Machine Learning Approach to Retrieving Physical Variables from Remotely Sensed Data

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MACHINE LEARNING APPROACH TO RETRIEVING PHYSICAL VARIABLES FROM REMOTELY SENSED DATA

by

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Abstract

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Scientists from all over the world make use of remotely sensed data from hundreds of satellites to better understand the Earth. However, physical measurements from an instrument is sometimes missing either because the instrument hasn’t been launched yet or the design of the instrument omitted a particular spectral band. Measurements received from the instrument may also be corrupt due to malfunction in the detectors on the instrument. Fortunately, there are machine learning techniques to estimate the missing or corrupt data. Using these techniques we can make use of the available data to its full potential.

We present work on four different problems where the use of machine learning techniques helps to extract more information from available data. We demonstrate how missing or corrupt spectral measurements from a sensor can be accurately interpolated from existing spectral observations. Sometimes this requires data fusion from multiple sensors at different spatial and spectral resolution. The reconstructed measurements can then be used to develop products useful to scientists, such as cloud-top pressure, or produce true color imagery for visualization. Additionally, segmentation and image processing techniques can help solve classification problems important for ocean studies, such as the detection of clear-sky over ocean for a sea surface temperature product. In each case, we provide detailed analysis of the problem and empirical evidence that these problems can be solved effectively using machine learning techniques.
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This thesis describes work that was previously published. The work for quantitative restoration for MODIS band 6 on Aqua described in Section 3.1 was previously published in [12], [13] and [14]. The statistical estimation of a 13.3 µm VIIRS channel using multisensor data fusion described in Section 3.2 was previously published in [11]. The estimation of true color imagery for GOES-R described in Section 3.3 was previously published in [17] and [18]. The improvement of VIIRS imagery using resampling described in Section 3.4 was previously published in [15]. The machine learning approach to clear-sky classification described in Chapter 4 was previously published in [16].
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Chapter 1

Introduction

The growing wealth of remote sensing data from hundreds of space-based sensors is providing us with enormous new opportunities to better understand the Earth at a time when that understanding may be critical. Government agencies such as NASA and NOAA strive to provide remote sensing data to better serve the public. One of NOAA’s mission support goals is to “provide a continuous stream of satellite data and information with the quality and accuracy to meet users requirements for spatial and temporal sampling, and for timeliness of delivery.” Yet there are various reasons why this critical priority is not always easy to meet.

Designing, building, and launching these sensors are enormous projects typically taking many years and costing billions of dollars. Unfortunately, these missions are sometimes canceled and often delayed. Even when the sensors are deployed, they may not provide data for the entire surface of the Earth, or they may not measure the precise spectral bands of interest, or they may not visit sites of interest frequently enough. Also, when remote sensing projects are successful, an instrument providing data may fail due to the hostile environment of space, or lacking funding to support the continuing operation and thus be retired.

Given the importance of these remote sensing instruments, it’s critical that techniques be in place and ready to reduce any potential risk from temporary or permanent non-functional
detectors. Fortunately, there are powerful statistically sound methods of estimating missing data. While none would suggest such estimations can completely replace the missing data, they can reduce risk by using all available information to provide a high quality estimation of the missing data. Growing computational power and statistical learning techniques provide a means to leverage the hundreds of satellites already observing the Earth, which produce multi-, hyper-, or ultra-spectral images. Statistical analysis and machine learning techniques can be used to produce virtual integrated sensors. These integrated sensors can help address some of the issues that cannot be addressed with hardware sensors alone. We will give examples below.

System failure in the Moderate Resolution Imaging Spectroradiometer (MODIS) instrument on Earth Observing System (EOS) Aqua satellite resulted in corruption of most of the values in the 1.6 $\mu$m band that it provides. We will show how to accurately restore these corrupted values by using the information in the non-corrupted values in the 1.6 $\mu$m band, and information from other MODIS bands [14, 27, 37, 40, 42]. Machine learning makes it possible to construct such algorithm.

The Advanced Baseline Imager (ABI) onboard the Geostationary Operational Environmental Satellite GOES-R provides visible band for red and blue, but does not provide a visible band for green. This makes it difficult to directly construct a color (RGB) image from the bands. Similar to the previous example, we can use machine learning to produce a RGB image based on other spectral bands [17, 18, 21, 30]. The end goals here is the production of a RGB image for visualization purposes, not necessarily the green band alone. Since GOES-R had not been launched at the time we developed this algorithm, and thus its data were not available yet, we constructed simulated ABI bands from MODIS bands at similar spectral range. This simulated data is used to develop and demonstrate the effectiveness of the algorithm.
Similar to how the ABI is missing a band, the Visible Infrared Imaging Radiometer Suite (VIIRS) onboard the Suomi National Polar-orbiting Partnership (S-NPP) satellite does not provide a band at 13.3\,\mu m, which is available on older platforms such as MODIS Aqua and Terra. This makes it difficult to compute cloud-top pressure (CTP) \[29\], a physical variable important to meteorologist and other scientists. However, S-NPP also carries the Cross-track Infrared Sounder (CrIS), which has a higher spectral resolution but lower spatial resolution than the imager VIIRS. CrIS covers the 13.3\,\mu m spectral response range through a multitude of narrow bands, which makes it possible to construct a 13.3\,\mu m band, albeit at a lower spatial resolution than VIIRS. We can develop a regression between the VIIRS bands and the CrIS-constructed 13.3\,\mu m band, and this regression can be used to estimate 13.3\,\mu m band at VIIRS resolution, which in turn is used to compute CTP \[11\].

Machine learning is also useful for issues which, unlike the previous three cases, doesn’t involve corrupt or missing measurements. The NOAA Advanced Clear Sky Processor for Oceans (ACSPO) sea surface temperatures (SST) product for VIIRS aims to provide an accurate clear-sky mask over ocean. However, there are many areas where this mask is too conservative and marks clear-sky conditions as cloud. The goal is to find these areas and mark them as clear-sky. It is possible to meet this goal by attempting to detect patterns in SST and other bands, and through the use of unsupervised learning and image processing tools \[16\]. Some image processing algorithms which rely on spatial context and patterns in the imagery require that the input is a continuous and non-distorted image. VIIRS in particular suffers from artifacts due to its scanning geometry and onboard processing. These instrument-specific data issues can be mitigated using a resampling procedure which permutes the pixels based on the scanning geometry and then uses interpolation such that a continuity of corresponding latitude and longitude arrays is ensured.

The rest of this thesis is organized as follows. In Chapter 2, we briefly introduce the remote sensing instruments. In Chapter 3, we present various virtual sensing approaches,
including the restoration of MODIS 1.6\textmu m band (Section 3.1), estimation of true color imagery for GOES-R (Section 3.3), estimation of VIIRS 13.3\textmu m band (Section 3.2), and improving VIIRS imagery using resampling (Section 3.4). In Chapter 4, we discuss how the ACSPO clear-sky mask can be improved using machine learning. Finally, we state our conclusions in Chapter 5.
Chapter 2

Remote Sensing Instruments

Remote sensing instruments onboard satellites orbiting the Earth continuously observe the Earth, measuring physical variables related to Earth’s surface, its atmosphere and the ocean. These measurements are sent back to ground stations and processed into products which are used by scientists to study the Earth. We briefly describe various remote sensing instruments that are discussed in the following chapters.

2.1 Polar Orbiting Satellites

Satellites which are in polar orbits around the Earth pass nearly above the poles of the Earth on each revolution. No spot of the Earth’s surface is sensed continuously by a polar orbiting satellite. However, these satellites can see virtually every part of the Earth over time as the Earth rotates underneath it. Examples of remote sensing instruments onboard polar orbiting satellites include MODIS (Section 2.1.1), VIIRS (Section 2.1.2), and Hyperion (Section 2.1.3).
2.1.1 Aqua and Terra

The Moderate Resolution Imaging Spectroradiometer (MODIS) is a key instrument aboard the Terra and Aqua satellites, part of the Earth Observing System (EOS) mission. It was designed to provide data for global monitoring of atmosphere, ocean, and land. MODIS has been in operation since the launch of Terra in December 1999. MODIS on Aqua became operational later in May 2002 when Aqua was launched. Terra (EOS AM) spacecraft orbits the globe and passes from north to south (descending) across the equator at 10:30 AM, and Aqua (EOS PM) spacecraft passes south to north (ascending) over the equator at 1:30 PM. MODIS observes the Earth using 36 spectral bands covering wavelengths from visible (VIS) to long-wave infrared. It has three different nadir ground spatial resolutions: 250 meters (bands 1 and 2), 500 meters (bands 3 to 7), and 1000 meters (bands 8 to 36). The 250-m spatial resolution band uses 40 detectors; the 500-m spatial resolution band uses 20 detectors; and the 1000-m spatial resolution band uses 10 detectors [37].

The Aqua satellite also carries the Atmospheric Infrared Sounder (AIRS)[2] instrument, designed to measure the Earth’s atmospheric water vapor and temperature profiles on a global scale. AIRS is a cross-track scanning instrument built by BAE SYSTEMS for NASA/JPL. It’s an infrared spectrometer/radiometer which covers the 3.7–15.4 µm spectral range with 2378 spectral channels, and produces a scan swath that extends roughly 800 km on either side of the ground track. The term “sounder” in the instrument’s name refers to the fact that measurements are effectively taken as a function of height, since each measurement in the infrared wavelength range is sensed by AIRS over a range of heights in the atmosphere, from the surface up into the stratosphere.
2.1.2 Suomi National Polar-orbiting Partnership

The Visible Infrared Imaging Radiometer Suite (VIIRS) is a scanning radiometer onboard the Suomi National Polar-orbiting Partnership (S-NPP) platform launched on 28 October 2011. It collects visible and infrared imagery and radiometric measurements of the land, atmosphere, cryosphere, and oceans. We give a detailed description of VIIRS scan geometry in Section 3.4.1. VIIRS will be also onboard two follow-on Joint Polar Satellite System (JPSS) satellites, J1 and J2, planned for launch in 2017 and 2023, respectively [16].

The S-NPP also carries the Cross-track Infrared Sounder (CrIS)[4] instrument, a Fourier transform spectrometer that produces high-resolution, three-dimensional temperature, pressure, and moisture profiles. CrIS provides soundings of the atmosphere with 1305 spectral channels, over 3 wavelength ranges: LWIR (9.14–15.38 µm); MWIR (5.71–8.26 µm); and SWIR (3.92–4.64 µm). CrIS scans a 2200km swath width (+/- 50 degrees), with 30 Fields of Regards (FORs). Each field consists of 9 Fields of View (FOVs), arrayed as 3x3 array of 14km diameter spots (nadir spatial resolution).

2.1.3 Earth Observing Mission 1

Hyperion on the Earth Observing Mission 1 satellite (EO-1) is a high resolution hyperspectral imager capable of resolving 220 spectral bands (from 0.4 to 2.5 µm) with a 30-meter resolution. The EO-1 satellite was launched on November 21, 2000 as part of a one-year technology validation/demonstration mission by NASA (National Aeronautics and Space Administration). The mission was successfully completed in November 2001. At the end of the mission, it was decided to continue acquisition of image data from EO-1 as part of EO-1 Extended Mission. Image data acquired by EO-1 are archived and distributed by the United States Geological Survey (USGS) Center for Earth Resources Observation and Science (EROS) and placed in the public domain [34].
2.2 Geostationary Satellites

Geostationary satellites are in circular orbit above the Earth’s equator and follow the direction of the Earth’s rotation. To an observer on the ground, the satellite appear motionless at a fixed position in the sky. Geostationary orbits allow the satellite to sense the Earth’s surface continuously, even a full hemisphere of the Earth. Examples of remote sensing instruments on geostationary satellites include the GOES-R ABI (Section 2.2.1) and Himawari AHI (Section 2.2.2).

