

Article

Gaussian Process and Deep Learning Atmospheric Correction

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Abstract: Atmospheric correction is the processes of converting radiance measured at a spectral sensor to the reflectance of the materials in a multispectral or hyperspectral image. This is an important step for detecting or identifying the materials present in the pixel spectra. We present two machine learning models for atmospheric correction trained and tested on 100,000 batches of 40 reflectance spectra converted to radiance using MODTRAN, so the machine learning model learns the radiative transfer physics from MODTRAN. We created a theoretically interpretable Bayesian Gaussian process model and a deep learning autoencoder treating the atmosphere as noise. We compare both methods for estimating gain in the correction model to the well-know QUAC method of assuming a constant mean endmember reflectance. Prediction of reflectance using the Gaussian process model outperforms the other methods in terms of both accuracy and reliability.

Keywords: atmospheric compensation; Gaussian process; hyperspectral

1. Introduction

Atmospheric correction of a hyperspectral or multispectral image is the process of converting the observed at-sensor radiance (the amount of light per wavelength measured at the sensor) to ground reflectance (the percent reflectance per wavelength of the material(s) located at on the ground). In this paper we present two methods for machine learning of atmospheric radiative transfer from collections of spectra from a hyperspectral image. Each method takes in a collection observed pixel spectra from a hyperspectral image and outputs the reflectance spectra for the pixels, providing coefficients for atmospheric correction that can be applied to the entire image.

A hyperspectral image is a digital image in which each pixel has more than the visual three color (red, green, blue) bands, but often hundreds of bands across wavelengths sufficient to get spectral information about the materials in each pixel. We focus on hyperspectral images that have band wavelengths from about 400nm to 2500nm - for comparison the visual colors occur around 450 (blue), 550nm (green) and 650nm (red) - and our spectra have 452 bands as collected with 375 bands after removing bands where the signal is absorbed by water vapor. For a hyperspectral image collected at these wavelengths, the measured light at the sensor is primarily reflected sunlight, having passed through the atmosphere, reflected off materials, and passed again through some amount of atmosphere (which may be small for a ground-based space or significant if the sensor is on board an aircraft or satellite.) Each band is typically 2nm to 10nm wide, and the bands are contiguous across the wavelength range. The reflectance for a material is important because it is the result of the interaction of photons at different wavelengths and the resonant frequencies of molecular bonds (for the wavelengths above the visible range) and the interaction of photons and electrons moving between quantum states (for wavelengths around the visible range). Specifically, important information about the constituents and bonds present in a material can be computed from reflectance spectra, for example distinguishing between different polymers, or distinguishing talcum powder from powdered sugar from dangerous white powdered substances.

As light propagates through the atmosphere, some light is absorbed by the particles and gases in the atmosphere, some light is scattered, and some light passes through the atmosphere. Light at lower wavelengths has greater probability of being scattered (the blue sky effect), and generally the fraction of light that is absorbed varies with wavelength, depending on the gasses and particles present. The percentage of light that passes through the atmosphere is called transmittance, which is a function of wavelength for a given atmosphere. This transmittance can be computed from physical measures for a given atmosphere (density of water vapor, sun and sensor angles, etc.) using MODTRAN [1] (MODerate resolution atmospheric TRANsmission) software. A plot of transmittance for two different atmospheric models created using the MODTRAN online interface¹ across our wavelength range with a spectral resolution (band width) of 5nm is shown in Figure 1. Observe that these two spectra differ in magnitude and in depth of the absorption features that occur at various wavelengths. Our main goal includes determining this transmittance fraction from spectra on the ground measured from a sensor even when the reflectance of the ground material is unknown.

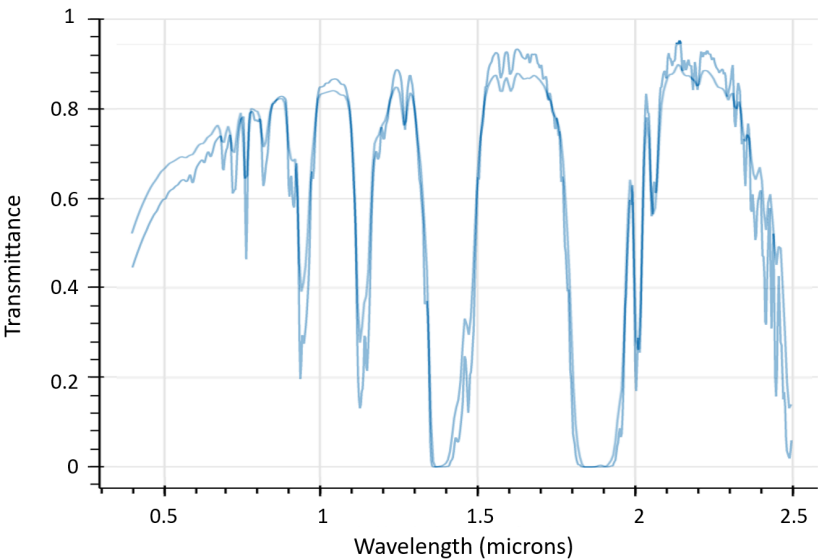


Figure 1. Two plots of transmittance for two different atmospheric models created using the MODTRAN online interface.

