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Estimating top-of-atmosphere thermal infrared radiance using
MERRA-2 atmospheric data

by

Tania Kleynhans

A thesis submitted in partial fulfillment of the
requirements for the degree of Master of Science
in the Chester F. Carlson Center for Imaging Science
College of Science
Rochester Institute of Technology

May 18, 2017

Signature of the Author _____

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CHESTER F. CARLSON CENTER FOR IMAGING SCIENCE
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CERTIFICATE OF APPROVAL

M.S. DEGREE THESIS

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has been examined and approved by the thesis committee
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by

Tania Kleynhans

Submitted to the
Chester F. Carlson Center for Imaging Science
in partial fulfillment of the requirements
for the Master of Science Degree
at the Rochester Institute of Technology

Abstract

Space borne thermal infrared sensors have been extensively used for environmental research as well as cross-calibration of other thermal sensing systems. Thermal infrared data from satellites such as Landsat and Terra/MODIS have limited temporal resolution (with a repeat cycle of 1 to 2 days for Terra/MODIS, and 16 days for Landsat). Thermal instruments with finer temporal resolution on geostationary satellites have limited utility for cross-calibration due to their large view angles. Reanalysis atmospheric data is available on a global spatial grid at three hour intervals making it a potential alternative to existing satellite image data. This research explores using the Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) reanalysis data product to predict top-of-atmosphere (TOA) thermal infrared radiance globally at time scales finer than available satellite data. The MERRA-2 data product provides global atmospheric data every three hours from 1980 to the present. Due to the high temporal resolution of the MERRA-2 data product, opportunities for novel research and applications are presented. While MERRA-2 has been used in renewable energy and hydrological studies, this work seeks to leverage the model to predict TOA thermal radiance. Two approaches

have been followed, namely physics-based approach and a supervised learning approach, using Terra/MODIS band 31 thermal infrared data as reference. The first physics-based model uses forward modeling to predict TOA thermal radiance. The second model infers the presence of clouds from the MERRA-2 atmospheric data, before applying an atmospheric radiative transfer model. The last physics-based model parameterized the previous model to minimize computation time. The second approach applied four different supervised learning algorithms to the atmospheric data. The algorithms included a linear least squares regression model, a non-linear support vector regression (SVR) model, a multi-layer perceptron (MLP), and a convolutional neural network (CNN). This research found that the multi-layer perceptron model produced the lowest error rates overall, with an RMSE of $1.22 \text{ W/m}^2 \text{ sr } \mu\text{m}$ when compared to actual Terra/MODIS band 31 image data. This research further aimed to characterize the errors associated with each method so that any potential user will have the best information available should they wish to apply these methods towards their own application.

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Dedication

Aan my Ma, wat my altyd ondersteun het, maak nie saak hoe moeilik haar eie lewe was nie.

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Chapter 1

INTRODUCTION

Thermal infrared satellite data have been widely used for cross-calibration studies [1] and climate research [2, 3]. However, thermal infrared satellites such as Landsat and Terra/MODIS have limited temporal resolution (Landsat has a revisit rate of up to 16 days while Terra/MODIS has a revisit rate of 1-2 days). Thermal instruments on geostationary satellites (e.g., GOES) have much finer temporal resolution, but have large view angles through the atmosphere for a significant portion of the disk, limiting their utility for cross-calibration. Reanalysis atmospheric data is available on a global spatial grid at three hour intervals making it a potential alternative to existing satellite image data.

This research describes two approaches to predict TOA thermal infrared radiance using the Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) reanalysis data product. MERRA-2 is produced by NASA's Global Modeling and Assimilation Office (GMAO), and it provides atmospheric data on a 0.5 degree latitudinal $\times$ 0.625 degree longitudinal world grid spacing (approximately 50×70 km at the equator). MERRA-2 variables are available every three hours for the past 37 years.

Figure 1.1: An example of the predicted TOA thermal infrared radiance world map on July 31, 2013 at 9am. Radiance in $W/m^2 sr \mu m$.

If TOA thermal infrared radiance can be predicted from MERRA-2 data, then it will be available worldwide at much greater temporal resolution than currently provided by thermal infrared satellites. Figure 1.1 displays one example of a predicted TOA thermal infrared radiance world map.

Broadly, this research used two approaches for predicting TOA thermal radiance from MERRA-2: 1) a physics-based approach, and 2) supervised machine learning. The details of each method will be described in Chapter 3. MERRA-2 data contains a series of atmospheric variables like air temperature, relative humidity, skin temperature, and the intent was to utilize these parameters to model the TOA radiance in a particular spectral band.

The results of this research are discussed along with sources that contribute to the prediction errors, e.g., the difference between MERRA-2 skin temperature and the Terra/MODIS Land Surface and Sea Surface Temperatures, and errors introduced by various data resampling methods. This research further aimed to characterize the errors associated with each method and land cover type, so that potential users will have the best information available should they wish to apply these methods towards their own application.

This document will provide an overview of the MERRA-2 data product, methodology to predict sensor reaching radiance from the atmospheric data, characterize model errors, and discuss the results and conclusions of the research.

Chapter 2

MERRA-2

MERRA-2 was developed by the Global Modeling and Assimilation Office as an Earth System reanalysis [4]. It was created to extend the 2004-2013 Goddard Earth Observing System Model, Version 5 (GEOS-5) operational data product. MERRA-2 provides worldwide atmospheric measurements from 1980 to present, and focuses on providing historical analysis of the hydrological cycle in a climate context [5]. It does this by integrating vast quantities of conventional weather observations, satellite-based data and other assimilation systems. The main strength of MERRA-2 lies with its continuous data record and global coverage. Depending on the application, the low spatial resolution of 0.5×0.625 degrees, which corresponds to about 50 km in the latitudinal direction, could be a limiting factor.

MERRA-2 consists of 42 collections (e.g., surface flux diagnostics, assimilated meteorological fields) containing several variables each (e.g. skin temperature, relative humidity, air temperature). An example of one collection (assimilated meteorological fields) can be seen in Table 2.1. The variables highlighted in bold, air temperature and relative humid-

Table 2.1: MERRA-2 collection: Assimilated Meteorological Fields

Frequency: 3-hourly from 00:00 GMT

Spatial Grid: 3D, pressure-level, full horizontal resolution

Dimensions: longitude(x) = 576, latitude(y) = 361, level(z) = 42, time(t) = 8

Name	Dim	Description	Units
EVP	tzyx	ertels potential vorticity	$K m^2 kg^{-1} s^{-1}$
H	tzyx	edge heights	m
O3	tzyx	ozone mass mixing ratio	$kg kg^{-1}$
OMEGA	tzyx	vertical pressure velocity	$Pa s^{-1}$
PHIS	tyx	surface geopotential height	$m^2 s^{-2}$
PS	tyx	surface pressure	Pa
QI	tzyx	mass fraction of cloud ice water	$kg kg^{-1}$
QL	tzyx	mass fraction of cloud liquid water	$kg kg^{-1}$
QV	tzyx	specific humidity	$kg kg^{-1}$
RH	tzyx	relative humidity after moist	1
SLP	tyx	sea level pressure	Pa
T	tzyx	air temperature	K
U	tzyx	eastward wind	$m s^{-1}$
V	tzyx	northward wind	$m s^{-1}$

ity, are two of the variables used in this research. The dimensions of the variables can be seen in the second column, where t represents the number of times per day that data is available, x and y represents the number of spatial locations, and z the vertical profile extending to 0.1 hPa (approximately 64 km above sea level). Variables without a z value have a horizontal resolution ($x \times y \times \text{time}$) only.

All variables are plotted on a world grid of $576(x) \times 361(y)$ pixels. Depending on the collection, the variables are available hourly, 3-hourly, 6-hourly or monthly mean ($t = 24$, $t = 8$, $t = 4$ or $t = 1$). Some variables have surface values only, resulting in a $576(x) \times 361(y)$ grid, while other variables have an atmospheric profile (z) with 42 layers where each layer represents a specific pressure level (ranging from 1000 hPa to 0.1 hPa which corresponds to 0 to approximately 64 km above seal level). The pressure levels are

Figure 2.1: MERRA-2 air temperature profile world map (Kelvin)

converted to distance above sea level by applying Equation 2.1.

$$alt = -\ln\left(\frac{p_a * 100}{p_0}\right) * h_0 \quad [m] \quad (2.1)$$

where p_a is the air pressure [hPa], p_0 is the atmospheric pressure at sea level [hPa] and h_0 is the scale height in meters (7000m).

These pressure level variables result in a data cube of $576 \times 361 \times 42$ pixels for every available 3-hourly period. Figure 2.1 displays the air temperature data cube for a given time and date. Figure 2.2 displays one air temperature profile in Kelvin against the associated altitude in km above sea level.

