large spike noise completely masks underlying signal components, and it is legitimate to interpret data elements corrupted by large spike noise as missing data. It should be replaced by a "good" estimate to minimize the effect of the extreme noise to model fitting and also for data integrity.

Fortunately, model fitting via the minimization using $\ell_{1}$-error is less affected by large spiky outliers, and therefore, the magnitude of the model fitting error,

$$
\left|\log \mathbf{Y}-\log \boldsymbol{t}^{(k)} \cdot\left(\boldsymbol{\beta}^{(k+1)}\right)^{\top}-\log \mathbf{A} \cdot \mathbf{X}^{(k+1)}-\overline{\mathbf{C}}^{-1} \mathbf{Z}\right|,
$$

would be a reasonable metric to detect the presence of large spiky outliers. ${ }^{7}$ I implement the large noise detection by hard-thresholding on the magnitude of the residual. If the element of the residual matrix is greater than a threshold value, it is considered to be corrupted by large spike noise. The threshold value is empirically determined to be 0.015 .

The best estimate for the missing data would be given by the signal model,

$$
\log \boldsymbol{t}^{(k)} \cdot\left(\boldsymbol{\beta}^{(k+1)}\right)^{\top}+\log \mathbf{A} \cdot \mathbf{X}^{(k+1)}+\overline{\mathbf{C}}^{-1} \mathbf{Z}^{(k+1)},
$$

and data elements with large noise spikes are replaced with these values after each denoising step.

### 3.4.3.4 Initialization

Since the minimization problem (3.49) is a non-convex optimization problem, it is heavily influenced by initialization. For example, let $\left(\log \boldsymbol{t}^{\star}, \boldsymbol{\beta}^{\star}, \mathbf{X}^{\star}, \mathbf{Z}^{\star}\right)$ be the minimizer

[^10]of the problem (3.49). Then following transformation:
\[

$$
\begin{aligned}
& \log t^{\star} \cdot \boldsymbol{\beta}^{\star \top}+\log \mathbf{A} \cdot \mathbf{X}^{\star}+\overline{\mathbf{C}}^{-1} \mathbf{Z}^{\star} \\
& =\left(\log t^{\star}+\overline{\mathbf{C}}^{-1} \boldsymbol{z}^{\prime}\right) \cdot \boldsymbol{\beta}^{\star \top}+\log \mathbf{A} \cdot \mathbf{X}^{\star}+\overline{\mathbf{C}}^{-1}\left(\mathbf{Z}^{\star}-\boldsymbol{z}^{\prime} \cdot \boldsymbol{\beta}^{\star \top}\right),
\end{aligned}
$$
\]

where $\boldsymbol{z}^{\prime} \in \mathbb{R}^{L \times 1}$ is an arbitrary vector that satisfies $\mathbf{Z}^{\star} \succeq \boldsymbol{z}^{\prime} \cdot \boldsymbol{\beta}^{\star \top}$, indicates that $\left(\log \boldsymbol{t}^{\star}+\right.$ $\left.\overline{\mathbf{C}}^{-1} \boldsymbol{z}^{\prime}, \boldsymbol{\beta}^{\star}, \mathbf{X}^{\star}, \mathbf{Z}^{\star}-\boldsymbol{z}^{\prime} \boldsymbol{\beta}^{\star \mathbf{\top}}\right)$ is also a solution since it achieves the same cost. In this solution, arbitrary concave components in the observed spectra are now integrated and considered as part of the transmission, which could make the shape of the transmission spectrum physically unreasonable. Therefore, it is crucial to initialize the transmission spectrum accurately enough to obtain a reasonable solution. My implementation utilizes the empirically obtained transmission spectra in the ADR that have been commonly used in the volcano scan correction as the starting point of the initialization of the transmission spectrum. While you could select a single transmission spectrum in the ADR data, I use a more flexible model for the transmission - a non-negative linear combination of the ADR transmission spectra. The flexibility created by the linear combination could represent more temporal and spatial variations of the atmospheric transmission. To be precise, I first solve the following minimization problem:

$$
\begin{align*}
& \underset{\mathbf{\Phi}, \mathbf{X}, \mathbf{Z}}{\operatorname{minimize}}\left\|\log \mathbf{Y}-\log \mathbf{T}_{\mathrm{ADR}} \cdot \boldsymbol{\Phi}-\log \mathbf{A} \cdot \mathbf{X}-\overline{\mathbf{C}}^{-1} \mathbf{Z}\right\|_{1,1}+\left\|\boldsymbol{\Lambda}_{\mathrm{A}} \odot \mathbf{X}\right\|_{1,1}  \tag{3.56}\\
& \text { subject to } \mathbf{X} \succeq \mathbf{0}, \mathbf{Z} \succeq \boldsymbol{\Gamma}, \boldsymbol{\Phi} \succeq \mathbf{0}
\end{align*}
$$

where $\mathbf{T}_{\mathrm{ADR}} \in \mathbb{R}^{L \times N_{T}}$ ( $N_{T}$ is the number of ADR transmission spectra) is the concatenation of all the transmission spectra in the $\operatorname{ADR}$ and $\Phi \in \mathbb{R}^{N_{T} \times N}$ is the weight of the linear model. The difference here from the signal model used for SABCOND is that the transmission component is expressed as the linear combination: $\log \mathbf{T}_{\mathrm{ADR}} \cdot \boldsymbol{\Phi}$.

After the solution is obtained, de-noising is performed using the absolute value of the residual, safeguarded with the standard deviation of the residual of each pixel. If the absolute value of the residual is greater than 0.1 and the standard deviation of the pixel is lower than 0.15 , then the pixel is marked as a bad entry and replaced with its model estimate. The rationale for the safeguarding with the standard deviation is to retain
pixels that show small random variation and huge constant bias due to calibration or processing errors.

Let the optimizers of the minimization $(3.56)$ be $\mathbf{X}^{\star}, \mathbf{Z}^{\star}$, and $\mathbf{\Phi}^{\star}$. I will use these solutions for initializing the transmission spectrum $\boldsymbol{t}$. This step is similar to the subproblem (3.53) that optimizes the transmission spectrum given the scale parameters and surface spectra of each observation. The initialization of the transmission spectrum can also be performed in a similar way. Assuming that each of the transmission spectra in $\log \mathbf{T}_{\mathrm{ADR}}$ have the same scale, the whole scale of the transmission component of the observed spectrum with respect to each $A D R$ transmission spectrum is obtained by the summation of the weight of the linear model: $\mathbf{1}_{1 \times N_{T}} \boldsymbol{\Phi}^{\star}$, where $\mathbf{1}_{1 \times N_{T}}$ is a $1 \times N_{T}$ vector with all the elements equal to unity. Then given the estimated scaling parameters $\mathbf{1}_{1 \times N_{T}} \boldsymbol{\Phi}^{\star}$ and the surface model, we can initialize the transmission spectrum by solving:

$$
\begin{equation*}
\underset{\log t}{\operatorname{minimize}}\left\|\log \mathbf{Y}-\log t \cdot\left(\mathbf{1}_{1 \times N_{T}} \mathbf{\Phi}^{\star}\right)-\log \mathbf{A} \cdot \mathbf{X}^{\star}-\overline{\mathbf{C}}^{-1} \mathbf{Z}^{\star}\right\|_{1,1} \tag{3.57}
\end{equation*}
$$

I note that the ADR transmission spectra are compensated with their artifact factors stored in the same data beforehand. The artifact spectra that correct the bowl-shape artifact around the $2.0 \mu \mathrm{~m}$ region are subtracted from the transmission spectra of the ADR. The artifact around the $2.0 \mu \mathrm{~m}$ wavelength region is too large and correlated with some endmember spectra of water ice or hydrated minerals, violating one of the assumptions of the proposed method. Integration of the artifact factors ahead of initialization prevents the large bowl-shape artifact, eliminating the violation.

### 3.4.3.5 Prior determination of $\Lambda_{A}$ and its update scheme

$\boldsymbol{\Lambda}_{\mathrm{A}}$ controls a trade-off between the sparsity of $\mathbf{X}$ and model fitting in the subproblem (3.52) (and (3.56) in the initialization step). Its optimal value depends on the amount of atmospheric residual and random noise. The elements of the parameter matrix $\boldsymbol{\Lambda}_{\mathrm{A}}$ for the initialization step are fixed to $\ell_{2}$-norm of their corresponding observation spectrum,
namely

$$
\boldsymbol{\Lambda}_{\mathrm{A}}=0.01 \cdot \mathbf{s q r t}\left(\mathbf{1}_{N_{A} \times L} \cdot(\log \mathbf{Y} \odot \log \mathbf{Y})\right),
$$

where $\mathbf{s q r t}()$ represents a function to perform element-wise square root operation of a matrix. Considering that I/F values normally range between $[0,1]$, larger trade-off parameters are assigned for darker I/F spectra because noise is enhanced in the logarithmic domain for low I/F values. It is found that this value is typical for a large set of images after being tested. In the mode with water ice aerosols, the entries of $\boldsymbol{\Lambda}_{\mathrm{A}}$ associated with the spectra of water ice is set to 0 . This is applied to the wavelength region over $1.0-2.6 \mu \mathrm{~m}$ (bands 3 to 244 ).

It is expected that the atmospheric residual is large in the initialization (3.56) and dramatically decreases after the initial $\log t$ is obtained by solving (3.57). The dramatic decrease of the atmospheric residual changes the balance between the sparsity term and the model fitting error. Using the same value $\boldsymbol{\Lambda}_{\mathrm{A}}$ in the subproblem (3.52) in the subsequent iteration would impose too much sparsity, leading to poor fitting. Therefore, it is important to adjust the trade-off parameters at the end of each iteration. To keep their balance, $\boldsymbol{\Lambda}_{\mathrm{A}}$ is updated using the ratio of the current model fitting error calculated with the updated transmission spectrum by that before updated:

$$
\begin{equation*}
\boldsymbol{\Lambda}_{\mathrm{A}} \leftarrow \boldsymbol{\Lambda}_{\mathrm{A}} \cdot\left\|\mathbf{R}_{\text {new }}^{(k)}\right\|_{1,1} /\left\|\mathbf{R}_{\text {old }}^{(k)}\right\|_{1,1}, \tag{3.58}
\end{equation*}
$$

where

$$
\begin{aligned}
& \mathbf{R}_{\text {old }}^{(k)}=\left|\log \mathbf{Y}-\log \boldsymbol{t}^{(k-1)} \cdot\left(\boldsymbol{\beta}^{(k)}\right)^{\top}-\log \mathbf{A} \cdot \mathbf{X}^{(k)}-\overline{\mathbf{C}}^{-1} \mathbf{Z}^{(k)}\right| \\
& \mathbf{R}_{\text {new }}^{(k)}=\left|\log \mathbf{Y}-\log \boldsymbol{t}^{(k)} \cdot\left(\boldsymbol{\beta}^{(k)}\right)^{\top}-\log \mathbf{A} \cdot \mathbf{X}^{(k)}-\overline{\mathbf{C}}^{-1} \mathbf{Z}^{(k)}\right|
\end{aligned}
$$

This update is performed after every iteration.

### 3.4.4 Modification of minimization problem and its update scheme for GPU processing

The SABCOND applies to wavelength bands that are not marked as bad pixels (BP) in the first stage of the bad pixel detection. In other words, such BPs are removed before processing. Since BPs are different for different columns, the number of bands $L$ varies for columns, making it difficult to process multiple columns at once by stacking together, and you need to process each column independently. (What I have in mind is pagefun in MATLAB. To use pagefun, you need to stack matrices/vectors in another dimension. There might be possible to use GPU by writing CUDA codes directly without any modification of the algorithm.) To overcome this issue, I instead solve the following problem

$$
\begin{align*}
\underset{\log t, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z}}{\operatorname{minimize}} & \left\|\boldsymbol{\Lambda}_{\mathrm{R}} \odot\left(\log \mathbf{Y}-\log \boldsymbol{t} \cdot \boldsymbol{\beta}^{\boldsymbol{T}}-\log \mathbf{A} \cdot \mathbf{X}-\overline{\mathbf{C}}^{-1} \mathbf{Z}\right)\right\|_{1,1} \\
& +\left\|\boldsymbol{\Lambda}_{\mathrm{A}} \odot \mathbf{X}\right\|_{1,1}+\left\|\boldsymbol{\Lambda}_{\mathrm{C}} \odot \mathbf{Z}\right\|_{1,1} \tag{3.59}
\end{align*}
$$

subject to $\quad \mathbf{X} \succeq \mathbf{0}, \mathbf{Z} \succeq \mathbf{\Gamma}$,
where two new trade-off parameters $\boldsymbol{\Lambda}_{\mathrm{R}} \in \mathbb{R}^{L \times N}$ and $\boldsymbol{\Lambda}_{\mathrm{C}} \in \mathbb{R}^{L \times N}$ are introduced. While $\boldsymbol{\Lambda}_{\mathrm{R}}$ and $\boldsymbol{\Lambda}_{\mathrm{C}}$ are generally considered as weight matrices, we can use them as one to flag bad pixels. Before processing, elements in $\boldsymbol{\Lambda}_{\mathrm{R}}$ that correspond to BPs are substituted by zeros, while the others are filled with ones. This operation allows to omit the contribution of the BP bands to the minimization. In addition, currently, corresponding elements of $\boldsymbol{\Lambda}_{\mathrm{C}}$ are set to infinity to disallow any contribution of the corresponding concave base. This operation is necessary for exactly ignoring the BP bands. You can create any concave curvature over non- BP bands without the concave base of BP bands. (the second operation might not be necessary. It might be better not doing so to produce better shape over band bands when interpolation is performed, however, this definitely causes instability in the processing since you can make up whatever background shape over BP bands as long as they are concave combined with non-BP bands.)

This way, users can mask bad pixels without changing the size of matrices, making
it easy to stack columns together. This is a formulation trick rather than improving the performance of the method. In addition, this method has another benefit. You can completely ignore any severe spike noise detected in the later processing by changing the value of its corresponding element of the flag matrices, while the version in Icarus paper approximately excludes the bands from the minimization by substituting such noise with its model values during the iteration.

The introduction of $\boldsymbol{\Lambda}_{\mathrm{R}}$ and $\boldsymbol{\Lambda}_{\mathrm{C}}$ does not add any significant computational cost to the algorithm. In the end, it is just replacing an identity matrix with flag matrices. You can still use the same framework, variable splitting and alternating minimization approach. Let $f_{\Lambda}(\log \boldsymbol{t}, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z})$ be

$$
\begin{align*}
f_{\Lambda}(\log \boldsymbol{t}, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z})= & \left\|\boldsymbol{\Lambda}_{\mathrm{R}} \odot\left(\log \mathbf{Y}-\log \boldsymbol{t} \cdot \boldsymbol{\beta}^{\boldsymbol{\top}}-\log \mathbf{A} \cdot \mathbf{X}-\overline{\mathbf{C}}^{-1} \mathbf{Z}\right)\right\|_{1,1} \\
& +\left\|\boldsymbol{\Lambda}_{\mathrm{A}} \odot \mathbf{X}\right\|_{1,1}+\left\|\boldsymbol{\Lambda}_{\mathrm{C}} \odot \mathbf{Z}\right\|_{1,1} . \tag{3.60}
\end{align*}
$$

The minimization problem (3.59) can be split into the two problems below:

$$
\left(\begin{array}{l}
\boldsymbol{\beta}^{(k+1)}  \tag{3.61}\\
\mathbf{X}^{(k+1)} \\
\mathbf{Z}^{(k+1)}
\end{array}\right)=\underset{\substack{\boldsymbol{\beta}, \mathbf{X}, \mathbf{Z} \\
\mathbf{x} \succeq \mathbf{0} \succeq \boldsymbol{Z} \succeq \boldsymbol{\Gamma}}}{\arg \min } f_{\Lambda}\left(\boldsymbol{\operatorname { l o g }} \boldsymbol{t}^{(k)}, \boldsymbol{\beta}, \mathbf{X}, \mathbf{Z}\right)
$$

and

$$
\begin{equation*}
\log \boldsymbol{t}^{(k+1)}=\underset{\log t}{\arg \min } f_{\Lambda}\left(\log \boldsymbol{t}, \boldsymbol{\beta}^{(k+1)}, \mathbf{X}^{(k+1)}, \mathbf{Z}^{(k+1)}\right) \tag{3.62}
\end{equation*}
$$

The minimization problem (3.61) can be formalized as the CS-WLAD problem:

$$
\begin{array}{ll}
\underset{\mathbf{S}}{\operatorname{minimize}} & \left\|\boldsymbol{\Lambda}_{\mathrm{R}} \odot\left(\log \mathbf{Y}-\mathbf{G}^{(k)} \mathbf{S}\right)\right\|_{1,1}+\|\hat{\boldsymbol{\Lambda}} \odot \mathbf{S}\|_{1,1}  \tag{3.63}\\
\text { subject to } & \mathbf{S} \succeq \hat{\boldsymbol{\Gamma}},
\end{array}
$$

where

$$
\begin{aligned}
& \mathbf{G}^{(k)}=\left[\begin{array}{ll}
\log \boldsymbol{t}^{(k)} & \log \mathbf{A} \\
\mathbf{C}^{-1}
\end{array}\right], \\
& \mathbf{S}=\left[\begin{array}{c}
\boldsymbol{\beta}^{\top} \\
\mathbf{X} \\
\mathbf{Z}
\end{array}\right], \quad \hat{\boldsymbol{\Lambda}}=\left[\begin{array}{c}
\mathbf{0}_{1 \times N} \\
\boldsymbol{\Lambda}_{\mathrm{A}} \\
\boldsymbol{\Lambda}_{\mathrm{C}}
\end{array}\right], \quad \text { and } \quad \hat{\boldsymbol{\Gamma}}=\left[\begin{array}{c}
\mathbf{0}_{1 \times N} \\
\mathbf{0}_{N_{A} \times N} \\
\boldsymbol{\Gamma}
\end{array}\right] .
\end{aligned}
$$

The CS-WLAD can be further transformed to the CBP format. Refer to Section 3.3.3.2 for further details.

The minimization problem (3.62):

$$
\underset{\log t}{\operatorname{minimize}}\left\|\boldsymbol{\Lambda}_{\mathrm{R}} \odot\left(\log \mathbf{Y}-\log \boldsymbol{t} \cdot\left(\boldsymbol{\beta}^{(k+1)}\right)^{\top}-\log \mathbf{A} \cdot \mathbf{X}^{(k+1)}-\overline{\mathbf{C}}^{-1} \mathbf{Z}^{(k+1)}\right)\right\|_{1,1},
$$

is straightforwardly regarded as the WLAD problem:

$$
\underset{\log t}{\operatorname{minimize}}\left\|\boldsymbol{\Lambda}_{\mathrm{R}} \odot\left(\left(\mathbf{R}_{\log t}^{(k+1)}\right)^{\top}-\boldsymbol{\beta}^{(k+1)} \cdot(\log t)^{\top}\right)\right\|_{1,1},
$$

where $\quad \mathbf{R}_{\log t}^{(k+1)}=\log \mathbf{Y}-\log \mathbf{A} \cdot \mathbf{X}^{(k+1)}-\overline{\mathbf{C}}^{-1} \mathbf{Z}^{(k+1)}$.

WLAD can be further transformed to a CBP problem. Refer to Section 3.3.3.3 for more details.

### 3.4.5 Results

I performed the proposed atmospheric correction and de-noising method on more than one hundred CRISM images in North East Syrtis Major, Jezero Crater, and Columbia Hills. In my environment (Intel Core i7 2.6 GHz (quad core) CPU and 16GB RAM), the computational time taken for each image is about one and half hours in the mode without water ice aerosols and two hours when they are included. This excludes the time for library convolution. I present some representative examples of the proposed method, comparing them with the outcome of the current CRISM processing pipeline: TER data products (when available) or TRR3 I/F images atmospherically corrected by CAT. I validate the SABCOND with three approaches. The first is a visual check of the spectra to investigate whether or not artifacts are removed or distortions introduced. In the case of severe corruption due to elevated noise, I also compare the corrected spectra with atmospherically corrected non-filtered I/F. Such I/F data can be obtained by using I/F conversion implemented in CAT on TRR3 RA (radiance) data. I also perform interimage comparison with the expectation that spectra of pixels from overlapping images at the same geographical locations should show similar spectral signatures if any overlapping images are available. All the atmospherically corrected spectra used for comparisons to
the proposed results are processed with CAT 7.4 using the empirical selection of the transmission spectra and artifact correction. Photometric correction is not applied.

### 3.4.5.1 Removal of atmospheric residuals

Fig. 3.7 shows the comparison of I/F spectra corrected by CAT and those obtained by the proposed method. From Fig. 3.7 (a) and (c), SABCOND significantly reduces the residuals over the $1.0-1.7 \mu \mathrm{~m}$ and $2.0 \mu \mathrm{~m}$ wavelength regions that are consistently observed for the spectra on the right. Furthermore, the $1.4 \mu \mathrm{~m}$ absorption feature is now clearly seen in the first and fourth spectra from the top on the left, while it is severely corrupted on their counterparts on the right. The appearance of that feature is plausible since it coincides with clear hydrated silica-like spectra that have bigger $1.9 \mu \mathrm{~m}$ hydration and $2.2 \mu \mathrm{~m} \mathrm{Al}-\mathrm{OH}$ bearing bands.

One may notice that the spectra in Fig. 3.7 (a) exhibit small high-frequency fluctuations that cannot be seen on the spectra in Fig. 3.7 (c). These are small zero-mean random noise components removed by TRR3 filtering for the input I/F of the CAT volcano scan, while not for the input I/F data to the proposed method. Fig. 3.7 (b) shows that such small Gaussian-like noise is significantly reduced by spatial averaging, which confirms these fluctuations are not systematic artifacts. On the other hand, the systematic artifacts in the spectra in Fig. 3.7 (c) and (d) are not reduced with spatial averaging.

The proposed method also mitigates some consistent features in other wavelength regions such as small spikes around $2.25,2.30,2.38$, and $2.48 \mu \mathrm{~m}$ wavelengths. These spikes could be calibration errors or systematic errors caused by the empirical volcano scan method or minor variation in atmospheric conditions and the shift of the central wavelength of CRISM spectral channels, but their exact origins are hard to precisely identify.

Next I show some examples where a significant amount of water ice aerosols are observed. Fig. 3.8 shows the comparison of corrected I/F spectra by the proposed method


Figure 3.7. Comparison of I/F spectra atmospherically corrected by the proposed method ((a) and (b)) and ones corrected using CAT 7.4 on TRR3 I/F data ((c) and (d)). (b) and (d) are the $5 \times 5$ spatial averages of (a) and (c), respectively. Spectra are in the column (156) in the observation FRT00009312_07 and their image coordinates are identical to the ones in Fig. 3.2.