The plot in Figure 2 shows more components involved in the radiative transfer model, also generated with the MODTRAN online interface. The Direct Solar (100km) gives the amount of sunlight measured at the top of the atmosphere. The main shape of this curve is from the blackbody radiation given the temperature of the sun. The Direct Solar (0km) is the amount of sunlight reaching the ground, which is the Direct Solar (100km) times a transmittance similar to that shown in Figure 1. The Downward Diffuse (0km) is the amount of light per wavelength that reaches the ground after scattering in the atmosphere; this is the indirect illumination on an object, for example on an object in a shadow from the sun. The upward Diffuse is the amount of upward light, which at 100km (top of atmosphere) is from atmospheric scattering and at 0km is from the blackbody radiation of the ground (which is insignificant given the wavelength range and ground temperature assumed in this model).

¹ http://modtran.spectral.com/modtran_home

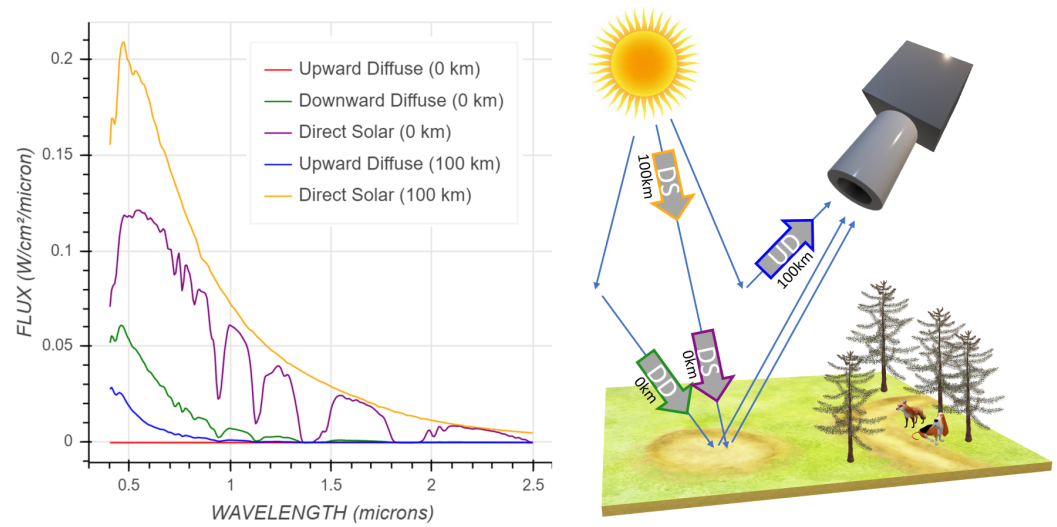


Figure 2. Components of the atmospheric radiative transfer model created using the MODTRAN online interface (left). The at-sensor radiance is the sum of all light entering the sensor, which is the result of these components and their interaction with the ground (right).

The at-sensor radiance is the Upward Diffuse (at the elevation of the sensor) plus the total illumination at the ground (Direct Solar + Downward Diffuse) times the percent reflectance per band of the material on the ground per wavelength Ref_{λ} ,

$$UD_{\lambda} + (DS_{\lambda} + DD_{\lambda})Ref_{\lambda} = Rad_{\lambda}.$$

There are additional nonlinear effects as well which are not shown in figure 2. Light that has passed through a leaf and reflected off the ground would have the leaf transmittance times ground reflectance in place of Ref_{λ} in this equation. In the lower wavelengths, especially blue and below, photons will take multiple bounces/scattering (collectively, 'haze' in the image) in the atmosphere. This multiple bounce haze causes additional upward diffuse and additional downward diffuse illumination on the ground. There are also photons that reflect off material at one ground location and then scatter in the atmosphere to enter the sensor at locations/directions for other pixels, causing an "Upward Diffuse" that varies across the image comprised of a nonlinear mixture of nearby ground material spectra and atmospherics, rather than the ideal Upward Diffuse from the atmosphere alone shown in figure 2. These nonlinear effects are minimal in most cases.

All of these values change with respect to atmospheric constituents, water vapor, CO₂, Ozone, CH₄, aerosols, sun angle, fraction of sun and sky visible to each pixel (shadow from objects, terrain, clouds, etc.), sensor angle, angle and roughness of the ground material, and other factors. The MODTRAN software can simulate these effects if they are known, and provide a modeled at-sensor radiance for reflectance spectra, or an approximated ground reflectance spectrum for a measured at sensor radiance.

The purpose of hyperspectral imaging is to perform spectroscopy writ large; that is, to be able to determine the materials in each pixel from the reflectance spectra for those pixels. As such, good atmospheric compensation is an essential step. The most accurate methods either use physics-based modelling with MODTRAN such as FLAASH [10] or using materials of known reflectance in the image, for example the empirical line method [11,12], in which case it is usually preferable to have materials that are spectrally flat, for example a set of five panels which are 5%, 30% 50% 80% and 95% reflectance across all wavelengths, which can be used to estimate a best fit regression line per wavelength to convert from radiance units to reflectance. However, both of these methods make approximations in their modelling of physical parameters. For example, a good ELM will estimate the upward diffuse as the intercept and the direct solar and downward diffuse as

the slope, but assume these are consistent values for every pixel in the image. FLAASH attempts to estimate the physical parameters from the image radiance spectra based on user input of parameters, even estimating water vapor content per pixel, and use a physics based model to compute the grouped reflectance from each at-sensor radiance measurement.