2.2.1 Geostationary Operational Environmental Satellites

The Geostationary Operational Environmental Satellites (GOES) line of satellites have existed since 1975 with GOES-1. On November 19, 2016, the National Oceanic and Atmospheric Administration (NOAA) launched the first satellite in a series of next-generation GOES called GOES-16. Since GOES satellites are assigned alphabetical values until placed into the proper geostationary orbit, whereupon they receive a numerical identifier, GOES-16 was previously known as GOES-R. GOES-16 represents a paradigm shift to the GOES program in terms of remote-sensing capabilities. Its suite of sensors include the first lightning mapper to fly in geostationary orbit (the GOES Lightning mapper, GLM), an improved imaging radiometer called the Advanced Baseline Imager (ABI) and several space weather sensors. The ABI contains 16 narrow-band channels spanning the optical spectrum (\(\sim 0.4–13.6 \mu m\)). Despite its many advances over the heritage GOES, the ABI does not provide all the color components necessary to render natural color imagery from its native channel suite. The ABI includes the red and blue bands, but it’s missing the green band at 0.55 \(\mu m\) [30].
2.2.2 Himawari

The Advanced Himawari Imager (AHI) [33] onboard the Himawari-8 geostationary satellite, operated by the Japan Meteorological Agency (JMA), has similar spectral and spatial characteristics to the GOES-16 ABI. It was launched on October 7, 2014, and started operation on July 7, 2015. The AHI is also onboard Himawari-9, which was recently launched on November 2, 2016. Himawari-8 and -9 are part of a dedicated meteorological mission, unlike the currently operational Multi-Functional Transport Satellite (MTSAT) 2 (also known as Himawari 7) which performs both meteorological and aeronautical functions. The currently operational AHI scans five areas: Full Disk (images of the whole Earth as seen from the satellites), the Japan Area, the Target Area and two Landmark Areas. In each 10-minute period, the AHI scans the Full Disk once, the Japan Area and Target Area four times, and the two Landmark Areas twenty times. The AHI observes 16 spectral bands. Color images will be derived by compositing three visible bands: blue at 0.47µm, green at 0.51µm, and red at 0.64µm.
Chapter 3

Virtual Sensing

Virtual sensing is a technique that uses existing information from other measurements to estimate a quantity of interest. It provides an economical alternative to costly physical sensing. Four examples are given below where virtual sensing is used to accurately estimate missing or corrupt measurements.

3.1 Restoration of the Aqua MODIS 1.6μm Band

System failures in a multispectral satellite imager may result in a loss of precious data about the Earth’s environment. Typically, an imager collects the data via many sensitive detectors. The launch process, deployment in the harsh environment of space, particle bombardment, and exposure to radiation and space dust can result in detector damage at any point in an imagers life cycle [14].

When a damaged detector produces noisy or distorted data in a scanning imager such as Moderate Resolution Imaging Spectroradiometer (MODIS), it results in periodic stripes. This is because, during every scan, the set of detectors produces a group of scanlines in the image. A single detector produces a single scanline, and as the groups of scanlines are built
up to produce an image, the broken detectors produce periodic noisy or dropped lines which appear as stripes.

A particularly important example of periodic line drop is the 1.6 µm band in the MODIS instrument on the Aqua satellite of the National Aeronautics and Space Administration (NASA). Fifteen out of 20 detectors in this band are broken, meaning that their data are missing or so noisy as to be considered unusable [37, 42]. Currently, the data are published with the locations of missing data recorded in the metadata. In addition, NASA publishes band 6 with the missing scanlines filled in using columnwise linear interpolation. This simple interpolation method results in artifacts due to the significant data loss, and it sometimes even fills pixels with statistically or physically implausible image values [14].

Interpolation is most effective when restoring scattered isolated missing pixels of scenes at points where it can be assumed that no edges or fine details are present, but this assumption does not apply to band 6 MODIS/Aqua images because they often contain fine cloud and land structural detail. In addition, rather than the lost pixels being isolated, many contiguous lines have been dropped, leaving large gaps in the data. The problem with columnwise interpolation is that there is not enough information coming from the good 25% of the detectors to restore the missing data; thus, this method introduces significant artifacts. Because of these artifacts, the image is smoother along columns than along rows. Since the columnwise interpolation dramatically corrupts image gradients, the image is unusable for any algorithm that uses gradients as input, such as edge detectors.

3.1.1 Background

There are several approaches to filling in missing scanlines in MODIS band 6 that gives better results than the columnwise interpolation method. In Wang et al. [42], the authors show that the missing data can be estimated by fitting, at good band 6 detectors, a cubic polynomial expressing the band 6 pixel values as a function of band 7. They then use this polynomial
to fill in the missing values. This approach is evaluated using MODIS/Terra bands 6 and 7 as proxies for the MODIS/Aqua band 7 and damaged band 6. It was shown that by using regression to find the polynomial coefficients, it’s possible to obtain a restoration that is significantly better than basic interpolation. A weakness in this approach is that, given the complex spectral reflectances of materials, there could be no true functional relationship between bands 6 and 7.

In Rakwatin et al. [37], a local cubic regression approach was proposed. This approach drops the unrealistically strong assumption that a global relationship between bands 6 and 7 exists and instead assumes that this relationship only exists locally. Thus, they let the parameters of a functional relation between bands 6 and 7 vary. To do this, they define a sliding window of pixels centered at the pixel to be filled in, and then use the working sensors of band 6, and the corresponding sensors of band 7 within the sliding window, to perform a locally varying cubic regression. This local regression is then applied to the band 7 data to restore the band 6 data at the damaged sensors. Each pixel is filled in using a cubic polynomial with a potentially different set of coefficients. Note that, although a window is used to find the coefficients of the polynomial regression, the input to the regression is just the band 7 value. In addition to allowing the regression to vary across the image, they also applied histogram matching destriping [19, 36] to the image as a pre-processing step to further improve the consistency of the regression and simultaneously reduce detector-to-detector striping artifacts.

Taking local fitting further, Shen et al. [40] proposed a within-class local fitting algorithm for restoring MODIS band 6. An unsupervised classification is first performed to separate various scene types, and then a within-class local fitting is performed based on the scene types. As in previous approaches, only band 7 is used to perform the prediction.

There are some recent work on restoration of MODIS Aqua band 6 that have come after the publication of our algorithm, Quantitative Image Restoration (QIR), described in
the next section. Published approximately two years after the publication of QIR, Li et al. describes an algorithm based on a Robust M-Estimator Multiregression (RMEMR) [27]. Similar to QIR, the regression is done locally in tiles of size $20 \times 20$ which are slided by a fixed step size (usually ten). This tile size is much smaller than the $200 \times 200$ sized tile used in QIR. The authors argue that since there are 20 detectors in total, the correlation is closer in most cases in a tile of size $20 \times 20$. For each tile $p$, it minimizes the error

$$\sum_{i,j} w_{i,j}(R_{i,j,6} - \hat{R}_{i,j,6})^2, \quad (i,j) \in \Omega_p \quad (3.1)$$

where $\Omega_p$ consists of all the values originating from non-broken detectors, $\hat{R}_{i,j,6}$ is the estimated value at band 6 at a pixel, and $R_{i,j,6}$ is the true value at the same pixel. This equation is identical to the error minimized by QIR in equation 3.4 except that it uses the weight $w_{i,j}$, which are calculated by a Huber M-estimator. Also, unlike QIR, RMEMR does not use sliding windows within a tile. However, it uses the bands 1–5 and band 7 for estimation as QIR does. This algorithm does some additional preprocessing compared to QIR. It fills in non-existing pixels similar to QIR, but it takes a different approach to destriping [32] and also corrects for odd-even pixels, called subframe stripes [28]. The RMEMR algorithm produces better restoration than QIR, and it also has faster running time than QIR [27].

Shen et al. [39] proposed a method (also approximately two years after publication of QIR) that restores band 6 based on adaptive spectrum-weighted sparse Bayesian dictionary learning with bands 1–5 and band 7. Compared to the other methods, the computational cost and complexity of this method are very high [27].

### 3.1.2 Algorithm

The fundamental problem with any approach that uses band 7 alone to determine band 6 is that these bands behave differently depending on surface and cloud composition; thus, while
there are special cases—such as generally uniform parts of the image—where a functional relationship between band 7 and band 6 may be approximately valid, it does not hold in general. Moreover, if it did, there would be little need for inclusion of band 6 in the MODIS imager. A single pixel value at the corresponding point in band 7 alone cannot provide enough information to restore band 6 [14].

Through the use of multiple bands and a local window as input (not just to train coefficients), much more information is available with which to perform the restoration [14]. We describe a quantitative image restoration (QIR) algorithm that is able to accurately estimate and restore band 6 using bands 1-5 and band 7 as input. In order to show that the new variable from band 5 provides additional information over that provided by band 7, we estimate the band 6 value using a cubic polynomial as in [42]. The difference between this estimated band 6 value and the actual band 6 value, which we call radiance error, is the part of the band 6 value not explained by band 7. If band 5 were not informative about this error, then the joint probability distribution of band 5 with the radiance error from band-7-estimated band 6 would be independent. This is not the case because as shown in Figure 3.1, this distribution does not match to the product of the single variable distributions. Thus, band 5 contains information about band 6 not captured by band 7. Similarly, as we add other spatial and spectral variables, we can improve the estimation of band 6.

We carefully balance the gain in information with potential overfitting by limiting the model to a multi-linear estimator and adjusting the window size according to results obtained on independent test data.

The outline of the QIR algorithm is presented in the diagram shown in Figure 3.2. QIR starts processing the data by attempting to fix out-of-valid-range values because pixels with values outside of the valid range will wreak havoc with regression since good band values provide input for the QIR algorithm. Then, similar to [37], the radiances are destriped using the histogram matching algorithm [19]. The restoration function is a composite (piecewise)
Figure 3.1: (a) Joint PDF of band 5 radiance and the residual of band 6 radiance with the portion predicted by band 7 subtracted; (b) Product of band 5 probability and residual of band 6 radiance with the portion predicted by band 7 subtracted.

Figure 3.2: Block diagram showing the overall structure of the QIR algorithm.
function built from smaller restoration functions defined on large overlapping portions of the image, which we refer to as tiles. The tiles are defined by first partitioning the image into a grid of nonoverlapping tiles, and for MODIS/Aqua, we used $200 \times 200$ pixel tiles. These grids of tiles are shifted horizontally by a half tile (100 pixels), vertically by a half tile, and diagonally by a half tile. Since a pixel may belong to several tiles, the restored value in the bad band is the average of the independent restoration functions for each tile to which it belongs.