Figure 2.2: MERRA-2 air temperature profile at a single grid point

MERRA-2 data is assimilated from a variety of sources. As an example, skin temperature over land is assimilated using in-situ observations from the National Oceanic and Atmospheric Administration (NOAA). There are 35,000 stations worldwide with 14,000 stations active daily. Figure 2.3 displays the worldwide stations where observations are collected.

Skin temperature over water is assimilated by NOAA’s International Comprehensive Ocean-Atmosphere Data Set (ICOADS) from ships, moored buoys, drifting buoys, C-MAN, coastal measurements, oil rigs, tide gauges and lightships [6]. Figure 2.4 displays the positions of these measurements taken in February 2017.

These conventional observations, together with satellite-based data from the Advanced Very High Resolution Radiometer (AVHRR) and the Advanced Microwave Sounding Unit-A (AMSU-A) are then assimilated using the Grid Point Statistical (GSI) Interpolation Scheme. The air temperature and relative humidity profiles are assimilated from ra-

Figure 2.3: Integrated surface database station distribution map. Image credit: NOAA

diosondes, dropsondes, aircraft, and temperature- and humidity-sensitive radiances from a variety of sounders and satellites (HIRS, SSU, MSU, SSM/I, AMSU-A, GOES, AIRS) [7].

Four MERRA-2 variables were used for this research: 1) instantaneous skin temperature (TS), 2) time-averaged skin temperature (TSH), 3) air temperature (T), and 4) relative humidity (RH). The air temperature and relative humidity variables are found in the “Assimilated Meteorological Fields” collection (see table 2.1) while the surface skin temperature is found in the “Single-Level Diagnostics” collection and effective surface skin temperature is found in the “Surface Flux Diagnostics” collection (see Appendix A). The instantaneous skin temperature variable is available hourly. Time-averaged skin temperature is available at 00:30 GMT, 01:30 GMT, 02:30 GMT, etc. Relative humidity and air temperature variables are available every three hours starting at 00:00 GMT. The time-

Figure 2.4: Ocean temperature measurements: February 2017. Image credit: ICOADS

averaged skin temperature was linearly interpolated to coincide with the same three hour periods as the relative humidity and air temperature variables.

The four variables used in this research were determined to be the most influential on TOA thermal radiance because, 1) in the thermal infrared region of the spectrum (8 - 14 microns), the most important gas species is water vapor due to the preferential absorption at these wavelengths, and 2) target self-emissions due to its temperature dominates effective radiance reaching the sensor in the thermal region.

Chapter 3

METHODS

To estimate TOA thermal infrared radiance, two approaches were taken, namely a physics-based approach and a machine learning approach. In total, seven models were built. Three models were developed using the physics-based approach, and four models using machine learning techniques. The first physics-based model used an atmospheric radiative transfer model with the MERRA-2 atmospheric variables mentioned in Chapter 2 as input to estimate TOA thermal radiance. Following this, a Cloud Inference Model (CIM) was evaluated which modified the physics-based model input to account for cloud formation. The last physics-based model was created using a parameterized version of the CIM model to minimize computation time. The machine learning models consisted of two regression, and two deep learning models. The first, a linear regression model (LR) was built as a baseline model for comparing against the other three supervised learning models, namely a Support Vector Regression model (SVR), a Multi-Layer Perceptron (MLP) and a Convolutional Neural Network (CNN).

All models were evaluated using the Moderate Resolution Imaging Spectroradiometer

(MODIS) [8] on-board the Terra satellite. MODIS repeatedly views regions of the Earth's surface every 1 to 2 days. Its thermal bands have a spatial resolution of 1 km at nadir. Six Terra/MODIS thermal infrared radiance scenes from band 31 (with range from 10.78 to 11.28 μm), were used for reference data. The test scenes were chosen to coincide temporally with the three-hourly air temperature and relative humidity fields in MERRA-2, and for their diverse cloud cover, land cover, and season.

Each scene was bi-linearly down-sampled to the same spatial resolution as MERRA-2 data and georegistered onto the respective predicted TOA radiance maps from the seven modeling methods. Figure 3.1 displays the Terra/MODIS test scenes (in RGB) that were used for evaluating all models.

3.1 Physics-based Approach

The first approach to derive TOA radiance from MERRA-2 data involved the use of a physics model. The MODerate resolution atmospheric TRANsmission model (MODTRAN) [9] was developed by Spectral Sciences, Inc (SSI) and the Air Force Research Laboratory (AFRL). It is used for the prediction and analysis of optical measurements through the atmosphere. MODTRAN uses absorption and scattering models to propagate radiance through the atmosphere. The atmosphere is modeled as a series of homogeneous layers, where the temperature of each layer is provided by user-supplied radiosonde data or one of six preset atmospheric profiles. Air pressure and relative humidity profiles are used to estimate the concentration of the permanent gases and water vapor (either pre-defined or user-specific profiles).

Figure 3.1: The Terra/MODIS test scenes in RGB

3.1.1 Atmospheric Radiative Transfer Model

The first method of calculating TOA radiance involved using MERRA-2 atmospheric parameters directly as input to MODTRAN. To specify the atmospheric profile, air temperature and dew point temperature profiles are needed. Since relative humidity is the ratio of how much moisture is in the atmosphere to how much moisture the atmosphere could hold at that temperature, the dew point was calculated using the MERRA-2 air temperature and the relative humidity variables. Using an approximation of the Clausius-Clapeyron equation [10] the dew point (DP) can be calculated by:

$$DP = \frac{237.3 * B}{1 - B} \quad [^{\circ}C] \quad (3.1)$$

where

$$B = \left(\ln \left(\frac{RH}{100} \right) + \left(\frac{17.27 * T}{237.3 + T} \right) \right) / 17.27 \quad (3.2)$$

and RH is the relative humidity in percent and T is the air temperature in degrees centigrade.

Initially the lowest level of MERRA-2 was used as ground elevation (pressure converted to distance above sea level). However, since MERRA-2 levels are of fixed pressure (and therefore height), the ASTER global 30 arc second digital elevation dataset (DEM) [11] was used for ground elevation. The DEM (approximately 1 kilometer spatial resolution) is produced by NASA's Earth Science Data Systems Program and available through the Spatial Data Access Tool (SDAT) [12]. The elevation ranges from -407 to 8752 meters with oceans masked as no data.

The importance of using the correct elevation was evaluated by changing only the altitude and skin temperature variables and keeping all other atmospheric variables the same for various MODTRAN simulations. Table 3.1 displays the difference in TOA thermal radiance between sea level and 1km above sea level at various temperature settings using MODTRAN.

Since the air temperature profiles start at 2 meters above ground level, the lowest air temperature values were updated to the skin temperature variables before entering the profiles into MODTRAN Card 3, along with the dew point profiles. The ground altitude, from ASTER's DEM, was entered into Card 2. The emissivity, taken from the ASTER global emissivity database [13], are converted to albedo and entered into Card 1, along

Table 3.1: Thermal radiance comparison at various altitudes and temperatures

Temperature Kelvin	Seal level $W/m^2 sr \mu m$	1 Km $W/m^2 sr \mu m$	Difference $W/m^2 sr \mu m$
240	4.91	4.02	0.89
260	5.95	5.34	0.61
280	7.27	7.02	0.25
300	8.87	9.05	-0.18
320	10.77	11.46	-0.69

with the skin temperature. MODTRAN simulations were run for wavelengths between 10.540 microns and 11.536 microns to coincide with the MODIS band 31 relative spectral response (RSR). The band-effective radiance was calculated by:

$$L = \frac{\int L_{\lambda} R(\lambda) d\lambda}{\int R(\lambda) d\lambda} \quad \left[\frac{W}{m^2 sr \mu m} \right] \quad (3.3)$$

where L_{λ} is the spectral radiance reaching the sensor, and $R(\lambda)$ is the MODIS band 31 normalized spectral response function.

3.1.2 Cloud Inference Model

At-sensor radiance when clouds are present, are challenging to predict. Several built-in cloud models are available in MODTRAN to assist in modeling TOA radiance when clouds are present. However, to use these functions, prior knowledge of cloud type, cloud thickness and base height is required.

To determine the characteristics of an air and dew point temperature profile that would produce a visible cloud in thermal infrared imagery, twenty MERRA-2 profiles were examined in which the corresponding location in MODIS imagery showed an obvious cloud. Figure 3.2 displays the profiles of two grid points where clouds were present. The MODIS

Figure 3.2: Air temperature and dew point profile for two grid points where cloud is present.