A heuristic and approximate but surprisingly effective method for atmospheric correction is to make the assumption that the mean spectrum of a significantly large diverse library of reflectance spectra will be constant (independent of the spectra used and varying only with wavelength, called the ideal mean reflectance), and use this assumption to compute a single gain and offset that is applied per wavelength across the image. A method based on this assumption is QUACC [6] (QUick Atmospheric Correction Code), which functions approximately as follows. First, the minimum measured radiance value across the image per wavelength is assumed to be the upwelling radiance at the sensor (offset), and is thus subtracted from the image. The top of atmosphere solar radiance (Direct Solar in Figure 2) is approximated using a plank function at the observed temperature of the sun, and this value is divided by the radiance values per band as a first step in correcting for illumination intensity. Then a sample of 50 different spectra (called endmembers) are selected from the radiance image, usually iteratively so each new endmember is optimally different than the previous ones, and the mean of these 50 endmembers is determined. Then the ratio between the ideal mean and mean of the endmembers is computed and used as a ‘gain’ and is multiplied by every upwelling-subtracted radiance value to convert to reflectance. This is often implemented with additional heuristic improvements such as removing spectra of mud or vegetation from the spectra, and is provided in QUACC [6]. There are other semi-heuristic methods for example SHARC [13].

The QUAAC method is faster than physics-based methods and unlike FLAASH requires no manual input. In tests, it often provides reflectance spectra that are generally $\pm 15\%$ in comparison to FLAASH generated reflectance spectra, and perhaps more importantly QUACC tends to generate reflectance spectra that retain the features of the true spectra, which is the most important factor for spectroscopy. The main assumptions in QUACC are:

1. Assuming that the atmospheric correction is linear, comprised of an offset (upward diffuse) and gain (transmittance per band).
2. Assuming the minimum radiance value observed in each band is the upward diffuse.
3. Assuming that the mean reflectance of a collection of spectral diverse spectra is always the universal mean

In this paper we provide a Gaussian process atmospheric correction process that does not make assumption 3, and a denoising autoencoder atmospheric correction process that can be used avoiding all 3 assumptions.

2. Materials and Methods

We developed and tested two machine learning models to transform the radiance data to reflectance. The first method, which showed exceptional performance, is a Gaussian process model. Our second method is a deep learning model using a denoising autoencoder, training the autoencoder as if the atmospheric effects are noise. These methods were trained and tested on reflectance spectra with associated radiance that were computed using MODTRAN.

2.1. Data

For this paper, we started with a set of about 1,200 reflectance spectra of known materials, each of which passed some basic quality checks. These spectra have 452 bands contiguous ranging from 400nm to 2400nm, resulting in 375 bands after removing bands in the 1340-1440-nm and 1800-2000nm ranges because light in these wavelengths is completely or nearly completely absorbed by water in the atmosphere. We then took random samples of size 39, randomly selected a set of parameters for MODTRAN (solar zenith angle from 0-85 in increments of 5, random selection from the 6 possible atmospheric models, random

selection from the 12 possible aerosol models) and created an associated set of 39 at-sensor radiance spectra. For each set, we then computed the mean spectrum and added this as a 40th spectrum. So our input data is a set of 40 radiance spectra each with 375 wavelengths, and our output data is a set of 40 reflectance spectra. Our software maintained the option to include the upwelling (offset) term, to to exclude it (approximating a situation where it was estimated in-scene for example by a darkest pixel per band method). In Figure 3 we show a plot of the 40 radiance spectra (left) and the associated reflectance spectra (right). We created a 100,000 such groupings of 40 reflectance spectra and applied the randomly selected atmospheric model to generate the associated radiance. The goal is to train a machine learning model to take the radiance spectra as an input and output the reflectance spectra. Two-thirds of our data was randomly selected for training and the remaining sets of spectra used for testing.