For each pixel from a scanline with a broken detector in band $K$, the restoration function $F$ must provide a value $I_{i_0,j_0,K} = z(q)$, with $q = (i_0, j_0)$, where we think of $z(q)$ as the dependent variable. For each pixel $q$, the independent variables are taken from the values in the image $I$ for an $m \times n$ spatial window, $w_q$ centered at $q$, with $m$ and $n$ odd, as shown in Figure 3.3. The $m \cdot n \cdot (K - 1)$ independent variables of $w_q$ are

$$x(q) = \{x_0(q), \ldots, x_{m\cdot n\cdot(K-1)}(q)\}$$

$$= \{I_{i,j,k}\}_{|i-i_0| \leq \frac{m-1}{2}, |j-j_0| \leq \frac{n-1}{2}, 1 \leq k \leq K-1}.$$  

Figure 3.3: Diagram showing the process of determining the restoration function for a tile.
To determine $F$, we separately and independently determine an $F_T$ for each tile $T$. We do this by first collecting a training set made up of the set of independent and dependent values $(x(p), z(p))_{p \in V_T}$, with $V_T$ being the set of all pixels $p$ corresponding to working detectors in the bad band, as shown at the top right of Figure 3.3. This is indicated in Figure 3.2 as the box “True Band 6 Value” which is $z(p)$ and as the box “Windows in Bands” which is the variable $x(p)$ for the window $w_p$. Every per-tile restoration function $F_T(x(p))$ has a training error defined as

$$\text{Error}(F_T) = \sum_{p \in V_T} |F_T(x(p)) - z(p)|^2.$$  

(3.4)

To determine $F_T$, we would like to find a function which minimizes this error without overfitting the training set $V_T$. We partially address the overfitting issue by restricting $F_T$ to one of the simplest possible families of functions, i.e., multi-linear functions of the form

$$F_{T,\alpha}(x(p)) = \sum_t \alpha_t x_t(p)$$

(3.5)

where parameters $\alpha_t = (\alpha_1, \ldots, \alpha_{m \cdot n \cdot (K-1)})$ minimize the training error $\text{Error}(F_T)$. The optimal solution for $\alpha_t$ is computed using a least squares solver. Once parameter $\alpha$ is found, it can be applied to windows centered at broken detector pixels to obtain the per-tile reconstruction for those band 6 pixels. Even without resorting to more general polynomial regression, multi-linear regression is good enough because the choices of window size and tile size provide the QIR algorithm the flexibility to trade off between improved fitting and generalizability, resulting in better estimation.
3.1.3 Evaluation

Although band 6 MODIS/Aqua has extensive damage, the corresponding band 6 MODIS/Terra is functioning normally. This makes it possible to evaluate QIR by simulating the damage to band 6 MODIS/Aqua on band 6 MODIS/Terra. The evaluation method compares restored images obtained from applying each of the algorithms on the simulated damaged bands to the original undamaged band 6 MODIS/Terra. This same method is used in all the articles discussed so far.

We chose ten granules with varied terrain containing snow, clouds, mountains, and vegetation in order to challenge all the algorithms. These representative ten granules were also chosen from many others because they could be restored with the prior work implementations without failure. We were unable to run the implementation that Rakwatin et al.[37] provided on many granules because it was not robust to the bad data that sometimes appear in the granules. This is only a problem with their implementation, not their algorithm. Since we wanted to minimize any modification to their code, we restricted the evaluation to granules on which their implementation ran smoothly.

The result of our evaluation, as seen in Figure 3.4a, was that all the algorithms do reasonably well. Among the algorithms that restores band 6 using a cubic polynomial function of the values in band 7, the local cubic regression in [37] does consistently and significantly better the global cubic regression in Wang et al. [37, 42]. The QIR algorithm, whether run on just the 500-m bands or with the 250-m bands included, performs better than the other algorithms. When the 250-m bands are included, there is a small improvement in performance. It is interesting to note that, while our restoration is more complex in the sense that we use more bands, it is also less complex in that we use a lower order model (linear versus cubic).[14, 27].
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Figure 3.4: (a) RMSE, in reflectances, of previous algorithms over ten test granules. (b) (Probability) Distribution of the QIR RMSEs in reflectances for the 82 granules using all the 500- and 250-m bands (the dashed line) and just the 500-m bands (the solid line). These are the errors only for the restored pixels using band 6 MODIS/Terra in which the damage was simulated.

Since the cross algorithm evaluation was done on only ten granules, we wanted to verify that the resulting range of errors was typical for QIR. To do this, we ran the QIR algorithm on 113 MODIS/Terra granules using just the 500-m bands. We then ran the QIR algorithm on 82 of those granules using all 500- and 250-m bands for restoration; the sample size was reduced because some of the 250-m bands failed the out-of-valid-range preprocessing step. Figure 3.4b shows the normalized histogram of root-mean-square errors (RMSEs) for QIR using all the bands and just the 500-m bands. The mean of the 82-granule sample (QIR using six bands) is around 0.004 RMSE, which is consistent with that of the 10-granule sample shown in Figure 3.4a. The mean RMSE of the 113-granule sample (QIR using only 500-m bands) is slightly higher, which is also consistent with that of the 10-granule sample. The overall improvement when compared to the restoration based on only the 500-m bands is consistent between the smaller and larger samples. However, we can see that there is a considerable variation in QIRs accuracy depending on the granule. Reflectances were used
Figure 3.5: (a) The scatter plots of band 6 radiances to its simulated band 6 radiances within a patch. (b) Probability distribution of errors (differences in radiance) for all ten considered granules.

in our evaluation since they were used in prior work[37, 42]. Note however, the calculation of reflectance uses the solar angle and intensity and involves further processing, potentially amplifying or even masking errors in the restoration. Thus, the remainder of our evaluation uses units of radiance.

When visually comparing a band 6 MODIS/Terra radiance image that was restored using the QIR algorithm with that of the original (undamaged) band 6 radiance image, it is virtually impossible to discern a difference. Using simulated damaged band 6, the scatter plot in Figure 3.5a shows how the restored band 6 values compare to the true band 6 values for a 200-by-200 patch. The distribution of errors for all of the ten considered granules, shown in Figure 3.5b, appears to be far from normal, with many of the errors being quite small.

In the case of MODIS/Aqua, we do not have ground truth available. However, we can visually compare QIR output to the results that are currently produced with interpolation. We see large differences between the interpolated image (left) and QIR restored image (right) in Figure 3.6. The interpolated images clearly show large distortions because columnwise
Figure 3.6: Crop of MODIS/Aqua band 6 image with basic interpolation (3.6a,3.6c) and restored using QIR (3.6b,3.6d).
Figure 3.7: Restoration error was computed over 51 granules (Wednesdays of each week in year 2016) near North East U.S. (a) Normalized RMSE per class. (b) Distribution of normalized RMSE per class.

interpolation introduces new edges which completely corrupt spatial derivatives of the image. We can see these distortions in the river in Figure 3.6a and the small clouds in Figure 3.6c. In contrast, the result of QIR lacks these strong artifacts, and even exposes details like cloud shadows on the ground.

The QIR algorithm performs slightly differently depending on the land type, geographical features, or atmospheric condition in the image. In Figure 3.7, we see the RMSE is fairly consistent between land/water and cloudy/clear sky. To obtain a representative sample of varying land features and atmospheric conditions, we used 51 granules uniformly distributed over one year near North East U.S. QIR performs best over smooth areas such as on clear-sky and water. When we encounter regions of high spatial gradient in the surface radiance, such as over cloud and land (which may have uneven snow accumulation) the performance is diminished.

The resulting images from our algorithm are high-quality restorations of the damaged bands, both qualitatively and quantitatively. Robustness of QIR has been accepted by
the wider remote sensing community. An implementation of it is currently being used in operation at NASA to provide more accurate MODIS/Aqua band 6 imagery to scientists.

3.2 Estimating a 13.3 $\mu$m VIIRS Band

Data collected from instruments aboard orbiting satellites are used by meteorologists and other scientists to create accurate estimates of physical parameters with important applications, such as cloud-top pressure (CTP) [29]. However, since the design of the instrument require technical and economical trade-offs, sometimes the data from a specific spectral band or wavelength is not directly available. This is the case for VIIRS, which does not have a band at 13.3 $\mu$m, which degrades its ability to determine semitransparent cloud properties (including CTPs/heights) compared to other sensors which include that band. One way to mitigate this deficiency is to combine information from available data sets and use machine learning techniques to estimate the values that are not directly observed [11].

Historically, the sensor used to make cloud related products has evolved or changed as satellite missions have been completed. Maintaining the consistency of long-term description of cloud trends in the face of sensor changes is a challenge. Cloud records have been created using data from Advanced Very High Resolution Radiometer (AVHRR) and the High Resolution Infrared Radiation Sounder (HIRS), as well as from the Moderate Resolution Image Spectroradiometer (MODIS) and the Atmospheric Infrared Sounder (AIRS). VIIRS is the current operational imager for the NOAA environmental polar satellite, and the Fourier transform spectrometer, the Cross-track Infrared Sounder (CrIS) is the operational sounder [11].

VIIRS and MODIS share some of the same bands. In particular, VIIRS bands M13, M14, M15, and M16 share similar characteristics to MODIS bands 23, 29, 31, and 32 (4, 8.5, 11, and 12 $\mu$m). However, unlike VIIRS, MODIS include a band centered at 13.3 $\mu$m, namely
band 33. Also, just as the Aqua satellite carries MODIS and the infrared sounder AIRS, the Suomi NPP satellite carries both VIIRS and CrIS. Both of these sounders cover the target spectral range around $13.3\mu m$ by using multitude of narrow bands, and at a much lower spatial resolution. For both pairs (MODIS/AIRS and VIIRS/Crs), the two instruments on the same satellite share largely overlapping observation areas, but in each case, the high spectral resolution sounder has less cross-track coverage than the high spatial resolution imager (see Figure 3.8). Therefore, if we develop a $13.3\mu m$ estimation algorithm that makes use of the bands shared by MODIS/AIRS and VIIRS/CrIS, we can evaluate the algorithm based on the ground truth provided by directly observed $13.3\mu m$ band on MODIS [11].

Estimation of VIIRS $13.3\mu m$ band also falls under the framework of virtual sensing. We present a technique to statistically construct a VIIRS channel at $13.3\mu m$ using measurements from VIIRS and CrIS measurements [11]. The CrIS sensor makes 1305 high spectral resolution measurements at $\sim15$-km resolution. These measurements are convolved with a spectral response function for the $13.3\mu m$ band (see Figure 3.9) at the lower 15-km CrIS.
Figure 3.9: The “+” markers indicate the spectral response values at 109 central wavelengths where AIRS measurements are available [11]. For our work, we have used the spectral response function for MODIS band 33 [11].

resolution. The resulting values are then used along with other infrared spectral bands on VIIRS at 750-m resolution to statistically estimate a virtual 13.3 µm channel at 750-m resolution. This virtual 13.3 µm channel is then used in a CTP algorithm, together with the observed VIIRS channels. The quality of the synthetic band is evaluated based on the accuracy of this derived product [11]. The goal of this approach is unlike the works presented in Section 3.3, where features from different sources are used to predict a band which is mainly used to produce a visualization.

The algorithm does not rely on any attributes specific to the 13.3 µm band. It is assumed that there exists an unknown function $F$ from bands available on VIIRS to the target 13.3 µm band, at least locally. It is also assumed that there exists a measure of scale invariance in the relationship between available source bands and the desired band. The validity of these assumptions are shown by testing them against MODIS and AIRS granules as a proxy for VIIRS and CrIS.
3.2.1 Algorithm

The steps in the algorithm described below are shown in Figure 3.10. First, the target 13.3 μm band is built at a lower resolution using the known 13.3 μm spectral response function and the CrIS data. We call this $\tilde{R}_\lambda^L$. Then, the high resolution VIIRS bands are spatially downsampled to the same low resolution as CrIS using geolocation information from both instruments. We call this $\tilde{R}_\nu^L$. We build a function $F$, where $\tilde{R}_\lambda^L = F(\tilde{R}_\nu^L)$. To estimate the 13.3 μm band at the higher 750-m resolution, we apply this function to the higher-resolution VIIRS measurements: $\tilde{R}_\lambda^H = F(\tilde{R}_\nu^H)$.

The estimating function $F$ was empirically determined to be essentially a smooth function. In order for $F$ to provide a meaningful approximation, the local variance of the 13.3 μm values should be small in a neighborhood of a fixed value for the input band. To demonstrate that this property indeed holds, we use MODIS data since it measures 13.3 μm as well as the input bands. Visualizing the relationship as a scatter plot would require four inputs and one output, or a total of five dimensions. To create a three-dimensional visualization (shown in Figure 3.11), we have taken the projections of the input variables into the first two principal
Figure 3.11: Scatter plot of the target 13.3 µm band radiance values (from MODIS) (z-axis) as a function of the four input bands radiances projected into two PCA components (x-y plane) for visualization. The fact that the points occur on or near the surface is evidence that the target band can be well estimated as a function of the input bands [11].