Cloud Mask was used as reference. The MODIS cloud mask (MOD35.L2), containing data collected from the Terra platform, is produced as an Earth Observing System (EOS) standard product. The cloud mask product consists of information regarding surface obstruction and various ancillary information affecting surface and cloud retrievals such as sun glint, land/water flag and non-terrain shadows. To determine if a cloud was present, only pixels indicating *cloudy* were used. Clouds were inferred to be present when: 1) the air temperature and dew point temperature were within 0.3 Kelvin of one another at any given point in the profile (left graph in Figure 3.2) and 2) the air temperature and dew point temperature were within 0.9 Kelvin of one another for a continuous 4 km in the atmosphere (right graph in Figure 3.2). These thresholds were determined by optimizing on various scenes using the MODIS cloud mask as reference. This was done by running simulations at various thresholds and using the threshold combination that yielded the lowest RMSE when compared to Terra/MODIS TOA radiance values.

When a cloud was present, the MERRA-2 atmospheric profile was adjusted such that

only the profile above the altitude where the cloud was inferred was used. These shortened profiles, along with the complete profiles of data where no clouds were found, were used as input for MODTRAN Card 3. The air temperature at the lowest level of the shortened profiles were used as skin temperature input in Card 1.

3.1.3 Parameterized Model

The forward modeling methods described in Sections 3.1.1 and 3.1.2 require running MODTRAN with the appropriate MERRA-2 values for every pixel in the scene of interest. Since a typical scene will have hundreds of thousands of pixels, running MODTRAN for each pixel can be computationally expensive. To reduce computational time, equations were created to model MODTRAN predictions. Hundreds of MODTRAN simulations at various temperature and altitude settings were plotted. A single atmospheric model was used for all simulations. Simulations were run for wavelengths between 10.540 microns and 11.536 microns to coincide with the MODIS band 31 relative spectral response (RSR). The lines in Figure 3.3 each represent a single altitude (ranging from 0 km to 12 km) with points on the lines representing different temperatures (ranging from 190K to 320K).

To create functions that can easily be applied to the MERRA-2 data, the slopes and intercepts of these lines were plotted and equations fitted to them. Figure 3.4 displays the fitted equations used to model the TOA radiance by:

$$L = m \times BB + b \quad [W/m^2 \text{ sr } \mu m] \quad (3.4)$$

Figure 3.3: Predicted MODTRAN TOA radiance vs. Blackbody radiance at various altitudes. Each line represent a different altitude. Points along each line represent different temperatures.

Figure 3.4: Equations fitted to the slopes and intercepts of the lines in Figure 3.3 where b represents the intercepts, m represents the slopes and x the altitude in km.

with

$$m = 0.6476 + 0.1992x - 0.0484x^2 + 0.006x^3 - 0.0004x^4 \quad (3.5)$$

$$b = 2.685e^{-0.7317x} + 0.025 \quad (3.6)$$

where x is the altitude above sea level in kilometer and BB is the blackbody radiance calculated using Planck's equation [14] for the given temperature and wavelength of $10.97\mu m$ (Terra/MODIS band 31, band center).

3.2 Machine Learning Models

Machine learning involves finding a mathematical model that relates a set of input variables (MERRA-2 air temperature, relative humidity and skin temperature variables) to

an output variable (TOA thermal infrared radiance). When machine learning models are trained with known output variables (labels), it is called supervised learning. The Terra/MODIS TOA thermal radiance values were used as labels to train all machine learning models.

The training set for all the machine learning models consisted of 44 temporally and spatially coincident Terra/MODIS and MERRA-2 scenes. At the MERRA-2 spatial resolution (of approx. 50 by 70 km) this led to 11255 training instances, of which a random 10% was used for validating (i.e., tuning hyper-parameters) the deep learning models. Reference data (training labels) consisted of the down-sampled Terra/MODIS band 31 radiance pixel values. Only data within ± 20 degree Field of View (FOV) of the MODIS scene center were used to minimize view-angle effects [15]. Models were validated by applying the trained models to 1756 disjoint test instances (not part of the training or validation set). These test instances were taken from the same six Terra/MODIS test scenes used in the physics-based model evaluations.

3.2.1 Linear Regression Model

The first machine learning approach used to estimate TOA thermal radiance was a least squares linear regression model, which serves as a simple baseline model for assessing the relative performance of the other methods. This regression model is given by

$$\hat{y} = \mathbf{w}^T \mathbf{x} + b, \quad (3.7)$$

where $\mathbf{x}$ is the input (i.e., MERRA-2 temperatures and relative humidity variables), b and $\mathbf{w}$ are parameters (or weights) learned from training data, and $\hat{y}$ is the predicted TOA

thermal radiance. Note that the bias (or intercept) term b can be incorporated into $\mathbf{w}$ by simply appending a ‘1’ to $\mathbf{x}$. The parameters are estimated by minimizing the expected error between the Terra/MODIS TOA thermal radiance reference data and the predicted radiance values over the complete training set:

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{i=1}^n \left((y_i - \mathbf{w}^T \mathbf{x}_i)^2 + \alpha \|\mathbf{w}\|_2^2 \right), \quad (3.8)$$

where n is the total number of $(\mathbf{x}_i, y_i)$ training data points and $\alpha \|\mathbf{w}\|_2$ incorporates L2 (ridge) regularization to prevent overfitting, with α controlling the strength of the regularization [16]. For simplicity, in Equation 3.8, the bias term b has been incorporated into $\mathbf{w}$. This optimization can be solved analytically using the Moore-Penrose pseudo-inverse [17]. Data used in this model was not normalized, thus all variables were left unchanged (i.e., temperature variables in Kelvin and relative humidity values between zero and one).

3.2.2 Support Vector Regression Model

SVR [18] is an extension of the Support Vector Machine (SVM) to regression problems, and it can make more complex predictions than the linear regression model. A one dimensional example of SVR is shown in Figure 3.5, where the data points represent the predicted values ($\hat{y}$) and the line represents the truth/reference/label (y) data. The two dashed lines are the bounds that are ϵ distance away from the reference data, where ϵ is a parameter chosen by the user. SVR uses only values outside the dashed lines to build the model. Training an SVR means solving:

$$\text{minimize} \quad \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n (\xi_i^* + \xi_i) \quad (3.9)$$

$$\text{subject to } \begin{cases} y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle - b \leq \epsilon + \xi_i^* \\ \langle \mathbf{w}, \mathbf{x}_i \rangle + b - y_i \leq \epsilon + \xi_i \end{cases}$$

where $\mathbf{w}$ is the learned weight vector, $\mathbf{x}_i$ is the i -th training instance, y_i is the training label, and ξ_i the distance between the bounds and predicted values outside the bounds. C is another parameter set by the user that is a constraint controlling the penalty imposed on observations outside the bounds to prevent overfitting.

To make the model capable of non-linear predictions, every dot/inner product $\langle \mathbf{w}, \mathbf{x}_i \rangle$ is replaced by a radial basis function (RBF) kernel to map the data to a higher dimensional feature space. Without the use of a kernel (i.e., linear SVR), the main difference between it and Linear regression is that SVR uses only a subset of the data, ignoring the points close to the model's prediction, and SVR's optimization does not depend on the dimensionality of the input space. The machine learning toolbox scikit-learn [19] implementation was used for the calculations.

Training and test data sets were the same as used in the Linear Regression model. Because of the distance calculation performed by the RBF kernel, the input features needed to be scaled to the same interval. Therefore, the data was normalized by dividing all temperature variables by the global maximum temperature, so that all training variables ranged in values between zero and one.

3.2.3 Multi-Layer Perceptron

While linear regression can only model linear functions, artificial neural networks (ANNs) are universal function approximators [20]. A feedforward Multi-Layer Perception (MLP) ANN consists of an input layer (i.e., the input variables), hidden layer(s), and an output layer. Each layer has a number of units (or neurons) within it, and these have learnable

Figure 3.5: Schematic of one dimensional SVR model. Only the points outside of the ‘tube’ are used for making predictions.

parameters (weights). Formally, the five-layer neural network model used here is given by:

$$\hat{y} = \sigma \left(\mathbf{w}^T \sigma \left(\mathbf{H}_5^T \sigma \left(\mathbf{H}_4^T \sigma \left(\mathbf{H}_3^T \sigma \left(\mathbf{H}_2^T \sigma \left(\mathbf{H}_1^T \mathbf{x} \right) \right) \right) \right) \right) \right), \quad (3.10)$$

where $\mathbf{H}_j$ are matrices containing the parameters for the hidden layers (the columns contain the weights for each unit), $\mathbf{x}$ is the input, and $\sigma(\cdot)$ is an ‘activation’ function that is applied element-wise, which enables the model to make non-linear predictions. Note that the bias term for each layer has been dropped to simplify the notation. If all hidden layers and activation functions are identity functions, then the MLP will be identical to the Linear Regression model. The rectified linear unit (ReLU) activation function [21], $\sigma(v) = \max(v, 0)$ was used, which sets all negative values to zero. ReLU is simple and tends to work significantly better than sigmoidal activation functions, and it was one of

Figure 3.6: The architecture of the MLP model used in this research.

the innovations that enabled deep neural networks. Figure 3.6 displays a schematic of the network architecture indicating the size of each fully connected layer.