Figure 3.8. Comparison of I/F spectra atmospherically corrected by the proposed method with water ice (in red) and by CAT (in blue). The spectra (a)-(d) are from FRT0000B573 and their image coordinates (sample, line) are (a) $(286,307)$, (b) $(550,202)$, (c) $(213,57)$, and (d) $(555,211)$ respectively. The spectra (e)-(k) are from HRL0000B8C2 and their image coordinates are (e) $(289,122)$, (f) $(149,364),(\mathrm{g})(83,433)$, (h) (111,415), (i) $(138,61),(\mathrm{j})(313,406)$, and (k) $(276,265)$ respectively. The spectra (l) are from FRT0000ABCB and their image coordinate is $(265,460)$. The blue spectra are shifted downward for ease of comparison.
with water ice aerosols and those atmospherically corrected on TRR3 filtered I/F. The images of these spectra are measured at low latitudes near aphelion. For a variety of spectra, the proposed method successfully mitigates the depression at $2.0 \mu \mathrm{~m}$ and the absorption at $1.5 \mu \mathrm{~m}$ caused by the water ice aerosol, together with other atmospheric residuals, and hydrated features at 1.4 and $1.9 \mu \mathrm{~m}$ are restored if they are present.

Validation process follows several steps. The first step is direct comparison with CAT corrected filtered TRR3 or TER3 images. Fig 3.9 (a) shows such a comparison. The spectrum corrected by the proposed method (in red) shows clearer absorption bands around 1.4, 1.9, and $2.0 \mu \mathrm{~m}$ wavelength regions than the CAT corrected spectrum in blue. Since the proposed method substitutes model values to bad channels there is the potential of creating fictitious absorptions if too many adjacent channels are bad. By comparing the red spectrum with the corresponding spectrum without substitutions (in orange) I can confirm the shape of the band at $2.3 \mu \mathrm{~m}$. Another validation method, illustrated in Fig. 3.9 (b), involves the spectra of a pixel at the same geographical location as the one in Fig. 3.9 (a) from an overlapping image. The spectrum corrected by the proposed method displays the same absorption bands as the one in Fig 3.9 (a). Furthermore, a similarly shaped $1.9 \mu \mathrm{~m}$ absorption seems to be present in the spectrum in Fig. 3.9 (b), where the corrupted wavelength channels for the spectrum in Fig. 3.9 (a) are non noisy, confirming the shape of the water band in the spectrum of Fig. 3.9 (a).

The advantage of the substitution method is also shown in the spatial domain. Fig. 3.10 shows a comparison of band images corrected by the proposed method and by CAT. The yellow rectangle highlights where such artifacts occur. In this highlighted area, sequential spatial columns are detected as BPs and are linearly interpolated with neighboring columns in the CRISM calibration, which causes a smear. In contrast in Fig. 3.10 (b), this type of smear cannot be seen and finer spatial patterns become distinguishable.


Figure 3.9. Comparison of I/F spectra atmospherically corrected by the proposed method with (red) or without (orange) bad entries substituted and with CAT on TRR3 I/F (blue) for the same (approximate) location in two overlapping images. (a) Spectra are from $(535,016)$ in FRT000174F4 and (b) Spectra are from $(276,432)$ in FRT0001821C. Spectra are shifted for ease of comparison.

### 3.4.5.2 Removal of noise and interpolation bias

This section investigates the performance of the proposed method in a scenario where detector noise is elevated and spectra are severely corrupted by interpolation bias. The first example in Fig. 3.11, shows a comparison of a spectrum corrected by the proposed method (red) and two other spectra by volcano scan with (blue) and without (purple) TRR3 filtering. Overall, the spikes around $2.0 \mu \mathrm{~m}$ are greatly reduced in the corrected spectrum by the proposed method and the hydration band at $1.9 \mu \mathrm{~m}$ becomes clearer. The observation ID 2422E indicates that the image was taken near aphelion. The small absorption at $1.5 \mu \mathrm{~m}$ and a smooth depression around $2.0 \mu \mathrm{~m}$ on the blue spectrum indicate the existence of water ice aerosols, which seems to be removed in the corrected spectrum by the proposed method in addition to severe noise. Compared to the CATcorrected filtered spectrum (blue), the red spectrum seems to add an absorption feature around $2.5 \mathrm{\mu m}$. The presence of this absorption is confirmed in the non-filtered spectrum


Figure 3.10. Comparison of two band images corrected with the proposed method (a) and with CAT on filtered I/F (b). They are the band $302(1.895 \mu \mathrm{~m})$ of FRT0001821C.
(purple). When only the non-BP bands are plotted, an absorption around $2.5 \mu \mathrm{~m}$ can be observed. Since this wavelength region is contaminated by many spikes due to interpolation bias, I speculate that TRR3 filtering smoothed out the signal around $2.5 \mu \mathrm{~m}$ while creating a band around $2.6 \mu \mathrm{~m}$.

Fig. 3.12 (a) and (b) show results of the proposed method on the two spectra introduced in Fig. 3.5 (b) and (c). The proposed method is only minimally affected by interpolation bias (Fig. 3.12(a)) and does not show a spurious absorption around $2.1 \mu \mathrm{~m}$ that is observed in the CAT corrected spectrum (Fig. 3.12(b)). The non corrupted spectrum (in purple) in Fig. 3.12(b) shows a depression around the $2.0 \mu \mathrm{~m}$ wavelength region. I show that the depression is also an artifact by investigating multiple kinds of ratioed I/F in the same manner as the method described in [84]. Under the assumption that the transmission spectrum is uniform along each column, the contribution of the atmospheric transmission could be removed by dividing a spectrum by another spectrally unremarkable in the same spatial column, whether or not they are atmospherically corrected. Fig. 3.12 (c) shows the ratios of four versions of the spectrum in Fig. 3.12 (b), with color coding as explained in the caption. In all cases, I use as a denominator the geometric mean spectrum of the same spatial column, which, as I carefully verified, only contains


Figure 3.11. Comparison of I/F spectra corrected with the proposed method (red) with those corrected with CAT on TRR3 I/F (blue) and with CAT on TRR3 I/F without filtering (gray/purple/yellow). Yellow dots represent bad channels (BPs). Purple dots represent non corrupted channels (non-BP). The image coordinate (sample line) of the spectrum is $(191,359)$ in HRL0002422E. Spectra are shifted for ease of comparison.
atmospheric contributions. The big absorption feature at $2.1 \mu \mathrm{~m}$ observed in the filtered I/F (blue) with atmospheric correction is also in the one (light blue) without atmospheric correction, indicating the feature is unlikely to be an artifact created by the volcano scan correction. However, the feature can not be observed in the ratioed spectrum (green) of the non-filtered I/F without atmospheric correction. The many downward spikes on the green spectrum are due to interpolation bias. Therefore, the big absorption feature at $2.0 \mu \mathrm{~m}$ on the upper two spectra are likely to be an artifact created by TRR3 filtering due to dense BPs. This artifact corresponds to the spurious feature observed by [84]. The ratioed spectrum (purple) of the non-filtered I/F with atmospheric correction shows an absorption around $2.0 \mu \mathrm{~m}$, which is an artifact caused by an error in the estimation of the scaling parameter for the volcano scan correction.

SABCOND can also perform reasonable corrections in small outcrops. Fig. 3.13 (a)(d) show a comparison of the atmospherically corrected spectra with the same three methods described in Fig. 3.11 of the same geographical location in four overlapping im-


Figure 3.12. (a-b) Comparison of I/F spectra corrected with the proposed method (red) with those corrected with CAT on TRR3 I/F (blue) and with CAT on TRR3 I/F without filtering (gray/purple/yellow). Yellow and purple dots represent bad channels (BPs) and non-BPs, respectively. (a) and (b) are from $(386,166)$ in FRT000174F4 and from $(90,318)$ in HRL0000C0BA, respectively. Spectra are shifted for ease of comparison. (c) Comparison of the ratioed I/F spectra performed in different ways. From the top to bottom, a ratioed spectrum of filtered I/F atmospherically corrected by CAT (blue), a ratio of filtered I/F (light blue), a ratio of non-filtered I/F (green), and a ratio of nonfiltered I/F atmospherically corrected by CAT (purple). These colors are only given for non-BPs. Yellow dots represent BPs for each plot and the whole spectra are plotted in gray. The image coordinate of these spectra is same as that of (b). Spectra are offset for ease of comparison.


Figure 3.13. Comparison of I/F spectra corrected with the proposed method (red) with those corrected with CAT on TRR3 I/F (blue) and with CAT on TRR3 I/F without filtering (gray/purple/yellow). Yellow dots represent bad channels (BPs). Purple dots represent non corrupted channels (non-BP). Spectra in (a), (b), (c), and (d) are from $(552,209)$ in FRT000161EF, $(294,163)$ in FRT000174F4, $(474,190)$ in FRT00018781, and $(295,119)$ in FRT00017103, respectively. The blue and purple spectra are shifted downward for ease of comparison. (e) a pseudo RGB map-projected image of FRT000161EF with a zoomed-in image into a location associated with the spectra.
ages. SABCOND consistently produces bland spectra while the CAT-corrected spectra shows a range of artifacts for different images. These spectra are affected by interpolation bias since this is a spatially small distinctive region as shown in Fig. 3.13 (e). The spectra corrected by the volcano scan using CAT exhibit anomalous shapes around the $2.0 \mu \mathrm{~m}$ wavelength region. The wide depression around $2.0 \mu \mathrm{~m}$ in the blue spectrum in Fig. 3.13 (a) and leftover spiky absorptions and a little depression around $2.0 \mu \mathrm{~m}$ in the blue spectra in Fig. 3.13 (b) and (c) is possibly a combination of the bowl-shape artifact and artifacts created by TRR3 filtering. A water ice like shape shown in the blue spectrum in Fig. 3.13 (c) is probably caused by uncorrected water ice aerosols. Indeed, the image with the observation ID 18781 from which the spectrum in Fig. 3.13 (c) is acquired
near aphelion. We can validate these products in a way similar to the multiple ratio method I previously described.


Figure 3.14. Comparison of I/F spectrum corrected with the proposed method (red) with those corrected with CAT on TRR3 I/F (blue) and with CAT on TRR3 I/F without filtering (gray/purple/yellow). Yellow dots represent bad channels (BPs). Purple dots represent non corrupted channels (non-BP). Spectra in (a), (b), (c), and (d) are from $(270,172),(269,194),(426,15)$, and $(161,170)$ in FRT000174F4, respectively. Spectra are offset for ease of comparison.

Fig. 3.14 shows additional comparisons from the image FRT000174F4. The proposed method still produces cleaner spectra, while the blue spectra are corrupted by atmospheric residuals and artifact due to interpolation bias.

Fig. 3.15 (a) shows the comparison of I/F spectra corrected by the proposed method
and CAT (identical to Fig. 11 (c) in the main text) and Fig. 3.15 (b) shows ratioed I/F spectra of the same pixel processed in the four different approaches. In Fig. 3.15, the corrected spectrum (red) is bland, while CAT correction creates a big depression around the $2.0 \mu \mathrm{~m}$ wavelength region whether or not TRR3 filtering is applied or not. Fig. 3.15 (b) shows that the depression present in I/F spectra corrected with CAT is an artifact. The ratioed filtered I/F (darker blue) with atmospheric correction exhibits a depression right at $2.0 \mu \mathrm{~m}$ while the ratioed filtered I/F (light blue) without atmospheric correction does not, indicating the center of the depression around $2.0 \mu \mathrm{~m}$ is likely to be an artifact caused by atmospheric correction. The 1.9 and $2.1 \mu \mathrm{~m}$ absorptions in the light blue spectrum are likely to be caused by interpolation bias because the absorptions are not observed in the ratioed non-filtered I/F (green) without atmospheric correction and BPs with moderate interpolation bias are concentrated around these wavelength regions. These 1.9 and $2.1 \mu \mathrm{~m}$ artifacts are likely to be identical to problematic spurious features reported in [84]. Therefore, we can conclude that the combination of these artifacts - the bow-shape one around at $2.0 \mu \mathrm{~m}$ and the spurious features at 1.9 and $2.1 \mu \mathrm{~m}$ - ends up in a broad depression around $2.0 \mu \mathrm{~m}$ in the blue spectrum in Fig. 3.15 (a).

Figs. 3.16 and 3.17 show another comparison of the spectra at the same location measured in different images. Those are inside the final candidate landing ellipses for 2020 Mars Rover in North East Syrtis and in Jezero crater. Fig. 3.16 shows that Mg/Fecarbonate features are seen on all the images. The interpolation bias is less problematic on those spectra because the unit spans 10 or more pixels around it. In contrast, the spectra in Fig. 3.17 shows smaller features. For different images, 1.9 and $2.3 \mu \mathrm{~m}$ absorptions are consistently seen, although those of (b) and (c) are quite small and the continua of the spectra look different. Such a difference may happen partly because those locations do not match perfectly and have subpixel shifts, or because of the different conditions of dust aerosols.

Finally, I compare spectra corrected by the proposed method and corrected by CAT


Figure 3.15. (a) Comparison of I/F spectra corrected with the proposed method (red) with those corrected with CAT on TRR3 I/F (blue) and with CAT on TRR3 I/F without filtering (gray/purple/yellow). Yellow dots represent bad channels (BPs). Purple dots represent non corrupted channels (non-BP). Spectra are from $(552,209)$ in FRT000161EF (same as Fig. 12 (a) in the main text). The blue and purple spectra are shifted downward for ease of comparison. (b) Comparison of the ratioed I/F spectra performed in different ways. From the top to bottom, a ratioed spectrum of filtered I/F atmospherically corrected by CAT (blue), a ratio of filtered I/F (light blue), a ratio of non-filtered I/F (green), and a ratio of non-filtered I/F atmospherically corrected by CAT (purple). These colors are only given for non-BPs. Yellow dots represent BPs for each plot and the whole spectra are plotted in gray. Spectra are shifted for ease of comparison.


|  | Our correction |
| :--- | :--- |
| $\square$ | CAT correction on TRR3 I/F |
|  | Good pixels of CAT correction on TRR3 RA I/F |
|  | Bad pixels of CAT correction on TRR3 RA I/F |
|  | CAT correction on TRR3 RA I/F |








Figure 3.16. Comparison of I/F spectra corrected with the proposed method (red) with those corrected with CAT on TRR3 I/F (blue) and with CAT on TRR3 I/F without filtering (gray/purple/yellow). Yellow dots represent bad channels (BPs). Purple dots represent non corrupted channels (non-BP). They are from (a) (342,231) in FRT000161EF, (b) $(632,190)$ in FRT0001642E, (c) $(604,177)$ in FRT000165F7, (d) $(46,127)$ in FRT00017103, (e) $(43,180)$ in FRT000174F4, and (f) $(217,207)$ in FRT00018781. The blue and purple spectra are shifted downward for ease of comparison.


Figure 3.17. Comparison of I/F spectra corrected with the proposed method (red) with those corrected with CAT on TRR3 I/F (blue) and with CAT on TRR3 I/F without filtering (gray/purple/yellow). Yellow dots represent bad channels (BPs). Purple dots represent non corrupted channels (non-BP). Spectra in (a), (b), (c), and (d) are from ( $25,154)$ in HRL000040FF, $(115,42)$ in FRT00005C5E, $(623,460)$ in FRT0001EAE0, and $(360,472)$ in FRT0001FB74, respectively. The blue and purple spectra are shifted for ease of comparison.
at some locations of particular interest reported in the literature. Fig. 3.18 shows the comparison of the spectra at the locations reported in [140] processed by the proposed method and by the volcano scan correction using CAT. The spectra shown in the figure are averaged within the same spatial windows provided in a supplemental table file in [140]. SABCOND produces spectral shapes comparable to ratioed spectra without ratioing, while non-ratioed CAT-corrected spectra exhibit more noise and artifacts. The comparison of ratioed spectra also shows that the proposed method removes some of the spiky noise, such as $1.2 \mu \mathrm{~m}$ in the ratio of CAT-corrected spectrum in Fig. 3.18 (a) and 1.65 and $1.9 \mu \mathrm{~m}$ in the ratio of CAT-corrected spectrum in Fig. 3.18 (d). A remaining concern would be the corrected spectra by SABCOND show slightly smaller absorption bands in the ratioed spectra. Another concern would be that the corrected spectra by SABCOND sometimes become unrealistically angular. For instance, the denominator spectrum of (a) jarosite shows an angular shape around $1.65 \mu \mathrm{~m}$.

### 3.4.6 Potential limitations

### 3.4.6.1 Too many bad pixels

Although SABCOND is robust to noise and less affected by BPs, the occurrence of too many adjacent BPs in a spectrum could be problematic. Fig. 3.19 (a) shows an example of such a case. The red spectrum has been corrected by the proposed method and the BPs have been substituted with the corresponding model values. The spectrum shows a $2.5 \mu \mathrm{~m}$ wavelength absorption, which is the shape suggested by the model. The orange spectrum, which has been corrected but with BP's that have been simply omitted, reveals that more than few sequential channels are bad. In such case, the shape of $2.5 \mu \mathrm{~m}$ cannot be easily corroborated. An image that contains a measurement of the same geographical location is shown in Fig 3.19 (b). The $2.5 \mu \mathrm{~m}$ wavelength region of that spectrum which does not require substitution shows no absorption features. The procedure leads us to reject the spectrum in Fig. 3.19 (a).


Figure 3.18. Comparison of atmospherically corrected I/F spectra and ratioed spectra corrected by the proposed method (red) and by volcano scan using CAT on TRR3 filtered I/F (blue) of (a) jarosite, (b) polyhydrated sulfate, (c) serpentine, and (d) saponite. (a1)(d1) are the comparisons of I/F spectra and (a2)-(d2) are those of ratioed I/F spectra. In (a1)-(d1), the two upper spectra (red and blue) are numerators and the two lower ones are denominators (red and blue). Spectra are shifted for ease for comparison. Their image coordinates and spatial average sizes are reported in [140].


Figure 3.19. Comparison of I/F spectra atmospherically corrected by the proposed method with (red) or without (orange) bad entries substituted and corrected with CAT on TRR3 I/F (blue). Spectra are from (a) $(255,270)$ in FRT000243C0 and (b) $(518,126)$ in FRS00029DA6. Spectra are shifted for ease of comparison.

Fig. 3.20 shows another potential limitation, by which actual spectral features could be removed by the proposed technique. In this figure, an absorption at $1.46 \mu \mathrm{~m}$, a depression around $2.0 \mu \mathrm{~m}$, and an absorption feature at $2.4 \mu \mathrm{~m}$ are removed by the proposed method. While the $2.0 \mu \mathrm{~m}$ depression correction can be justified as a bowl-shape distortion, $1.46 \mu \mathrm{~m}$ and 2.4 mm are more problematic. However, those features are present everywhere along the column, which makes SABCOND consider them as systematic column-dependent artifacts. While I cannot confirm that the features are atmospheric, the fact that they are present through the columns suggests that they are not due to surface contributions and therefore they can be corrected.

### 3.4.6.2 Unrealistic spectral edge drop

The background component $\overline{\mathbf{C}}^{-1} \mathbf{Z}$ in the spectral model can model any concave curvature. When you encounter a downward spike around the edge of a spectrum, the spike is unlikely to be detected. Rather, it is well modeled as a part of the background


Figure 3.20. Comparison of I/F spectra corrected with the proposed method (red) with those corrected with CAT on TRR3 I/F (blue) and with CAT on TRR3 I/F without filtering (gray/purple/yellow). Yellow dots represent bad channels (BPs). Purple dots represent non corrupted channels (non-BP). Spectra are from $(391,449)$ in FRT00003192. Spectra are shifted for ease of comparison.
component. Figure 3.21 shows such an example.

### 3.4.6.3 Problems related to the initial transmission spectrum

Since the SABCOND uses the transmission spectra in the ADR to initialize the image transmission spectrum, an image transmission spectrum that is dramatically different from those in the ADR library could also be an issue. The non-convex optimization may not recover from a poor initialization. So far on all the images I have tested initialization using the ADR transmission appears to work well on many images; however, in some cases, problems are found.

### 3.4.6.3.1 Kiserite issue

Kieserite has a big and broad absorption band around $2.0 \mu \mathrm{~m}$, which significantly conflicts with the triplet absorption of $\mathrm{CO}_{2}$ in the Martian atmosphere. The current collection of initial transmission spectra often causes a big hash artifacts in the first iteration; therefore, you need to do something aggressive, using a relatively large sparsity


Figure 3.21. An example of edge drop
constraint to satisfactory ignore this feature. On the other hand, the large constraint also causes the underestimation of important mineral absorption features. The big absorption feature of Kieserite around $2.0 \mu \mathrm{~m}$ is strongly affected by this problem. Since any common residual is considered as a column-dependent artifact, features that are commonly present and cannot be properly modeled via the surface model are absorbed into the estimated transmission spectrum, causing inverted features on the corrected spectra.

This problem is pointed out by Dr. Milliken in the collaboration research [141]. The problem especially happened in FRT00017D33. The data used there was produced instead by modifying the current algorithm; atmospheric transmission is obtained by processing only lines $1-100$ where kieserite is scarcely present, instead of using all the lines. Fig. 3.22 shows the example of the inverted kieserite feature. You can see the feature is inverted for the red and blue spectra. The blue has the inverted version of kieserite feature. To overcome this issue, you need a better atmospheric transmission spectrum in the first place. That allows users to use a milder sparsity constraint, mitigating the


Figure 3.22. An example of inverted kieserite feature
underestimation of mineral features.

### 3.4.6.3.2 Detector edge issue

Toward cross-track edge columns of the detector array, the transmission spectra in the ADR looks to deviate more from what it should be, causing mismatch in the absorption features over $1.2-1.6 \mu \mathrm{~m}$ wavelength region. The absorption over there is underestimated, causing angular shape over this region, or you might see slight absorption there. Fig. 3.23 shows examples of this issue.

### 3.4.6.3.3 Overcorrection in half resolution images

You need to aggressively remove the artifacts in the first iteration by using the large sparsity promoting parameter $\boldsymbol{\Lambda}_{\mathrm{A}}$. This might overcorrect underlying mineral absorptions as we saw in the kieserite inverting feature issue.