In practice, the estimation performs best when the estimating function $F$ is a piecewise approximation which varies with geographic location. Thus, $F$ was extended to take the latitude and longitude as input arguments in addition to requiring the source radiance values. To estimate the target radiance at a given pixel, the vector of radiance values for the source bands at high resolution and its corresponding geographic coordinates are used to query the component analysis (PCA) components as the x-y plane, and corresponding value in the 13.3 µm band as the z-axis. It is clear from the figure that, indeed, the relationship of the input bands to the target band is essentially a function. It should also be noted that for the estimation algorithm to work, the function $F$ must be invariant across different spatial resolutions. The consistency of least-square coefficients describing this relationship at various spatial resolutions, which can be seen in Figure 3.12, illustrates that this is the case.
Figure 3.12: Least-square coefficients describing the relationship between four MODIS bands (known on VIIRS) to the 13.3 µm band at various spatial resolutions [11].
database. The query is efficiently executed using the k-d tree data search algorithm to find k-nearest neighbors. The scale factor combining radiance and coordinates into distance, as well as \( k = 5 \), was determined empirically. For each input pixel, the query finds the five pixels among the low-resolution training data set, which are closest to the input values in the six-dimensional space representing the four input bands and two additional geographic dimensions. The corresponding 13.3\( \mu \text{m} \) values for these neighbors are then averaged to create an estimated value for each pixel at the higher resolution in the target 13.3\( \mu \text{m} \) band.

### 3.2.2 Evaluation

To evaluate our algorithm, we require truth values \( R^H_\lambda \) since the error of our estimates is given by the mean square errors \( |R^H_\lambda - \tilde{R}^H_\lambda|^2 \). Since the 13.3\( \mu \text{m} \) values are unavailable for VIIRS, we use MODIS/AIRS data as a proxy for VIIRS/CrIS data. Our evaluation is done on seven instances of this proxy, which demonstrates consistent results across a variety of granules, with the statistical estimation of a 13.3\( \mu \text{m} \) band at MODIS resolution providing a very close estimate of the actual MODIS 13.3\( \mu \text{m} \) band.

Figure 3.13 shows the normalized RMSE (NRMSE) computed between the estimated and actual 13.3\( \mu \text{m} \) data for each of the seven test cases and Figure 3.14 shows the relative error distributions among all seven test instances. These results show that the performance of the algorithm is consistent for both when all pixels are included and when considering only pixels where MODIS and AIRS overlap.

In addition to testing the 13.3\( \mu \text{m} \) values produced by our estimation against the known MODIS 13.3\( \mu \text{m} \) band, we tested it as input values to an algorithm which estimates CTP using data from 11-, 12-, and 13.3\( \mu \text{m} \) bands. While it’s possible to compute CTP using the VIIRS algorithm which doesn’t require 13.3\( \mu \text{m} \) values, the state of the art algorithm we used was developed for the GOES-R ABI instrument and it requires 13.3\( \mu \text{m} \) values. Figure 3.15 shows one example of CTP values created with actual and synthesized 13.3\( \mu \text{m} \) data, as well
Figure 3.13: Normalized RMSE (NRMSE) in radiance for the estimated 13.3μm channel when compared to the actual MODIS 13.3μm channel, for seven test cases [11].

Figure 3.14: Histogram of errors among all pixels for MODIS/AIRS 13.3μm estimation [11].
Figure 3.15: Cloud-top pressure (CTP) product based on MODIS Aqua granule on January 20, 2012, 5:00 UTC (MYD021KM): (a) original 13.3µm band, (b) estimated 13.3µm band, and (c) difference [11].

as their difference. These tests showed that similarly synthesized data from VIIRS and CrIS would allow VIIRS/CrIS to match GOES-R in terms of CTP determination, to within the GOES-R specifications.

A quantitative evaluation of 13.3µm estimation directly on VIIRS/CrIS measurements is not possible due to the lack of VIIRS 13.3µm ground truth data. However, if MODIS and VIIRS data are available covering the same area at around the same time of day, as in Figure 3.16, a qualitative evaluation between MODIS and VIIRS is possible. We can evaluate the difference between CTP values created from VIIRS using the reconstructed 13.3µm values and those created from MODIS with the ABI algorithm using true 13.3µm values (the state of the art). Both can then be compared to the CTP values made from those data sets using the VIIRS algorithm, which requires no 13.3µm values. The CTPs for the four cases show in Figure 3.17 appear very similar, although the slight discrepancies may provide valuable information to meteorological experts.
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3.3 Estimating True Color Imagery for GOES-R

The GOES before the currently operational GOES-R provided panchromatic visible image every 15 (or 30) minutes. The ABI on GOES-R improves this to at least 5 minutes (over the Continuous United States) and provides two narrow visible bands (red, blue), but it is not sufficient to directly produce color (RGB) images. As a result, GOES-R cannot directly produce color images despite the widespread demand for such images for use as decision aids by meteorologists and for visualization by the public [17].

3.3.1 Background

The issue of generating a synthetic green band has been investigated by both Cooperative Institute for Meteorological Satellite Studies (CIMSS)\(^1\) and Cooperative Institute for Research

\(^1\)Space Science and Engineering Center / University of Wisconsin-Madison
Figure 3.17: CTPs over Korean peninsula on August 28, 2012. (a-b) MODIS measurements at 04:30 UTC; (c-d) VIIRS/CrIS measurements at 04:40 UTC. CTPs derived using (a) MODIS data and VIIRS algorithm; (b) MODIS data and ABI algorithm, the state of the art; (c) VIIRS data and VIIRS algorithm; and (d) VIIRS data (with estimated 13.3 µm band from CrIS) and ABI algorithm.
in the Atmosphere (CIRA)\textsuperscript{2} using a look-up table (LUT) method [21, 30]. The starting point is a large collection of data gathered from remote sensing data and generated from models, which we refer to as “training” data because the LUT is trained using this data, before it is used. Since GOES-R ABI data was not available at the time these algorithms were developed, this training data typically consisted of simulated ABI constructed from similar MODIS bands as proxy. MODIS also contains a green band, which makes it possible to build a LUT to determine the green values for GOES-R.

Two algorithms presented in [21] and [30] differ at what point Rayleigh-correction is done. It is either done on the reflectances before populating/consulting the LUT ([30] shown in Figure 3.18) or on the resulting RGB values after the LUT has been consulted ([21] shown in Figure 3.19). Both LUT use values from 470 nm (blue), 640 nm (red), and 860 nm (near

\textsuperscript{2}Research department within Colorado State University’s College of Engineering
infra-red (NIR)) bands as inputs and predicts 550 nm green band value. The reflectance value in each blue, red, and NIR are quantized into one of $N$ evenly spaced bins per band. The number stored in that entry is the average reflectance value $G$ restricted to those pixels in the training data whose blue, red, and NIR values fall into the range determined by the entry in the 3D data-tables. In [21], the number of quantization levels $N$ for the LUT is 200 and in [30] it is 250. The lookup table is applied to new data by finding the nearest blue, red and NIR reflectance values, and looking up the corresponding green value. As a further refinement in [30], the images can be first segmented by surface type. A separate LUT can then be built for pixels in that surface type. Since the surface type is assumed unknown, the selection of LUT is done through geo-location process. A typical result of applying these algorithms to generate a true color RGB image such as is shown in Figure 3.20. A comprehensive analysis on which of the LUT algorithm has better performance has not been completed. There are indications that the results depend on the image [17].
3.3.2 Algorithm

We propose some improvements over building a lookup table on three bands to predict green values. The improvements involve refinements in the following three areas [17]:

1. The approximation function for green will depend on five spectral parameters as opposed to the three that was employed in [21, 30].

2. The piecewise constant green approximation is replaced by a piecewise linear approximation over the Voronoi cells associated with the sampling points.

3. A variably spaced sampling points is employed, as opposed to the lattice-spaced sampling points used in [21, 30].

The first area is based on the idea that there may be different valued green pixels which have similar associated R, G, and NIR triplets, but can be disambiguated by the values in other bands. The MODIS bands 1 (Red), 2 (NIR), 3 (Blue), 6 and 7 corresponding to the ABI 470 nm, 640 nm, 865 nm, 1.64 µm, and 2.25 µm center wavelengths were used for the approximation function. In Figure 3.21, we see the mutual information of these bands with band 4 (Green) and it shows that there is significant amount of mutual information that support the inclusion of these bands. MODIS band 5 was not considered because it does not have a direct match to the ABI [17].

One challenge in using more channels is that the size of LUT increases exponentially with the number of channels, requiring more data to populate the LUT. The size of the LUT is $N^d$ where $N$ is the number of bins for quantization in each dimension and $d$ is the number of channels. Because a larger input space is used, a fully non-parametric lookup table becomes infeasible. Instead, we argue that a locally parametric method, that of piecewise multi-linear function, is able to maintain enough flexibility to handle nonlinear variations in the surface but still able to cope with relative data sparsity due to the large input space. While an
LUT is piecewise constant function, by moving to a piecewise multi-linear function we can reduce the number of pieces without reducing accuracy. By reducing the number of pieces we effectively reduce the number of parameters, using less memory, and requiring less data [17].

The third point makes it possible for the predictor function to change rapidly in part of the input space where there is more variation, while efficiently remaining simple in parts of the input space where multi-linear prediction works well. The variable spacing is based on nearest neighbor classifier, which results in regions defined by Voronoi cells (seen in Figure 3.22).

The general outline of the approach we propose is presented in the diagram shown in Figure 3.23a. The proposed approach falls into three components. The first component is obtaining and building ground truth training and testing data sets. The second is development of an effective parameterized predictor, along with an efficient method of estimating
the predictor parameters. Finally, the third component is the development of our testing
and evaluation of the predictor.

The first component, data preparation, starts with selection of the MODIS bands 1, 2,
3, 6, and 7, followed by two preprocessing steps for each band. We start processing the data
by attempting to fix out-of-valid range values in each of the considered MODIS bands. We
preprocess out-of-range values using an adaptive mean value filter, which replaces isolated
missing pixels with the mean value of the valid pixels in a window with an adaptive size.
The adaptive window size is the minimum size such that the majority of the pixels in the
window are within valid range. Note that the window is limited to a fixed maximum size.
The file is abandoned if more than half of the pixels in the input bands are bad.

The next step when working with the data is destriping the radiances. As observed in
Rakwatin et al.[37], destriping can significantly improve regression. In theory, an image of
properly calibrated radiances should not have stripes, nevertheless some striping artifacts
remain and can be removed using histogram specification as is commonly done [19]. We
apply destriping to all bands, but if a band’s detectors are well matched so that destriping
is not required then the algorithm essentially returns the unstriped values.
The second component, training, begins with six preprocessed MODIS bands listed above, which can be thought of as a collection of points in six dimensional space, one of which represents green value. The point of the training component algorithm is to formulate an accurate model of the functional relationship between the green band and the other five bands, which can then be used by the predictive algorithm. The process we used to create our predictive green value is presented in Figure 3.23b.

1. For each training granule, we randomly select $N$ points in the domain space $\mathbb{R}^5$, where $N$ is empirically determined. We use these random points to initialize the K-means clustering algorithm which we run on the input data to determine a set of clusters for a single granule.

2. The union of all the cluster centers for all granules is combined, and the aggregated list of centers is used to build Voronoi domains.

Figure 3.23: (a) Block diagram of the algorithm and (b) Block diagram of the training algorithm.
3. For each such Voronoi domain we find a least squares best linear approximation for the green value expressed as a multi-linear function of the remaining five parameters.

The prediction function, following this method, takes a tuple with values from bands 1, 2, 3, 6, and 7 as input. The first step is to use a nearest neighbor classifier to assign this pixel to a Voronoi domain by finding the closest cluster center. Since each center has an associated multi-linear function, this function is applied to the tuple of bands to predict band 4 (green). Again, for the ABI the corresponding bands would be used.