To find values for MLP’s parameters that produce a good fit to the training data, the error between the model’s predictions and the training data must be minimized, which is described by a loss function. However, unlike SVR and Linear Regression, it is not possible to find the global minima, but a local optima can be found using error backpropagation. To do this with the MLP model, mean squared loss was minimized. The initial learning rate used with backpropagation (how much to update the weights in the direction to decrease the gradient) of 0.001 was reduced ($\times 0.1$) when the validation loss did not decrease for five consecutive epochs (iteration of going through the whole dataset). To train and run the network, Keras [22] with the Theano [23] back-end was used in Python.

Each training instance consisted of the air temperature and relative humidity profiles (27 layers each), and instantaneous and time-averaged skin temperature.

Because many applications need higher spatial resolution, the MLP model was trained at three different spatial resolutions. The low-resolution model was trained at the same spatial resolution as the MERRA-2 data. The medium-resolution model was trained at 10 times higher spatial resolution than the low-resolution model, which corresponds to a pixel size of about 5×7 km at the equator. Since Terra/MODIS has a higher spatial resolution (1×1 km) than the medium-resolution model, Terra/MODIS still needed to be down-sampled, but to a lesser extent. The high-resolution model was trained at Terra/-

MODIS resolution, which was done by up-sampling the MERRA-2 data to Terra/MODIS resolution.

3.2.4 Convolutional Neural Network

MLP's do not explicitly encode spatial information, i.e., the features neighboring a particular latitude/longitude are ignored. The neighborhood information may improve the model's ability to make predictions. Convolutional neural networks (CNNs) are capable of including neighboring spatial information in a computationally efficient manner. A CNN is similar to an MLP. However, the hidden units are replaced by learnable filters that are convolved with the input from the previous layer. The training and test instances for the CNN were created using a 9×9 window around the spatial location of interest.

The CNN model, shown in Figure 3.7, consisted of only two convolutional layers, and then a fully-connected output layer. After each hidden layer, the output was down-sampled with mean pooling, reducing its dimensionality. The mean pooling layer performs down-sampling by dividing the input into rectangular pooling areas and computing the average of each area. Two regularization techniques were used to prevent overfitting: batch normalization [24] and drop-out [25]. Both were applied only after the first convolutional layer for both models. All zero air temperature values (where no data exists due to land above sea level) were replaced with the instantaneous skin temperature. More convolutional layers added to the second CNN did not improve the model in experiments.

Figure 3.7: Architecture of CNN with lowest RMSE.

3.3 Methods summary

To estimate sensor reaching thermal radiance, seven models were developed using both physics-based and machine learning approaches with MERRA-2 variables as input to the models. The first physics-based approach used the atmospheric radiative transfer model MODTRAN to predict TOA radiance. The next model accounted for clouds by calculating dew point depressions to infer the presence of clouds for each atmospheric profile, before using MODTRAN to predict TOA thermal radiance with the adjusted cloud profiles. Next, since running MODTRAN for all pixels in a scene is computationally expensive, a parameterized model was created to estimate MODTRAN predictions given a certain skin temperature and altitude. The machine learning models were trained using 44 Terra/MODIS band 31 scenes with the temporally and spatially coincident MERRA-2 data as input to the models. The first machine learning model, Linear regression, was used as a baseline model for comparison to the other supervised training models, namely a support vector regression, multi-layer perceptron and convolutional neural network. Since Terra/MODIS band 31 was used as reference, models were built to predict TOA thermal radiance with center wavelength $10.97\mu m$ (corresponding to Terra/MODIS band 31 band center).

Chapter 4

RESULTS AND DISCUSSION

This research used the four MERRA-2 variables (described in Chapter 2) as input to the 7 methods (described in Chapter 3) to predict TOA thermal infrared radiance. Terra/MODIS thermal data band 31 was used as a reference since it is well calibrated [26] with a calibration uncertainty of less than 0.13%. Therefore, predicted TOA radiance images were produced for each of the Terra/MODIS scenes displayed in Figure 3.1. The RMSE, standard deviation, and mean error was calculated between the MODIS reference and the predicted TOA for each model to assess the accuracy of each model over a range of scene content and atmospheric types. Another error metric used to analyze the models was the percent error in the prediction. The percent errors were divided into seven radiance ranges based on the reference data radiance values (ranging from between 1.5 and 14 $W/m^2 sr \mu m$).

4.1 Model assessment on six test scenes

For each of the Terra/MODIS test scenes, the predicted TOA radiances from the seven methods were compared to the Terra/MODIS band 31 radiance product. The six Terra/MODIS scenes spanned a range of material type (land, water, clouds) and atmospheric type to assess the models' performance on representative Earth scenes. Errors are reported in root-mean-square-error (RMSE) as this represents the difference between predicted and observed thermal infrared radiance values in $W/m^2 sr \mu m$. To visualize the results, Figures 4.2 to 4.7 display predicted TOA thermal infrared data for each of the test images for the various models. The Terra/MODIS reference image resampled to MERRA-2 resolution is displayed top left, followed by the predicted TOA thermal infrared radiance images of the atmospheric radiative transfer model (ARTM), the Cloud Inference Model (CIM) and on the right the Parameterized Model (PM). The bottom row displays the Linear Regression Model (LR), the Support Vector Regression (SVR), the Multi-Layer Perceptron (MLP), and on the bottom right the Convolutional Neural Network (CNN) predicted thermal radiance images.

All images are displayed for the model predictions at the MERRA-2 spatial resolution (approx. 50 by 70 km). Please note the images display the full scene but statistics are only calculated on the ± 20 degree field-of-view (FOV) from nadir of the MODIS scene center to minimize effects due to view-angle through the atmosphere. Tables 4.1 to 4.6 display the RMSE, standard deviation and mean error for each of the test scenes. The mean error was calculated by subtracting the predicted model values from the Terra/MODIS radiance values. Therefore, when the mean value is negative, the model over predicted the radiance. The second column of the tables reports the total errors for each scene. Columns three to

Figure 4.1: Terra/MODIS RGB image on the left with Terra/MODIS thermal image on the right.

five display the errors for the various land cover classifications. Columns without results are due to no land/water evaluated in that specific scene (e.g. the Indian ocean scene in Figure 4.7 did not produce any results over land since the ± 20 degree FOV of this scene only consisted of water pixels).

The MODIS Land Cover maps [27] and Cloud Mask were used to classify land, water and cloud cover. For example, to calculate the errors where clouds were present, only test instances were evaluated where the MODIS Cloud Mask indicated *cloudy*. To calculate errors over land and water, only test instances where the MODIS Cloud Mask indicated *probably clear* and *confident clear* were evaluated.

Darker pixels in thermal imagery are due to low radiance values. As mentioned in Chapter 2, target self-emissions due to its temperature dominates effective radiance reaching the sensor in the thermal region. Therefore, low pixel values can be interpreted as clouds present in the scene due to the cold temperature of clouds. An example can be seen in Figure 4.1 where the Terra/MODIS RGB image is displayed on the left and the Terra/MODIS thermal band 31 image is displayed on the right.

Table 4.1: RMSE, Standard deviation (STD) and Mean error [Mean] in $W/m^2 sr \mu m$ for scene Middle East, 08:55 GMT, 31 July 2013.

Model	Total RMSE (STD) [Mean]	Land RMSE (STD) [Mean]	Water RMSE (STD) [Mean]	Cloud RMSE (STD) [Mean]
ARTM	1.61 (1.50) [-0.58]	0.84 (0.77) [0.36]	0.85 (0.75) [-0.41]	3.24 (1.45) [-2.90]
CIM	1.55 (1.46) [-0.52]	0.83 (0.75) [0.37]	0.85 (0.75) [-0.41]	3.10 (1.57) [-2.68]
PM	1.62 (1.58) [-0.34]	1.02 (0.83) [0.58]	0.64 (0.63) [-0.07]	3.26 (1.61) [-2.84]
Linear Reg	1.14 (1.13) [-0.17]	0.86 (0.78) [0.36]	0.58 (0.58) [-0.07]	2.11 (1.41) [-1.58]
SVR	1.36 (1.31) [-0.38]	1.06 (0.87) [0.60]	1.22 (0.78) [-0.94]	2.05 (1.43) [-1.49]
MLP-low-res	1.25 (1.24) [0.20]	1.33 (0.85) [1.02]	0.89 (0.86) [-0.23]	1.60 (1.38) [-0.83]
CNN	1.36 (1.26) [-0.51]	0.74 (0.73) [0.14]	0.73 (0.66) [-0.30]	2.72 (1.43) [-2.31]

Figure 4.2: Visualization of scene in Middle East, 08:55 GMT, 31 July 2013. Top row: Terra/MODIS reference image, ARTM, CIM, and PM model predictions. Bottom row: LR, SVR, MLP-low-res, and CNN model predictions.