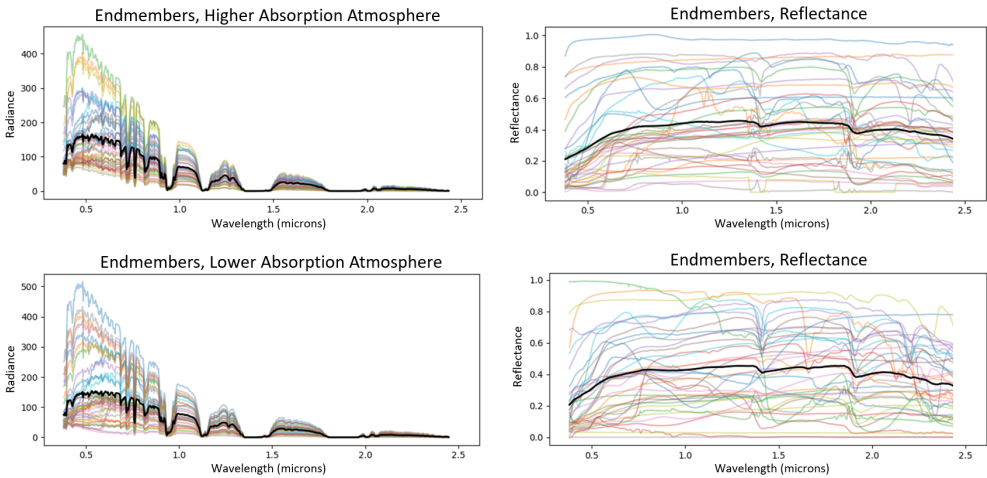


Figure 3. At-sensor radiance for 39 spectra and the mean plotted in black (left-hand plots) along with the true reflectance for these materials and the mean of their reflectance in black (right-hand plots). The top row of plots have a atmosphere with greater absorption and the lower pair has less absorption.

Figure 4 shows reflectance and radiance values from different endmember means, showing that there is significant variant in both the radiance and reflectance values for different groupings and atmospheres.

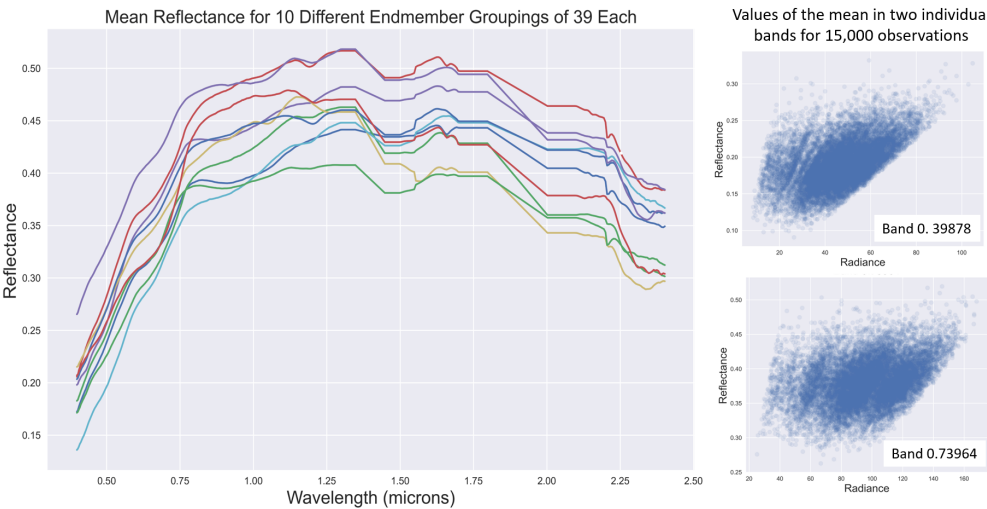


Figure 4. The mean reflectance spectrum for 10 different groupings of 39 endmembers (left) and the reflectance and radiance values in two different bands over 15,000 of our observations.

2.2. Gaussian Process Atmospheric Compensation

The Gaussian process model can be described using conditional probabilities as follows. Let $\mathbf{x} = (\text{Rad}_{\lambda_1}, \dots, \text{Rad}_{\lambda_N})$ denote the N -dimensional vector of values for the mean for a set of radiance endmembers, and let $\mathbf{y} = (\text{Ref}_{\lambda_1}, \dots, \text{Ref}_{\lambda_N})$ be the N -dimensional mean vector of the reflectance for these endmembers. Let $\mathbf{z}$ be the $2N$ -dimensional concatenation of $\mathbf{x}$ and $\mathbf{y}$,

$$\mathbf{z} = (\text{Rad}_{\lambda_1}, \dots, \text{Rad}_{\lambda_N}, \text{Ref}_{\lambda_1}, \dots, \text{Ref}_{\lambda_N}).$$

We use capital letters $\mathbf{X}$, $\mathbf{Y}$, and $\mathbf{Z}$ for the arrays consisting of k observations of each type, which are of size $k \times N$, $k \times N$, and $k \times 2N$ respectively.

Making the assumption that $\mathbf{Z}$ is a multivariate normal random variable, we can compute the mean μ_z and covariance Σ_z . Let μ_x and μ_y be the means for the radiance and reflectance so that μ_z is the concatenation of μ_x and μ_y . If we denote the covariance of the $\mathbf{Z}$ by Σ_z , the covariance of X by Σ_{xx} , and the covariance of Y by Σ_{yy} , then the covariance matrix $\mathbf{Z}$ can be written in block form as

$$\begin{bmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{bmatrix}.$$

Then for a given radiance x_0 which is the mean of endmembers, we get the conditional probability distribution for the reflectance as the multivariate normal distribution [7]

$$P(\mathbf{y}|\mathbf{x} = \mathbf{x}_0) = \mathcal{N}(\bar{\mu}; \bar{\Sigma})$$

where

$$\bar{\mu} = \mu_y + \Sigma_{yx}\Sigma_{xx}^{-1}(\mathbf{x}_0 - \mu_x) \quad (1)$$

$$\bar{\Sigma} = \Sigma_{xx} - \Sigma_{yx}\Sigma_{xx}^{-1}\Sigma_{xy}. \quad (2)$$