This is also potentially problematic for other HRL images. HRL images are binned, so the random noise present the data would be smaller that in full resolution images. This would change the balance between the residual term and sparsity term in the cost


Figure 3.23. Examples of Cross track edge issue
function controlled by the sparsity promoting trade-off parameter. However, the artifacts caused by the atmospheric transmission using ADR data are not any smaller. Therefore, still you need to aggressively remove the artifacts in the first iteration by using the large sparsity promoting parameter. If you do not use a strong enough sparsity promoting parameter, the model overfits to the atmospheric residual and it cannot be removed, while you can keep surface features.


Figure 3.24. An example of 40FF problem

Fig. 3.24 illustrates this problem. The yellow spectrum is the original TRRB I/F before atmospheric correction and de-noising is applied, the blue and red spectra are processed with

$$
\begin{aligned}
& \boldsymbol{\Lambda}_{\mathrm{A}}=0.01 \cdot \operatorname{sqrt}\left(\mathbf{1}_{N_{A} \times L} \cdot(\log \mathbf{Y} \odot \log \mathbf{Y})\right) \\
& \boldsymbol{\Lambda}_{\mathrm{A}}=0.001 \cdot \operatorname{sqrt}\left(\mathbf{1}_{N_{A} \times L} \cdot(\log \mathbf{Y} \odot \log \mathbf{Y})\right),
\end{aligned}
$$

respectively. The blue spectrum crawls under the yellow spectrum over the $1.4-2.0 \mu \mathrm{~m}$ wavelength region since the trade-off parameter is so large that some "olivine" features are underestimted, while the red spectrum has the same level at $1.8 \mu \mathrm{~m}$, but causing a hump-shape artifact over $2.0 \mu \mathrm{~m}$. If you find any overcorrection, it may be a good idea to play around with smaller $\boldsymbol{\Lambda}_{\mathrm{A}}$ to see if there is any better optimal solution that alleviates overcorrection while sufficiently removing the atmospheric residual.

### 3.4.6.4 Presence of water and carbon dioxide ice

Finally, SABCOND could lead to erroneous results in scenes where water and carbon dioxide ice are present on the surface. In particular, in the presence of water ice aerosols, the proposed method cannot discriminate ice aerosols from surface ice. The extension of the technique to such images will be the subject of a future publication.

### 3.5 Two-step SABCOND

This section describes the two-step SABCOND, a methodology for higher fidelity correction using SABCOND.

### 3.5.1 Motivation

SABCOND initializes the transmission spectrum using the empirically derived transmission spectra that are also used in volcano scan method. As shown in Section 3.4.6.3,
this causes several problems. More accurate initialization of the transmission spectrum would solve these problems. Fortunately, it is possible to simulate the transmission spectrum through the Martian atmosphere for a specific time and geographical location using atmospheric statistics obtained from Mars Climate Database (MCD) $[142,143]$ and universal absorption line parameters of gaseous molecules in the atmosphere from the HITRAN (High Resolution Transmission) database [88].

Unfortunately, I experimentally found that the original simulated transmission spectrum is insufficient to accurately represent the CRISM absorption spectrum since it turns out to create another multiplicative error in the correction. In order to resolve this problem, a two-step approach is proposed. First, a spectrally bland image that has atmospheric statistics and calibration residuals similar to those of the image of interest is selected. The simulated transmission spectrum is first created for the bland image using the HITRAN and the MCD, and then optimized by running the SABCOND on it. This optimized spectrum is then used as an initial estimate of the atmospheric transmission for the image to correct.

### 3.5.2 Background

### 3.5.2.1 MCD

MCD is a database of atmospheric statistics computed from the Global Climate Model (GCM) of the Martian atmosphere. The GCM models various kinds of atmospheric processes on Mars, is extensively validated with observational data, and is considered to be the compilation of the state-of-the-art knowledge of the Martian atmospheric conditions. MCD v5.3 is the latest version at this time of writing, and its full version is available upon request from its developers. MCD allows us to obtain atmospheric statistics at a given time and a geographical location up to the altitude of 300 km .

### 3.5.2.2 HITRAN

HITRAN database is the compilation of the molecular spectroscopic parameters derived from experiments and computations. The central component of the database is line-by-line spectroscopic parameters of gaseous molecules to derive high resolution molecular absorption and radiance over microwave to ultraviolet region through atmospheric paths. Its comprehensive coverage of the molecular spectroscopic data enables modeling of transmission, absorption, and radiance through atmospheric paths in different environments, and extensively deployed for dealing with radiative transfer problems in the atmosphere of Earth, Mars, and other planets.

### 3.5.3 Methodology

### 3.5.3.1 Bland image selection and inter-image spectral ratioing

A bland image is a spectrally unremarkable image where no or little absorption features diagnostic to mineral detection are observed throughout the image and only continuum components are present. Such spectrally unremarkable continuum components would be well modeled by the concave background. You can ignore absorption components on such a bland image, allowing SABCOND to perform aggressive correction without being careful not to overcorrect absorption features.

Spectral blandness can be evaluated by looking at the spectra directly or by spectral parameter maps. We can transfer the idea used for deriving the atmospheric transmission spectra for volcano scan correction. The regions at the top and bottom of the Olympus Mons are assumed to be spectrally bland in the volcano scan correction. Spectra of these regions are characterized by the upward slope towards from $1.0 \mu \mathrm{~m}$ and to $2.3 \mu \mathrm{~m}$ region and expected only to have concave curvature without absorption features. Images that have the same spectral characteristic would indicate spectral blandness and become candidates.

A bland image that can be paired with the image of interest should have not only
the same atmospheric statistics, but also the same multiplicative errors as the image of interest so that its optimized atmospheric transmission spectrum can sufficiently remove both the residual of atmospheric correction and the calibration errors. The bland image needs to be carefully selected since absorption features present in the bland image and the mismatch of the atmospheric transmission or calibration errors could be the source of new artifacts. I currently select the bland image in an empirical way.

First, candidates of the bland image are pre-selected using the meta information of the images. Geographical proximity (including latitude, longitude, and elevation) and seasonal proximity are indicators of the similarity of the atmospheric statistics. The similarity of calibration errors can be evaluated by the temporal proximity of the acquisition of the two images. If the two images are taken within a short interval of time, it also means they are in the same season. Therefore, spatially and temporally close images become candidates of the bland image. In addition, elevation should be close as it is related to the path length of the transmission.

Once the candidates are selected, we can utilize the spectral ratioing technique to more quantitatively determine the similarity of the atmospheric condition and the calibration errors of the image to be corrected and the candidates of the bland image. If ratioing of spectra of the same column from the two images shows no atmospheric residual features, and only features relevant to surface are observed, it is reasonable to say the atmospheric transmission and calibration errors of the two images are similar and canceled out by the ratioing. A scaling might be applied on the spectrum of the bland image to consider the difference in the path length.

### 3.5.3.2 Simulation of the atmospheric transmission spectrum on the bland image

The atmosphere is first divided into 30-40 vertical layers, and the atmospheric statistics - pressure, temperature, volume mixing ratios of the molecules, carbon dioxide, car-
bon monoxide, and water vapor, that are dominant in the Martian atmosphere and have significant absorption are obtained from the MCD. For each layer, the atmospheric statistics are assumed to be constant, and gaseous absorption coefficient $\alpha(\lambda)$ ( $\lambda$ : wavelength) is computed based on the Voigt profile using the line-by-line parameters of the molecules obtained by the HITRAN database. In order to accurately model the absorption coefficient, I set the resolution to be ultra high at $0.0001 \mathrm{~cm}^{-1}$. Then optical of each layer is computed by $e^{-\alpha l}(l$ : the thickness of the layer), and the total absorption is obtained by multiplying the optical depths of all the layers. Currently the effects of dusts and aerosols are not considered. Once the ultra high resolution transmission spectrum is obtained, it is then convolved with CRISM channels using the instrument's spectral response functions.

### 3.5.3.3 Two-step atmospheric correction

The simulated transmission spectrum at CRISM resolution is now used as an initial estimate of the transmission spectrum, and SABCOND is performed on the bland image. Because the little amount of spectral absorption features is expected on the bland image and its unremarkable surface spectra would be well modeled by the background concave function $\overline{\mathbf{C}}^{-1} \mathbf{Z}$, it is expected that the contribution of the library in the mixing model (??) is minimal. To avoid overfitting the library endmembers to the surface mixing model, I utilize large values for the trade-off parameters $\boldsymbol{\Lambda}_{\mathrm{A}}$ for the sparsity constraint in the cost function $f_{\Lambda}$ in Eq. (3.60) in the optimization problem (3.49). The optimized transmission spectrum on the bland image is expected to have much less errors for the correction of the image of interest even at the first iteration. The output transmission spectrum is then used as the initial estimate for the correction using SABCOND on the image of interest.

### 3.5.4 Preliminary results

I tested the new approach for the correction of HRL000040FF (40FF) acquired over Jezero crater where the NASA Perseverance rover touched down this year.

### 3.5.4.1 Bland image selection



Figure 3.25. Inter-image spectral ratioing with scaled dividends. Logarithmic ratioed I/F spectra are shown. Three figures show the subtraction of the mean logarithmic spectrum over lines 1 to 400 at column 148 of 40 FF by the mean of ones from all lines of the same column of the candidate bland images ( (a) 40A2, (b) 3D3C, and (c) 37AE). 3D3C and 37AE are FRT images and binned to the half resolution beforehand. The gray spectra demonstrate the logarithmic ratioed I/F spectra obtained by incrementing the scale of bland image spectra from 0.8 to 1.2 by 0.025 from bottom to top. The red spectra are the subtraction associated with the optimally scaled bland image spectra, where the optimal scaling values are manually determined to (a) 0.975 , (b) 0.8875 , (c) 1.125 by visual inspection.

The scene 40 FF is located at $77.418^{\circ} \mathrm{E} 18.505^{\circ} \mathrm{N}$ and covers the west side of the Jezero crater near Nili Fossae, located around the boundary of Isidis Planitia and Syrtis Major. The elevation is around -2400 m , intermediate value of the low land, Isidis Plantia, and a high land, Syrtis Major.

From the meta information of the 40FF image, three images, HRL000040A2, FRT00003D3C, and FRT000037AE are pre-selected as candidates of the bland image. FRT00003D3C is located at $90.889^{\circ}$ E $11.764^{\circ} \mathrm{N}$ inside the Isidis Planitia, while HRL000040A2 scenes is located at $155.919^{\circ} \mathrm{E} 8.790^{\circ} \mathrm{N}$ in Elysium Planitia. FRT000037AE is at $74.688^{\circ} \mathrm{E} 24.694^{\circ} \mathrm{N}$
in Nili Fossae.
It is almost impossible in many cases to select a perfect bland image. One might need to compromise some aspects. 40A2 is measured just one Earth day before 40FF and almost perfectly satisfies the condition of the temporal and seasonal proximity. In addition, 40A2 is the mean altitude of -2600 m , quite close to the mean elevation of 40 FF , and it is spectrally quite bland, while it is not geographically close to 40 FF . 3D3C is much closer to 40 FF than 40 A 2 , and spectral blandness and uniformity is at extreme. However, its mean elevation -3580 m is much lower than that of 40 FF . In addition, it is taken 20 Earth days before 40FF, and thus the temporal proximity condition may be violated. 37AE best meets the spatial proximity condition, while temporal proximity condition (more than 30 Earth days in advance) may be violated and its mean elevation -800 m is a little deviated from that of 40FF. In addition, spectral blandness may be violated.

Among these candidates, the best bland image is then selected using the inter-image spectral ratioing. Fig. 3.25 demonstrates the spectral ratioing of a spectrum obtained from 40 FF by the scaled column means from the three candidates of the bland image. All operations, such as averaging and scaling are performed after the logarithmic transformation of I/F spectra. Note that ratioing operation, namely division, is equivalent to subtraction and scaling is simply performed by multiplication after the logarithmic conversion. The gray spectra show that changing the scale of the bland image spectra changes the shape of residuals and indicates an optimal scaling that minimizes the residual would exist. The red spectra are the logarithmic ratioed I/F spectra obtained by the optimally scaled bland image spectra. The optimal scaling values are determined to minimize atmospheric contribution, mainly the triplet shape around at $2.0 \mu \mathrm{~m}$ wavelength. The optimal values for 40A2, 3D3C, and 37AE are $0.975,0.8875$, and 1.125 , respectively. These values generally agree with our intuition; the 3D3C scene covers an area at much lower altitude than the 40 FF scene and has more atmospheric absorption. Therefore,


Figure 3.26. The vertical profile of atmospheric statistics at the scene 40A2.
scaling by the value well below 1 is necessary to match the atmospheric transmission of 40 FF . The 37 AE scene covers an area at higher altitude than 40 FF and has less atmospheric absorption. Thus, scaling by the value well above 1 is required. The 40A2 scene covers an area at altitude close to 40 FF and thus only a little scaling is required.

Overall 40A2 seems to be the best bland image. After the subtraction by the optimal scaling, the red spectrum in Fig. 3.25 (a) shows the least amount of errors. In particular, the triplet at $2.0 \mu \mathrm{~m}$ is almost perfectly canceled out, much less significant than the waterbearing band at $1.91 \mu \mathrm{~m}$. On the other hand, the red spectra in Fig. 3.25 (b) and (c) show more errors, and residuals here and there obscure the underlying absorption bands and spectral shapes. These residuals is possibly caused by the mismatch of calibration errors. In particular, the red spectrum in Fig. 3.25(b) shows that the triplet at $2.0 \mu \mathrm{~m}$ are still present and as significant as the water-bearing band, indicating the mismatch of the absorption around this wavelength range.


Figure 3.27. Simulated transmission spectrum. Blue: the original simulated transmission spectrum at $0.0001 \mathrm{~cm}^{-1}$ wavenumber resolution. Red: convolution using the spectral response function of CRISM at column 148.

### 3.5.4.2 Creation of transmission spectrum for the bland image

Fig. 3.26 shows the vertical profile of the atmospheric statistics - pressure, temperature, and the volume mixing ratio of carbon dioxide, water vapor, and carbon monoxide at the center of the geographical location of 40A2. The profile is obtained until the pressure drops small enough since the pressure indicates the density of the atmosphere. The sufficiently small atmospheric density indicates little contribution to atmospheric absorption that can be ignored. You might notice that the vertical slicing may look rough. This is a compromise of the computational time versus accuracy. Using these parameters and absorption line parameters obtained from HITRAN database, I simulate the transmission spectrum (Fig. 3.27). Absorption line broadening depends on temperature and pressure, so it is important to divide the atmosphere into the vertical layer so that each layer has approximately constant statistics. The figure shows that the original simulated transmission spectrum has extremely narrow absorption bands compared to the CRISM wavelength sampling.

### 3.5.4.3 Processing on the bland image

Fig. 3.28 shows the atmospheric correction of the bland image 40A2 using the simulated transmission spectrum. The simulated transmission spectrum cause a significant artifacts at $2.0 \mu \mathrm{~m}$. In addition, it seems that the over-correction occurs around $1.35 \mu \mathrm{~m}$. After the update of the transmission spectrum, these artifacts are successfully removed.


Figure 3.28. Correction of the spectra CRISM at column 148 of 40A2. Spectra are averaged over lines 1 to 480 . Gray: the I/F spectrum before atmospheric correction. Blue: the corrected I/F spectrum at the first iteration using transmission spectrum optimized on 40A2. Red: the corrected I/F spectrum after the update of the transmission spectrum

Fig. 3.29 shows the result of the correction of the image of interest, 40FF, using the transmission spectrum optimized on 40A2, compared with the correction using the ADR transmission spectrum. Although you see a small triplet residuals over $2.0 \mu \mathrm{~m}$ in the correction using the 40A2-optimized transmission, residualistic features are much smaller and less frequent. In addition, the potential under-correction at $2.6 \mu \mathrm{~m}$ is also addressed. Fig. 3.30 shows correction results after the second iteration. The new two-step approach retains the overall spectral continuum absorption band shapes and only correcting minor errors, while the original SABCOND using the ADR transmission spectra is doing rather


Figure 3.29. Correction of the CRISM spectra at column 148 of 40FF. Spectra are averaged over lines 1 to 400 . (a) Gray: the I/F spectrum before atmospheric correction. Blue: the corrected I/F spectrum at the first iteration using transmission spectrum optimized on 40A2. (b) Gray: the I/F spectrum before atmospheric correction. Blue: the corrected I/F spectrum at the first iteration using ADR transmission spectra.


Figure 3.30. Correction of the spectra CRISM at column 148 of 40FF. Spectra are averaged over lines 1 to 480. (a) Gray: the I/F spectrum before atmospheric correction. Blue: the corrected I/F spectrum at the first iteration using transmission spectrum optimized on 40A2. (b) Gray: the I/F spectrum before atmospheric correction. Blue: the corrected I/F spectrum at the first iteration using ADR transmission spectra.
drastic - changing the spectral continuum shape and absorption bands. It also smooths out the water vapor absorption around $2.6 \mu \mathrm{~m}$, changing the continuum level, leading to a potential underestimation of any absorption around at $2.5 \mu \mathrm{~m}$ if present.

### 3.6 Summary

This chapter proposed a new atmospheric correction and de-noising method (SABCOND) for CRISM IR images of non-icy surfaces over the $1.0-2.6 \mu \mathrm{~m}$ wavelength range. SABCOND estimates the atmospheric transmission spectrum from the image itself by solving the minimization problem that unifies light propagation through the atmosphere and surface mixing, while large random noise spikes are simultaneously detected and removed. Experimental results show that SABCOND significantly mitigates columndependent systematic artifacts that could be caused by the volcano scan method using CAT, while successfully detecting and removing severe noise. Compared with CATcorrection, SABCOND provides a significant improvement over the $1.1-1.7 \mu \mathrm{~m}$ and $1.9-2.1 \mu \mathrm{~m}$ wavelength regions where the strong atmospheric absorptions of carbon dioxide are present. SABCOND has been applied to a large number of images of non-icy surfaces. The technique is also able to contend well with adverse conditions like elevated detector temperatures and water ice aerosols. Validations reveal that SABCOND retrieves consistent spectral shapes for the same location in different overlapping images even in the presence of elevated noise. Another validation using ratioed spectra clarified that SABCOND corrects for artifacts created in the calibration, such as interpolation bias. Second, this chapter proposed two-step SABCOND, aiming for more accurate correction with higher fidelity. The two-step SABCOND is applied to an image in Jezero crater and shows its potential in correcting images with more fidelity, further solving some problems encountered in the SABCOND.

This chapter also provided an advancement in the optimization algorithm by introducing the formulation of alternating direction method of multipliers using generalized augemented term (ADMM-GAT) together with associated residual balancing.

This chapter also advanced the understanding of noise and artifacts present in the CRISM IR images. We discovered the mechanism of the occurrence of interpolation bias formally reported by [84]. We also succeeded in extracting three different kinds of noise
patterns present in CRISM scene images - an autoregressive pattern, random spikes and a telegraph pattern. We presented a new theoretical limitation of the empirical volcano scan method.

# CHAPTER 

# MUTUAL MAP PROJECTION OF CRISM AND MASTCAM IMAGES VIA HIGH-RESOLUTION DIGITAL ELEVATION MODEL 

### 4.1 Introduction

Martian ground rover missions heavily rely on orbital measurements/images, including selecting the initial touchdown locations, designing their traverses to achieve scientific goals, and ensuring the safety of operations [144]. The Mars Science Laboratory (MSL) Curiosity Rover, which landed on the floor of the Gale crater on Mars in 2012, is the NASA's rover for the MSL mission, aiming for investigating the modern and past habitability environment of Mars [145]. This mission takes full advantage of ultra-high spatial resolution images acquired by the High Resolution Imaging Science Experiment (HiRISE) [146], and hyperspectral images acquired by the CRISM [4] (both on the MRO) for mission planning, safety assessment, and scientific analysis [144,145]. HiRISE images have the spatial resolution as fine as 0.25 m and their derived elevation model has 1 m resolution. These ultra-high resolution images are even useful for determining a more precise traverse to guide rovers even after they landed. Besides, the CRISM spectroscopic images provide the abundant information of surface mineralogy, guiding scientific measurements and analysis.

These orbital images are also often introduced and compared to complement the geol-
ogy, mineralogy, geochemistry, or organics investigations at the ground for post scientific analysis. In order to incorporate orbital images to ground observation, it is necessary to geographically link both data to each other accurately. Furthermore, an automatic and systematic method for resolving the geographic matching problem would help increase the efficiency of the scientific analysis. This chapter investigates one of such methods, in particular, presenting a method for pixel-level mapping between ground images acquired by Mast camera (Mastcam) [147] installed on the Curiosity rover and hyperspectral images acquired by CRISM via the HiRISE-derived digital terrain model (DTM).

The new method takes full advantage of the camera model of the Mastcam instrument and the sensor model of CRISM. The camera/sensor models allows us to find a precise location of each pixel in the geographic map when surface topography is given. The projection that mutually maps CRISM and Mastcam image pixels is achieved by combining the projection of Mastcam images and CRISM images onto the surface. MSL_Gale_DEM_Mosaic_10m.tif (MSL Gale DEM Mosaic), available on the Annex of the PDS Cartography \& Imaging Sciences Node USGS website [148], is used as a surface model in this research. The field-of-view of Mastcam images on the MSL Gale DEM Mosaic is evaluated with the camera model. A novel method to compute the viewshed of the Mastcam image is introduced. Additionally, the precise footprints of CRISM pixels are computed from its sensor model and the DEM Mosaic. The two projections are finally combined together to build the mutual map projection between the Mastcam and CRISM images.

The contribution of this chapter is as follows:

1. I propose a novel pixel-to-pixel projection of Mastcam images using a high resolution DEM model using the camera model.
2. I introduce a general viewshed algorithm for a camera based on CAHV model is introduced.
3. To the best of our knowledge, our proposed approach is the first to project the footprint of CRISM pixels onto the high resolution DEM model.
4. To the best of our knowledge, our proposed approach is the first to provide a precise map projection of CRISM image pixels onto Mastcam images.

### 4.2 Background

### 4.2.1 Mastcam cameras

The Mastcam instrument suite $[147,149]$ consists of a set of two mega-pixel cameras (left and right) mounted on the 2 m mast of the Curiosity rover. It consists of two optical megapixel CCD cameras, one on the left and the other on the right of the mast. Both of the cameras can take RGB images and also have the capability of taking multispectral images over visible to near infrared wavelength regions. The acquisition mode - either RGB or multispectral modes - are switched by rotating their internal filter-wheel. In the multispectral mode, multiple images are collected with different filters. Users are required to merge them by themselves. Right and Left cameras have different focal lengths and different spatial resolution. The right camera has higher spatial resolution, but the lower spatial field-of-view (FOV), while the Left camera has lower spatial resolution and a wider FOV.