Looking at the results of the first scene (the Middle East imaged at 08:55 GMT in summer) in Table 4.1, the MLP model performed the best when clouds were present, with the linear regression (LR) model having the lowest overall RMSE. Visual inspection of Figure 4.2 suggests that the ARTM model did not predict clouds well since no built-in cloud models were applied to MODTRAN simulations as discussed in Chapter 3.

Table 4.2: RMSE, Standard deviation (STD) and Mean error [Mean] in $W/m^2 sr \mu m$ for scene Chilean Coast, 15:00 GMT, 15 January 2014.

Model	Total RMSE (STD) [Mean]	Land RMSE (STD) [Mean]	Water RMSE (STD) [Mean]	Cloud RMSE (STD) [Mean]
ARTM	0.69 (0.64) [-0.24]	1.00 (0.64) [0.78]	0.45 (0.45) [0.02]	0.76 (0.37) [-0.67]
CIM	0.61 (0.62) [0.01]	1.00 (0.64) [0.78]	0.63 (0.57) [0.26]	0.47 (0.33) [-0.34]
PM	0.64 (0.62) [0.15]	1.01 (0.59) [0.83]	0.74 (0.64) [0.37]	0.39 (0.36) [-0.16]
Linear Reg	0.79 (0.66) [0.44]	1.42 (0.79) [1.18]	0.83 (0.59) [0.59]	0.54 (0.52) [0.16]
SVR	0.83 (0.79) [-0.24]	1.59 (0.98) [1.26]	0.64 (0.64) [-0.04]	0.76 (0.27) [-0.71]
MLP-low-res	0.66 (0.65) [0.08]	1.33 (0.87) [1.02]	0.59 (0.53) [0.28]	0.47 (0.40) [-0.26]
CNN	0.86 (0.86) [-0.07]	1.77 (0.89) [1.54]	0.67 (0.67) [0.10]	0.73 (0.51) [-0.52]

Figure 4.3: Visualization of scene Chilean Coast, 15:00 GMT, 15 January 2014. Top row: Terra/MODIS reference image, ARTM, CIM, and PM model predictions. Bottom row: LR, SVR, MLP-low-res, and CNN model predictions.

All models performed nearly the same on the next scene off the Chilean coast at 15:00 GMT (results in Table 4.2 and Figure 4.3) since there were not many clouds present. The CIM model had the lowest RMSE followed closely by the parameterized model, the MLP model and the ARTM model. All models displayed high errors over land which might be due to large temporal temperature fluctuations in this desert scene in summer.

Table 4.3: RMSE, Standard deviation (STD) and Mean error [Mean] in $W/m^2 sr \mu m$ for scene Egypt, 09:00 GMT, 12 March 2014.

Model	Total RMSE (STD) [Mean]	Land RMSE (STD) [Mean]	Water RMSE (STD) [Mean]	Cloud RMSE (STD) [Mean]
ARTM	1.59 (1.56) [0.33]	1.00 (0.61) [0.80]	- (-) [-]	4.01 (1.82) [-3.59]
CIM	1.59 (1.56) [0.33]	1.00 (0.61) [0.80]	- (-) [-]	4.01 (1.82) [-3.59]
PM	1.67 (1.64) [0.34]	1.06 (0.66) [0.83]	- (-) [-]	4.15 (1.94) [-3.69]
Linear Reg	1.51 (1.32) [0.73]	1.22 (0.48) [1.12]	- (-) [-]	3.11 (1.75) [-2.60]
SVR	1.32 (1.30) [-0.02]	0.61 (0.59) [0.16]	- (-) [-]	3.78 (1.72) [-3.38]
MLP-low-res	1.25 (1.24) [0.14]	0.72 (0.53) [0.49]	- (-) [-]	3.32 (1.59) [-2.93]
CNN	1.52 (1.41) [0.58]	1.13 (0.51) [1.01]	- (-) [-]	3.42 (1.71) [-2.98]

Figure 4.4: Visualization of scene Egypt, 09:00 GMT, 12 March 2014. Top row: Terra/MODIS reference image, ARTM, CIM, and PM model predictions. Bottom row: LR, SVR, MLP-low-res, and CNN model predictions.

Both the ARTM and CIM models performed the same on the desert scene in Egypt (09:00 GMT, winter), since the CIM model inferred no cloud presence (see Table 4.3). This could be due to incorrect MERRA-2 temperature and relative humidity profiles, or incorrect assumptions made by the CIM model. Clouds are slightly visible in the LR, SVR and MLP models in Figure 4.4. The MLP-low-res model performed the best.

Table 4.4: RMSE, Standard deviation (STD) and Mean error [Mean] in $W/m^2 sr \mu m$ for scene Southern Africa, 08:55 GMT, 1 October 2014.

Model	Total RMSE (STD) [Mean]	Land RMSE (STD) [Mean]	Water RMSE (STD) [Mean]	Cloud RMSE (STD) [Mean]
ARTM	0.86 (0.77) [0.38]	0.93 (0.7) [0.61]	0.50 (0.49) [-0.14]	1.18 (1.01) [-0.67]
CIM	0.86 (0.77) [0.38]	0.93 (0.7) [0.61]	0.50 (0.49) [-0.14]	1.18 (1.01) [-0.67]
PM	1.04 (0.89) [0.55]	1.16 (0.76) [0.88]	0.46 (0.42) [-0.21]	1.26 (1.02) [-0.81]
Linear Reg	1.10 (0.73) [0.83]	1.18 (0.73) [0.93]	0.82 (0.52) [0.63]	1.11 (1.16) [0.09]
SVR	0.71 (0.70) [-0.11]	0.70 (0.68) [-0.18]	0.65 (0.64) [0.12]	1.19 (1.21) [-0.28]
MLP-low-res	0.70 (0.67) [0.22]	0.67 (0.64) [0.19]	0.72 (0.64) [0.34]	1.10 (1.15) [-0.02]
CNN	0.85 (0.77) [0.37]	0.89 (0.76) [0.46]	0.63 (0.61) [0.19]	1.26 (1.26) [-0.39]

Figure 4.5: Visualization of scene Southern Africa, 08:55 GMT, 1 October 2014. Top row: Terra/MODIS reference image, ARTM, CIM, and PM model predictions. Bottom row: LR, SVR, MLP-low-res, and CNN model predictions.

The next scene was imaged at 08:55 GMT during summer in Southern Africa. Even though clouds are visible in this scene (Figure 4.5) in both the CIM and PM models, the 20 degree FOV constraint did not include cloudy areas in the data, thus the ARTM and CIM model had the same predictions. Most models produced errors less than $1 W/m^2 sr \mu m$ (corresponding to approx. 10 Kelvin).

Table 4.5: RMSE, Standard deviation (STD) and Mean error [Mean] in $W/m^2 sr \mu m$ for scene Russia, Mongolia and China, 03:00 GMT, 1 April 2015.

Model	Total RMSE (STD) [Mean]	Land RMSE (STD) [Mean]	Water RMSE (STD) [Mean]	Cloud RMSE (STD) [Mean]
ARTM	1.18 (1.18) [-0.10]	0.77 (0.60) [0.49]	- (-) [-]	1.85 (1.14) [-1.46]
CIM	1.36 (1.24) [0.57]	1.11 (0.84) [0.73]	- (-) [-]	1.79 (1.79) [0.16]
PM	1.32 (1.28) [0.33]	1.02 (0.90) [0.48]	- (-) [-]	1.81 (1.82) [-0.07]
Linear Reg	1.61 (1.14) [1.14]	1.45 (0.80) [1.21]	- (-) [-]	1.85 (1.63) [0.89]
SVR	1.49 (1.44) [-0.38]	1.13 (1.03) [-0.48]	- (-) [-]	2.09 (2.08) [-0.27]
MLP-low-res	1.09 (1.01) [-0.41]	0.74 (0.69) [-0.27]	- (-) [-]	1.61 (1.43) [-0.83]
CNN	1.03 (1.00) [0.26]	0.86 (0.68) [0.53]	- (-) [-]	1.34 (1.28) [-0.39]

Figure 4.6: Visualization of scene Russia, Mongolia and China, 03:00 GMT, 1 April 2015. Top row: Terra/MODIS reference image, ARTM, CIM, and PM model predictions. Bottom row: LR, SVR, MLP-low-res, and CNN model predictions.

Figure 4.6 displays the test scene over Russia, Mongolia and China at 03:00 GMT in spring with prediction errors in Table 4.5. The CNN performed better both overall, and where clouds were present. However, the CNN produced a blurred (averaged) estimated radiance image, which could be explained by the use of spatial information around the pixel of interest to train the model. Like the other test scene results, all models over-estimated cloud radiance (higher/warmer) compared to the Terra/MODIS reference values. Since this scene were taken over land only, no results are reported over water.