CIE-XYZ colorspace

We propose another approach to producing quantitative true color imagery from ABI which attempts to produce more perceptually accurate RGB image [18]. While the LUT method above does provide a good statistical regression of the 550 nm green channel, it does not take into account that human perception is not based on a narrow band red, green and blue channel responses. The human visual system does not respond to only narrow red, green and blue bands, but has three broadband color responses; these responses have been standardized and quantified through the CIE 1931 XYZ color space defined by CIE (International Commission on Illumination) [7]. The XYZ color space provides the functions $x$, $y$, and $z$ shown in Figure 3.24, which when applied to the measured spectral radiance curve, give parameters $X$, $Y$, and $Z$ called the tristimulus values:

$$X = \int_0^{\infty} I(\lambda)x(\lambda)d\lambda, \quad Y = \int_0^{\infty} I(\lambda)y(\lambda)d\lambda, \quad Z = \int_0^{\infty} I(\lambda)z(\lambda)d\lambda,$$

(3.6)

Here, the spectral radiance distribution $I(\lambda)$ is given in watts/meter$^2$ per unit wavelength $\Delta\lambda$. The tristimulus values were chosen based on experimental measurements with human subjects to establish an international standard (color) observer. If any normal observer is asked to distinguish two patches of color, having spectral radiance $I_1$ and $I_2$ respectively,
they will be impossible to distinguish if and only if \( X(I_1) = X(I_2) \), \( Y(I_1) = Y(I_2) \), and \( Z(I_1) = Z(I_2) \). There exists calibration tools which can convert XYZ to the RGB of a specific computer monitor, or the CMYK (Cyan, Magenta, Yellow and Black) of a specific printer. Thus, the determination of the XYZ color for an ABI granule, unlike the estimation of a narrow green band, makes it possible to able to produce an accurate color representation for any viewing device.

This approach is demonstrated using data from the hyper-spectral imager Hyperion, from which training and verification data sets are obtained. The training set consisting of many pixels where we have coincident values for \( X \), \( Y \), and \( Z \) as well as values for the 6 visible and near visible bands of ABI. These values are produced from a spectral radiance distribution at each pixel derived from the Hyperion data. We then apply a non-linear regression method which produces a predictor of the values of \( X \), \( Y \), and \( Z \) from the ABI data. We then can use this predictor to produce \( X \), \( Y \), and \( Z \), given new ABI data [18].
a separate multi-linear model per K-means cluster. The only difference here is that instead of predicting one parameter (green value), we’re predicting three parameters: $X$, $Y$, and $Z$.

### 3.3.3 Evaluation

The evaluation of the first algorithm presented is done using ABI bands simulated from MODIS data. In the second, CIE-XYZ colorspace based algorithm, we used Hyperion sample granules from the EO-1 obtained from the USGS website. To evaluate the algorithm we used one large continuous region of the Hyperion granule for training and a separate, non-overlapping region for testing. The error in prediction, measured as the root mean square errors (RMSE) in radiance between the true $v_p = [X_p, Y_p, Z_p]$, and the predicted $v'_p = [X'_p, Y'_p, Z'_p]$ at a pixel $p$, is given as $||v'_p - v_p||$. Note that the XYZ are broadband responses, thus that radiance levels, and consequently the errors, are much larger than radiance levels for a narrow band responses.

Both algorithms presented break the data into separate data clusters and fit a separate multi-linear model per cluster. Since a cluster is a subset of the data, the fitting (training) error will at worst be the same, and typically will decrease. The fitting error will continue to decrease with an increasing number of clusters. Potential over-fitting can be evaluated by testing the model on test data produced in the same way as for the training data, but not used for fitting. This error of the fit on this test approximates the generalization error, i.e., the error of the model on new data. What we expect is that as we increase the number of clusters $K$ the generalization error will, in general, drop for a while, and then as we begin over-fitting, the generalization error will not improve or even climb.

The RMSE for XYZ color estimation using the method of K-means clustering, followed by a model fit on each cluster is shown in Figure 3.25. Because K-means is a random seeded iterative algorithm, the clustering followed by fitting was run on training data many (100) times, and the best result on testing data was used. This should be seen as part of the
optimization. The RMSE shown in the figure was taken from the training set because too little data was available in the testing set for it to be considered statistically representative. The local increases and decreases in the RMSE have to do with the peculiarities of the data set and the interaction of the local models with the changes in the clustering. In general, as expected, there is a decrease in RMSE with increasing number of clusters. It can be seen, however, that after 10 clusters little or no improvement is seen. This suggests using more than 10 clusters would result in over-fitting.

Similarly, the number of clusters used in K-means for the first algorithm, based on ABI bands simulated from MODIS, is also determined empirically. To explore how the algorithm is impacted by changing the number of Voronoi domains, we first set the per-granule number of clusters to $N = 50$ training using 40 training granules, resulting in 2000 clusters total. When the clusters were aggregated, very small clusters were eliminated. Note $N$ is much larger in this case compared to the first algorithm where Hyperion data was used because we choose to use a bigger training data set, thus we have lower risk of overfitting to the data.
Figure 3.26: Relative error of green band using multi-linear piecewise approximation (ABI simulated using MODIS/Terra) with $N$ clusters (a,b,d) and using LUT method (c). The locations of errors that are above 0.15 threshold are shown in red in (a) and (b).
We have picked a test granule (not part of the training granules) shown in Figure 3.26 which illustrates smoke-over-vegetation case in the midwestern U.S., collected by MODIS/Terra on June 28\textsuperscript{th}, 2002 at 16:40 UTC. The portions where the relative error (the absolute error divided by original value) is over 15% are mapped in the Figure 3.26(a,b). The largest errors seem to be located on the boundaries, mostly likely because more Voronoi cells are needed on the boundaries in order to handle pixels of mixed type. If we increase the per-granule number of initial clusters to $N = 200$ the result improves dramatically. Further increases in the number of clusters used in training do not seem to result in improvements in the testing, but perhaps increasing the number of training granules could.

The results of piecewise multi-linear regression appears to compare quite favorably with results obtained by LUT. The relative error for LUT-based prediction is shown in Figure 3.26c, and the relative error from the piecewise multi-linear prediction (with $N = 200$) is shown in Figure 3.26d. The error in the upper left portion and over the lake in the middle improves dramatically. Figure 3.27 shows the RGB image produced using the original green band 4 and that produced using the green channel predicted from the piecewise multi-linear
method. Visually they look nearly identical and any minor differences are not noticeable without very close inspection.

To render a highly accurate color satellite image to a computer display or to a printer, device specific profiles must used to implement the transformation from XYZ to RGB. However, since we intended to equalize the images to emphasize the contrast between original and predicted, we used a generic profile. Figure 3.28 shows three original-predicted image pairs using this profile followed by histogram equalization of each band (independently) to maximize the visual differences. As can be seen in the pairs Figure 3.28(a,b) and Figure 3.28(c,d) the agreement for RGB is excellent although the irrelevant equalization process does introduce some unnatural colors (purple haze). The image pair in Figure 3.28(e,f) shows a failure case. While in most parts of the image the predicted image is quite close, the brown region in the middle right of the image in Figure 3.28(e) is yellow in the image in Figure 3.28(f). One problem is that because the K-means is performed independent of the multi-linear prediction, pixels requiring different predictors are sometimes grouped together [18].

The XYZ values allows us to get a better understanding of what colors are most problematic by moving the errors to the 2-dimensional chromaticity. This space normalizes by the luminance or more informally the “grey component.” This is done by projecting the XYZ into two variables $x$, and $y$ where

$$x = \frac{X}{X + Y + Z}, \quad y = \frac{Y}{X + Y + Z}. \quad (3.7)$$

The plot of color pixels into this color space is called the chromaticity diagram, as shown in Figure 3.29. The curve bounding the color region shows the limits of color perception. The bounding curve represents pure spectral curves where the center fades to a “white point” where the colors are desaturated. Overlaid on the chromaticity diagram are the $x$, and $y$ values computed from the actual XYZ values of our data. The dots are colored by the RMSE
Figure 3.28: Original and predicted XYZ images converted to RGB then color equalized to increase contrast. The pairs (a)-(b) and (c)-(d) show excellent agreement while the pair (e)-(f) was a challenging case.
Areas with high error

Figure 3.29: Size of per pixel XYZ-RMSE overlaid on a chromaticity diagram.

of the predicted XYZ values. As seen in the figure, the large errors are concentrated in the desaturated red/purple region with some deep green pixels also being challenging. Still, the majority of the color have small error.

3.4 Improving VIIRS Imagery using Resampling

More than a dozen Advanced Very High Resolution Radiometers (AVHRRs) onboard National Oceanic and Atmospheric Administration (NOAA) satellites have been in operational use since 1978. The Visible Infrared Imaging Radiometer Suite (VIIRS) is a new generation US imager, developed to succeed the AVHRR in NOAA operations. The first VIIRS sensor was launched on October 2011 onboard the Suomi National Polar-orbiting Partnership (S-NPP). Four more instruments are set to launch onboard the Joint Polar Satellite System (JPSS) satellites, J-1 to J-4 from 2017-2026.
CHAPTER 3. VIRTUAL SENSING

The NOAA VIIRS sensor builds upon the NASA Moderate Resolution Imaging Spectroradiometers (MODIS) flown onboard the two Earth Observation System (EOS): Terra and Aqua. Both VIIRS and MODIS carry a comprehensive set of spectral bands, and take measurements in a wide swath to provide (near) global daily coverage, with high spatial resolution and low radiometric noise. Although the design and performance of both sensors can support accurate monitoring of atmosphere, ocean, land and cryosphere from space, VIIRS improves on MODIS upon all performance metrics [22, 23].

Nevertheless, both VIIRS and MODIS are affected by two major imagery artifacts: striping and bow-tie distortions. Both have multi-detector push-broom design and double side rotating mirror, introduced to improve spatial resolution and reduce radiometric noise. The VIIRS imagery is further affected by two irreversible processing steps applied onboard—pixel deletion and aggregation, which are applied to reduce the data volume prior to its down-linking to the ground.

These artifacts should be corrected before VIIRS imagery can be used for visual analysis or downstream processing. Currently, the burden of correcting the artifacts specific to the instrument fall to the users of the satellite imagery. Most users and even satellite data producers may be unfamiliar with the details of the lower-level data processing, that require the knowledge of the instrument design and the specifics of the onboard processing. Thus, there is a growing need for intermediate user-friendly data products such as Level 1.5 [38], in which some of the instrument-specific data issues have been mitigated.

There are various destriping algorithms [5, 19, 32, 36] that have been proposed to correct the striping artifact, and we are satisfied with the destriping results from [5]. In this section, we explore the other three artifacts in VIIRS imagery: (1) onboard aggregation; (2) bow-tie distortions; and (3) onboard deletions in the bow-tie regions. We describe a simple and computationally fast methods for approximating the values deleted onboard, and for resampling VIIRS imagery, while preserving the originally-observed data and associated
geo-locations nearly intact. The original geophysical values will be slightly adjusted so that the corresponding VIIRS imagery is physically continuous. The longitudes in the overlapping portions of the scans are adjusted, and only at the sub-pixel level. Typically, the imagery continuity requirement is only met after remapping, in the Level 3 and higher processing level products, such as the VIIRS Level 3 Uncollated sea surface temperature (SST) Product at NOAA [26].

The proposed bow-tie correction algorithm [15] was adopted in the NOAA Advanced Clear-Sky Processor for Oceans (ACSPO), the NOAA SST retrieval system which uses Level 2 data as input. It is currently set to be in operation as part of ACSPO version 2.50, for both MODIS and VIIRS. We only describe the resampling algorithm for VIIRS. For MODIS, the algorithm is very similar and even, in fact, simpler, as there are no pixel aggregations or onboard deletions in MODIS.