The primary task of the Mastcam is to record the images of landscapes or atmosphere to study the geology, topography, geomorphology, mineralogy, and meteorology of the field site. The high resolution of the Mastcam (left: $450 \mu \mathrm{~m}$ at 2 m distance and 22 cm at 1 km and right: $150 \mu \mathrm{~m}$ at 2 m and 7.4 cm at 1 km ) enables the observation of fine details of the Martian surface that cannot be obtained from orbits over a wide range of distances. The acquired Mastcam images are also used for supporting rover operations, including the selection of interesting locations.

### 4.2.2 CAHV/CAHVOR models

CAHV [150] and its extension, CAHVOR [151] are camera models extensively deployed in planetary rover missions, such as the 1997 Mars Pathfinder (MPF) Mission, the 2003 Mars Exploration Rover (MER) mission, 2012 MSL Rover Curiosity, and Mars 2020 Perseverance rover.

CAHV encodes internal and external camera parameters, simplifying the projection of points onto the image plane. CAHV model consists of four camera parameters ( $\boldsymbol{c}$, $\boldsymbol{a}, \boldsymbol{h}, \boldsymbol{v}) ; \boldsymbol{c} \in \mathbb{R}^{3}$ is the position vector for the camera center position in the reference coordinate system, $\boldsymbol{a} \in \mathbb{R}^{3}$ is the unit direction vector for the line of sight of the camera in the reference coordinate system, and $\boldsymbol{h} \in \mathbb{R}^{3 \times 1}$ and $\boldsymbol{v} \in \mathbb{R}^{3 \times 1}$ are the vectors relating to horizontal and vertical information of the image plane of the camera. For a given object position vector, $\boldsymbol{p}$ defined in the reference coordinate system, the projection onto the camera image expressed as $(x, y)$ is performed by

$$
\begin{equation*}
x=\frac{\boldsymbol{h} \cdot(\boldsymbol{p}-\boldsymbol{c})}{\boldsymbol{a} \cdot(\boldsymbol{p}-\boldsymbol{c})} \quad \text { and } \quad y=\frac{\boldsymbol{v} \cdot(\boldsymbol{p}-\boldsymbol{c})}{\boldsymbol{a} \cdot(\boldsymbol{p}-\boldsymbol{c})}, \tag{4.1}
\end{equation*}
$$

where • represents the inner product of two vectors. Yakimovsky and Cunningham [150] provide a decomposition of $\boldsymbol{h}$ and $\boldsymbol{v}$ with physical understandable parameters:

$$
\boldsymbol{h}=h_{s} \boldsymbol{h}^{\prime}+h_{c} \boldsymbol{a} \quad \text { and } \quad \boldsymbol{v}=v_{s} \boldsymbol{v}^{\prime}+v_{c} \boldsymbol{a},
$$

where $\boldsymbol{h}^{\prime} \in \mathbb{R}^{3 \times 1}$ and $\boldsymbol{v}^{\prime} \in \mathbb{R}^{3 \times 1}$ are the unit direction vectors in the reference coordinate system, respectively pointing in the $x$ and $y$ direction of the image plane, $h_{s}$ and $v_{s}$ are the focal length expressed as the number of pixels, and $\left(h_{c}, v_{c}\right)$ is the coordinate in the camera image plane where the line of sight intersects with the plane. Note that $\boldsymbol{a}, \boldsymbol{h}^{\prime}$, and $\boldsymbol{v}^{\prime}$ are orthogonal to each other. Fig. 4.1 illustrates the geometric relationship of these parameters.

There exist identity relationships between the parameters, $h_{c}, v_{c}, h_{s}$, and $v_{s}$, which


Figure 4.1. CAHV model
can be written as follows [152]:

$$
\begin{array}{r}
\boldsymbol{a} \cdot \boldsymbol{h}=\boldsymbol{a} \cdot\left(h_{s} \boldsymbol{h}^{\prime}+h_{c} \boldsymbol{a}\right)=h_{s} \cdot\left(\boldsymbol{a} \cdot \boldsymbol{h}^{\prime}\right)+h_{c} \cdot\|\boldsymbol{a}\|_{2}^{2}=h_{c} \\
\boldsymbol{a} \cdot \boldsymbol{v}=\boldsymbol{a} \cdot\left(v_{s} \boldsymbol{v}^{\prime}+v_{c} \boldsymbol{a}\right)=v_{s} \cdot\left(\boldsymbol{a} \cdot \boldsymbol{v}^{\prime}\right)+v_{c} \cdot\|\boldsymbol{a}\|_{2}^{2}=v_{c} \\
\left\|\boldsymbol{a} \times\left(h_{s} \boldsymbol{h}^{\prime}+h_{c} \boldsymbol{a}\right)\right\|_{2}=\left\|h_{s} \cdot\left(\boldsymbol{a} \times \boldsymbol{h}^{\prime}\right)+h_{c} \cdot(\boldsymbol{a} \times \boldsymbol{a})\right\|_{2}=h_{s} \\
\left\|\boldsymbol{a} \times\left(v_{s} \boldsymbol{v}^{\prime}+v_{c} \boldsymbol{a}\right)\right\|_{2}=\left\|v_{s} \cdot\left(\boldsymbol{a} \times \boldsymbol{v}^{\prime}\right)+v_{c} \cdot(\boldsymbol{a} \times \boldsymbol{a})\right\|_{2}=v_{s},
\end{array}
$$

where $\times$ represents the cross product of the vectors, and orthogonality between $\boldsymbol{a}, \boldsymbol{h}^{\prime}$, and $\boldsymbol{v}^{\prime}$ is used and the fact that $\boldsymbol{a}, \boldsymbol{h}^{\prime}$, and $\boldsymbol{v}^{\prime}$ are all unit vectors. These relations are identities obtained by the definition of the parameters. $\boldsymbol{h}^{\prime}$ and $\boldsymbol{v}^{\prime}$ can be also easily obtained once the above scalar parameters are obtained from the definition:

$$
\boldsymbol{h}^{\prime}=\frac{\boldsymbol{h}-h_{c} \boldsymbol{a}}{h_{s}} \quad \text { and } \quad \boldsymbol{v}^{\prime}=\frac{\boldsymbol{v}-v_{c} \boldsymbol{a}}{v_{s}} .
$$

The inverse projection of the equation (4.1), namely recovering the vector $\boldsymbol{p}$ given the image coordinate ( $x, y$ ), was discussed in [150] and described here. Let $\boldsymbol{p}_{C}=(\boldsymbol{p}-\boldsymbol{c})$,
representing a direction vector associated with the image plane coordinate $(x, y)$. Then we can express the relation (4.1) with $\boldsymbol{P}_{C}$ :

$$
\begin{array}{cccc} 
& x \boldsymbol{a} \cdot \boldsymbol{p}_{C}=\boldsymbol{h} \cdot \boldsymbol{p}_{C} \quad \text { and } \quad y \boldsymbol{a} \cdot \boldsymbol{p}_{C}=\boldsymbol{v} \cdot \boldsymbol{p}_{C} \\
\Leftrightarrow \quad & (x \boldsymbol{a}-\boldsymbol{h}) \cdot \boldsymbol{p}_{C}=0 \quad \text { and } \quad(y \boldsymbol{a}-\boldsymbol{v}) \cdot \boldsymbol{p}_{C}=0 . \tag{4.2}
\end{array}
$$

The equations (4.2) indicate that $\boldsymbol{p}_{C}$ is orthogonal to both of the vectors $(x \boldsymbol{a}-\boldsymbol{h})$ and $(y a-\boldsymbol{v})$. Such a vector can be obtained by taking a cross product of these vectors. Namely, we have

$$
\begin{equation*}
\boldsymbol{p}_{C}=\boldsymbol{a}+\frac{x-h_{c}}{h_{s}} \boldsymbol{h}^{\prime}+\frac{y-v_{c}}{v_{s}} \boldsymbol{v}^{\prime} . \tag{4.3}
\end{equation*}
$$

You might need to normalize the derived pointing vector. The normalization factor is just the squared sum of the coefficients of the mutually independent vectors:

$$
\sqrt{1+\frac{\left(x-h_{c}\right)^{2}}{h_{s}^{2}}+\frac{\left(y-v_{c}\right)^{2}}{v_{s}^{2}}} .
$$

The equation (4.3) indicates that $\boldsymbol{p}_{C}$ points in the same direction as $\boldsymbol{a}$ with respect to the plane defined by the camera image plane basis vectors $\boldsymbol{h}^{\prime}$ and $\boldsymbol{v}^{\prime}$.

CAHVOR [151] is an extension of the CAHV model with two additional parameters (the optical axis unit vector $\boldsymbol{o}$, and the radial distortion parameter $\boldsymbol{r}=\left(\rho_{0}, \rho_{1}, \rho_{2}\right)$ ). Consideration of the distortion of the optical axis and the radial distortion are integrated into the camera projection operation. The operation is as follows. First, the pointing vector $\boldsymbol{p}_{C}=(\boldsymbol{p}-\boldsymbol{c})$ is decomposed into two components - one parallel to the optical axis unit vector $\boldsymbol{o}$ and its perpendicular one $\boldsymbol{\lambda}$ :

$$
\boldsymbol{p}_{C}=\xi \boldsymbol{o}+\boldsymbol{\lambda},
$$

where $\xi$ is the scalar coefficient of the optical axis component. $\xi$ and $\boldsymbol{\lambda}$ are obtained by the following relationships:

$$
\xi=\boldsymbol{p}_{C} \cdot \boldsymbol{o} \quad \text { and } \quad \boldsymbol{\lambda}=\boldsymbol{p}_{C}-\xi \boldsymbol{o} .
$$



Figure 4.2. CAHV model

The radial distortion occurs along the vector $\boldsymbol{\lambda}$, and its magnitude depends on that of the radial component. Precisely, CAHVOR model defines it by the tangent of the angular distance, $\left(\tan \alpha=\lambda / \xi\right.$, where $\left.\lambda=\|\boldsymbol{\lambda}\|_{2}\right)$, of $\boldsymbol{p}_{C}$ from the optical axis $\boldsymbol{o}$. Then, the amount of distortion $\mu$ is obtained by

$$
\begin{equation*}
\mu=\rho_{0}+\rho_{1} \tau+\rho_{2} \tau^{2}, \tag{4.4}
\end{equation*}
$$

where $\tau=\tan ^{2} \alpha$. Finally, the pointing vector is modified as

$$
\begin{equation*}
\boldsymbol{p}_{C}^{\prime}=\boldsymbol{p}_{C}+\mu \boldsymbol{\lambda}=\xi \boldsymbol{o}+(1+\mu) \boldsymbol{\lambda}, \tag{4.5}
\end{equation*}
$$

and the projection of the CAHV model (4.1) is applied to $\boldsymbol{p}_{C}^{\prime}$. Note that $\mu$ represents the ratio factor of the distortion on the radial component. Fig. 4.2 illustrates the geometric relationship of the CAHVOR model parameters.

It is possible to perform the projection operation above without introducing the pa-
rameter $\xi$ by normalization along the optical axis:

$$
\hat{\boldsymbol{p}}_{C}=\frac{\boldsymbol{p}_{C}}{\left(\boldsymbol{p}_{C} \cdot \boldsymbol{o}\right)} .
$$

$\hat{\boldsymbol{p}}_{C}$ lies on the ray that originated from $\boldsymbol{c}$ in the direction of $\boldsymbol{p}_{C}$. Therefore, it is still projected onto the same coordinate in the camera image plane as $\boldsymbol{p}_{C}$. This normalization operation sets $\xi=1$, and its radial component is obtained by simple subtraction

$$
\hat{\lambda}=\hat{\boldsymbol{p}}_{C}-\boldsymbol{o} .
$$

Then, using $\hat{\lambda}^{2}=\|\hat{\boldsymbol{\lambda}}\|_{2}^{2}$, the magnitude of optical distortion is obtained by

$$
\mu=\rho_{0}+\rho_{1} \hat{\lambda}^{2}+\rho_{2} \hat{\lambda}^{4}
$$

Finally, the projection (4.1) is applied to the modification $\hat{\boldsymbol{p}}_{C}^{\prime}$ of $\hat{\boldsymbol{p}}_{C}$ :

$$
\begin{equation*}
\hat{\boldsymbol{p}}_{C}^{\prime}=\hat{\boldsymbol{p}}_{C}+\mu \hat{\boldsymbol{\lambda}}=\boldsymbol{o}+(1+\mu) \hat{\boldsymbol{\lambda}} . \tag{4.6}
\end{equation*}
$$

Inverse projection for CAHVOR model, namely recovering the pointing vector $\boldsymbol{p}_{C}$ from the camera image coordinate, is not as straightforward as that for the CAHV model. An analytical solution may not exist, but a numerical solution can be obtained. It is also discussed in [151] and described here in two different ways.

First, $\hat{\boldsymbol{p}}_{C}^{\prime}$ is obtained by the same way used for the inverse projection of the CAHV model (4.3):

$$
\begin{equation*}
\boldsymbol{p}_{C}^{\prime}=\boldsymbol{a}+\frac{x-h_{c}}{h_{s}} \boldsymbol{h}^{\prime}+\frac{y-v_{c}}{v_{s}} \boldsymbol{v}^{\prime} \tag{4.7}
\end{equation*}
$$

Recall from equation (4.5), that distortion can also be expressed using any $\boldsymbol{\lambda}^{\prime}$ such that $\boldsymbol{\lambda}^{\prime}=k \boldsymbol{\lambda}$ where $k$ is a nonzero scalar,

$$
\begin{equation*}
\boldsymbol{p}_{C}^{\prime}=\boldsymbol{p}_{C}+\mu \boldsymbol{\lambda}=\boldsymbol{p}_{C}+\mu^{\prime} \boldsymbol{\lambda}^{\prime} \tag{4.8}
\end{equation*}
$$

where $\mu^{\prime}=\mu / k$. Considering that this distortion operation does not change the magnitude of the component in the optical axis direction, we have

$$
\xi=\boldsymbol{p}_{C} \cdot \boldsymbol{o}=\boldsymbol{p}_{C}^{\prime} \cdot \boldsymbol{o}
$$

Let us consider a specific $\boldsymbol{\lambda}^{\prime}$, the radial component of $\boldsymbol{p}_{C}^{\prime}$, obtained by $\boldsymbol{\lambda}^{\prime}=\boldsymbol{p}_{C}^{\prime}-\xi \boldsymbol{o}$. By definition, we have $\boldsymbol{\lambda}^{\prime}=(1+\mu) \boldsymbol{\lambda}$. The equation (4.8) indicates $\mu \boldsymbol{\lambda}=\mu^{\prime} \boldsymbol{\lambda}^{\prime}$ and therefore we have $\mu \boldsymbol{\lambda}=\mu^{\prime}(1+\mu) \boldsymbol{\lambda}$. Comparing the coefficients on its both sides we obtain $\mu+1=\frac{1}{1-\mu^{\prime}}$. Thus, substituting this into $\boldsymbol{\lambda}^{\prime}=(1+\mu) \boldsymbol{\lambda}$, we have $\boldsymbol{\lambda}=\left(1-\mu^{\prime}\right) \boldsymbol{\lambda}^{\prime}$. Let $\tau^{\prime}=\frac{\lambda^{\prime} \cdot \lambda^{\prime}}{\xi^{2}}$, we have $\tau=\left(1-\mu^{\prime}\right)^{2} \tau^{\prime}$. Finally, we obtain the following by substituting the above results back into the equation (4.4)

$$
\begin{gathered}
\frac{1}{1-\mu^{\prime}}-1=\rho_{0}+\rho_{1} \tau^{\prime}\left(1-\mu^{\prime}\right)^{2}+\rho_{2} \tau^{\prime 2}\left(1-\mu^{\prime}\right)^{4} \\
\Leftrightarrow\left(1+\rho_{0}\right)\left(1-\mu^{\prime}\right)+\rho_{1} \tau^{\prime}\left(1-\mu^{\prime}\right)^{3}+\rho_{2} \tau^{\prime 2}\left(1-\mu^{\prime}\right)^{5}-1=0 .
\end{gathered}
$$

Solving this with respect to $\mu^{\prime}$ by any numerical method such as a Newton method or a bisection method, we have $\boldsymbol{p}_{C}=\boldsymbol{p}_{C}^{\prime}-\mu^{\prime} \boldsymbol{\lambda}^{\prime}$.

This could be simpler when normalization along optical axis is performed in the first place. First, $\boldsymbol{p}_{C}^{\prime}$ is obtained by the equation (4.7). Then normalize this vector with respect to $\boldsymbol{o}$ :

$$
\hat{\boldsymbol{p}}_{C}^{\prime}=\frac{\boldsymbol{p}_{C}^{\prime}}{\boldsymbol{p}_{C}^{\prime} \cdot \boldsymbol{o}}
$$

Since $\hat{\boldsymbol{p}}_{C}^{\prime}$ is the outcome of the equation (4.6), we can express it as

$$
\begin{aligned}
\hat{\boldsymbol{p}}_{C}^{\prime} & =\boldsymbol{o}+(1+\mu) \boldsymbol{\lambda} \\
\Leftrightarrow \hat{\boldsymbol{p}}_{C}^{\prime}-\boldsymbol{O} & =\left(1+\rho_{0}+\rho_{1} \lambda^{2}+\rho_{2} \lambda^{4}\right) \boldsymbol{\lambda} .
\end{aligned}
$$

The right hand side is the vector in the direction of $\boldsymbol{\lambda}$ and so is the left hand side. Therefore, by taking the magnitude on both sides, we have

$$
\left\|\hat{\boldsymbol{p}}_{C}^{\prime}-\boldsymbol{o}\right\|_{2}=\left(1+\rho_{0}+\rho_{1} \lambda^{2}+\rho_{2} \lambda^{4}\right) \lambda .
$$

Subsequently, any numerical method can be used to get $\lambda$ and $\hat{\boldsymbol{p}}_{C}$ is obtained by

$$
\hat{\boldsymbol{p}}_{C}=\boldsymbol{o}+\lambda \frac{\hat{\boldsymbol{p}}_{C}^{\prime}-\boldsymbol{o}}{\left\|\hat{\boldsymbol{p}}_{C}^{\prime}-\boldsymbol{o}\right\|_{2}} .
$$



Figure 4.3. Illustration of different types of DTMs. The bottom row illustrates the discrete sampling of each type of DTMs together and the interpolation of the surface using the samples, and the upper row shows the 3D view of the DTMs.

### 4.2.3 Digital terrain model (DTM) / Digital elevation model (DEM)

Terrain is a continuous topographical surface, expressed as a function defined on a geographical coordinate system. A digital terrain model (DTM) (or digital elevation model $(\mathrm{DEM}))^{1}$, commonly deployed in the geographical information system, is a representation of terrain using a finite set of discrete elevation data on a two-dimensional space associated with a certain geographical map projection [153,154]. DTM/DEM models the terrain/surface by some interpolation using the set of elevation data points. Two sub classes of the DTM model are usually considered, triangulated irregular network (TIN) and regular squared grid (RSG), based on how the discrete elevation data are sampled and on how the terrain is modeled [154]. TIN is a class of the DTM model, where the

[^11]elevation samples are arbitrarily scattered on the 2-D map-projected space and forms the terrain by making the samples being vertices of triangles (see Fig. 4.3(a)). The RSG model is the other, where the elevation data is uniformly sampled on the regular grid on the map-projected space. The interpolation of the surface could be achieved in different ways (see Fig. 4.3 (b-c)).

DEM data used in this study is MSL_Gale_DEM_Mosaic_10m.tif (MSL Gale DEM Mosaic), available on the Annex of the PDS Cartography \& Imaging Sciences Node USGS website [148]. The MSL team created the MSL Gale DEM Mosaic for facilitating science and engineering operations by combining multiple kinds of DEM products generated from High Resolution Stereo Camera (HRSC) [155], Mars Reconnaissance Orbiter (MRO) Context Camera (CTX) [156], and HiRISE by stereo vision [157], which are all tied to a Mars Orbiter Laser Altimeter (MOLA) DTM [158]. The elevation $h_{\text {Mars }}$ are calculated from the MOLA areoid and it is considered as topography defined in [158] as:

$$
h_{\text {Mars }}=R_{\text {Mars }}-R_{\text {areoid }},
$$

where $R_{\text {Mars }}$ is the radius at the terrain of Mars, the length from the center of the Mars, and $R_{\text {areoid }}$ is the radius of the areoid, considered as the radius at the sea level of Mars. This DEM Mosaic uses the RSG model and saved in a single-layered raster image format. Equirectangular projection, which projects a body onto a plane with the grid of latitudes and longitudes, is used for the creation of the grid of the image. Standard parallel, which is the only parameter of the equirectangular projection and defines the latitude where the no distortion is achieved, is set to zero. The vertical and horizontal axes of the image represent northing and easting, respectively, counting coordinate values by meter from the zero longitude and latitude point in the projected map. The resolution of the image is one meter per pixel in each direction, same as that of HiRISE-based DEM products, the highest resolution obtained from the orbit at the time of this writing. The projection information for converting to a geographic coordinate is stored in the image header or its LABEL file (with the extension .LBL) accompanied with the image.

### 4.2.4 Geographic and projected coordinate systems

The correct interpretation of the DEM/DTM requires the understanding of geographic and projected coordinate systems. A geographic coordinate system (GCS) is a coordinate system that defines the location of a celestial body in the three dimensional space. Most common representation is a spherical coordinate system using planetocentric latitude, longitude, and elevation. The elevation is defined as the radius subtracted by a reference radius, such as geoid and areoid. Geoid is the earth surface that has the constant gravitational potential equal to that at the sea level, which defines the zero elevation. The mass distribution of the earth creates the variation of the radius on the geoid around the earth body. Areoid is the analogue of the geoid to Mars. The planetocentric latitude and longitude define the north-south and east-west location in the geographic coordinate system. The spherical coordinate system can converted to a Cartesian coordinate system. Let the spherical coordinate of a point $p$ be $(r, \varphi, \theta)$ where $r$ is the radius, $\varphi$ is the planetocentric latitude, and $\theta$ is the planetocentric longitude. The Cartesian coordinate $(x, y, z)$ of $p$ is computed as follows:

$$
\begin{aligned}
& x=r \cos \varphi \cos \theta \\
& y=r \cos \varphi \sin \theta \\
& z=r \sin \varphi,
\end{aligned}
$$

where $+x$ looks in the direction to $(\varphi, \theta)=(0,0),+y$ to $(\varphi, \theta)=(0, \pi / 2)$, and $+z$ to $\varphi=\pi / 2$.