This conditional probability density function is depicted in the case where x is one dimensional and $\mathbf{y}$ is two dimensional in Figure 5. The predicted mean reflectance is then the expected value of the reflectance given the observed radiance,

$$E[\mathbf{y}|\mathbf{x} = \mathbf{x}_0] = \bar{\mu}.$$

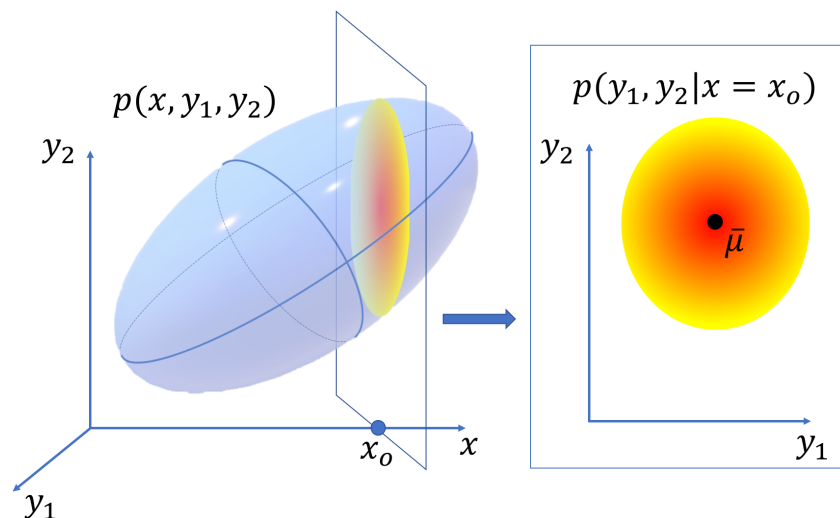


Figure 5. The conditional probability density function for a multivariate normal distribution is a lower dimensional multivariate normal distribution.

This predicted mean reflectance can be used in atmospheric correction similar to how the 'universal mean' is used in QUACC, as follows. First, for each band the minimum value over all pixels in the image for that band is determined, and this minimum value is used as the offset, which is an estimate for the upwelling radiance. This offset is subtracted from every pixel in the image, and then a collection of endmembers is collected from the image. The mean of these endmembers is the radiance vector x_0 , and the predicted reflectance is $\bar{\mu}$. The gain for the atmospheric conversion is $\bar{\mu}/y$, which is multiplied per-band by every spectrum in the image to complete conversion to reflectance. Two examples of mean of the radiance endmembers (left) and predicted reflectance (right) are shown in Figure 6 using observations from our test data. Observe that the method accurately predicts the mean reflectance spectra even though these means differ from each other significantly. This enables us to perform accurate atmospheric correction in situations where the assumption in QUACC of a universal mean is not a reasonable assumption.

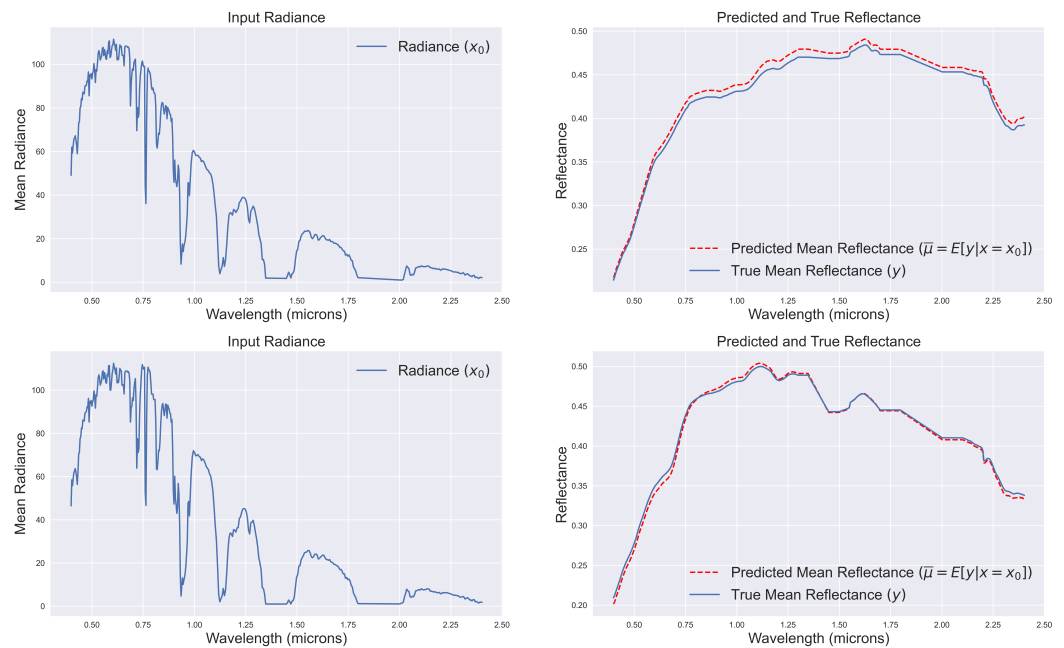


Figure 6. The autoencoder neural network used for converting from radiance to reflectance. Details for the network architecture are included in the labels.