ACSPO uses some uniformity filters (within an \( n \times n \) pixel spatial window) for clear-sky identification, and a more comprehensive pattern recognition algorithm (discussed in Chapter 4) perform other processing requiring spatial continuity (e.g., computation of the gradient field). A continuous, non-distorted imagery in a swath projection is a prerequisite to these algorithms. We will show how resampling brings improvements of the cloud mask in ACSPO. The proposed resampling should also improve other applications that use spatial information at the L2 processing, such as ocean color, cloud properties, etc.

### 3.4.1 VIIRS Scan Geometry

The VIIRS Rotating Telescope Assembly (RTA) sweeps in a cross-track direction a 112.56° Earth view sector corresponding to the view zenith angle (VZA) range of ±70° on the ground and a swath of ∼3040 km in the cross-scan direction. In the along-scan direction, the 16 detectors cover a strip of approximately 11.9 km at nadir and 25.9 km wide at the end of each scan. This increase is attributed to the scan geometry and Earth’s shape, resulting
Figure 3.30: Top-left: Example of bow-tie deletions when the Visible Infrared Imaging Radiometer Suite (VIIRS) sea surface temperature (SST) image is displayed in the original swath projection. Deleted pixels are rendered in black and the land is shown in brown. Top-right: Location of the 10-min Advanced Clear-Sky Processor for Oceans (ACSPO) granule (18 October 2015 UTC) is shown by blue rectangle and its portion, displayed in the top-left, is shown in magenta. Bottom: Schematic representation of the left half of a single scan, showing bow-tie distortions, on-board deletions and aggregation for a single-gain M-band.
in a panoramic “bow-tie” segment. A schematic of the VIIRS half-scan projection on the Earth surface from nadir to swath edge is shown in Figure 3.30.

The neighboring whiskbrooms do not overlap at nadir but start overlapping at scan angles greater than approximately 19°. The overlap increases with scan angle and reaches ~12 km at the swath edge. However, in a swath projection, the overlapping pixels from the neighboring scans appear in the order they were acquired onboard, rather than according to their position on the Earth’s surface. As a result, the L1 imagery appears distorted.

The constant angular resolution of the sensor field-of-view results in an increasing pixel “footprint” projected onto the Earth for the view directions away from the nadir. Therefore, the resolution of the image is degraded for pixels further away from nadir. The decision was made to employ an onboard aggregation algorithm, to reduce the variation of the pixel size across swath. At nadir, three ~0.24 km footprints are aggregated to form a single VIIRS “pixel” with a size of ~0.74 km. The aggregation changes from 3×1 to 2×1 at the scan angle ~31.589° and to 1×1 at 44.680° as shown in Figure 3.30. The discontinuities in the pixel size due to the change in the aggregation scheme can cause artifacts during re-projection or resampling and should be treated properly.

The consecutive whiskbrooms overlap resulting in “duplicate” data, progressively more so away from nadir. On VIIRS, unlike MODIS, the decision was made to delete onboard the radiances measured in the overlapping portions of the scan, in order to reduce the data volume to be transmitted to the ground. The data in black in the VIIRS imagery in Figure 3.30 show pixels deleted onboard the S-NPP. Simple estimates suggest that this onboard data deletion reduces the data volume by ~12.9%. When the VIIRS Raw Data Record (RDR; L0) and corresponding sensor data record (SDR; L1b) are created on the ground, the radiances in the deleted pixels are populated with fill values (whereas the corresponding geographical coordinates and angles are calculated and written to the RDR and SDR data files). These missing data on VIIRS complicate de-bowtizing and should be filled in.
The bow-tie effect can be effectively removed by re-projecting the swath image onto a map. Therefore, users of Level 3 and higher level products never have to worry about the bow-ties. However, re-projection is computationally expensive and there were no fast off-the-shelf algorithms easily available that preserve both the array dimensions and the corresponding geo-information. Our resampling algorithm aims to de-bowtize L1 and/or L2 imagery without expensive re-projection operations and preserve the original swath projection.

3.4.2 Algorithm

Our objective is a resampling that satisfies the following major requirements:

(I) Ensures spatial continuity of the imagery;

(II) Provides minimal deviation from the original swath geo sampling grid;

(III) Is computationally fast and appropriate for real time L2 processing.

Intuitively, what is minimally required is an unfolding procedure that reorganizes the footprints according to their geolocation, rather than in the order they were acquired by the instrument and reported in the RDR/SDR swath data files. Unfolding is a re-ordering according to the geometry of the instrument’s swath projection and the footprint locations of the scan on the Earth surface. This pattern is specific to the particular instrument and can be estimated using sorting procedures on a per-column basis for individual scan and then statistically determined based on the large set of scan-based re-ordering patterns. There are two types of VIIRS geolocation files—ellipsoid based (GMODO) and terrain corrected (GMTCO). Since the unfolding of the bow-tie distortions is performed in conjunction with the near elliptical Earth’s shape, we use the ellipsoid geolocation file.

Figure 3.31a demonstrates the effect of unfolding for three consecutive scans (only the left half-scan is shown). The detectors are shown with 16 distinct colors, ranging from yellow
Figure 3.31: Three consecutive VIIRS whiskbrooms for the left half of the scan (from the edge of the swath to the nadir): (a) in swath projection (along with sorting patterns); (b) in the mapped projection. The detectors are shown with distinct colors ranging from yellow (detector 1) to blue (detector 16); and (c) reordering scheme corresponding to the left half of the VIIRS swath.
to blue. The center of the swath (the nadir) has no overlap, so the original order remains the same, but away from nadir the rows become interleaved after re-ordering. The unfolding pattern corresponding to Figure 3.31a,b is illustrated in Figure 3.31c, for one scan $S_k$. Only the left half-scan is shown; to extend the unfolding procedure to the right side, the table should be reflected symmetrically with respect to the nadir. The rows in the Figure 3.31c correspond to VIIRS detectors and the columns define the column ranges with identical re-ordering pattern. Numbers in each cell represent the amount of shift for each of 16 rows in the scan $S_k$ during the reordering. Positive values correspond to an increase of the row index and negatives correspond to the decrease of the row index. Zeros represent no change (no re-ordering). Note that the blue colored cells correspond to a propagation of detectors from scan $S_{k-1}$ into $S_k$, and the yellow-to-orange colored cells correspond to propagation from scan $S_{k+1}$.

There are a total of 21 reordering zones determined by 20 break points, $N_i$, corresponding to column indexes where the reordering pattern changes. The break points are the positions where the grid lines of $S_k$ intersect with the grid lines of $S_{k-1}$ and $S_{k+1}$. The upper (detectors 1 through 8) and the lower (detectors 9 through 16) parts of the table can have different break points, as the middle scan $S_k$ can have different overlaps with the neighboring scans, caused by a slight variation in the sub-satellite track. Our analysis of VIIRS data suggest that such scan-to-scan variations of the sub-satellite track are small but sufficient to affect the reordering positions derived as one static set. The reordering pattern is thus general, but the break points $N_i$’s need per-scan adjustments. The break points are adjusting iteratively by moving them in the direction where the grid lines between the two scans intersect until the intersection point is found.

Re-ordering procedure described so far is computationally cheap, meets the requirements (II) and (III) and almost meets the requirement (I). The last component of the resampling procedure is the adjustment of the longitude values in the bow-tie regions, which satisfies
requirement (I) and fulfills all three requirements, (I)-(III). This last step is necessary due to the relative displacement of the consecutive scans, caused by Earth rotation. As the VIIRS instrument completes its $S_k$'th scan and gets ready for $S_{k+1}$'th one, the Earth has rotated by a certain amount, depending on the latitude and on the instrument scan rate. This causes the grid displacements between consecutive scans by the amount of this rotation.

The relative grid displacement with respect to the grid width is what really matters for the continuity assumption of requirement (I). The largest relative displacement is at the nadir for the scan that sweeps through the equator. For the VIIRS instrument, this displacement can exceed the pixel width, since the nominal VIIRS scan rate of 1.7864 s/scan and the speed of the Earth rotation at the equator is $2 \times \pi \times \frac{6380}{(24 \times 3600)}$ km/s, resulting in the shift of $\sim 0.828$ km between the scans, which is larger than the 0.75 km pixel width at the nadir.

In Figure 3.32, the latitude and longitude values are plotted for one column in the transition area from the 2:1 to the 1:1 sample aggregation scheme, zoomed into two scan’s overlap. The blue line in the latitude plot corresponds to the original scan order. The black dotted line (top plot) shows the latitude values after reordering, which makes the plot monotonic. Reordered longitudes, shown in a black solid line (bottom plot) have a zigzagging pattern, as expected due to the described relative scan displacement.

One possible alternative to preserve the values of the original geo-grid and to mitigate the zigzagging effect is to additionally reorder columns. However, this would require a change of the original 3200 column setting to allow for the shifts persistently present between consecutive scans. A more attractive approach was deemed to (slightly) adjust the longitudes, which also ensures the spatial continuity while preserving the swath width intact. Simple (and computationally fast) 1D per-column interpolation, preserving the longitudes that have not been reordered (cf. cells with “0” entries in 3.31c), results in the monotonic longitude val-
Figure 3.32: Latitude and longitude values for a column in the transition area from the 2:1 to the 1:1 sample aggregation scheme. The unfolding order for this region corresponds to the $N_5 + 1:N_6$ columns in Figure 3.31. Top: Blue line represents original latitude and black line corresponds to latitudes reordered according to Figure 3.31. Bottom: Black line corresponds to longitudes reordered according to Figure 3.31. Zigzagging effect caused by Earth rotation is present at the bow-tie regions after reordering. Magenta line, representing adjusted longitudes, is monotonic. The adjustments are performed only at the overlapping portions of the consecutive scans.
ues shown in magenta in Figure 3.32 (bottom plot). Note that adjustments to the longitudes are only done for the reordered pixels while the latitudes are reordered but not modified.

With all the reordering work done, the estimating of the missing values at the onboard deleted pixels is a straightforward task: in the resampled imagery, the index-based neighbors are now also geo-neighbors, which makes distance-based weighted averaging a simple and well-justifiable option. For each onboard deleted value, we use the four closest (±1 row/column) neighbors and compute the Gaussian-weighted average with standard deviation proportional to the corresponding vertical footprint size.

An example of resampled brightness temperature BT at 12 µm with estimated values in the deleted zones is shown in Figure 3.33c. For comparison, the original BT at 12 µm is given in Figure 3.33a. “Repeats” typical for bow-tie distortions, which were apparent in Figure 3.33a, are not present in the unfolded reordered image shown in Figure 3.33b. The reordered image in Figure 3.33b also reveals the variation of the break-points and a zigzagging pattern is noticeable along edges. Corrections to the longitude values undo the zigzagging artifacts caused by the shifts, as can be seen from resampled image in Figure 3.33c. The image shown in Figure 3.33c now meets all the requirements (I)–(III) above.
Figure 3.34: Number of clear sky observations for one day (18 October 2015) of global ACSPO SST data as a function of view zenith angle (VZA) for S-NPP VIIRS. (a) Original data are shown in light gray and resampled in dark gray. Day and night data are combined together. (b) Corresponding percent increase separated by night and day.

3.4.3 Evaluation

We evaluate the impact of the proposed resampling on the performance of the current ACSPO clear-sky mask (ACSM)[35]. In the resampled data, we expect ACSPO to reduce the number of clear-sky pixels falsely detected as cloud (“false alarms”), and increase the number of clear-sky ocean pixels, CN, and the corresponding clear-sky fraction, CF (defined as a ratio of clear-sky to the total number of ocean pixels). To verify this expectation, we generated global ACSPO products from S-NPP VIIRS (144 10-min granules) for one full day (18 October 2015). Two ACSPO runs were performed: with the original sensor data record (SDR) data and with the resampled SDRs.