A projected coordinate system is a map representation of a three dimensional celestial body projected onto a two dimensional flat plane. The most common projected coordinate system to represent the region of Mars at low latitudes is the equirectangular coordinate system. The equirectangular projection projects a body onto a plane with the grid of latitudes and longitudes with auxiliary spacing. As mentioned in the last section, the MSL Gale DEM Mosaic is also saved using this projection. A point $p=(r, \varphi, \theta)$ in
the geographic coordinate system is projected onto the coordinate (northing, easting) obtained by:

$$
\begin{aligned}
\text { northing } & =R \cdot\left(\varphi-\varphi_{\mathrm{ref}}\right) \\
\text { easting } & =R \cdot\left(\theta-\theta_{\mathrm{ref}}\right) \cdot \cos \theta_{\mathrm{sp}},
\end{aligned}
$$

where $R$ is a reference radius, $\varphi_{\text {ref }}$ and $\theta_{\text {ref }}$ are reference latitude and longitude at which northing and easting become zeros, respectively, and $\theta_{\text {sp }}$ is a standard parallel, a latitude at which pixel smearing do not happen. Parameters used for the projection, such as the reference radius and the standard parallel, are usually attached with the data. It is easy to obtain the associated latitude and longitude given northing and easting.

The Curiosity Rover orientation is defined on the map coordinate system of the equirectangular projection whose $+x,+y$, and $+z$ directions represent northing, easting, and nadir directions, respectively. It can be converted into the geographic Cartesian coordinate system. Suppose that the Martian body is modeled as a sphere. Northing, easting, and nadir directions in the equirectangular projection are equivalent to north, east, and negative radial direction in the local tangential coordinate system at latitude $\varphi$ and longitude $\theta$ on the sphere. The nadir looking vector is identical to the negative of the normal vector of the tangential plane. Its representation in the Cartesian coordinate system is obtained as:

$$
\boldsymbol{e}_{\text {nadir }}=-\boldsymbol{e}_{\mathrm{r}}=-\left(\begin{array}{lll}
\cos \varphi \cdot \cos \theta & \cos \varphi \cdot \sin \theta & \sin \varphi
\end{array}\right)
$$

Next, the north looking vector on the tangential plane is derived. Consider when $\theta=0$, and the north direction of the local tangential plane is evaluated simply in the $z x$ plane in the Cartesian coordinate system: $(-\sin \varphi, 0, \cos \varphi)$. By rotating $\theta$ about $+z$ axis, the north looking vector is obtained as:

$$
\boldsymbol{e}_{\text {north }}=\left(\begin{array}{lll}
-\sin \varphi \cdot \cos \theta & -\sin \varphi \cdot \sin \theta & \cos \varphi
\end{array}\right) .
$$

Finally, the basis vector in the east direction is the one perpendicular to both:

$$
e_{\text {east }}=\left(\begin{array}{lll}
-\sin \theta & \cos \theta & 0
\end{array}\right) .
$$

Then the Curiosity Rover orientation is converted to the geographic Cartesian coordinate by multiplying a $3 \times 3$ matrix $\left[\begin{array}{lll}\boldsymbol{e}_{\text {north }} & \boldsymbol{e}_{\text {east }} & \boldsymbol{e}_{\text {nadir }}\end{array}\right]$ from the left.

The shape of Mars may be modeled as a spheroid with an equatorial radius and a polar radius. First I derive the difference of the local tangential plane of the sphere and the spheroid. The tangential plane of the sphere is perpendicular to the planetocentric latitude, and that of the spheroid is perpendicular to the planetodetoic latitude. Since both of the sphere and spheroid are rotation invariant around the $z$-axis, I only consider it in the vertical cross section. Let the equatorial and polar radii be $R_{e}$ and $R_{p}$, respectively, and the vertical cross-section of the sphere and spheroid that passes through the origin is an ellipse, expressed as

$$
\frac{x^{\prime 2}}{R_{e}^{2}}+\frac{y^{\prime 2}}{R_{p}^{2}}=1,
$$

where $x^{\prime}$ and $y^{\prime}$ axes represent the horizontal and vertical axes, respectively. Taking the derivative, we have

$$
\frac{x^{\prime}}{R_{e}^{2}} d x^{\prime}+\frac{y^{\prime}}{R_{p}^{2}} d y^{\prime}=0 \Leftrightarrow\left[\begin{array}{ll}
\frac{x^{\prime}}{R_{e}^{2}} & \frac{y^{\prime}}{R_{p}^{2}}
\end{array}\right]\left[\begin{array}{l}
d x^{\prime} \\
d y^{\prime}
\end{array}\right]=0
$$

Therefore, the tangential line at $\left(x_{1}^{\prime}, y_{1}^{\prime}\right)$ on the ellipse is

$$
\left[\begin{array}{ll}
\frac{x_{1}^{\prime}}{R_{e}^{2}} & \frac{y_{1}^{\prime}}{R_{p}^{2}}
\end{array}\right]\left[\begin{array}{c}
x^{\prime}-x_{1}^{\prime} \\
y^{\prime}-y_{1}^{\prime}
\end{array}\right]=0 \quad \Leftrightarrow \quad\left[\begin{array}{ll}
\frac{x_{1}^{\prime}}{R_{e}^{2}} & \frac{y_{1}^{\prime}}{R_{p}^{2}}
\end{array}\right]\left[\begin{array}{l}
x^{\prime} \\
y^{\prime}
\end{array}\right]=1
$$

This indicates that $\left[\begin{array}{ll}\frac{x_{1}^{\prime}}{R_{e}^{2}} & \frac{y_{1}^{\prime}}{R_{p}^{2}}\end{array}\right]$ is the normal vector for the tangential plane. Any point on the ellipse is expressed with a parameter $\psi$ as $\left(R_{e} \cos \psi, R_{p} \sin \psi\right)$. For the planetocentric latitude $(\varphi)$, we have the following relationship:

$$
\tan \varphi=\frac{R_{p} \sin \psi}{R_{e} \cos \psi}=\frac{R_{p}}{R_{e}} \tan \psi .
$$

The planetodetoic latitude $\left(\varphi^{\prime}\right)$ is the angle between the normal vector to the tangential plane with the $x$-axis and we have

$$
\tan \varphi^{\prime}=\frac{\frac{y_{1}^{\prime}}{R_{p}^{2}}}{\frac{x_{1}^{\prime}}{R_{e}^{2}}}=\frac{\frac{R_{p} \sin \psi}{R_{p}^{2}}}{\frac{R_{p} \cos \psi}{R_{e}^{2}}}=\frac{R_{e}}{R_{p}} \tan \psi .
$$

By combining the two equations above, we have the relationship between the planetocentric and planetodetoic latitudes:

$$
\begin{equation*}
\tan \varphi^{\prime}=\left(\frac{R_{e}}{R_{p}}\right)^{2} \tan \varphi \tag{4.9}
\end{equation*}
$$

For the spheroidal Mars, the rover orientation on the equirectangular map projection coordinate system is converted to the geographic Cartesian coordinate system as follows. First, the planetodetoic latitude $\varphi^{\prime}$ is obtained from the planetocentric latitude $\varphi$ by the equation (4.9). Similarly performed for the spherical Mars, northing, easting, and nadir direction on the map projection are equivalent to the north, east, and nadir directions on the local tangential plane of the spheroid. These are simply obtained by replacing the latitude of the result of the spheroid:

$$
\begin{aligned}
& \boldsymbol{e}_{\text {nadir }}=\left(\begin{array}{lll}
-\cos \varphi^{\prime} \cdot \cos \theta & -\cos \varphi^{\prime} \cdot \sin \theta & -\sin \varphi^{\prime}
\end{array}\right) \\
& \boldsymbol{e}_{\text {north }}=\left(\begin{array}{lll}
-\sin \varphi^{\prime} \cdot \cos \theta & -\sin \varphi^{\prime} \cdot \sin \theta & \cos \varphi^{\prime}
\end{array}\right) \\
& \boldsymbol{e}_{\text {east }}=\left(\begin{array}{lll}
-\sin \theta & \cos \theta & 0
\end{array}\right) .
\end{aligned}
$$

### 4.2.5 Viewshed algorithms

It is important to address the visible area on the surface from the camera position to know geographical locations imaged at camera pixels. Identifying viewshed, the region that is visible from a certain viewpoint, is a classical and essential research problem in the fields of geographic information systems (GIS) data processing since 1980s. The evaluation of the viewsheds from Martian rovers is also important in facilitating exploration on Mars and the analysis of acquired images [159].

Viewsheds can be represented in a continuous way or in a discrete way $[153,154]$. The continuous viewshed representation partitions the entire continuous terrain into visible and invisible regions. This requires gap filling between the finite elevation samples to be explicitly defined. This representation is well-suited with the TIN model, where a terrain is modeled as a polyhedron created by the tessellation of triangles. Continuous visibility
can be obtained by solving how the triangles intersect and overlay to each other when viewed from a viewpoint. The analytical solution exists for this problem since the visible area of a triangle obstructed by any planar triangle is always expressed as a polygon.

The discrete viewshed representation is simpler. It also partitions the continuous terrain into the finite number of areas, and the visibility of each partitioned area is represented by that of one or multiple representative points in it. In other words, point visibility is evaluated on the representative points to determine the visibility of each partitioned area. This representation is commonly used for the RSG model since its grid is dense and each area is small enough relative to the scale of the whole region of interest, and therefore, testing the visibility of discrete elevation data points would be sufficient to determine that of their whole occupying square cell areas, pixels.

The discrete visibility algorithm has drawn huge interests in the field of GIS data processing, partly because more and more RSG DTM data become available in the raster image format, and partly because the orderly structure of the RSG can be taken advantage of. Blelloch's method [160] and R3 algorithm [161] are the oldest of such methods, which evaluate if the line-of-sight (LOS), a line segment from the viewpoint to each pixel center of the DTM, is obstructed by the surface topography. R3 assesses the line of sight projected onto the 2 d grid and if the LOS is above or below of the grid at all the intersections. Blelloch described a method, similar to the one later called R2 algorithm [162], that evaluates all the LOS's to the boundary pixels first, and estimates the visibility of the inside pixels by that of the intersections of the LOS's to the boundary pixels with the inside pixels. R3 algorithm is considered as the most ideal algorithm due to its exhaustive evaluation of LOS's at the expense of computational cost. Researchers have developed viewshed algorithms, such as R2 [163], XDraw [163], and reference plane method [164] that run faster than R3 by approximation. Van Krevald [165] developed a radial sweeping algorithm with a dedicated tree data structure to reduce a computational complexity. Viewshed algorithms are also available in commercial softwares such as in

Viewshed tool in ArcGIS ${ }^{\circledR}$ deployed in [159].
Some refinements of the traditional algorithms [166-168] are all in the realm of the traditional algorithm Family. In addition, most of development on the algorithmic aspects of viewshed computation occurred back in 1990s, and most of the recent advancement of the viewshed algorithms is related to the efficient implementation of the algorithms by optimizing I/O-efficiency [169-174] and by parallelization [173-180]. I/O efficiency refers to the optimization of data transfer between the external storage to main memory. As DTM data keep increasing in size, it may be impossible to load and keep all the DTM data of interest into main memory. In such a case, the data transfer operation from the storage to the main memory is required during the computation. Access to the external storage is generally much slower than accessing main memory; therefore, the minimization of the number of times of accessing the storage is necessary to reduce the computational time. Parallelization of the algorithms is also a key in reducing the amount of the computational time.

### 4.2.6 SPICE system

The SPICE system [181, 182], developed at NASA's Navigation and Ancillary Information Facility (NAIF), provides NASA's standard integrated platform that facilitates the computation of observation geometry parameters of measurements in space missions and the production and archiving of source and derived ancillary data files. The SPICE system consists of the low-level data files, called SPICE kernel files, and SPICE Toolkit, the application interface (API) that allows us handling of the files and retrieving observation geometry parameters from them. The SPICE Toolkit, originally written in Fortran 77, is now available in multiple computer programming languages (C, IDL, MATLAB, and Java Native language). The software is freely available, and the archived SPICE data files of many space missions are publicly accessible at the NASA PDS NAIF node
website. ${ }^{2}$
The computation of observation geometry is a complex and challenging task [182]. First both observers and targets are moving; they may be rotating, or revolving. In addition, it is required to load correct ephemerides, a table that records the trajectory of astronomical bodies or satellites over time. Furthermore, light time and stellar aberration corrections needs to be assessed, and you must deal with the conversion of multiple different coordinate systems between an observing instrument centered system, one for the spacecraft/body that boards the instrument, target body centered coordinate system, etc. SPICE system provides a simple interface to deal with such a complicated problem. For example, with the UTC time of a measurement and several parameters such as the spacecraft and instrument identification numbers given, the position and orientation of the spacecraft and onboard instruments, and the measurement geometry on the observation target is calculated with the simple interface by loading appropriate SPICE kernel files.

### 4.2.7 Related works

The Mastcam cameras has been used for acquiring the images of landscapes or atmosphere on the ground. Mastcam image products are not accompanied with image data that associate pixels with geographic coordinates. Thus, the map projection between Mastcam images and orbital images requires additional custom processing. Researchers have partially attempted map projection between Mastcam and geo-referenced HiRISE images in the literature. Stack et al. [183] attempted the overlay of geological units evaluated from HiRISE images on Mastcam images. The projection is performed by manually matching features on the orbital images to the rover images. Nachon et al. [184] proposed a more systematic way using the ArcGIS ${ }^{\circledR}$ software and the information of the camera position and orientation attached to each Mastcam image product. Nachon's method

[^12]outputs a viewshed, a union of visible areas by the camera given its position, though pixel-level matching is not supported.

CRISM spectroscopic images have been giving an additional dimension to scientific analysis. Mineralogical maps derived from CRISM images have been taking a significant role in rover operations and determining its traverse, for example, by identifying and mapping clay and sulfate layers in the Gale crater. Since the pixel footprints of the CRISM on the ground is no smaller than 18 m , quite large relative to a scale observed at the ground, they were normally only interpreted at a regional scale.

Recently, the more precise comparison of the CRISM mineral detections with ground measurements is undertaken. Fraeman et al. [185] compared CRISM spectral measurements with the Mastcam images to show the confirmation of mineral detection from the orbit and at the ground. Frizzell et al. [186] further attempted matching CRISM image pixels with Mastcam images, although the work seems immature. The difficulty of the mapping of the CRISM spectral measurements onto the ground lies in the differences in the viewing angle and in the spatial resolution. Gold et al. [187] address this problem by developing an interactive virtual reality system, Planetary Visor, that integrates orbital images on the simulated terrain observed from the ground. It projects CRISM pixel footprints obtained from Derived Data Record (DDR) [4], on the 3D terrain, and allows users to view the terrain from arbitrary perspectives including any virtual rover perspective, helping the integrative understanding of surface using both ground and orbital CRISM observations. DDR data provides the latitude and longitude coordinate and elevation of each pixel center of the CRISM image and Planetary Visor approximates a pixel footprint with a polyhedron shape.

### 4.3 Mutual map projection of Mastcam images using DTM

This section describes a new method to perform mutual map projection between Mastcam image coordinate and the MSL Gale DEM Mosaic image. The projection of a Mastcam image to DTM is composed of several steps. The first step is to prune DTM pixels that are projected to outside of the image using the CAHV/CAHVOR model. The second step is to eliminate pixels hidden by topographical surface occlusions. This step is closely related to so called visibility problem (or, viewshed) and could be computationally intensive due to the high resolution of DTM data. To reduce the computation, only the DTM pixels selected in the first step are tested for visibility. It is essential to reduce the number of pixels to be tested for visibility in the first step as many as possible.

The third step is to construct a mapper data structure that allows us to point a corresponding DTM pixels given Mastcam camera image pixels, or a corresponding camera image pixels given DTM pixels. The mapper is based on the nearest neighbor method. Nearest neighbor may not give precise footprints; if a camera image pixel is much smaller than the resolution of DEM, the precise footprint of the camera image pixels on the DTM image may be much smaller than one pixel. However, the eventual goal for this chapter is to perform mutual mapping between Mastcam image pixels and CRISM image pixels. Since CRISM pixel footprints are much larger than the pixel size of HiRISE DEM pixels, such errors are less problematic.

### 4.3.1 Pruning of DEM pixels outside of the camera image

Here I start with the first step: the pruning of DTM pixels that are projected outside of the camera image. I take the full advantage of the CAHV/CAHVOR model parameters attached with all the Mastcam images. As described in Section 4.2.2, the CAHV/CAHVOR model allows us a simple way to project a point in geographic coordinate system onto the camera image plane coordinate system. It not only provides information on whether a point is inside the field of view (FOV) of the acquired image,


Figure 4.4. Illustration of the valid image region and the image pixel coordinate system on the camera image plane. The rectangle region surrounded by the solid black line segments are the valid image region.
but also which pixel in the image the point falls into. Let $C$ be a camera center point and denote its positional vector by its lowercase bold type $\boldsymbol{c}$. Let $P$ be a point in the geographic coordinate (I denote its positional vector by $\boldsymbol{p}$ ). Let $(x, y)$ be the coordinate in the camera image plane and $\left(x_{P}, y_{P}\right)$ be the xy coordinate associated with the projection of $P$. With the CAHV model, the equation (4.1) is performed to obtain $\left(x_{P}, y_{P}\right)$. In case of CAHVOR model, a series of the operations described in Section 4.2.2 is performed. Let the number of horizontal and vertical pixels be $S_{\text {cam }}$ and $L_{\text {cam }}$, respectively. A point $P$ is projected inside or on the border of the image if its projection $\left(x_{P}, y_{P}\right)$ satisfies the following three conditions:

$$
\left\{\begin{array}{l}
-0.5 \leq x_{P} \leq S_{\mathrm{cam}}-0.5  \tag{4.11a}\\
-0.5 \leq y_{P} \leq L_{\mathrm{cam}}-0.5 \\
(\boldsymbol{p}-\boldsymbol{c}) \cdot \boldsymbol{a}>0
\end{array}\right.
$$

where I assume the coordinate of the center of the most upper left pixel in the camera image is $(0,0)$ and the pitch of pixels is equal to 1 (see Fig. 4.4). The first two conditions test whether the projection falls within the valid rectangle region of the image, inside or on the border of the black rectangle in Fig. 4.4. The additional constraint $(\boldsymbol{p}-\boldsymbol{c}) \cdot \boldsymbol{a} \geq 0$ ensures that $P$ is in the same side as $\boldsymbol{a}$ is pointing with respect to the plane that passes $C$ and is perpendicular to $\boldsymbol{a}$. Also note that rounding $\left(x_{P}, y_{P}\right)$ tells you the image pixel bin that $P$ falls into.

Let us define the set of points that satisfy the the above projection as $S$. The set $S$ may be insufficient as the set of all the contributing pixels. Since I construct topographic surface by the triangulation of the HiRISE DEM based on the RSG model, a pixel projected outside of the region defined by (4.10a) and (4.11a) is considered to be contributing the camera image, if it is one of the vertices of a triangle partially inside the camera image region. Such points are retrieved using the set $S$. Precisely, any point at least one of eight surrounding neighbors of which belongs to the set $S$ needs to be added as a potentially contributing pixels. Figure 4.5 (a) shows potential DEM pixels contributing a Mastcam image (0475ML001888). The pixels in the half-transparent yellow region satisfy the conditions (4.10a) and (4.11a). This region has a cone-like shape topped at the camera center. Figure 4.5 (b) gives us a close look of this region. The yellow region are surrounded by half-transparent orange and blue pixels. The orange pixels are the pixels one/some of whose vertices is/are vertex(es) of the potentially contributing triangles. Slightly more pixels are marked by the bluish color for evaluating the visibility of the pixels in the edge area.

### 4.3.2 Viewshed computation

Next, the visibility of the points are tested. The problem here is a partial viewshed algorithm restricted within the field of view (FOV) of the camera on the RSG DEM model. Here I propose a new method for detecting viewshed of the Mastcam image. First, it assumes a specific model for the terrain. All of the previous methods descended from the R3 algorithm evaluate only the intersection of the LOS's to the grid, the part of the terrain that is not on the grids is not defined. The method here explicitly defines the terrain by the triangulation of the RSG DEM and rigorously assesses if the LOS's is obstructed by any of the triangles. The proposed method can be used with geographic coordinate systems, including a celestial body centered rectangular coordinate system, allowing us a rigid handling of the curvature of the body. In contrast, all the previous


Figure 4.5. A viewshed on the MSL DEM Mosaic of the image associated with sequential ID 1888 taken by the Mastcam Left camera on sol 475 : (a) a whole viewshed and (b) a close look around the camera. The cross represents the position of the Rover, and the solid yellow regions are visible from the Mastcam. The semi-transparent color indicates the potentially visible regions based only on the camera projection. The background gray scale image is Mars MSL Gale Merged Orthophoto Mosaic 25 cm v3 available on the Annex of the PDS Cartography \& Imaging Sciences Node USGS website. The bottom region in (a) that do not have valid DEM data is masked in black.
viewshed algorithm on the RSG model assume that elevations are considered as heights measured vertically from the base plane where the projected coordinate system is defined. The curvature of the planetary body could be only approximately applied as vertical displacements to elevation data points. This method is as accurate as the R3 algorithm and even more restrictive since it is equivalent in testing more intersections of the LOS's with diagonal line segments created by the tessellation.