The covariance matrices computed from the radiance and reflectance training data for the parameters computations in 1 are shown in Figure 7. From this figure we can see that Σ_{xx} is a covariance matrix for reflectance spectra, Σ_{yy} is a covariance for radiance spectra, and the off diagonal matrices indicate a conversion between units.

2.3. Denoising Autoencoder Atmospheric Compensation

An autoencoder is a deep learning neural network that passes data through a series of layers that decrease in size leading to a dimensionally smaller representation of the data (encoding), and then passing the data through a symmetric series of layers back to the original data shape (decoding). When trained well, the process learns a representation of the data in the reduced dimensional space so that the encoding stage removes noise and the decoding stage recovers the data in the original space [2–5]. A diagram of the architecture of our autoencoder is shown in Figure 8.

Our autoencoder is trained on the reflectance and radiance data described previously (removing the last 3 bands to provide an appropriate even number for the autoencoder), providing the full 40×372 2-D array of endmembers and mean for each rather than just the mean. One training data observation with both radiance (input for the autoencoder)

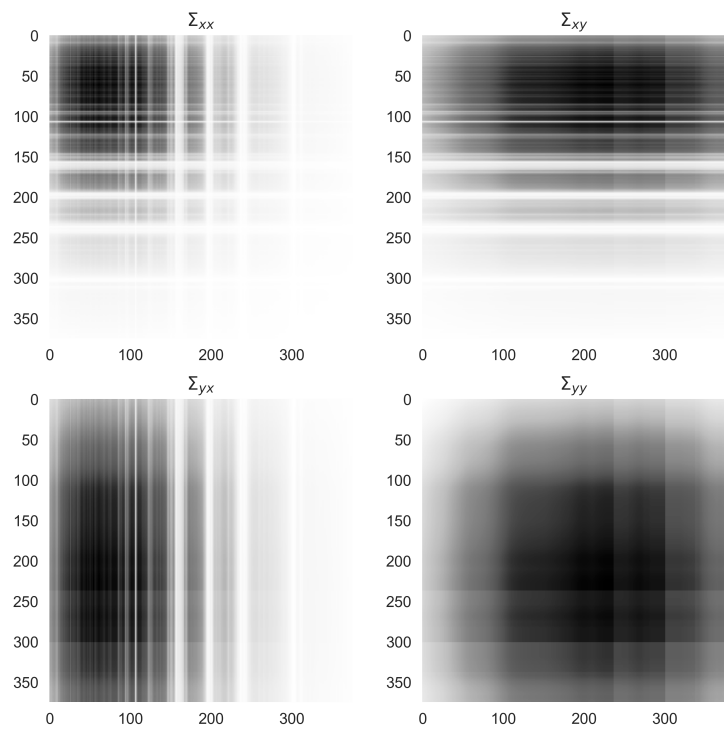


Figure 7. The covariance matrices computed from the radiance and reflectance data for the parameters for the conditional probability.

and reflectance (output) is shown in Figure 10. All of our data and methods are provided open access².

3. Results

We tested all three methods: Gaussian process (GPAC), universal mean regression (UMR), and our denoising autoencoder (DA) for atmospheric correction on out test data. The data consisted of 100,000 observations, where each observation has an X input array of 40 radiance spectra and a Y output variable of these 40 spectra in reflectance. The radiance was created from the reflectance by apply a MODTRAN atmospheric absorption. For each observation, the reflectance spectra were a random selection from a library of over 1000 spectra and the parameters for the MODTRAN atmosphere were randomly selected. The data was randomly split into 66,667 training observations and 33,333 test observations. The test set is then $33,333 \times 39 = 1,299,987$ unique radiance-reflectance pairs of spectra (We exclude the mean for scoring, so each group has 39 rather than 40).

We applied each method to the each test observation to determine a predicted reflectance spectrum for each radiance. (The GPAC and UMR methods each produce a mean reflectance which is used to determine a gain, which is then applied to each radiance spectrum to obtain the reflectance, while the DA directly provides a predicted reflectance for each radiance spectrum.) We then computed the following metrics.

1. *Mean Correlation:* The mean of the correlations between each predicted reflectance spectrum with the corresponding true reflectance.
2. *Standard Deviation in Correlation:* The standard deviation of the correlations between each predicted reflectance spectrum with the corresponding true reflectance.