As expected, the CN derived from the original SDRs was found to be smaller than from the resampled SDRs because 12.9% of VIIRS pixels which had been deleted onboard were filled in by resampling. The change in the CF is guided by two mutually offsetting mechanisms. First, the deleted pixels are filled in from the four neighbors, and there is a high probability that at least one of them is cloudy. As a result, the filled pixels are expected to have a “cloudy” bias, which should lead to a decrease in the CF. On the other hand, the improved spatial uniformity due to resampling is expected to result in the improved ACSM,
and larger CF. We found that improvements in the ACSM tends to outweigh the “cloudy” bias in the filled pixels. Figure 3.34 (left panels) shows the CF (day and night combined) as a function of view zenith angle (VZA). For both sensors, the CF is largest around nadir (\(\sim 22\%-24\%\)) and drops off to \(\sim 10\%-15\%\) at the swath edges. The resampled data always have a comparable or larger CF, in all bins. The relative differences between the two gray curves are shown on the right. The improvement is insignificant around nadir, and progressively increases towards swath edges, where it reaches from 6\% to 8\%. The increment is a little larger at night, likely due to the use of reflectances during the daytime, which may be more subject to artifacts in visible imagery and result in higher screening rate.
Chapter 4

Machine Learning Approach to
Clear-sky Classification

Discriminating clear-ocean from cloud in the thermal IR imagery is challenging, especially at night. Thresholds in automated cloud detection algorithms are often set conservatively leading to underestimation of domain over which variables such as Sea Surface Temperature (SST) is computed. Yet an expert user can visually distinguish the cloud patterns from such variables. In this chapter, we present the problem of detecting clear-sky for the VIIRS SST product, discuss the currently operational algorithm, and propose improvements which restores clear-sky pixels misclassified as cloud.

4.1 Background

The NOAA Advanced Clear Sky Processor for Oceans (ACSPO) [35], developed at the National Environmental Satellite, Data, and Information Service (NESDIS), generates clear-sky ocean products. One example of such product is the ACSPO sea surface temperatures (SSTs) product retrieved from the Visible Infrared Imaging Radiometer Suite (VIIRS) sensor on-
board S-NPP. This product contains the ACSPO clear-sky mask (ACSM) which identify the clear-sky pixels, which are the only pixels relevant to SST. The ACSM is created from comparisons of retrieved SST with a first guess (reference) SST, reflectance thresholds, and spatial uniformity tests [35]. The reference SST is obtained from the daily Canadian Meteorological Centre CMC product [6], interpolated from 0.2° CMC grids to VIIRS pixels.

The ACSM generally performs well on a global scale. However, it tries to be conservative when assigning to the clear-sky class in an attempt to avoid cloud leakages (cloud misclassified as clear-sky). This leads to over-screening some highly dynamic areas with strong currents, cold upwellings, and eddies, as well as some coastal zones. It is these areas that are of the most interest to SST users for various applications, including fishing, ship navigation, ocean dynamics analyses, marine biology studies, and recreation activities. Another large group of Level 2 SST users are producers of Level 4 SST analyses. Those also need more data in data sparse dynamic and coastal areas, to accurately reproduce SST gradients and fine structure of the SST fields.

Despite attempts to avoid cloud leakages, they still exist in ACSM, along with even more false alarms (clear sky misclassified as cloud). There is no easy fix to this conservative nature of the ACSM within its current conceptual framework, e.g. by a simple adjustment of its thresholds, without triggering massive cloud leakages.

We propose some pattern recognition approaches to further minimize false alarms in ACSM [16]. It’s based on the idea that visual inspection of the retrieved Sea Surface Temperature (SST) in typical false alarm regions suggests that such problematic areas are typically uniform, contiguous, with well-defined boundaries, and often located in the vicinity of ocean thermal fronts. Determination of ocean thermal fronts is a well-studied area, which has been extensively explored with SST imagery [8, 9, 24]. Note that customary practice is to analyze thermal fronts under clear sky conditions, after having the cloudy pixels removed. However, non-uniform scenes associated with ocean fronts and coastal zones, are typically
the most challenging for the current clear sky masks including the ACSM, often leading to misclassification of cold water spots adjacent to thermal fronts as cloud, and thus limiting the ability of thermal front detection in clear-sky SST imagery.

The proposed algorithm attempts to mimic some intuitive visual perception of SST imagery by a human eye and help distinguish typical uniform and contiguous ocean patterns from ragged structures typical of clouds. Even when the ocean is dynamic, it exhibits slow-meandering and swirl-like contiguous patterns. Difference between ocean and cloud patterns is more pronounced in the SST gradient magnitude domain. Viewed as a terrain, the dynamic areas of the ocean appear as sharp mountain ridges (corresponding to ocean thermal fronts) towering over flat valleys (corresponding to slowly changing ocean temperatures) (see Figure 4.2) [20]. In the proposed SST Pattern Test (SPT) algorithm, we first identify such SST gradient ridges and adjacent contiguous areas with similar SST values, and then make ocean versus cloud decision based on the statistics of the whole region, rather than on a per pixel basis.

The current implementation of the SPT algorithm does not use any information other than patterns in the VIIRS retrieved SST field. In particular, albedo channels in the daytime data are very informative, but they are reserved for an independent verification of the algorithm. This is intentional and aimed at facilitating the desired consistency and continuity at day-night transition.

4.2 Algorithm

Here we describe the proposed algorithm to restore clear sky areas into ACSM. The steps of the algorithm are demonstrated using a representative example of ACSPO misclassification of two types: “false alarms” (i.e., clear sky regions that have been mistakenly identified as
cloud by the ACSM), and cloud leakages (i.e., clouds missed by the ACSM). This study focuses on false alarms and does not discuss cloud leakages.

The proposed SPT algorithm uses local spatial characteristics of the SST field, and requires that the underlying 2D SST surface is continuously differentiable. This requirement is not satisfied for the unprocessed VIIRS imagery in the original swath projection [23]. We assume the VIIRS granule is already preprocessed using a destriping and resampling procedure such that the input is a continuous, non-distorted imagery in a swath projection. Without this preprocessing, the performance of the SPT degrades towards bow-tie areas, and the zones with deleted pixels cannot be processed. For destriping, the method described in [5] was used and the resampling procedure we used is described in Section 3.4.

A case study from the VIIRS granule acquired on 16 February 2013 from 22:00–22:10 UTC was selected to demonstrate the proposed approach. Retrieved SST values in all pixels of the selected scene are shown in Figure 4.1a, and with the ACSM overlaid in Figure 4.1b. There are three false alarms in this scene (circled in red). Two are found in the coastal zones, one in the Kagoshima Bay and the other around the Tanegashima Island. A third false alarm is found in a dynamic region to the south of the Yakushima Island, where different masses of water mix in a swirly pattern. There are also two cloud leakages (circled in blue). Those are beyond the scope of this study and will be analyzed later.

Unlike a human operator, automated cloud detection algorithms such as the ACSM, may misclassify the dynamic ocean as cloud. Recall that the human eye does not perceive absolute pixel values, but instead relies on the local contrasts, ratios, and gradients in an image. To illustrate this, the magnitude of the gradient field is shown in Figure 4.2. The sharply-defined strands of SST gradient are likely thermal fronts on the ocean surface while the less regular mixed patterns of high and low gradients are associated with clouds. The proposed SST Pattern Test (SPT) explores the gradients and their lower order local statistics
to resolve this misclassification in the ACSM and comprises the following steps (illustrated in Figure 4.3):

**Step 1: Narrow down the search domain.** In order to save time on computations, we first narrow down the search domain by removing the most obvious cloudy regions while keeping in the analysis all potential “clear-sky” pixels. In our implementation, this was accomplished by excluding pixels satisfying any of the following conditions:

- \( \text{SST} < 270 \text{ K} \),
- Gradient magnitude of SST > 1 K,
- \( \Delta \text{SST} = \text{Retrieved SST} - \text{Reference SST} > -15 \text{ K} \),
- Local standard deviation of Laplacian of SST > 1/3 K.

Figure 4.3a confirms that Step 1 successfully eliminates many “ACSM cloudy” pixels. At the same time, it keeps the “warm clouds” (including false alarms circled in red and the cloud leakages circled in blue in Figure 4.1a) in the search space. The following Steps 2–5 are performed only within this restricted domain.
Step 2: Determine *SST gradient ridges* (*SGR*). Identification of the SGRs is a major component of the algorithm. The SGRs are found in the SST gradient magnitude domain where the difference between ocean and cloud patterns is very pronounced, using image processing tools such as morphological dilation, erosion, thinning, and connected components. The SGRs detected by our algorithm are shown in Figure 4.3b.

Step 3: Determine spatially connected regions with retrieved SST smaller than the reference SST. This step is accomplished using an image processing segmentation procedure applied to $\Delta$SST = Retrieved SST − Reference SST. We use the watershed algorithm [3, 10, 41]. The purpose is to find contiguous regions with $\Delta$SST below specified threshold. It is those clear areas that are most often misclassified by the ACSM as cloud. There are different implementations of the watershed approach, including watershed by flooding, topographic distance, inter-pixel watershed, and optimal spanning forest algorithms. The one used in this study is the watershed by flooding. Its principle can be illustrated by viewing the image of $\Delta$SST as a topographic relief, where the gray level of a pixel is interpreted as its altitude. A drop of water falling on a topographic relief flows along a path to finally reach a local
Figure 4.3: Steps of the SST Pattern Test (SPT); (a) Step 1: Search over white pixels only; (b) Step 2: SST gradient ridge (SGR) test; (c) Step 3: Spatially-connected segments; (d) Step 4a: Segments with overlaid SGRs; (e) Step 4b: Clouds adjacent to SGRs; (f) Step 5: Rejecting corner cases.
Figure 4.4: (a) $\Delta$SST = retrieved SST − reference SST; (b) $\Delta$SST as a topographic relief (rotated for improved visual perception). Areas with $\Delta$SST < −1 K (corresponding to starting flooding level) are rendered in gray.

minimum. Intuitively, the watershed corresponds to the limits of the adjacent catchment basins. Figure 4.4a and 4.4b maps $\Delta$SST as a false color image and as a topographic relief, respectively. The “water” level in the watershed interpretation was set to $\delta_0 = -1 K$ in Figure 4.4b.

In our application, the over-segmentation is acceptable and actually preferred over the under-segmentation scenario, when a mix of clear sky and cloudy pixels appears in the same segment. Since the decision is made on a per-cluster basis, we require segments to be large enough to be considered as a potential ocean pattern. We use 100 pixels as a lower bound for the segment size (approximately equivalent to a 10 by 10 km region). Segments identified by segmentation procedure, are shown in Figure 4.3c where the distinct contiguous segments are rendered in different colors.

**Step 4:** *Ridge Adjacency Test.* Visual analysis of typical ACSM misclassifications suggests that most of such false alarms take place in the proximity of ocean thermal fronts and often correspond to retrieved SST being colder than the reference SST. Therefore, the segments with negative $\Delta$SST adjacent to SGRs are considered as potential risk regions for the
ACSM misclassification. The purpose of this step is to check which segments are adjacent to SGRs and labeled as cloudy by ACSM. Figure 4.3b–d as compared to Figure 4.1b shows that the spots misclassified by the ACSM as cloud, are adjacent to fairly long portions of the ridges found in Step 2. There are also some clouds adjacent to SGRs. However, four such segments circled in Figure 4.3e are all adjacent to very short ridges. As a result, the SPT may add new cloud leakages to those already present in the ACSM. To prevent these new cloud leakages, one can increase the minimum number of pixels in the SST Local Ridge Test. In the current implementation, it is set to 10, which may not be sufficient to confidently decide whether the region adjacent to a short ridge is ocean or cloud. On the other hand, increased threshold may lead to losing some small cold spots of the ocean, especially in the coastal areas, where many ACSM false alarms are found. The following tests for corner cases were added to identify and reject potential SPT cloud leakages.