When the topographic surface is constructed by the tessellation of triangles, the LOS test, the visibility of a point $\boldsymbol{p}$, can be tested by assessing if the line segment $P C$ intersects

```
Algorithm 4.1 Naïve viewshed algorithm on the triangulated RSG DEM model
    for all Triangles in \(\{T\}\) do
        Get \(\mathbf{M}^{-1}\) from Eq. (4.12)
        for all Points in \(\{P\}\) do
            Get ( \(s, t, u\) ) by Eq. (4.13)
            if \(s, t, u>0\) and \(s+t+u>1\) then
                \(P\) is marked as invisible
            end if
        end for
    end for
```

any triangle. This problem is broken down into a series of test, whether a line segment intersects with a triangle. Let us denote the triangle by $T$, and its vertices by $V_{1}, V_{2}, V_{3}$ and their 3 -D position vectors by $\boldsymbol{v}_{1}, \boldsymbol{v}_{2}, \boldsymbol{v}_{3} \in \mathbb{R}^{3 \times 1}$, respectively. Let us also express the triangle $T$ by $T=\triangle V_{1} V_{2} V_{3}$ and define a $3 \times 3$ matrix:

$$
\mathbf{M}=\left[\begin{array}{lll}
\boldsymbol{v}_{1}-\boldsymbol{c} & \boldsymbol{v}_{2}-\boldsymbol{c} & \boldsymbol{v}_{3}-\boldsymbol{c} \tag{4.12}
\end{array}\right],
$$

Line segment $P C$ intersects with $\triangle V_{1} V_{2} V_{3}$ if

$$
s, t, u>0 \quad \text { and } \quad s+t+u>1
$$

where

$$
\left[\begin{array}{c}
s  \tag{4.13}\\
t \\
u
\end{array}\right]=\mathbf{M}^{-1}(\boldsymbol{p}-\boldsymbol{c})
$$

$s, t, u>0$ guarantees that a ray $C P$ intersects $\triangle V_{1} V_{2} V_{3}$, and $s+t+u>1$ confirms that the $P$ is the other side of $\triangle V_{1} V_{2} V_{3}$ with regard to $C$.

Let us denote the whole set of DEM sample points after pruning by $\{P\}$ and the whole set of triangles created by these DEM sample points by $\{T\}$. Using the above test, one may come up with a naïve algorithm (Algorithm 4.1) by performing the above test for all combinations of triangles and Points. It is tedious to perform this test for all the combinations of points and triangles. I here propose a novel method to reduce the computational burden by prior-binning of the points using CAHV model projection. Consider linear projection using a CAHV model. The projection of any triangle onto the
image plane defined by the CAHV parameters is a triangle. A line $P C$ passes through a triangle $\triangle V_{1} V_{2} V_{3}$ if and only if the projection of $P$ onto the image plane falls within that of the triangle. Therefore, you do not need to test all the points for each triangle. It is sufficient to test all the points within the rectangle that minimally encloses the triangle. The coordinate $\left(x_{V_{i}}, y_{V_{i}}\right)$ of the projection of $V_{i}$ in the image plane defined in the CAHV model is obtained by the CAHV projection (4.1)

$$
\begin{equation*}
x_{V_{i}}=\frac{\boldsymbol{h} \cdot\left(\boldsymbol{p}_{V_{i}}-\boldsymbol{c}\right)}{\boldsymbol{a} \cdot\left(\boldsymbol{p}_{V_{i}}-\boldsymbol{c}\right)} \quad \text { and } \quad y_{V_{i}}=\frac{\boldsymbol{v} \cdot\left(\boldsymbol{p}_{V_{i}}-\boldsymbol{c}\right)}{\boldsymbol{a} \cdot\left(\boldsymbol{p}_{V_{i}}-\boldsymbol{c}\right)}, \tag{4.14}
\end{equation*}
$$

where $\boldsymbol{p}_{V_{i}}$ is the positional vector associated with $V_{i}$. The rectangular region minimally enclosing $\triangle V_{1} V_{2} V_{3}$ is then expressed as

$$
\operatorname{MinEncRect}_{\triangle V_{1} V_{2} V_{3}}=\left\{(x, y) \mid x_{V \min }<x_{P}<x_{V \max } \text { and } y_{V \min }<y_{P}<y_{V \max }\right\}
$$

where

$$
\begin{array}{ll}
x_{V \text { min }}=\min \left(x_{V_{1}}, x_{V_{2}}, x_{V_{3}}\right), & x_{V_{\text {max }}}=\max \left(x_{V_{1}}, x_{V_{2}}, x_{V_{3}}\right)  \tag{4.15}\\
y_{V_{\text {min }}}=\min \left(y_{V_{1}}, y_{V_{2}}, y_{V_{3}}\right), & y_{V_{\text {max }}}=\max \left(y_{V_{1}}, y_{V_{2}}, y_{V_{3}}\right) .
\end{array}
$$

Using the results above, one may come up with Algorithm 4.2 by inserting a screening operation before performing the LOS test. Line 9 is simply performed by testing $x_{v \min } \leq$ $x_{P} \leq x_{v \max }$ and $y_{v \min } \leq y_{P} \leq y_{v \max }$. It is worth noting that only the CAHV part of the model is used even when you use CAHVOR model. This is because the the radial distortion in the CAHVOR model projection could change the geometric relationship of a line and a triangle. Algorithm 4.2 is still inefficient because the screening test at Lines 8-9 need to be performed on all of the points. Therefore, its computational complexity is not reduced from Algorithm 4.1.

In order to effectively use this idea, I first segment the camera image region into two dimensional pixel bins. Let us define the pixel bin structure Bin with the size of $L \times S$ and represent the $(i, j)$ bin with $\operatorname{Bin}[i][j]$. $\operatorname{Bin}[i][j]$ occupies a rectangular region satisfying $i-0.5 \leq x<i+0.5$ and $j-0.5 \leq y<j+0.5$ on the $x y$ image plane. In the prior binning step, all the points are binned according to their projection coordinates as a

```
Algorithm 4.2 Viewshed algorithm with image plane screening
    for all Triangles \(\{T\}\) do
        for \(V_{i} \in\left\{V_{1}, V_{2}, V_{3}\right\}\) do
            Get \(\left(x_{V_{i}}, y_{V_{i}}\right)\) by Eq. (4.14)
        end for
        MinEncRect \(\triangle V_{1} V_{2} V_{3}\) is obtained by Eq. (4.15)
        Get \(\mathbf{M}^{-1}\) from Eq. (4.12)
        for all Points \(\{P\}\) do
            Get \(\left(x_{P}, y_{P}\right)\) by Eq. (4.1)
            if \(\left(x_{P}, y_{P}\right) \in\) MinEncRect \(_{\Delta V_{1} V_{2} V_{3}}\) then
                    Get \((s, t, u)\) by Eq. (4.13)
                    if \(s, t, u>0\) and \(s+t+u>1\) then
                    \(P\) is marked as invisible.
                    end if
            end if
        end for
    end for
```

pre-processing. A point $P$ is first projected on the camera image plane and its projection coordinate $\left(x_{P}, y_{P}\right)$ is obtained. The coordinate are then rounded to:

$$
\left(i_{P}, j_{P}\right)=\left(\left\lfloor x_{P}+0.5\right\rfloor,\left\lfloor y_{P}+0.5\right\rfloor\right)
$$

where $\lfloor x\rfloor$ rounds down to its nearest integer, and $P$ is sorted to $\operatorname{Bin}\left[j_{P}\right]\left[i_{P}\right]$. Note that points that falls outside of the binned region are collected to the closest bins by rounding their coordinate values on the projected plane. Then, instead of performing the screening operation as performed in Algorithm 4.2, only the points in the bins that intersect the rectangle minimally enclosing each triangle are tested for the visibility. After MinEncRect ${ }_{\triangle V_{1} V_{2} V_{3}}$ is obtained by the operation (4.15), the minimum and maximum indices of intersecting bins are obtained simply by rounding the edge coordinates of MinEncRect $\triangle V_{1} V_{2} V_{3}$. The LOS test is performed on only the points in $\operatorname{Bin}[j][i]$ for all $i \in \mathcal{R}_{T i}$ and $j \in \mathcal{R}_{T j}$, where

$$
\begin{aligned}
& \mathcal{R}_{T i}=\left[\left\lfloor x_{V \min }+0.5\right\rfloor,\left\lfloor x_{V \max }+0.5\right\rfloor\right] \\
& \mathcal{R}_{T j}=\left[\left\lfloor y_{V \min }+0.5\right\rfloor,\left\lfloor y_{V \max }+0.5\right\rfloor\right] .
\end{aligned}
$$

The whole processing is summarized in Algorithm 4.3. While Algorithm 4.2 performs a

```
Algorithm 4.3 Viewshed algorithm with CAHV model prior binning
Prior Binning
    for all Points \(\{P\}\) do
        Get \(\left(x_{P}, y_{P}\right)\) by Eq. (4.1)
        \(\left(i_{P}, j_{P}\right)=\left(\left\lfloor x_{P}+0.5\right\rfloor,\left\lfloor y_{P}+0.5\right\rfloor\right)\) and add \(P\) to \(\operatorname{Bin}\left[j_{P}\right]\left[i_{P}\right]\)
    end for
Main Loop
    for all Triangles \(\{T\}\) do
        for \(V_{i} \in\left\{V_{1}, V_{2}, V_{3}\right\}\) do
            Get \(\left(x_{V_{i}}, y_{V_{i}}\right)\) by Eq. (4.14)
        end for
        Get \(x_{V \text { min }}, x_{V \text { max }}, y_{V \text { min }}, y_{V \text { max }}\) by Eq. (4.15)
        Get \(\mathrm{M}^{-1}\) from Eq. (4.12)
        for \(j \in\left[\left\lfloor y_{V \text { min }}+0.5\right\rfloor,\left\lfloor y_{V \text { max }}+0.5\right\rfloor\right]\) do
            for \(i \in\left[\left\lfloor x_{V \min }+0.5\right\rfloor,\left\lfloor x_{V \text { max }}+0.5\right\rfloor\right]\) do
                for \(P \in \operatorname{Bin}[j][i]\) do
                    Get ( \(s, t, u\) ) by Eq. (4.13)
                    if \(s, t, u>0\) and \(s+t+u>1\) then
                            \(P\) is marked as invisible and removed from \(\operatorname{Bin}[j][i]\)
                    end if
                end for
            end for
        end for
    end for
```

for loop over all points independently for each triangle, Algorithm 4.3 just does it over points in the bins whose indices are in the ranges $\mathcal{R}_{T i}$ and $\mathcal{R}_{T j}$. Since the sizes of the triangles composing surface are expected to be small, the range $\mathcal{R}_{T i}$ and $\mathcal{R}_{T j}$ should be much smaller than the image size, so is the number of points inside these bins. This is especially beneficial when the camera is looking at a distant target, where the surface triangles look even smaller. This way, prior binning can effectively reduce the number of points to be tested for each triangle.

This method is more efficient than R3, yet more restrictive in the sense that it also tests for a diagonal line segment of the RSG DEM model. While the R3 algorithm is equivalent to divide the image by azimuth angles to reduce the number of intersections to be tested by taking advantage of the regular DEM structure, this proposed method divides also in the vertical direction, reducing the number of points to be tested for
the triangle more effectively. In addition to that, this method does not use the regular grid structure; therefore, the algorithm can be used even after the conversion to another coordinate system, such as a body centered rectangular coordinate system, allowing us to rigorously deal with the celestial body curvature. Once a point is marked as visible, then the points do not need to be assessed for visibility again. This dynamic removal of invisible points may also be implemented for the former naïve algorithms and help speeding up the processing.

Algorithm 4.3 can be further generalized by allowing arbitrary size for bins. Let us define two factors $K_{S}$ and $K_{L}$ such that $1 / K_{S}$ and $1 / K_{L}$ become the horizontal and vertical side length of the bins, respectively. Given a projection coordinate $(x, y)$, the index $(i, j)$ of the bin which $(x, y)$ is sorted into is obtained by:

$$
\begin{equation*}
(i, j)=\left(\left\lfloor K_{S}(x+0.5)\right\rfloor,\left\lfloor K_{L}(y+0.5)\right\rfloor\right), \tag{4.16}
\end{equation*}
$$

which and given MinEncRect $\Delta V_{1} V_{2} V_{3}$, the range of the indices associated with its intersecting bins are

$$
\begin{align*}
& \mathcal{R}_{T i}=\left[\left\lfloor K_{S}\left(x_{V \min }+0.5\right)\right\rfloor,\left\lfloor K_{S}\left(x_{V \max }+0.5\right)\right\rfloor\right]  \tag{4.17}\\
& \mathcal{R}_{T j}=\left[\left\lfloor K_{L}\left(y_{V \min }+0.5\right)\right\rfloor,\left\lfloor K_{L}\left(y_{V \max }+0.5\right)\right\rfloor\right] . \tag{4.18}
\end{align*}
$$

A generalized version of Algorithm 4.3 can be obtained by replacing Line 3 with Eq. (4.16) and Lines $7-8$ with Eqs. (4.18) and (4.17).

Until here, we have focused on point visibility. Namely, visibility is only tested at the center of the pixel. DEM pixels are not points, but rather occupy square areas in the map centered at their discrete samples. Fig. 4.6 shows an illustration of the surface of one pixel when the terrain is modeled by triangulation. The surface within a pixel may be partially visible, and the visibility of the center of the pixel may not represent the visibility of the whole pixel. Thus, it would be more appropriate to assess the visible region of the surface in the pixel. However, such an approach is computationally intensive on the highly dense RSG DEM model. I use an approximation of the pixel visibility. Not


Figure 4.6. Illustration of continuous representation of the terrain of a single pixel.
only the center of the pixel, four vertices of the pixel on the topographic surface are tested for point visibility, and I consider a pixel to be visible if one of the five points are visible from the surface. Fig. 4.5 shows the viewshed of a Mastcam image. The solid yellow regions are the visible pixels from the camera.

### 4.3.2.1 Implementation

It is necessary to construct an appropriate data structure to realize the prior binning. When implementing in C , the structure can be realized via a linked list containing the two-dimensional bins as elements. First a 2-D array is created, where each element corresponds the bins, and points to the linked list of DEM samples falls in it. The element of the linked list has the column and row indices of the DEM samples in the DEM image, and its radius value as members. The implementation using the linked list is convenient for adding and removing its bin elements. Since the number of DEM samples for each bin is not known in advance and removal operation is performed in the algorithm, the linked list is best suited for the algorithm.

### 4.3.3 Geo-referencing of camera image pixels

Until now, I consider the projection from the DEM pixels to camera image pixels. This section considers the opposite - projection from camera image pixels to the DEM surface. It is assumed that each camera pixel is represented by its center point and we can consider geo-referencing of the center of the pixels. For the pointing vector associated with each pixel center, its depth - distance from the camera center to the geo-location of the pixel - is evaluated. The depth of a pixel is obtained as the distance to the closest intersection of its associated pointing vector/ray starting from the camera center with the terrain. This operation requires similar problems encountered in the viewshed algorithm, testing if the ray intersects with triangles of the surface. Applying a similar strategy used for computing a viewshed, a ray needs to be tested for intersection only with some triangles among all. In case of CAHVOR model, prior binning is employed and the pixel index associated with pointing vectors are stored in the bins. In the main iteration, the intersection all the pointing vectors stored in the bins intersecting the rectangle minimally enclosing the triangle projected on the image plane is tested. If the obtained distance is smaller the current value in the distance matrix, distance is updated. Let us consider the pixel index $\left(i^{\prime}, j^{\prime}\right)$. Let $\boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)$ be its associated pointing vector. By applying CAHV projection (4.1), we have its coordinate $\left(x_{\left(i^{\prime}, j^{\prime}\right)}, y_{\left(i^{\prime}, j^{\prime}\right)}\right)$ on the CAHV image plane as

$$
\begin{equation*}
x_{\left(i^{\prime}, j^{\prime}\right)}=\frac{\boldsymbol{h} \cdot \boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)}{\boldsymbol{a} \cdot \boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)} \quad \text { and } \quad y_{\left(i^{\prime}, j^{\prime}\right)}=\frac{\boldsymbol{v} \cdot \boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)}{\boldsymbol{a} \cdot \boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)} \tag{4.19}
\end{equation*}
$$

The binning operation is performed with this coordinate value. Testing the intersection of the ray with a triangle $\triangle V_{1} V_{2} V_{3}$ is performed as follows. First M is obtained by the equation (4.12). Second, the computation similar to the equation (4.13) is performed:

$$
\left[\begin{array}{c}
s  \tag{4.20}\\
t \\
u
\end{array}\right]=\mathbf{M}^{-1} \boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)
$$

The ray $\boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)$ intersects if and only if $s, t, u>0$, and if so, the intersection is expressed as

$$
\boldsymbol{c}+\frac{1}{s+t+u} \boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)
$$

```
Algorithm 4.4 Map projection of camera pixel centers (CAHVOR)
Prior Binning
    for all Image pixel indices \(\left(i^{\prime}, j^{\prime}\right)\) do
        Get \(\left(x_{P_{C}\left(i^{\prime}, j^{\prime}\right)}, y_{P_{C}\left(i^{\prime}, j^{\prime}\right)}\right)\) by Eq. (4.19)
        \(\left(i_{\left(i^{\prime}, j^{\prime}\right)}, j_{\left(i^{\prime}, j^{\prime}\right)}\right)=\left(\left\lfloor x_{P_{C}\left(i^{\prime}, j^{\prime}\right)}+0.5\right\rfloor,\left\lfloor y_{P_{C}\left(i^{\prime}, j^{\prime}\right)}+0.5\right\rfloor\right)\)
        Add \(\left(i^{\prime}, j^{\prime}\right)\) to \(\operatorname{Bin}\left[j_{\left(i^{\prime}, j^{\prime}\right)}\right]\left[i_{\left(i^{\prime}, j^{\prime}\right)}\right]\)
    end for
Main Loop
    for all Triangles \(\{T\}\) do
        for \(V_{i} \in\left\{V_{1}, V_{2}, V_{3}\right\}\) do
            Get \(\left(x_{V_{i}}, y_{V_{i}}\right)\) by Eq. (4.14)
        end for
        Get \(x_{V \text { min }}, x_{V \text { max }}, y_{V \text { min }}, y_{V \text { max }}\) by Eq. (4.15)
        Get \(\mathbf{M}^{-1}\) from Eq. (4.12)
        for \(j \in\left[\left\lfloor y_{v \min }+0.5\right\rfloor,\left\lfloor y_{v \max }+0.5\right\rfloor\right]\) do
            for \(i \in\left[\left\lfloor x_{v \min }+0.5\right\rfloor,\left\lfloor x_{v \max }+0.5\right\rfloor\right]\) do
                for \(\left(i^{\prime}, j^{\prime}\right) \in \operatorname{Bin}[j][i]\) do
                        Get \((s, t, u)\) for \(\boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)\) by Eq. (4.20)
                        if \(s, t, u>0\) then
                        \(d=1 /(s+t+u)\)
                                if \(d<D\left[j^{\prime}\right]\left[i^{\prime}\right]\) then
                                    \(D\left[j^{\prime}\right]\left[i^{\prime}\right]=d\)
                                    end if
                                    end if
                end for
            end for
        end for
    end for
```

Suppose $\boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)$ has the unit length, its coefficient $\boldsymbol{p}_{C}\left(i^{\prime}, j^{\prime}\right)$ becomes the depth. Computation is performed for all the triangles and the depth of pixels are updated in the pre-allocated depth map $D[\cdot][\cdot]$ if the newly obtained distance is shorter than the current value. The whole algorithm is summarized in Algorithm 4.4.

The prior binning step is unnecessary for the CAHV model since camera pixel centers are exactly aligned on the CAHV image plane. The potentially intersecting pixel center rays are selected by directly rounding the coordinate at the border of the minimally enclosing rectangle of triangles. The whole procedures are shown in Algorithm 4.5.

Using depth, it is easy to calculate the geo-location of the pixel in the reference

```
Algorithm 4.5 Map projection of camera pixel centers (CAHV)
Main Loop
    for all Triangles \(\{T\}\) do
        for \(V_{i} \in\left\{V_{1}, V_{2}, V_{3}\right\}\) do \(\quad \triangleright\) The three vertices of the triangle
            Get \(\left(x_{V_{i}}, y_{V_{i}}\right)\) by Eq. (4.14)
        end for
        Get \(x_{V \text { min }}, x_{V \text { max }}, y_{V \text { min }}, y_{V \text { max }}\) by Eq. (4.15)
        Get \(\mathrm{M}^{-1}\) from Eq. (4.12)
        for \(j \in\left[\left\lceil y_{V \text { min }}+0.5\right\rceil,\left\lfloor y_{V \text { max }}+0.5\right\rfloor\right]\) do
            for \(i \in\left[\left\lceil x_{V \text { min }}+0.5\right\rceil,\left\lfloor x_{V \text { max }}+0.5\right\rfloor\right]\) do
                Get \((s, t, u)\) for \(\boldsymbol{p}_{C}(i, j)\) by Eq. (4.20)
                \(d=1 /(s+t+u)\)
                    if \(d<D[j][i]\) then
                    \(D[j][i]=d\)
                end if
                end for
        end for
    end for
```

coordinate system. It is also possible to obtain other photometric parameters, such as emission angles. The emission angle is the angle between the normal vector of the reflected surface in the zenith direction and the vector of reflected light. If you approximate the emission angle associated with the measurement of each pixel by the angle of the normal of the triangle that intersect the pointing vector of the pixel center with the negative of the pointing vector, it is easily obtained. The emission angle is useful for recognizing the topography captured by the camera especially for distant targets. Fig. 4.7 shows an example of the result of geo-referencing of the camera pixels. It is observed that the MSL Gale DEM Mosaic captures the topography quite well especially for distant targets, although there might be large errors at a close range. Using the geo-reference, it is also simple to get the nearest DEM pixel for each camera image pixel.

### 4.3.4 Correction of the orientation of the Curiosity rover

Although the position of the Curiosity rover is corrected in the localization effort, the correction of the orientation is not performed. The uncorrected error causes the angular difference of the Mastcam image and estimated range or emission angle maps using the

(a) RGB image

(b) Image of depth

(b) Image of emission angles

Figure 4.7. Geo-referencing of the MASTCAM image

DTM model. The orientation can be corrected by using manually selected ground control points (GCP) between the Mastcam image and the range/emission angle maps. Once GCPs are obtained, pixel pointing vectors are obtained from the camera imgage pixels of GCPs on the Mastcam image and on the range/emission angle maps, respectively. The camera orientation is fixed so that the associated pixel pointing vectors match as much as possible. Let the true coordinate of the GCPs in the Mastcam image be ( $\left.x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)$ and that obtained by the projection with the uncorrected orientation be $\left(x_{n}^{\mathrm{proj}}, y_{n}^{\mathrm{proj}}\right)$ for $n=1, \ldots, N_{\mathrm{GCP}}$, where $N_{\mathrm{GCP}}$ is the number of GCPs. Their corresponding pointing vector are $\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)$ and $\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)$. The correction is considered in the

I consider the correction of the orientation first in the 3-D camera coordinate system where the $+x,+y$, and $+z$ directions correspond $\boldsymbol{a}, \boldsymbol{h}^{\prime}$, and $\boldsymbol{v}^{\prime}$, respectively. The horizontal and vertical correction angles around the $\boldsymbol{v}^{\prime}$ and $\boldsymbol{h}^{\prime}$, respectively, are evaluated.