² <https://www.kaggle.com/code/billbasener/autoencoder-atmospheric-compensation/notebook>

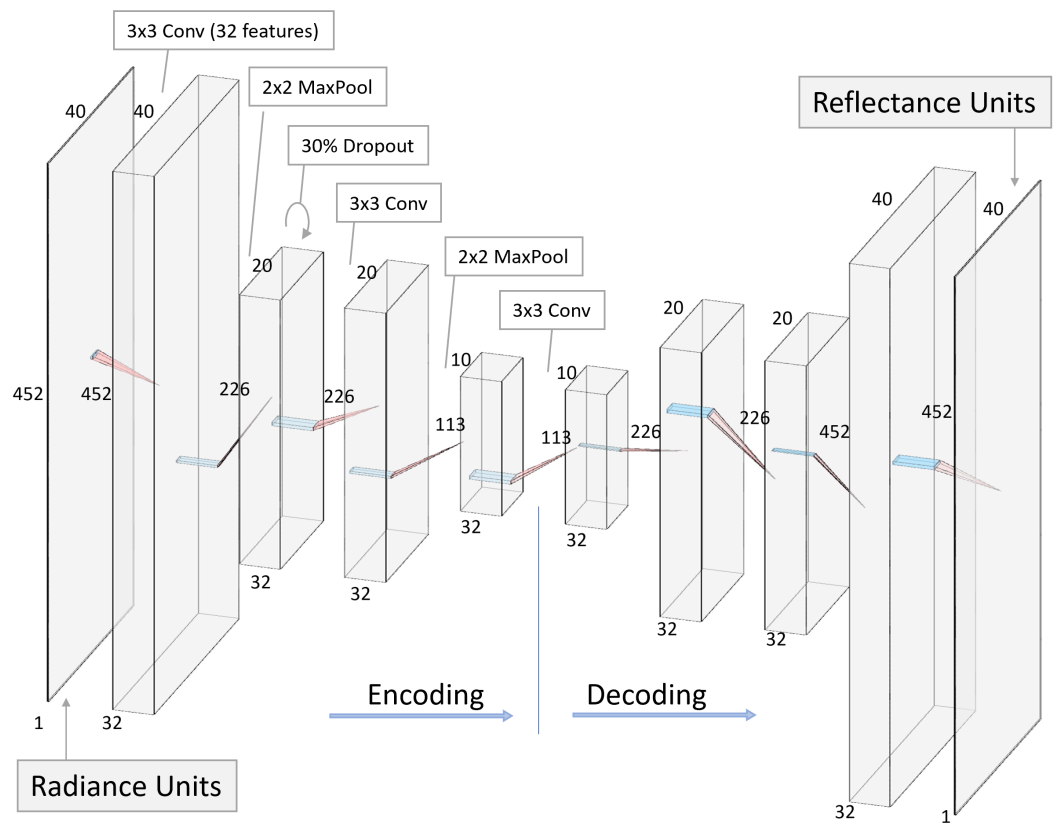


Figure 8. The autoencoder neural network used for converting from radiance to reflectance. Details for the network architecture are included in the labels.

3. *Percent with all bands in $\pm 15\%$ of True:* The percent of spectra (out of the 1,299,987) for which the predicted reflectance is within $\pm 15\%$ of the true reflectance for all bands.
4. *Percent with $> 98\%$ of bands in $\pm 15\%$ of True:* The percent of spectra (out of the 1,299,987) for which the predicted reflectance is within $\pm 15\%$ of the true reflectance for at least 98% of the bands.

The mean correlation between the predicted and true spectra is an important metric because most material detection and identification process incorporate correlation (in native or PCA space), and moreover the chemical bonds in materials appear as features (minima, maxima, slopes, etc.) in the spectra, and correlation between spectra captures these better than absolute difference. It is clear from our test that the GPAC method provides the most accurate (highest mean) and most consistent (lowest standard deviation) results when measured in by correlation between predicted reflectance and true reflectance.

The two metrics measuring how well the predicted reflectance stays within plus or minus 15% of the true reflectance provide additional import information on accuracy. This type of comparison has been used to justify the accuracy of QUACC [14]. Often, the predicted reflectance will be close to the true reflectance except for a small number of bands near the water band regions, where high absorption from a particular atmosphere can result in low signal in the radiance spectra and unnaturally high values in predicted reflectance for GPAC and UMR. The GPAC method performed the best by these metrics as well. Notably, for 73% of spectra the predicted reflectance with was within 15% of the true reflectance for at least 98% of the bands, while this was true for UMR for only 41% of the spectra.

Six reflectance endmembers along with their approximated reflectance from GPAC are shown for two different observations sets in Figure ?? . Observe that along the edges

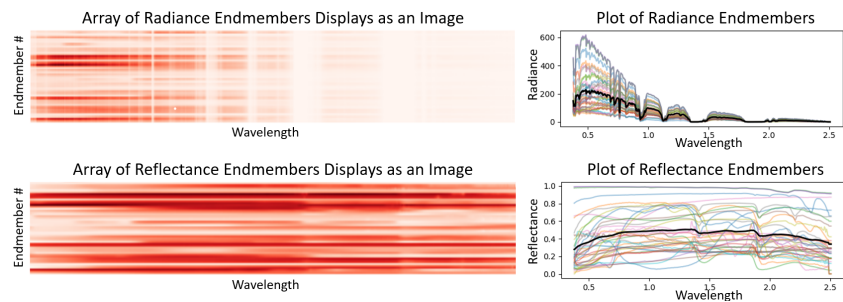


Figure 9. The training data for the auto encoder is an array of the radiance endmembers (upper-left) and array of the reflectance endmembers (lower-left). The plots for each of these is shown to the right.

Table 1. Evaluation metrics for the Gaussian process prediction, universal mean regression, and denoising autoencoder methods.