**Step 5: Corner Cases Test.** Many cold clouds are eliminated in Steps 2-4, but yet, some may go uncaptured (see Figure 4.3e). Also, there are cases when the segmentation procedure fails to separate cloudy and clear pixels, leaving them in one cluster. In such cases, the whole segment adjacent to the ridge would be accepted as “clear sky”. Another scenario is when a short SGR corresponds to a flaky cloud boundary, rather than to an ocean thermal front. Such cases prove difficult even for visual identification from the VIIRS SST field alone. However, identification can be improved when the texture (context) of the surrounding zones is considered, on a larger scale. In this step of the algorithm, we apply some tests to identify segments that should be eliminated. The tests include check for segment stability after morphological variation, the relative length of the adjacent SGR compared to the total segment border, and smoothness of the segment border [16].

Finally, the output of the SPT is only applied to those pixels excluded by the ACSM as cloudy, and the resulting pixels are restored back into the SST domain. Currently, no
change is made to the ACSM “clear sky” pixels, even though the SPT output may suggest that they are cloudy.

4.3 Evaluation

At the initial stage of the SPT algorithm development, 48 cropped images representative of typical ACSM misclassifications had been selected, visually inspected and hand-marked. This data set was used to train the proposed algorithms, and evaluate its performance—how accurately it restores clear-sky in the ACSM domain. The SPT was additionally tested using more than 600 10-min ACSPO VIIRS granules. This included two days of global data in July 10-11, 2014 (288 granules, since one full day contains 144 granules) and 3 weeks over the Gulf Stream area collected from June 11 to July 4, 2014 (77 granules). Other days and granules have also been analyzed, to ensure stability and reproducibility of the SPT performance in time. We discuss below the typical examples of SST imagery and some statistical summaries for two data sets—the global set, and the Gulf Stream (crop) sample which represents the most dynamic subset of the 77 regional granules over the area from 39° to 43° N, 59° to 67° W.

An example daytime ACSPO SST image over the Mediterranean Sea on July 11, 2014 is shown in Figure 4.5. Three upwellings are circles: one off the west coast of Italy in the Tyrrhenian Sea (between Rome and Naples), the other off the south coast of Sicily in the Strait of Sicily, and the third off the south-east coast of Calabria in the Ionian Sea. These areas where classified as cloud in ACSM because they are colder than the reference SST and the ambient waters by 3–4° C. In Figure 4.5b, we see that SPT classifying these areas as clear-sky and successfully restores them back into SST domain. The corresponding reflectances in the VIIRS band centered at 1.61 μm (shown in Figure 4.5c) and several SST images over the same area later in July (not shown) confirm that these sub-regions remained
Figure 4.5: Cold upwellings in the Mediterranean Sea on July 11, 2014 (day-time). Land is rendered in brown and cold upwellings are circled in red. (a) SST without any cloud mask; Pixels with out-of-scale cold SST values is in black. (b) SST with cloud mask overlaid; Pixels restored by the SPT back in SST domain is shown in gray; Areas where ACSM and SPT agree on it being cloud is in Magenta. (c) VIIRS reflectance in band M10 centered at 1.61 $\mu$m.
Figure 4.6: Same as in Figure 4.5 but for the Kuroshio Current in the vicinity of Honshu Island on April 27, 2014 (day-time).

Figure 4.7: Same as in Figure 4.5 but for Gulf of California on May 11, 2013 (night-time).

largely cloud free. The upwellings did show some minor evolution over time, but they largely remained in the same locations and retained comparable SST contrasts.

Figure 4.6 shows SST imagery of the Kuroshio Current on April 27, 2014, which is another daytime example. This very dynamic area is characterized by high SST contrasts. Circled are the three largest regions restored by the SPT: one in the coastal Honshu and the other two areas offshore. The visual inspection of the SST patterns and comparison with corresponding measurements in the solar reflectance bands (not shown) confirm that the restored areas are indeed SST features and not cloud.
A night example of restoration in the coastal zone of the Gulf of California is shown in Figure 4.7. Most of the coastal zone was misclassified by the ACSM. Unlike the previous two examples, there are no corresponding measurements in the solar reflectance bands at night. However, comparison between the SST image and the SPT cloud mask, and analyses of the corresponding daytime and nighttime observations for several consequent overpasses, suggest that the restored areas are indeed SST features and not cloud.

A daytime image of the Gulf Stream, is shown in Figure 4.8. This is an example of the ACSM misclassification in the glint area, where the performance of the clear sky mask usually degrades [25]. This is a challenging and complex case for SPT. However, as we can see in the cloud mask, numerous pixels are successfully restored by the SPT.

The geographical distribution of SPT restorals in the Gulf Stream area during the three weeks in June–July 2014 is summarized in Figure 4.9. Regionally, the SPT restores up to 15% of pixels misclassified by the ACSM as cloudy, into ACSPO clear-sky domain, as shown in Figure 4.9a and b. Additionally, as seen in Figure 4.9c and d, the ACSM tends to be progressively more conservative in the areas with the highest density of ocean fronts. This is exactly where the SPT is most needed and at the same time most useful.
Figure 4.9: Percentage of SPT restored pixels in the Gulf Stream area (77 ACSPO granules from June 11 to July 4, 2014): (a) percent of SPT additions to the ACSM clear-sky domain; (b) zoomed into the area of the Gulf Stream with the largest percent of ACSPO misclassifications and SPT restorals (note that the color-bar is quantized at 3%); (cd) same as (ab) but with SPT additions rendered in gray, and corresponding SGRs overlaid in black.
Figure 4.10: Percent of clear-sky ocean pixels (relative to total ocean pixels) during day and night, for the global data set and the Gulf Stream data set (restricted to 39° to 43° N, 59° to 67° W). The light-gray colored bars are for ACSM and the dark-gray colored bars are for SPT.
CHAPTER 4. CLEAR-SKY CLASSIFICATION

Figure 4.10 summarizes the ACSM and SPT performance statistics, over the globe and over the selected Gulf Stream crop. Globally, the ACSM identifies approximately 18.4% of total ocean pixels. The percent increase in SPT clear sky over the ACSM clear-sky domain, not noticeable from the figure, are approximately 0.25%. The high percentage of clear sky SST pixels, remarkable consistency between day and night, and a relatively small fraction of the ACSM false alarms (i.e. SPT additions) confirm that overall the ACSM is a globally well tuned and balanced mask.

Over the Gulf Stream (crop) domain, the fraction of ACSM clear-sky pixels is 37.43% during the daytime and 32.47% at night. The day and night clear-sky fractions are somewhat out of balance, likely suggesting a more conservative ACSM screening at night, when reflectance bands are missing over this complex area. Compared to the global numbers, the clear-sky domain is approximately two times larger. This is consistent with known cloud free bias during the local summer in this area [1]. The SPT adds to the ACSM domain 2.82% during the daytime, and 4.27% at night. These additions are from $10 \times$ (day) to $20 \times$ (night) larger than the global average numbers. Note that these are the average numbers over the Gulf Stream area, but locally, the added domain may be as large as 15% as seen in Figure 4.9. Despite SPT restoring more data at night—attempting to make up for the lack of day/night balance in the original ACSM—the ACSM + SPT fractions (38.5% during the daytime and 33.9% at night) remain out of balance. This may be due to the diurnal cycle of cloud coverage in the Gulf Stream area [31].

Based on these observations we can say SPT additions to the ACSM are highly non-uniform in space and in time. Globally, the SPT increases the ACSPO clear-sky domain from 0.2-0.3%. However, in dynamic areas of the ocean and coastal zones such as the Gulf Stream, SPT may add up to 15% (cf. Figure 4.9) to the ACSPO clear-sky SST domain. ACSM is tends to be more conservative in these highly dynamic areas but SST users for various applications have greater interest in these areas. SPT was able to restore more clear-
sky in these areas compared to other areas. If handling of false alarms in the ACSM by the current SPT proves successful, then the next step may be to increase the conservativeness of the ACSM (to minimize its cloud leakages) and process a larger “cloudy” ACSM domain with the SPT. The current plan is to include the pattern recognition improvements in SPT into a future version of ACSPO (version 2.60).
We’ve presented various machine learning approaches to retrieving physical variables from remotely sensed data. The evaluation on the QIR algorithm for MODIS band 6 estimation shows that our results outperform previous results which were based purely on band 7. We tested across granules with different surface types well separated over time and obtained consistent improvement. We also verified the error rates of our QIR algorithm on the granules that we used to compare with the prior work by using a comprehensive sample of granules. The algorithm is a general approach which uses neighboring pixels, both spectral and spatial, to quantitatively estimate missing values even when the damage to a target band is severe [14].

We demonstrated that we can accurately estimate 13.3\,\mu m broadband radiance data from the high spectral resolution infrared sounder data and high spatial resolution imager radiances measures, for both Aqua MODIS and AIRS data as well as VIIRS and CrIS. We found a good agreement between VIIRS and MODIS CTPs when VIIRS has the assistance from the estimated 13.3\,\mu m channel. These example results suggest that synergistic use of VIIRS and CrIS measurements can overcome the absence of a 13.3\,\mu m channel on VIIRS.
CHAPTER 5. CONCLUSION

The central assumption required by the algorithm is that the functional relationship between the input and output bands are scale invariant [11].

We have shown that despite the fact that the future ABI on GOES-R will not have a 550nm green band, it is possible to obtain a good estimate of true color imagery using all the visible and Near IR bands. Our approach improves upon previous LUT-based approaches which uses only a Red, Blue and single Near IR band. We achieved this by combining a multi-linear regression, with K-means clustering to achieve selectable level of flexibility. This provided a compromise between the robust multi-linear regression whose performance is limited due to its inability to adapt to different kinds of scenes, and a multi-dimensional lookup table which can provide arbitrary flexibility but whose data requirements explode with the number of input variables. We note that this same method could be used to approximate a virtual sensor with any desired spectral response. In our case, we’ve used it to approximate bands that are used to construct a RGB image: the green band and the CIE 1931 XYZ color space.

We have shown that the SST Pattern Test (SPT) was able to improve the ACSPO clear-sky mask by using pattern recognition and image processing techniques. SPT was able to restore significant amount of clear-sky regions in ACSPO, both globally and in highly dynamic areas such as the Gulf Stream. We also saw how resampling was able to correct distortions in VIIRS imagery, creating a continuously differentiable 2D space on which SPT was able to make the best use of spatial features. The restoration of clear-sky in highly distorted areas was improved due to resampling.

The MODIS band 6 estimation, GOES-R color image estimation, and VIIRS 13.3\(\mu\)m band estimation problems are similar in that we’re trying to estimate missing data. In all three cases we have training data either from the same instrument or simulated data from a proxy instrument. The approaches taken involve creating a function from the training data, which is then used to predict the missing data. The techniques used here include
multi-linear regression, polynomial fitting, and nearest neighbor search. Sometimes a global approximation function for an image is not a good enough predictor and we must take into consideration spatially local features or different surface types. In this case, the prediction function can be build on a local patch (e.g. QIR) or it can be done on different clusters (e.g. GOES-R RGB prediction).

The problem of restoring the false alarms in ACSPO clear-sky mask is a very different problem than the other three problems because the classifier was not built directly from the training data. The variables that must be used for classification is experimentally determined based on image processing results. Unsupervised learning is used here to detect spatially similar regions, but not to train a predictor exclusive to these regions. Overall, this problem seems to be more challenging than the others. It is easier to evaluate the results when we have some ground truth. In MODIS band 6 restoration, we were able to use Terra as benchmark, and in GOES-R color image prediction and VIIRS 13.3\,\mu m band estimation we were able to use MODIS as proxy. For ACSPO clear-sky prediction, evaluation was done manually or through aggregated statistics on restoration.
Bibliography