The horizontal correction angle $\alpha$ is obtained by the horizontal angular deviation between $\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)$ and $\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)$. Let the component of $\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)$ that does not include vertical component be $\left[\boldsymbol{p}_{C}(\cdot, \cdot)\right]_{v_{\perp}^{\prime}}$, we have

$$
\begin{aligned}
& {\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)\right]_{v_{\perp}^{\prime}}=\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)-\left(\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right) \cdot \boldsymbol{v}^{\prime}\right) \boldsymbol{v}^{\prime}} \\
& {\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)\right]_{v_{\perp}^{\prime}}=\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)-\left(\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right) \cdot \boldsymbol{v}^{\prime}\right) \boldsymbol{v}^{\prime} .}
\end{aligned}
$$

Then the vertical deviation angle $\alpha_{n}$ derived from the GCP indexed by $n$ is:

$$
\alpha_{n}=\frac{\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)\right]_{v_{\perp}^{\prime}} \cdot\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)\right]_{v_{\perp}^{\prime}}}{\left\|\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)\right]_{v_{\perp}^{\prime}}\right\|\left\|\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)\right]_{v_{\perp}^{\prime}}\right\|}
$$

$\alpha$ is estimated from $\alpha_{n}\left(n=1, \ldots, N_{\mathrm{GCP}}\right)$ :

$$
\alpha=\frac{1}{N_{\mathrm{GCP}}} \sum_{n=1}^{N_{\mathrm{GCP}}} \alpha_{n} .
$$

Finally, the sign of $\alpha$ is obtained by

$$
\operatorname{sgn}\left(\left(\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)\right]_{v_{\perp}^{\prime}}-\left[\boldsymbol{p}_{C}\left(x_{n}^{\mathrm{proj}}, y_{n}^{\mathrm{proj}}\right)\right]_{v_{\perp}^{\prime}}\right) \cdot \boldsymbol{h}^{\prime}\right)
$$

where $\operatorname{sgn}(\cdot)$ is the function to get the sign of the input. Similarly, the vertical correction angle $\beta$ is obtained. Let the component of $\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)$ that does not include horizontal
component be $\left[\boldsymbol{p}_{C}(\cdot, \cdot)\right]_{h_{\perp}^{\prime}}$, we have

$$
\begin{aligned}
& {\left[\boldsymbol{p}_{C}\left(x_{n}^{\mathrm{proj}}, y_{n}^{\mathrm{proj}}\right)\right]_{h_{\perp}^{\prime}}=\boldsymbol{p}_{C}\left(x_{n}^{\mathrm{proj}}, y_{n}^{\mathrm{proj}}\right)-\left(\boldsymbol{p}_{C}\left(x_{n}^{\mathrm{proj}}, y_{n}^{\mathrm{proj}}\right) \cdot \boldsymbol{h}^{\prime}\right) \boldsymbol{h}^{\prime}} \\
& {\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)\right]_{h_{\perp}^{\prime}}=\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)-\left(\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right) \cdot \boldsymbol{h}^{\prime}\right) \boldsymbol{h}^{\prime} .}
\end{aligned}
$$

Then the horizontal deviation angle $\beta_{n}$ derived from the GCP indexed by $n$ is:

$$
\beta_{n}=\frac{\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)\right]_{h_{\perp}^{\prime}} \cdot\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)\right]_{h_{\perp}^{\prime}}}{\left\|\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)\right]_{h_{\perp}^{\prime}}\right\|\left\|\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)\right]_{h_{\perp}^{\prime}}\right\|}
$$

$\beta$ is estimated from $\beta_{n}\left(n=1, \ldots, N_{\mathrm{GCP}}\right)$ :

$$
\beta=\frac{1}{N_{\mathrm{GCP}}} \sum_{n=1}^{N_{\mathrm{GCP}}} \beta_{n}
$$

The sign of $\beta$ is obtained by

$$
\operatorname{sgn}\left(\left(\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {true }}, y_{n}^{\text {true }}\right)\right]_{h_{\perp}^{\prime}}-\left[\boldsymbol{p}_{C}\left(x_{n}^{\text {proj }}, y_{n}^{\text {proj }}\right)\right]_{h_{\perp}^{\prime}}\right) \cdot \boldsymbol{v}^{\prime}\right) .
$$

The correction angles are then converted to the ones for the rover's pitch, yaw, and roll angles. Using $\alpha$ and $\beta$, you could easily form a rotation matrix for the orientation correction in the 3d camera coordinate system:

$$
\mathbf{R}_{\mathrm{cam}}^{\mathrm{corr}}=\left(\begin{array}{ccc}
\cos \alpha & -\sin \alpha & 0 \\
\sin \alpha & \cos \alpha & 0 \\
0 & 0 & 1
\end{array}\right)\left(\begin{array}{ccc}
\cos \beta & 0 & \sin \beta \\
0 & 1 & 0 \\
-\sin \beta & 0 & \cos \beta
\end{array}\right) .
$$

Let the rotation matrix $\mathbf{R}_{\text {nav }}^{\text {corr }}$ in the Rover navigation frame, we have a following relationship:

$$
\mathbf{R}_{\mathrm{nav}} \mathbf{R}_{\mathrm{nav}}^{\mathrm{corr}} \mathbf{R}_{\mathrm{cam}}=\mathbf{R}_{\mathrm{nav}} \mathbf{R}_{\mathrm{cam}} \mathbf{R}_{\mathrm{cam}}^{\mathrm{corr}} \quad \Leftrightarrow \quad \mathbf{R}_{\mathrm{nav}}^{\mathrm{corr}}=\mathbf{R}_{\mathrm{cam}} \mathbf{R}_{\mathrm{cam}}^{\mathrm{corr}} \mathbf{R}_{\mathrm{cam}}^{\top},
$$

where $\mathbf{R}_{\text {cam }}$ is the rotation matrix from the camera frame to the rover navigation frame defined by $\mathbf{R}_{\text {cam }}=\left[\begin{array}{lll}\boldsymbol{a} & \boldsymbol{h}^{\prime} & \boldsymbol{v}^{\prime}\end{array}\right]$. The corrected rotation matrix from the rover navigation frame to its reference frame is $\mathbf{R}_{\text {nav }} \mathbf{R}_{\text {nav }}^{\text {corr }}$ and the corrected yaw, pitch, and roll angles are obtained from this rotation matrix. Figure 4.8 shows an example of the correction using the method presented here. You can see that a significant displacement occurs with


Figure 4.8. Orientation correction of the MASTCAM image using GCPs
the projection when not correction is performed. The blue crosses in Figure 4.8 (a) and red crosses in Figure 4.8 (b) are the manually obtained GCPs. Figure 4.8 (c) shows the image of emission angles after correction. The image now matches well the RGB image.

### 4.3.5 Mutual mapper structure

Now we have the viewshed of the Mastcam image on the MSL Gale DEM Mosaic, and the centers of pixels of the Mastcam image are geo-referenced with the DEM. Two types of mutual mapping are considered - point-to-point and area-to-are mutual map projections. Point-to-point mutual map projection defines a one-to-one correspondence
between a single point in the camera image plane and a single point on the DEM model. It can be implemented by directly using the formula and the CAHV/CAHVOR model projcetion (refer Section 4.2.2). Given a point on the visible region of the terrain defined by the DEM, we can easily obtain its camera image coordinate by performing the CAHV/CAHVOR model projection. On the other hand, given a camera image pixel, you can easily obtain the geo-location of the center of the pixel as an outcome from the algorithms in Section 4.3.3, although it might be computationally intensive to obtain the geo-location of arbitrary points on the camera image.

Area-to-area mutual mapping interprets each pixel as a square area and locates a corresponding area of the other image given a pixel of one image. This is more complicated since a pixel of the camera may corresponds to discontinuous regions on the DEM. An image pixel pointing to a surface at a close distance may be smaller than a DEM pixel, which requires a polygonal expression to rigorously handle its corresponding area on the DEM. Instead of such a rigorous area-to-area mapping, I consider mutual mapping of two images at pixel level, pixel-to-pixel mutual map projection. Given a pixel of one image, the pixel-to-pixel mutual map projection resolves the corresponding pixels of the other. There exists an asymmetry in this projection; a pixel of DEM does not have one-to-one correspondence with a pixel of the camera image. A single DEM pixel close to the camera center may correspond to multiple camera image pixels, while multiple DEM pixels may correspond to a single camera image pixel when the DEM pixels are far from the camera. This asymmetry in the nearest pixel projection needs to be properly handled.

I propose a pixel-to-pixel mapper structure that facilitates the mapping operation. I first create two 2D-arrays, DEM2Mastcam for the projection from the DEM to a Mastcam image and Mastcam2DEM for that from the Mastcam image to the DEM. DEM2Mastcam has the size of the DEM image, and each element stores its corresponding camera pixels. Mastcam2DEM has the size of the Mastcam image, and each element stores its corresponding DEM pixels. The 2-D arrays DEM2Mastcam and

Mastcam2DEM could not be implemented with the standard layered image format as each element is likely to be different in length. In my implementation with MATLAB ${ }^{\circledR}$, cell arrays are used. For interoperability, a binary format may be necessary. Using this nearest mapper data structure, a mapping operation is performed by simply selecting camera image pixels of the given DEM pixel, or selecting DEM pixels image pixels of the given camera image pixel.

In order to perform the pixel-to-pixel mutual map projection, you might want to a forward-backward projection. Consider a projection of a Mastcam image pixel with a small depth. You can easily locate its corresponding DEM pixel by selecting a element of Mastcam2DEM. It is likely that the DEM pixel is associated with multiple Mastcam image pixels. The pixels of the Mastcam image corresponding to the DEM pixel are obtained by referring DEM2Mastcam. This forward-backward projection gives pixel-to-pixel matching between two images.

The construction of this data structure is performed as follows. The CAHV/CAHVOR projection of the visible DEM pixels returns you camera image pixel indices that they belong to. The nearest camera image pixels for each of the DEM pixel centers are obtained by rounding the coordinate values in the projected image plane, and first stored into the array structure of DEM2Mastcam. In order to solve the asymmetry, the nearest DEM pixels for the camera image pixels obtained in Section 4.3.3 are used. The camera image pixels are then sorted by their nearest DEM pixels and added to the element of DEM2Mastcam. Mastcam2DEM is created in a similar way. First, the nearest DEM pixels of the camera image pixels obtained in Section 4.3.3 are first stored into the element of Mastcam2DEM. Then the visible DEM pixels are sorted with respected to their nearest camera pixels and added to the element of Mastcam2DEM.

### 4.4 A new CRISM map projection on MSL Gale DEM Mosaic

CRISM map projection is traditionally performed using the information of geographic coordinates stored in the DDR data [4]. The DDR data is a multi-layer image whose layers have the same size as the observation image, containing latitude, longitude, emission angles, incident angles, elevation from MOLA, etc., of the center of pixels. The latitude and longitude can be directly used for the map projection of CRISM images. Commonly, the CRISM images are projected to a map of their expected spatial resolution, 18 m per pixel for full resolution images and 36 m for half resolution images.

However, since the platform of the CRISM instrument is moving and also experiencing the rotation around the Gimbal axis during the acquisition, pixel footprints may be different in size for different lines and may be overlapping for a series of lines, depending on its motion and rotation. Such variations of the pixel footprints and overlapping are not considered with the projection using DDR data. It may be less problematic to capture the regional/broad-scale mineralogy of the Martian surface, but it may be a significant problem when matching the CRISM observation with ground rover measurements.

Kreisch et al. [103] handle the overlapping of CRISM image pixels using the pixel spread function of the CRISM image to derive a higher resolution image map projected image. They target CRISM along-track oversampled (ATO) observation products that intentionally acquire highly overlapping pixels. They model the terrain using the latitude, longitude, and elevation in the DDR data.

This section considers projecting the CRISM image directly onto the high-resolution MSL Gale DEM Mosaic and assesses the footprint on the high resolution DTM. The direct projection of the CRISM image onto such a high-resolution DEM model has never been attempted. A new method and representation of CRISM map projection that could allows more precise map projection are presented. The fine sampling of the DEM also
allows more accurate representation of the footprint of CRISM pixel.
Kreisch et al. [103] defines the pixel spread function on the plane that is perpendicular to the line-of-sight and passes the pixel center in the geographic coordinate system. The proposed method simplifies the processing by the use of the CAHV model.

This idea is similar to "inverse-orthorectification" [188], which was also applied to the map projection of a CRISM image [189]. Rice et al. [189] shares the same objective as my method - improving the accuracy of the map projection of the CRISM image.

### 4.4.1 Overall methodology

The movement of the CRISM instrument is approximately handled by equally dividing one exposure time into $N$ small periods. At each small period, the position and orientation of the CRISM are assumed to be fixed, and the spatial footprints of CRISM pixels at each period $n \in(n=1,2, \ldots, N)$ are evaluated by map projection using its sensor model. The total spatial footprint of each CRISM pixel over one exposure is then obtained by summing up its spatial footprint of $N$ periods. Let us call the total spatial footprint of one exposure a pixel footprint function (PFF) and that of one small period an instantaneous PFF (IPFF). In my implementation, $N=7$ is typically used.

The computation of IPFF on the DEM is performed by projecting DEM samples onto the image plane of the CRISM. The reference DEM model, MSL Gale DEM Mosaic has one meter spatial resolution, significantly higher that of CRISM; therefore, it would be sufficient to assess the projection of its center of DEM pixels to represent them to approximate the IPFF at the DTM pixel resolution.

The projection onto the CRISM image plane is achieved by a pseudo CAHV model derived from the sensor model of the CRISM recorded in SPICE instrumental kernel (ik). The pseudo CAHV model consists of four basic camera parameters ( $\boldsymbol{c}, \boldsymbol{a}, \boldsymbol{h}, \boldsymbol{v}$ ) and the coordinate of the center of arbitrary sampled pixels on the image plane coordinate system to consider the non-linearity of the pixel sampling of the CRISM pixels. The sampling


Figure 4.9. Illustration of the pseudo CAHV model for CRISM and the IPFF of each pixel sample.
is defined based on the angular distance from the boresight vector, and therefore, all the pixel centers are not exactly aligned on the integer grids at the same time for any CAHV parameters, although the non-linearity is small since the FOV of the CRISM is quite small. Section 4.4.2 describes the derivation of the pseudo CAHV model in detail.

Each IPFF is modeled as a Gaussian function on the image plane of the pseudo CAHV model. For DEM pixels whose projection falls within the IPFF of a CRISM pixel, its response value is calculated based on their image plane coordinate. Section 4.4.3 describes the derivation of the Gaussian IPFF and the calculation of IPFF on the DEM in detail.

Fig. 4.9 illustrates the psuedo CAHV for CRISM and IPFF. The boresight vector is the axis vector $(\boldsymbol{a})$, the cross-track and along-track directions represent the horizontal and vertical axes of the image plane. The pointing vectors of the pixel centers are equally sampled according to their (line-of-sight) angles from the boresight vector around the vertical axis, and their horizontal coordinates are computed by CAHV projection. The CRISM imager is a pushbroom imager and the vertical coordinate values of these pixel centers are considered to 0 .

The projection using the pseudo CAHV model is repeated $N$ times for one line of the image, which is then repeated for all lines. I develop an adhoc method to effectively narrow the DEM region on which the CAHV projection is performed. Section 4.4.4 describes the detail of the narrowing method.

Finally, in order to store the PFF of CRISM pixels of the multiplie lines, a dedicated data structure needs to be constructed. Section 4.4.5 introduces such a structure convenient for storing the PFFs of CRISM image pixels.

Additionally, there might exist a mismatch between the pointing of CRISM and the referenced DEM model. Such a mismatch can be observed as a displacement between a scene image registered with the DEM and a CRISM map projected image based on the pointing of CRISM and the DEM model. Normally the residual displacement are corrected by a general image registration method as a post processing. The map projected image, which is derived from the pointing of CRISM and the DEM model, are warped to another image with interpolation, using a distortion model with ground control points (GCP). However, this post-processing do not tell how to correct the PFF of each CRISM. Section 4.4.6 describes a method to directly correct the pointing of CRISM instrument during the measurement using GCPs.

### 4.4.2 Pseudo CAHV model for CRISM

To construct the pseudo-CAHV model for the CRISM image, CAHV parameters are derived by trigonometric geometry. CAHV parameter is defined on the CRISM instrument-fixed coordinate, and converted later to another coordinate system when necessary. According to the SPICE ik kernel, the CRISM instrument-fixed coordinate defines the camera center as the origin, the boresight vector as the positive Z direction, and detector cross-track direction as the X axis, and the X axis is determined to satisfy right-hand rule, which corresponds to the along-track direction, the parameter FOV_REF_VECTOR in the ik kernel file. By definition, the camera center $\boldsymbol{c}=(0,0,0)$, and the camera axis


Figure 4.10. Trigonometry of the pseudo CAHV model for CRISM
$\boldsymbol{a}=(0,0,1)$. The horizontal and vertical directions of the camera image is defined as $\boldsymbol{h}^{\prime}=(1,0,0)$ and $\boldsymbol{v}^{\prime}=(0,1,0)$.

Let us remind $\boldsymbol{v}=v_{s} \boldsymbol{v}^{\prime}+v_{c} \boldsymbol{a} . v_{c}$ is the vertical index in the camera image where the camera Axis intersects. It is reasonable to set $v_{c}=0$ so that the camera axis passes the pixel vertical center. $v_{s}$ is determined from the parameter FOV_REF_ANGLE in the SPICE ik kernel by

$$
v_{s}=\frac{0.5}{\tan (\text { FOV_REF_ANGLE) }} .
$$

This makes the size of the vertical size of the pixel one, and ( $-0.5,0.5$ ) is considered as the vertical region of the CRISM pixels. Refer to Fig. 4.10(a) for the sketch of the geometric relationship.

The horizontal direction is more complicated. Similarly, we have $\boldsymbol{h}=h_{s} \boldsymbol{h}^{\prime}+h_{c} \boldsymbol{a}$. The pixel sampling in the cross-track direction is slightly different for different wavelength bands of the CRISM image cube, so it may require different CAHV models for different bands. Here I take a reference band $b_{\text {ref }}$ (by default it would be 223 for VNIR and 247 for IR in detector row numbers). According to the SPICE ik kernel file, the line-of-sight angle of sample $s$ from the boresight vector is modeled as $a_{0}^{\text {ref }}+a_{1}^{\text {ref }} s$, where $a_{0}^{\text {ref }}$ and $a_{1}^{\text {ref }}$ are the constants for each wavelength band recorded in the kernel file. $h_{c}$ is obtained
where the line-of-sight angle becomes zero:

$$
h_{c}=-\frac{a_{0}^{\text {ref }}}{a_{1}^{\text {ref }}} .
$$

It is reasonable to set $h_{s}$ so that the pixel center is sampled approximately at the interval of one in the camera image plane. This is accomplished by taking a reference sample $s^{\text {ref }}$

$$
\begin{gathered}
\theta_{\text {ref }}=a_{0}^{\text {ref }}+a_{1}^{\text {ref }} s^{\text {ref }} \\
h_{s}=\frac{s^{\text {ref }}-h_{c}}{\tan \theta_{\text {ref }}} .
\end{gathered}
$$

This makes the projection of sample $s^{\text {ref }}$ exactly to $\left(s^{\text {ref }}, 0\right)$. See Fig. 4.10(b) for the sketch of the geometric relationship.

With this model, the center of CRISM pixel $s$ is projected onto the image plane as follows. First, the line-of-sight angle of pixel $s$ is obtained by

$$
\theta_{s}=a_{0}^{\text {ref }}+a_{1}^{\text {ref }} s
$$

Next, the pointing vector $\boldsymbol{p}_{C}(s)$ associated with the center of pixel $s$ is obtained by a simple rotation from the boresight vector $\boldsymbol{a}$ around the Y axis:

$$
\boldsymbol{p}_{C}(s)=R_{Y}\left(\theta_{s}\right) \boldsymbol{a}
$$

where $R_{Y}(\theta)$ is a rotation matrix around the Y axis defined as

$$
R_{Y}(\theta)=\left(\begin{array}{ccc}
\cos \theta & 0 & \sin \theta \\
s d 0 & 1 & 0 \\
-\sin \theta & 0 & \cos \theta
\end{array}\right)
$$

Then the coordinate of the center of CRISM pixel $s$ is obtained by CAHV model projection

$$
m_{s}=\frac{\boldsymbol{h} \cdot \boldsymbol{p}_{C}(s)}{\boldsymbol{a} \cdot \boldsymbol{p}_{C}(s)} \quad \text { and } \quad y_{s}=0
$$

### 4.4.3 IPFF

The spatial transfer function (STF) for the CRISM is modeled as a Gaussian function. Kreisch et al. [103] estimated it from the spectral transfer function recorded in the preflight calibration data. I derived it from the modulation transfer function (MTF) shown in [4, Fig. 28]. I model the STF of pixel $s$ in the image plane of the pseudo CAHV model as the Gaussian centered at the coordinate of the center of the pixel. The variance is estimated from the MTF function since it represents the Fourier transform of the STF in the pixel coordinate domain. The unit length in the image plane is almost equivalent to the pixel pitch, so the estimated variance would be a good approximation of that of STF in the image plane. I refer the MTF of VNIR in at 1000 nm [4, Fig. 28]. Considering that the pixel pitch of CRISM detectors is $27 \mu \mathrm{~m}, 9.25$ cycle $/ \mathrm{mm}$ means that the period of the target sinusoidal curve has $1000 / 9.25 \cong 108 \mu \mathrm{~m}$, equivalent to the length of four detectors. Since the unit length of the pseudo image plane coordinate is approximately equivalent to one pixel pitch, 9.25 cycle $/ \mathrm{mm}$ is equivalent to 0.25 Hz . Similarly, 18.5 cycle $/ \mathrm{mm}$ is equivalent to 0.5 Hz . The point spread function (PSF) at pixel $s$ can be modeled as a two dimensional isotropic Gaussian function on the image plane [103]:

$$
\operatorname{PSF}_{s}(x, y)=\frac{1}{2 \pi \sigma^{2}} \exp \left(\frac{1}{2 \sigma^{2}}\left(\left(x-m_{s}\right)^{2}+y^{2}\right)\right)
$$

where $\sigma$ is the standard deviation of the Gaussian function. The line spread functions (LSF) in both of the $x$ and $y$ directions are also Gaussians with the same sigma. MTF is the modulus of the Fourier Transform of the LSF:

$$
\operatorname{MTF}_{s}(k)=e^{-2 \pi^{2} \sigma^{2} k^{2}}
$$

From [4, Fig. 28], we have $\operatorname{MTF}(1 / 4)=0.8$ and $\operatorname{MTF}(1 / 2)=0.4$. Then $\sigma$ is approximately obtained as $\sigma=0.43$.