Metric	GPAC	UMR	DA
Mean Correlation	0.96	0.94	0.86
Std. Deviation in Correlation	0.11	0.14	0.19
percent with all bands in $\pm 15\%$ of True	43%	23%	0.3%
percent with $> 98\%$ of bands in $\pm 15\%$ of True	73%	41%	1.4%

of the water band regions, that $1/\text{SNR}$ (where SNR for a bands λ is the max radiance over all bands divided by the radiance value for band λ) is higher and there are poor approximations for the individual bands. This is a problem that arises in all atmospheric correction methods where the low SNR water bands result in poor reflectance estimates.

4. Conclusions

The most common automated atmospheric compensation method is QUACC [6], described in Section 1. In this method, after estimating and removing an offset (upwelling diffuse), a set of endmembers is selected and the UMR method is used to estimate a gain (transmittance), which is then applied to the whole image. Some additional heuristics are used, such as excluding vegetation or mud from the endmembers and choosing a subset of bands for endmember selection. Despite the approximations, this method generates reasonable reflectance spectra that are within 15% of those generated with physics-based methods such as FLASH [14].

The theoretical design of the Gaussian process mean from GPAC should be a better approximation to the mean reflectance of a set of endmembers than a constant universal mean, and our test indicate that this is robustly true. While we trained and tested on MODTRAN data rather than image data, we expect that incorporating GPAC in place of UMR in QUACC would provide substantial significant robust improvement in atmospheric compensation. Moreover, our Gaussian process framework could similarly be used to predict the offset from an estimate based on the QUACC minimum-value approximation.

While our denoising autoencoder method does not perform well in comparison to the other methods we tested, we believe that it is an important first step in applying the growing field of deep learning of physical principles to atmospheric compensation in hyperspectral imagery and remote sensing. We expect, based on the trajectories of other efforts in deep learning of physical phenomena, that better inclusion of physical principles in the architecture of the autoencoder could substantially improve the quality of output. For example, the inclusion of skip connections in the ResNet Network enables layers that learn functions closer to the identity, leading to the ability to train much larger, more

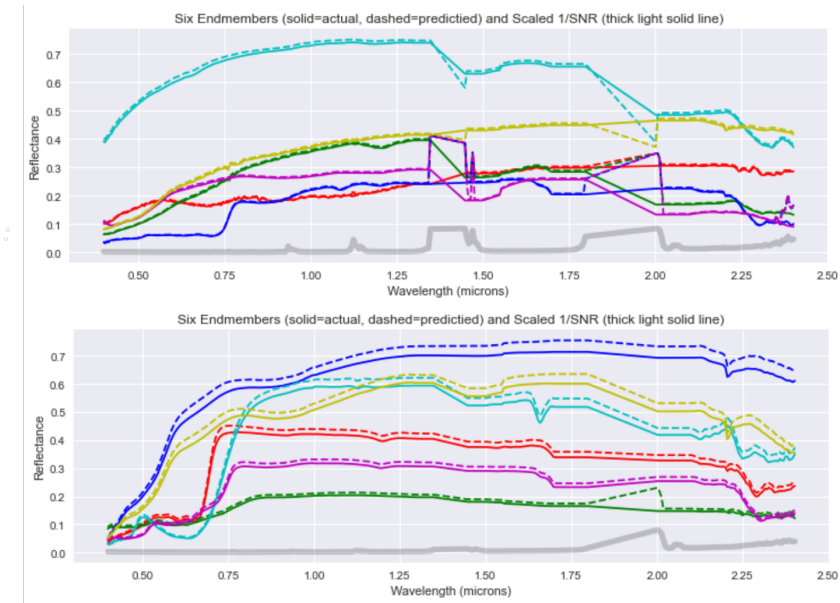


Figure 10. For two different observations endmeber sets and atmospheres, the true and predicted reflectance spectra for six endmembers are shown. Also shown is 1/SNR for each band, with the SNR is the radiance value for the given band divided by the maximum radiance.

complex, networks [8] with a smoother loss function that has fewer local minima [9]. It is possible that similar architecture modifications, or maybe a hybrid approach with a Gaussian process, could aid a deep learning model to approximate the physics involved and/or train to learn the physics better.

5. Patents

The University of Virginia is considering filing a patent based on the GPAC method described in this paper

Author Contributions: Conceptualization, B.B. and A.B.; QUACC software written in C++, A.B.; validation, A.B. and B.B.; formal analysis, B.B. and A.B.; data curation, B.B.; writing—original draft preparation, B.B.; writing—review and editing, B.B. and A.B.; visualization, A.B. and B.B.; supervision, B.B.; All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: Code in Python for all algorithms in this paper are available at <https://www.kaggle.com/code/billbasener/autoencoder-atmospheric-compensation/notebook>. Some data is available with that resource, but some reflectance spectra used are in the public domain. The MODTRAN coefficients can be accessed via <http://modtran.spectral.com/> and <http://modtran.spectral.com/m>

Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

MDPI	Multidisciplinary Digital Publishing Institute
MODTRAN	MODerate resolution atmospheric TRANsmission
GPAC	Gaussian Process Atmospheric Correction
UMR	Universal Mean Regression
DA	Denoising Autoencoder

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