Table 4.6: RMSE, Standard deviation (STD) and Mean error [Mean] in $W/m^2 sr \mu m$ for scene Indian Ocean, 05:55 GMT, 22 May 2014.

Model	Total RMSE (STD) [Mean]	Land RMSE (STD) [Mean]	Water RMSE (STD) [Mean]	Cloud RMSE (STD) [Mean]
ARTM	2.65 (2.23) [-1.45]	- (-) [-]	0.37 (0.32) [-0.19]	3.91 (2.60) [-2.93]
CIM	3.17 (3.17) [0.28]	- (-) [-]	2.43 (2.33) [0.74]	3.84 (3.84) [-0.31]
PM	2.77 (2.77) [-0.16]	- (-) [-]	1.90 (1.83) [0.53]	3.50 (3.36) [-1.03]
Linear Reg	2.03 (2.02) [0.18]	- (-) [-]	1.32 (0.79) [1.06]	2.64 (2.51) [-0.86]
SVR	1.94 (1.93) [-0.27]	- (-) [-]	0.93 (0.74) [0.56]	2.69 (2.40) [-1.25]
MLP-low-res	2.03 (2.02) [0.20]	- (-) [-]	1.31 (0.56) [1.19]	2.65 (2.47) [-0.97]
CNN	2.04 (2.05) [-0.01]	- (-) [-]	1.17 (0.69) [0.94]	2.75 (2.51) [-1.15]

Figure 4.7: Visualization of scene Indian Ocean, 05:55 GMT, 22 May 2014. Top row: Terra/MODIS reference image, ARTM, CIM, and PM model predictions. Bottom row: LR, SVR, MLP-low-res, and CNN model predictions.

Figure 4.7 displays the last test scene taken over the Indian ocean between India and Africa at 05:55 GMT in spring. Looking at the results of this scene in Table 4.6, it is interesting to note that the ARTM model performed significantly better than the CIM

Figure 4.8: MODIS cloud mask on the left with the CIM model cloud predictions for scene Indian Ocean, 05:55 GMT, 22 May 2014 on the right.

model. This was investigated and found that the inference of cloud in this scene by the CIM model was rather inaccurate. Figure 4.8 displays the MODIS cloud mask on the left with the predicted clouds of the CIM model on the right for this scene. Since clouds were incorrectly predicted, the error over water was also high for the CIM model. None of the models estimated TOA thermal infrared radiance well for this scene, with the SVR having the lowest RMSE of $1.94 \text{ W/m}^2 \text{ sr } \mu\text{m}$.

Comparing the RMSE's (total column) of the six test scenes, five of the seven models produced the lowest RMSE per scene (namely the LR, CIM, MLP, CNN and SVR models). However, the MLP-low-res model produced the lowest errors on two scenes and were closely second on three other scenes. Radiance values over water were generally best estimated by the ARTM model with an RMSE of $0.58 \text{ W/m}^2 \text{ sr } \mu\text{m}$, compared to the MLP-low-res model with an RMSE of $0.95 \text{ W/m}^2 \text{ sr } \mu\text{m}$. Over land and cloudy scenes the MLP-low-res model produced the lowest errors.

Table 4.7 displays the RMSE, standard deviation and mean error associated with the combined results of all six test scenes for all models. Overall, the MLP-low-res model has

Table 4.7: RMSE, Standard deviation (STD) and Mean error [Mean] in $W/m^2 sr \mu m$ for various land and cloud cover for the combined 6-scene dataset.

Model	Total RMSE (STD) [Mean]	Land RMSE (STD) [Mean]	Water RMSE (STD) [Mean]	Cloud RMSE (STD) [Mean]
ARTM	1.52 (1.50) [-0.26]	0.90 (0.67) [0.59]	0.58 (0.55) [-0.19]	2.67 (1.89) [-1.88]
CIM	1.67 (1.66) [0.18]	0.99 (0.74) [0.67]	1.44 (1.43) [0.14]	2.59 (2.49) [-0.71]
PM	1.60 (1.60) [0.15]	1.04 (0.81) [0.70]	1.16 (1.14) [0.20]	2.51 (2.33) [-0.92]
Linear Reg	1.41 (1.30) [0.55]	1.25 (0.76) [1.00]	0.94 (0.77) [0.54]	1.95 (1.93) [-0.30]
SVR	1.34 (1.31) [-0.27]	0.93 (0.93) [-0.01]	0.92 (0.92) [-0.10]	2.10 (1.86) [-0.98]
MLP-low-res	1.22 (1.22) [0.04]	0.86 (0.81) [0.29]	0.95 (0.86) [0.41]	1.86 (1.68) [-0.79]
CNN	1.31 (1.31) [0.10]	0.97 (0.75) [0.62]	0.85 (0.82) [0.24]	2.03 (1.76) [-1.01]

the lowest RMSE errors over land and cloudy scenes respectively.

For most scenes, clouds (dark pixels) are clearly visible in the Cloud Inference Model and the parameterized model, but not in the ARTM model. Clouds are also visible in the Linear Regression, SVR and MLP-low-res models. However, the CNN produced estimated radiances that are more averaged over the scene, which can be explained by the use of spatial information around the pixel of interest to train the model.

Overall, the machine learning models performed better than the physics-based models. The final supervised training models all used only 27 layers of air temperature and relative humidity profile data. This corresponds to about 21 km above sea level which is in the lower stratosphere. Models with fewer layers (just troposphere) did not perform as well which could indicate that the atmospheric profiles into the lower stratosphere affect TOA thermal radiance.

No data normalization techniques applied resulted in a lower error for the MLP-low-res model and thus the training data were not normalized. Various architectures and data normalization techniques tested with resulting RMSE, are displayed in Appendix B.

Since some applications may require higher spatial resolution, the final MLP low resolution model was rebuilt at different spatial resolutions. Overall, the MLP-low-res model

Table 4.8: MLP results at various resolutions ($W/m^2 sr \mu m$)

Model	Resolution	RMSE
MLP-low-res	$0.5^\circ \times 0.625^\circ$	1.22
MLP-med-res	$0.05^\circ \times 0.0625^\circ$	1.24
MLP-high-res	$0.01^\circ \times 0.01^\circ$	1.48

had the lowest RMSE of $1.22 W/m^2 sr \mu m$. The MLP-med-res model had slightly higher errors than the MLP-low-res model, while the MLP-high-res model performed the worst. This could be due to the significant up-sampling of the MERRA-2 data (interpolating each pixel from approx. 50×70 km to 1×1 km gsd). Table 4.8 displays the RMSE for the MLP models at the various resolutions. In the best MLP-med-res and MLP-high-res models, all zero air temperature values were replaced with the instantaneous skin temperature values, as described in Section 3.2.4.

4.2 Prediction error percentage

The percent prediction error was also used as an error metric. The percent error was calculated for the combined dataset as the absolute value of the difference between Terra/MODIS radiance and Model Predicted, divided by Terra/MODIS radiance, as per Equation 4.1.

$$\text{error} = \frac{|\text{Terra/MODIS} - \text{Model Predicted}|}{\text{Terra/MODIS}} \quad [\%] \quad (4.1)$$

This was calculated for several radiance ranges as can be seen in Table 4.9. The apparent (blackbody) temperature ranges corresponding to the radiance ranges at wavelength 10.97 microns (Terra/MODIS band 31 center wavelength) are displayed in the table below

Table 4.9: % error per radiance band

Radiance Range	1.5 to <2 $W/m^2 sr \mu m$	2 to <4 $W/m^2 sr \mu m$	4 to <6 $W/m^2 sr \mu m$	6 to <8 $W/m^2 sr \mu m$	8 to <10 $W/m^2 sr \mu m$	10 to <12 $W/m^2 sr \mu m$	12 to <14 $W/m^2 sr \mu m$
Blackbody Temperature	211 to <221 Kelvin	221 to <250 Kelvin	250 to <271 Kelvin	271 to <288 Kelvin	288 to <303 Kelvin	303 to <316 Kelvin	316 to <328 Kelvin
# of pixels	12	90	141	405	696	398	14
ARTM	395 %	107 %	37 %	10 %	6 %	8 %	10 %
CIM	176 %	74 %	44 %	10 %	9 %	8 %	10 %
PM	210 %	75 %	45 %	9 %	8 %	10 %	14 %
Linear Reg	267 %	74 %	43 %	10 %	10 %	10 %	10 %
SVR	290 %	71 %	38 %	12 %	8 %	5 %	11 %
MLP-low-res	281 %	64 %	27 %	9 %	8 %	6 %	8 %
CNN	286 %	64 %	36 %	8 %	9 %	8 %	10 %

the radiance range for reference. The number of pixels used in each range to calculate the percent error are also displayed. From the table it can be seen that very large errors occur when the radiance values are below $6 W/m^2 sr \mu m$ (below 271 Kelvin). This is consistent with the results in Table 4.7 where clouds (which are cold and therefore have low radiance values) have the highest RMSE's. The ARTM model had the highest RMSE for radiance values below $4 W/m^2 sr \mu m$ which confirms the assumption made in the analysis that radiance values where clouds are present are poorly estimated by MODTRAN when no cloud specific parameters are set. If previous knowledge of cloud cover is available, and land/water temperatures are above 271 Kelvin, the percent error in TOA thermal prediction is less than 10% for cloudless scenes.