The instantaneous pixel footprint function (IPFF) is obtained by the convolution of
the PSF with a rectangular area of a detector element:

$$
\begin{aligned}
\operatorname{IPFF}_{s}(x, y) & =\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \operatorname{PSF}_{s}(x-\alpha, y-\beta) \operatorname{Rect}_{s}(\alpha, \beta) d \alpha d \beta \\
\operatorname{IPFF}_{s}(x, y) & =\int_{-0.5}^{0.5} \int_{m_{s}-0.5}^{m_{s}+0.5} \operatorname{PSF}_{s}(x-\alpha, y-\beta) d \alpha d \beta \\
& =\left\{\phi\left(\frac{x^{\prime}+0.5}{\sigma}\right)-\phi\left(\frac{x^{\prime}-0.5}{\sigma}\right)\right\}\left\{\phi\left(\frac{y+0.5}{\sigma}\right)-\phi\left(\frac{y-0.5}{\sigma}\right)\right\},
\end{aligned}
$$

where $\operatorname{Rect}_{s}(x, y)$ is a rectangular shape function associated with pixel $s$

$$
\operatorname{Rect}_{s}(x, y)=\left\{\begin{array}{l}
1 \text { if } m_{s}-0.5 \leq x \leq m_{s}+0.5 \text { and }-0.5 \leq y \leq 0.5 \\
0 \text { otherwise }
\end{array}\right.
$$

$x^{\prime}=x-m_{s}$ and $\phi(x)$ is the cumulative normal distribution function. With $\sigma=0.43$, I experimentally verified that the $\operatorname{IPFF}_{s}(x, y)$ is well approximated by a Gaussian with $\tilde{\sigma}=0.53$.

$$
\begin{equation*}
\operatorname{IPFF}_{s}(x, y) \approx \frac{1}{2 \pi \tilde{\sigma}^{2}} \exp \left(\frac{1}{2 \tilde{\sigma}^{2}}\left(\left(x-m_{s}\right)^{2}+y^{2}\right)\right) \tag{4.21}
\end{equation*}
$$

The IPFF decays away from the center. It is reasonable to cut-off the IPFF if its response is sufficiently small. The valid region of $\mathrm{IPFF}_{s}$ is defined as

$$
S_{\mathrm{IPFF}_{s}}=\left\{(x, y)| | y_{P} \mid<k \tilde{\sigma} \text { and }\left|x_{P}-m_{s}\right|<k \tilde{\sigma}\right\}
$$

where $k$ is a coefficient defining the valid region. I use $k=4$ for my implementation.
Using this definition of IPFF on the image plane, IPFF on the MSL Gale DEM Mosaic is evaluated by projecting the center of DEM pixels onto the plane. First, the coordinate on the camera image plane of the center of DEM pixels is obtained by the projection, and IPFF is computed if it falls within the valid area of the IPFF function. This process is summarized in Algorithm 4.6.

### 4.4.4 Pre-processing of the DEM image

The CRISM instrument collects one line of an image at one time. With its position and orientation fixed, the FOV of CRISM covers a long and narrow area of the surface.

```
Algorithm 4.6 Evaluation of IPFF
Input: \(P(\boldsymbol{p})\) : DEM sample point (positional vector); \(k\) : parameter for valid IPFF region
Output: \(\operatorname{IPFF}_{s}\left(x_{P}, y_{P}\right)\) : IPFF value at \(P\)
    \(x_{P}=\boldsymbol{h} \cdot(\boldsymbol{p}-\boldsymbol{c}) / \boldsymbol{a} \cdot(\boldsymbol{p}-\boldsymbol{c})\) and \(y_{P}=\boldsymbol{v} \cdot(\boldsymbol{p}-\boldsymbol{c}) / \boldsymbol{a} \cdot(\boldsymbol{p}-\boldsymbol{c})\)
    If \(\left(x_{P}, y_{P}\right) \in S_{\mathrm{IPFF}_{s}}\) then Get \(\operatorname{IPFF}_{s}\left(x_{P}, y_{P}\right)\) by Eq. (4.21), otherwise
    \(\operatorname{IPFF}_{s}\left(x_{P}, y_{P}\right)=0\).
```

In order to speed up the projection, it is necessary to effectively restrict the region of the DEM image for evaluating IPFF beforehand. I develop a practical method for pre-processing that restricts the search region. First I start from a simple statement. Let the upper and lower bounds of the radius of the region of interest as $r_{\text {max }}$ and $r_{\text {min }}$ respectively. Let us consider two pointing vectors $\boldsymbol{p}_{1}$ and $\boldsymbol{p}_{2}$ from a camera associated with their projection $p_{1}^{(\mathrm{cam})}$ and $p_{2}^{(\mathrm{cam})}$ onto the camera image plane. Define the intersection of a vector from the camera pointing in the direction of $\boldsymbol{p}_{i}$ with a celestial body of radius $r$ be $p_{i}(r)$ and its equirectangular projection is $p_{i}^{(\text {equi })}(r)$. Any point on the line segment on the camera image plane determined by $p_{1}^{(\mathrm{cam})}$ and $p_{2}^{(\mathrm{cam})}$ would be projected within or on the rectangular region minimally enclosing $p_{1}^{(\text {equi })}\left(r_{\min }\right), p_{1}^{(\text {equi })}\left(r_{\max }\right), p_{2}^{\text {(equi) }}\left(r_{\min }\right)$, and $p_{2}^{(\text {equi) }}\left(r_{\max }\right)$ in the map of the equirectangular projection. This statement is theoretically inaccurate considering the spherical or ellipsoidal body of a celestial body and the nonlinearity of the equirectangular projection. Practically, around the Gale crater region, this statement holds due to the low degree of non-linearity of the projection at a low latitude.

Based on this assumption, we can effectively restrict the search region of the DEM image. The valid regions of the $\mathrm{IPPF}_{s}$ on the CAHV image plane is a rectangle region defined by

$$
m_{s}-k \tilde{\sigma}<x<m_{s}+k \tilde{\sigma} \quad \text { and } \quad-k \tilde{\sigma}<y<k \tilde{\sigma} .
$$

Let the vertices composing this rectangle be $v_{i}(i=1,2,3,4)$. Given $r_{\text {max }}$ and $r_{\text {min }}$, the search region of the DEM image for getting $\mathrm{IPPF}_{s}$ is the rectangle region of the DEM image minimally enclosing eight points: $v_{i}^{(\text {equi })}\left(r_{\text {min }}\right), v_{i}^{(\text {equi })}\left(r_{\max }\right)(i=1,2,3,4)$. The


Figure 4.11. Pre-processing of the DEM image for the projection of CRISM
union of these rectangles for all CRISM pixels becomes the total region to be evaluated for IPFF.

Figure 4.11 displays the result of the pre-processing using the upper and lower bounds and subsequent projection for obtaining IPFF $_{s}$ for all CRISM samples. The background image is the DEM image in the gray scale. The blue region is the union of the minimally enclosing rectangles obtained from the upper and lower bounds of the radius. The yellow region is the union of the actual IPFFs for all CRISM samples. The yellow region is completely placed inside the blue region with some margins, showing that the preprocessing is not overcutting the region for the evalution of IPFF. The CRISM FOV on the ground is a narrow long area and due to its observation geometry, the slip looks slanted on the equirectangular projection map, which makes the assumption made for this pre-processing more likely to be valid.

### 4.4.5 A new representation of CRISM image map projection on hiresolution DEM model

A standard image format is inconvenient for recording the PFF-based projection of a CRISM image as there are likely to exist overlaps betweem PFFs, and one DEM pixel may belong to the PFF of an arbitrary number of CRISM pixels.

I propose a new data format for storing the new structure of the map projection result based on PFF. In the new data format, the PFF of each pixel of the CRISM image is retained independently. Each PFF image would be a small one layer image storing the response of PFF, rectangular minimally enclosing the PFF, attached with supporting information of the vertical and horizontal range. This can be realized by three binary image. The first image is multilayer image storing the sample and line offset from the original reference DEM image where each PFF starts and the number of samples and lines of each PFF. The second image is the vector format of the PFF concatenated. The third image stores the byte offset of each PFF in the second image.

### 4.4.6 Correction of CRISM instrument pointing

One may observe displacement of the CRISM map projected image with respect to the MSL Gale Ortho Mosaic image since they are processed using different pipelines. I consider adjusting displacement by correcting the pointing direction of the CRISM instrument. Using a map projected image, we could get ground control points (GCP) that relate pixels of a CRISM image to ones in the MSL Gale Ortho Mosaic whose geographic coordinates are retrieved by MSL Gale DEM Mosaic. For each GCP, the orientation of the CRISM at the time associated with the GCP of CRISM is corrected by rotation to point the geographical coordinate of the GCP of the MSL Gale Ortho Mosaic. The correction of the orientation of the CRISM at the other times are interpolated (extrapolated) using bilinear spherical interpolation(extrapolated). Due to the resolution difference between MSL Gale Ortho Mosaic and the CRISM image, accurate GCPs may be difficult to
obtain. More accurate correction would be necessary. Let the areographic coordinate (planetocentric latitude, longitude) of the GCPs in the reference MSL Ortho Mosaic image be $\left(\varphi_{n}^{\text {true }}, \theta_{n}^{\text {true }}\right)$ and that obtained by the projection with the uncorrected orientation be ( $\varphi_{n}^{\mathrm{proj}}, \theta_{n}^{\text {proj }}$ ) for $n=1, \ldots, N_{\mathrm{GCP}}$, where $N_{\mathrm{GCP}}$ is the number of GCPs. Let the CRISM pixel (sample, line) associated with the GCP be $\left(x_{n}, y_{n}\right)$. Let the start time of the measurement of line $l$ be $t_{l}^{\text {(start) }}$ and the exposure time be $t_{\exp }$. Assume that the GCP is associated with the center of the CRISM sample pixel at the time of its half exposure, namely at $t_{n}=t_{y_{n}}^{\text {(start) }}+t_{\exp } / 2$. By definition, we have

$$
\boldsymbol{p}_{C}\left(x_{n}, 0, t_{n}\right) \| \boldsymbol{p}\left(\varphi_{n}^{\mathrm{proj}}, \theta_{n}^{\mathrm{proj}}\right)-\boldsymbol{c}\left(t_{n}\right),
$$

where $\boldsymbol{p}_{C}\left(x_{n}, 0, t_{n}\right)$ is the pointing vector associated with the center of the CRISM sample $x_{n}$ at time $t_{n}, \boldsymbol{p}\left(\varphi_{n}^{\text {proj }}, \theta_{n}^{\text {proj }}\right)$ is the positional vector at the areographic coordinate ( $\left.\varphi_{n}^{\text {proj }}, \theta_{n}^{\text {proj }}\right)$, and $\boldsymbol{c}\left(t_{n}\right)$ is the camera center at time $t_{n}$. The true pointing vector is

$$
\boldsymbol{p}_{C}^{\text {true }}\left(x_{n}, 0, t_{n}\right) \| \boldsymbol{p}\left(\varphi_{n}^{\text {true }}, \theta_{n}^{\text {true }}\right)-\boldsymbol{c}\left(t_{n}\right) .
$$

The orientation of the CRISM instrument is corrected to align $\boldsymbol{p}_{C}\left(x_{n}, 0, t_{n}\right)$ to $\boldsymbol{p}_{C}^{\text {true }}\left(x_{n}, 0, t_{n}\right)$.
This rotation is defined by the unit-length rotation axis vector $\boldsymbol{\omega}_{n}$ :

$$
\boldsymbol{\omega}_{n}=\frac{\boldsymbol{p}_{C}\left(x_{n}, 0, t_{n}\right) \times \boldsymbol{p}_{C}^{\text {true }}\left(x_{n}, 0, t_{n}\right)}{\left\|\boldsymbol{p}_{C}\left(x_{n}, 0, t_{n}\right) \times \boldsymbol{p}_{C}^{\text {true }}\left(x_{n}, 0, t_{n}\right)\right\|},
$$

and the rotation angle $\alpha_{n}$ :

$$
\alpha_{n}=\cos ^{-1}\left(\frac{\boldsymbol{p}_{C}\left(x_{n}, 0, t_{n}\right) \cdot \boldsymbol{p}_{C}^{\text {true }}\left(x_{n}, 0, t_{n}\right)}{\left\|\boldsymbol{p}_{C}\left(x_{n}, 0, t_{n}\right)\right\|\left\|\boldsymbol{p}_{C}^{\text {true }}\left(x_{n}, 0, t_{n}\right)\right\|}\right) .
$$

Let us denote the quaternion ${ }^{3}$ obtained from the axis vector $\boldsymbol{\omega}_{n}$ and the angle $\alpha_{n}$ by $\boldsymbol{q}_{n}$. Assume that the GCPs are sorted with respect to their time stamps $t_{n}$. The rotation quaternion for correcting the orientation of the CRISM instrument at arbitrary time $t$ is obtained by bilinear spherical interpolation/extrapolation using the collection of reference rotation quaternions $\left\{\left(t_{n}, \boldsymbol{q}_{n}\right)\right\}$ for $n=1, \ldots, N_{\mathrm{GCP}}$ of the GCPs. Special attentions must be paid on the frame in which each vector, quaternion, and rotation matrix are defined.

[^13]

Figure 4.12. Example of the PFF of one CRISM pixel.

### 4.4.7 Presentation of the results

Fig. 4.12 shows an example of the PFF of one pixel of CRISM on the MSL Gale DEM Mosaic. The Gaussian is slightly smeared along the direction of the movement. This way, it is possible to precisely pinpoint the pixel footprints of the CRISM. The PFF of the CRISM pixels is a fundamental result of the map projection for deriving geo-referenced images of associated CRISM images or its derived map products. Fig. 4.13 shows the PFFs of one line of CRISM measurements.

One way to geo-reference the CRISM detector image is highest PFF mapping, where each of the pixel of the DEM grid is filled with the CRISM pixel that has the highest PFF value. Fig. 4.14 shows the result of the highest PFF mapping, compared with the common DDR-based projection. While the DDR-projection suffers from pixel aliasing, the proposed method shows CRISM pixel shapes perpendicular to the movement of the imager, more accurate footprints of pixels, although information regarding the Gaussian spatial response function is lost.

Fig. 4.15 (a) shows the displacement of the map projection of CRISM image using the raw SPICE observation geometry together with the DTM data. It clearly shows a displacement between the map-projected CRISM image and MSL Ortho Mosaic image.


Figure 4.13. PFF of one line of a CRISM image

Such a displacement is usually addressed after the image is geo-referenced, but this does not correct the PFF of CRISM pixels. In order to obtain more accurate PFFs, we can fix the mismatch by directly correcting the orientation of the CRISM using manually selected ground control points (GCP). Fig. 4.15 (b) shows the geo-referenced CRISM image using the corrected orientation and that the correction clearly improves the accuracy of map projection.

### 4.5 Mutual map projection between CRISM and Mastcam

Using the mutual map projection between the CRISM and MSL Gale DEM Mosaic and that between the Mastcam image and the DEM Mosaic, the PFF of CRISM pixels on the Mastcam image will be derived. The PFF of CRISM pixels on the MSL Gale DEM Mosaic is projected onto the Mastcam image using the map projection structure from the MSL DEM Mosaic to the Mastcam image. Denote the PFF of the CRISM pixel $(s, l)$ at DEM pixel $\left(x_{\mathrm{dem}}, y_{\mathrm{dem}}\right)$ as $\mathrm{PFF}_{s, l}\left(x_{\mathrm{dem}}, y_{\mathrm{dem}}\right)$ and the PFF of the CRISM pixel $(s, l)$ at Mastcam image pixel $\left(x_{\mathrm{mst}}, y_{\mathrm{mst}}\right)$ as $\mathrm{PFF}_{s, l}\left(x_{\mathrm{mst}}, y_{\mathrm{mst}}\right)$. Denote the $\left(x_{\mathrm{dem}}, y_{\mathrm{dem}}\right)$ element


Figure 4.14. Comparison of the geo-referencing of CRISM data using the proposed method (a) and using DDR data on an 18 m grid (b). Band $13(1.08 \mu \mathrm{~m})$ of the CRISM FRT0000B6F1 image is used.
of the mapper structure DEM2Mastcam by DEM2Mastcam $\left(x_{\mathrm{dem}}, y_{\mathrm{dem}}\right)$. Then the value of $\operatorname{PFF}_{s, l}\left(x_{\mathrm{dem}}, y_{\mathrm{dem}}\right)$ is assigned to all the Mastcam pixels in DEM2Mastcam $\left(x_{\mathrm{dem}}, y_{\mathrm{dem}}\right)$. If multiple $\operatorname{PFF}_{s, l}\left(x_{\mathrm{dem}}, y_{\mathrm{dem}}\right)$ are assigned to one Mastcam pixel, then the value of $\operatorname{PFF}_{s, l}\left(x_{\mathrm{mst}}, y_{\mathrm{mst}}\right)$ is obtained by averaging all the values of $\mathrm{PFF}_{s, l}\left(x_{\mathrm{dem}}, y_{\mathrm{dem}}\right)$ to that Mastcam pixel.

Fig. 4.16 shows an integrated system that relates the CRISM measurement to Mastcam data together with a geo-referenced map projection view. Using the PFF of the CRISM on the DEM and on the Mastcam image, it is easy to match the CRISM image pixel both on the map-projected image and on the Mastcam image. This automatic processing facilitates matching the CRISM measurement to the pixels in the Mastcam image, potentially aiding the scientific analysis.


Figure 4.15. Evaluation of the displacement of the CRISM image FRT0000B6F1 geo-referenced to the MSL Gale DEM Mosaic without (a) and with (b) orientation correction. The background image is the MSL Ortho Mosaic image registered with MSL Gale DEM Mosaic down-sampled to 10 m resolution and the front color-scaled image is band $13(1.08 \mu \mathrm{~m})$ of the geo-referenced CRISM.


Figure 4.16. Concept of the interactive view of the mutual map projection of CRISM and Mastcam.

## C H A P T ER

## CONCLUSION

This dissertation explored different aspects of hyperspectral unmixing. First, I investigated a theoretical aspect of sparse unmixing, a semi-supervised unmixing method that identifies endmembers present in the observation from the large collection of spectra in the spectral database. In specific, I derived a theoretical conditions that guarantee the correct recovery of endmembers for the sparse unmixing formulated as a non-negative lasso (NLasso) problem. I further introduced approximately perfect recovery condition (APMRC) that practically performs as a necessary and sufficient condition of Nlasso. A rigorous mathematical proof of the necessity and sufficiency of the APMRC is also provided.

Then I explored the application of hyperspectral unmixing. First, I applied it to the processing of hyperspectral image acquired by the Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) onboard the Mars Reconnaissance Orbiter (MRO). In specific, I developed a new atmospheric correction and de-noising method for CRISM images, simultaneous atmospheric correction and de-noising for CRISM (SABCOND). SABCOND models light interaction through the Martian atmosphere by the Beer-Lambert's law and surface reflection using an unmixing model. An optimal atmospheric transmission spectrum is estimated by solving a minimization problem that also takes noise into account. A dedicated solver in which a generalized version of ADMM is developed to efficiently solve the SABCOND. I showed that SABCOND successfully removed most of the problematic systematic artifacts in CRISM images that would have been caused by
the traditional atmospheric correction, volcano scan correction, and accurately detects and removes large noise spikes. It can also remove the contribution of water ice aerosols, and successfully works on noisy images. In addition, I further introduced a two-step SABCOND to overcome some of the problems still left for the SABCOND. The two-step SABCOND requires manual processing, but I showed that the two-step SABCOND can further improve the signal quality and fidelity of the corrected spectral signals.

Lastly, I investigated how hyperspectral images acquired from orbits can be precisely combined with ground observation. In specific, I mapped hyperspectral images obtained by the CRISM onto ground mega-pixel images acquired by the Mast Camera (Mastcam) installed on the Curiosity rover on Mars at pixel level. I project both of the CRISM and Mastcam images onto a high resolution digital elevation model, and successfully link the images at pixel level. In this procedure, I devise a new fast and exact algorithm to detect invisible surface points from the Mastcam camera that takes most advantage of the CAHV/CAHVOR model, and a new map projection method for CRISM data using their sensor model and ephemerides using the psuedo CAHV model projection. The projection involves some manual corrections since the required accuracy of surface topography, their localizations, spacecraft trajectories and instrumental orientation is quite demanding. However proposed map projection methods shows what could be achieved in the future when more and more accurate and high-resolution data become available.

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[^0]:    3.10. Comparison of two band images corrected with the proposed method (a) and with CAT on filtered I/F (b). They are the band $302(1.895 \mu \mathrm{~m})$ of FRT0001821C.

[^1]:    ${ }^{1}$ This chapter is the compilation of the two pieces of research work [7] and [8].

[^2]:    ${ }^{2}$ Micro-Hyperspec ${ }^{\circledR}$ is a registered trademark of Headwall Photonics, Inc.

[^3]:    ${ }^{3}$ Spectralon ${ }^{\circledR}$ is a registered trademark of Labsphere, Inc.

[^4]:    ${ }^{1}$ This chapter includes my research contribution [55], [56], and [57].

[^5]:    ${ }^{2}$ The residual of the proposed atmospheric correction method, obtained by removing estimated atmospheric and surface components from I/F signal, is considered to be a suitable approximation of the noise in CRISM signals.

[^6]:    ${ }^{3}$ https://github.com/scottprahl/miepython

[^7]:    ${ }^{4}$ http://ghosst.obs.ujf-grenoble.fr

[^8]:    ${ }^{5}$ Technically, it would be more precise to ignore these bands by removing their corresponding rows, but I found that it only have minor effects and I just choose this approximation for simpler implementation.

[^9]:    ${ }^{6}$ https://www.ibm.com/analytics/cplex-optimizer

[^10]:    ${ }^{7}$ Fitting with more commonly used $\ell_{2}$-error would be affected by large spike noise and proximal bands to the spike may also have large residual values.

[^11]:    ${ }^{1}$ This dissertation does not differentiate DTM and DEM and they are used interchangeably.

[^12]:    ${ }^{2}$ naif.jpl.nasa.gov/naif/

[^13]:    ${ }^{3}$ Quaternion is a numbering system extended from the complex number. It is useful to represent 3-D rotation without any singularity point unlike euler angles.