4.3 Results summary

The models developed in Chapter 3 were used to predict sensor reaching thermal infrared radiance with band center $10.97 \mu m$ (corresponding to Terra/MODIS band 31 band center). All models were evaluated using the same six test scenes. Results are reported in RMSE, standard deviation and mean error for all six test scenes individually, as well as combined.

For the combined results, the MLP-low-res model predicted TOA thermal radiance better than all other models over land, cloud and total scene. The ARTM model had the lowest RMSE for scenes over water. However, running MODTRAN for every pixel in a scene is computationally expensive compared to the fast implementation of the machine learning models. Individually, the MLP model had the lowest RMSE in two of the six test scenes. Except for one scene, the machine learning models produced the lowest individual total, land and cloud errors. To understand how much the predicted thermal radiances differed from the reference data, the percent prediction error was also calculated and reported in seven radiance ranges (between 1.5 and 14 $W/m^2 sr \mu m$). Where the reference data were above 6 $W/m^2 sr \mu m$ (apparent temperature above 271 Kelvin), most models predicted thermal radiance to within 10%.

Chapter 5

ERROR ANALYSIS

To understand the models' prediction errors (as observed in Table 4.7), research into possible sources of error in the input variables as well as the methodology were conducted. The largest expected error sources were investigated through a series of parallel studies and are listed in the sections of this chapter.

5.1 Accuracy of MERRA-2 skin temperature

As discussed in Chapter 2, the target self-emissions due to its temperature dominates effective radiance reaching the sensor in the thermal region. Due to this, the MERRA-2 skin temperature used in this research were evaluated as a possible source of error.

To validate MERRA-2 skin temperatures, coincident MODIS Sea Surface Temperature (SST) [28] and MODIS Land Surface Temperature (LST) measurements down-sampled to the MERRA-2 grid were used. The quality of the MERRA-2 skin temperature over land was assessed using MODIS LST (MOD11.L2) product where the MODIS QA and

Figure 5.1: Histogram of the difference between MERRA-2 TS and MODIS LST in Kelvin.

Data quality flag of the MODIS LST was applied, as described in the MODIS LST user guide [29].

A histogram of the difference between the MERRA-2 instantaneous skin temperature and the down-sampled MODIS LST can be seen in Figure 5.1. Differences ranged from -6.3 Kelvin to 5.6 Kelvin with an RMSE of 2.15 Kelvin, a standard deviation of 2.06 Kelvin and a mean error of -0.66 Kelvin. Note that 2.15 Kelvin is approximately $0.2 \text{ W/m}^2 \text{ sr } \mu\text{m}$ in Terra/MODIS band 31, thus approximately 25% of the error displayed in Table 4.7 (MLP-low-res), can be attributed to the use of the MERRA-2 skin temperature.

MERRA-2 skin temperature over water was also evaluated using two separate scenes. MODIS Sea Surface Temperature (SST) [28] was used as validation. MODIS SST quality bands indicates the quality of a measurement, and only the 0-flag (highest quality) data was used in comparisons. According to the MODIS SST Guide document [30], data with a 0-flag are considered accurate to ± 0.4 degrees Celsius.

Figure 5.2: Histograms of the differences between MERRA-2 TS and MODIS SST in Kelvin for two scenes.

Figure 5.2 displays histograms of the errors for both scenes, with Figure 5.3 displaying the associated RGB images of the MODIS scenes used for this analysis. The scene on the left correspond to the histogram on the left and the scene on the right correspond to the histogram on the right. There is significant variation between the scenes. The scene on the left has an RMSE of 2.67 Kelvin, a standard deviation of 2.21 Kelvin and a mean error of 0.84 Kelvin. The scene on the right has smaller errors with an RMSE of 0.47 Kelvin, standard deviation of 0.46 Kelvin and a mean error of 0.10 Kelvin. The large difference in RMSE between the two scenes might be due to the differences in the scenes used. The graph on the left relates to the scene that was part land, part water, while the scene on the right was completely over water, see Figure 5.3. The large variation in water temperature differences (compared to the reference data) could explain between 5% and 23% of the error over water, based on the RMSE of the MLP-low-res model.

Figure 5.3: RGB images of the scenes used to compare MODIS SST and MERRA-2 skin temperature. The scene on the left corresponds to the histogram on the left.

5.2 Comparing differences in spatial resolution

Another possible source of error in the model prediction could be due to the large difference in spatial resolution between the training data (MERRA-2) and the reference data (Terra/MODIS). Various interpolation techniques yielded different results. A comparison between a Terra/MODIS scene down-sampled to the MERRA-2 spatial resolution using nearest neighbor and bilinear interpolation respectively resulted in differences in radiance values with an RMSE of $0.177 \text{ W/m}^2 \text{ sr } \mu\text{m}$. Figure 5.4 displays the difference image between the two resampling methods for the Middle East scene (first test scene described in Chapter 4). Bilinear interpolation was used throughout this work to mitigate this effect.

To emphasize the effect of down-sampling Terra/MODIS to MERRA-2 resolution, three different regions of interest in a Terra/MODIS scene were inspected. Each region of interest (one over water, one over land and the last with water, land and cloud in the area) corresponded to the same size as one MERRA-2 pixel (approximately $50 \times 70 \text{ km}$).

Figure 5.4: Difference image between resampling methods used with MODIS data with values in radiance units.

The minimum, maximum and average radiance values, as well as the standard deviation of each region of interest is reported in Table 5.1. Bilinear interpolation, when down-sampled from 1×1 km to 50×70 km pixel size, is equivalent to averaging the pixels. Over water, the down-sampling had little effect on the averaged TOA thermal radiance value. However, over mixed land cover, radiance values in the Terra/MODIS region of interest ranged between 3.23 and $10.77 W/m^2 sr \mu m$, which resulted in a standard deviation of $1.52 W/m^2 sr \mu m$. Thus, part of the RMSE in the various models can be explained by the effect of down-sampling Terra/MODIS to MERRA-2 resolution.

Table 5.1: Comparing regions in a Terra/MODIS scene that has the same spatial dimensions as one MERRA-2 pixel. Values displayed are in $W/m^2 sr \mu m$.

Land Cover	Min	Max	Mean	Std Dev
Water	8.76	8.99	8.90	0.04
Land	9.10	12.43	11.44	0.90
Water/Land/Cloud	3.23	10.77	7.67	1.52

5.3 Predicting in-between MERRA-2 times

Since MERRA-2 variables used in this research are only available every three hours, the MLP-low-res model was used to predict in-between the available three hourly window. This was done by linearly interpolating the MERRA-2 variables that bracket the chosen scene time. Three scenes were tested with mixed results. One scene, imaged 31 July 2013 at 14:15 over Argentina and both the Atlantic and Pacific oceans, is displayed in Figures 5.5 and 5.6. The image on the left is the Terra/MODIS reference image and on the right the MLP-low-res TOA prediction. For this scene, the RMSE was $0.99 W/m^2 sr \mu m$. Another scene imaged on 31 July 2015 at 00:55 GMT, Northern Australia, had a high RMSE of $1.64 W/m^2 sr \mu m$. This result was investigated and is displayed in Figure 5.7. The image on the left is Terra/MODIS band 31 thermal radiance at 00:55 GMT followed by the MLP-low-res model prediction for the same time. The predicted scene did not represent clouds well. However, looking at the TOA thermal radiance predictions at 00:00 GMT and 03:00 GMT (two rightmost scenes), it is clear that the atmospheric data at 00:00 GMT and 03:00 GMT did not indicate clouds either. Thus, the in-between radiance estimation could not have predicted correct radiance values where clouds were present.

This is a limitation of using reanalysis data. If a phenomena is varying faster than the MERRA-2 times, then it probably cannot be modeled by MERRA-2 data.

Figure 5.5: Terra/MODIS band 31 at 14:15 GMT

Figure 5.6: MLP TOA thermal radiance prediction at 14:15 GMT

Figure 5.7: Terra/MODIS reference data on the left with the MLP-low-res TOA prediction at 00:55 GMT, followed by the MLP-low-res prediction at 00:00 GMT and on the right the MLP-low-res prediction at 00:30 GMT.

5.4 Cloud and No-cloud models

Since the largest prediction errors occurred when clouds were present in a scene, one model was created to predict sensor reaching radiance only when clouds were present, and another to predict TOA radiance when no clouds were in a scene. These two separate MLP-low-res models were built using only training instances where the training labels were either

cloud or no-cloud (based on the MODIS cloud mask). Both models, when compared to the single MLP-low-res model results for cloud and no-cloud cover individually (see Table 4.7), performed better when tested on all six test scenes combined. The Cloud model RMSE was $1.68 \text{ W/m}^2 \text{ sr } \mu\text{m}$ compared to the results of the MLP-low-res model for cloud cover ($1.86 \text{ W/m}^2 \text{ sr } \mu\text{m}$). The No-cloud model had an RMSE of $0.71 \text{ W/m}^2 \text{ sr } \mu\text{m}$ compared to the cloudless pixels in the MLP-low-res model ($0.91 \text{ W/m}^2 \text{ sr } \mu\text{m}$). However, these models can only be used if prior knowledge of cloud cover is available. One method to infer the presence of cloud based on these models, was to apply both No-cloud and original MLP-low-res models to the test dataset, and then subtract the results from each other. Pixels with large differences (based on a chosen threshold), would be flagged as a pixel where cloud is present. The input data where clouds were inferred would then be modeled by the cloud model, and the rest by the no-cloud model. The results were combined, but initial errors were still higher than the original MLP-low-res model for various thresholds.

5.5 Total cloud area fraction variable

Another MERRA-2 variable that was investigated for the prediction of TOA thermal infrared radiance was the 2D *total cloud area fraction* variable (from the Aerosol Diagnostics collection) with continuous values between zero and one. Visual comparison between the MODIS cloud mask, the MERRA-2 total cloud area fraction variable, and the cloud predictions of the CIM model for all six test scenes suggested that the MERRA-2 cloud area fraction variable did not present a better cloud model than the CIM cloud predictions. Figures 5.8 and 5.9 display the MODIS cloud mask, the MERRA-2 cloud area fraction variable and the CIM cloud prediction images for two of the test scenes. In both scenes

the MERRA-2 total cloud area fraction variable does not predict clouds well compared to the MODIS cloud mask. In Figure 5.9 the CIM model cloud prediction presented the clouds better than the MERRA-2 total cloud area fraction variable.

Figure 5.8: Comparison of cloud masks, with the MODIS cloud mask on the left, the MERRA-2 total cloud area fraction variable in the center, and the CIM cloud prediction on the right.

Figure 5.9: Comparison of cloud masks, with the MODIS cloud mask on the left, the MERRA-2 total cloud area fraction variable in the center, and the CIM cloud prediction on the right.

One MLP-low-res model was built to include the MERRA-2 total cloud area fraction

variable but this model did not perform better than the final model. Thus, this variable was not used in the main research.

5.6 MERRA-2 coastline anomalies

Another variable available in MERRA-2 is the water skin temperature (TSKINWTR) variable in the Ocean Surface Diagnostics collection. This 2D variable has values over water only. A difference image was produced between this variable and the skin temperature variable used in this research to see if the water skin temperature should replace the skin temperature values over water. Figure 5.10 displays the difference image between the two skin temperatures. The skin temperature values over land (where TSKINWTR had no values) were set to zero. From this difference image it is clear that some error occurs at the coastlines. For offshore water, the mean error is approximately 0.003 Kelvin (standard deviation of 0.12 Kelvin). However at the coast it varies between -20 and +34 Kelvin. This might be explained by the large gsd of MERRA-2 (approx. 50×70 km). It is possible that those coastal pixels are a combination of land and water, therefore the water skin temperature assigns the coastline pixel a water temperature value and the skin temperature assigns that same pixel a land temperature value. However, looking at the difference image, it is unclear why the coastlines of Africa and Europe have warmer water skin temperature (TSKINWTR) than skin temperature (TS), but the coastlines of the Americas have colder water skin temperature (TSKINWTR) than skin temperature (TS).

Figure 5.10: Difference image between skin temperature and water skin temperature variables in MERRA-2 for 12:00 GMT on July 31, 2013.

5.7 MLP input variables

The same four MERRA-2 variables used with the linear regression and SVR models, i.e., air temperature, relative humidity, instantaneous skin temperature, and time-averaged skin temperature, were used as input to the MLP models. In addition, variables indicating land cover, season, and latitude were included in some of the MLP models. Land cover was used to simulate emissivity. The MODIS global land cover map consists of 17 land cover labels and has a spatial resolution of 0.0833 deg. Table B.2 displays the labels and associated variables used for the land cover classification. The land cover classification map is generated [27] using the System for Terrestrial Ecosystem Parameterization (STEP) database as training data for the MCD12Q1 product algorithm. The seasonal indicator,

a discrete value from 1 to 4, was used to provide information about seasonal atmospheric trends. It was surprising that by removing the land cover variable and seasonal indicator from the input data, the MLP model performance improved, since the land cover variable was thought to assist modeling emissivity, and the seasonal indicator was thought to account for large scale seasonal atmospheric conditions.

No data normalization techniques applied resulted in a lower error for the MLP-low-res model and thus the training data were not normalized. Various architectures and data normalization techniques tested with resulting RMSE, are displayed in Appendix B. In the best MLP-med-res and MLP-high-res models, all zero air temperature values were replaced with the instantaneous skin temperature values.

5.8 MODTRAN without MERRA-2 atmospheric profile

There are six pre-defined atmospheric profiles that can be used for MODTRAN simulations. However, this research provided MODTRAN with user-defined atmospheric profiles (MERRA-2 air temperature and relative humidity profiles). To investigate the model performance between using a built-in profile and the MERRA-2 profiles, all six test scenes were evaluated. Table 5.2 displays the results of both MODTRAN simulations for all scenes combined. MODTRAN with the MERRA-2 profile performed better than MODTRAN predictions with the generic built-in mid-lat summer profile, which provides merit to this research.

Table 5.2: RMSE, Standard deviation (STD) and Mean error [Mean] in $W/m^2 sr \mu m$ for various land and cloud cover to compare MODTRAN with the MERRA-2 profiles and MODTRAN with a standard atmospheric profile.

Model	Total RMSE (STD) [Mean]	Land RMSE (STD) [Mean]	Water RMSE (STD) [Mean]	Cloud RMSE (STD) [Mean]
MODTRAN built-in	1.73 (1.72) [0.23]	1.12 (0.80) [0.77]	1.41 (1.40) [0.23]	2.66 (2.55) [-0.78]
MODTRAN with M2 profile	1.52 (1.50) [-0.26]	0.90 (0.67) [0.59]	0.58 (0.55) [-0.19]	2.67 (1.89) [-1.88]

5.9 Error Analysis summary

It was found that the difference between MERRA-2 skin temperature and MODIS LST could account for 25% of the RMSE over land. For water, 5% to 23% of the error could be explained by the accuracy of MERRA-2 skin temperature. The somewhat low spatial resolution of MERRA-2 (compared to MODIS) also accounts for roughly $0.117 W/m^2 sr \mu m$ when resampling MODIS to MERRA-2 resolution. When predicting in-between the available MERRA-2 three hourly window, results show that when atmospheric conditions vary faster than the three hourly MERRA-2 window, accurate predictions might not be possible. Visual inspection of the MERRA-2 total cloud area fraction variable compared to the MODIS cloud mask and CIM model cloud predictions resulted in the variable not being used in this research. Mean errors between the MERRA-2 skin temperature and skin water temperature varied between -20 and +34 Kelvin near or on the coastline, and less than 0.003 Kelvin over water (not near the coast). ARTM predictions produced lower RMSE over all land cover types compared to using MODTRAN with built-in atmospheric profiles.

Chapter 6

SUMMARY

Thermal infrared data from satellites is widely used in environmental studies and cross-calibration of other thermal sensors. However, thermal satellites have limited temporal resolution. The objective of this research was to investigate the use of the Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) to predict TOA thermal infrared radiance. This investigation also sought to identify the major error sources and limitations of using reanalysis data in predicting TOA radiance.

To estimate sensor reaching thermal radiance, seven models were developed using both physics-based and machine learning approaches with MERRA-2 variables as input to the models. The first two physics-based models used the atmospheric radiative transfer model MODTRAN to predict TOA radiance, while the third model was created to estimate MODTRAN predictions to minimize computation time. The machine learning models was trained using 44 Terra/MODIS band 31 scenes with the temporally and spatially coincident MERRA-2 data as input. Two regression models and two deep learning models were built. Since Terra/MODIS band 31 was used as reference, all models were built to predict TOA

thermal radiance with center wavelength $10.97\mu m$ (corresponding to Terra/MODIS band 31 band center).

The models developed in Chapter 3 was used to predict sensor reaching thermal infrared radiance. All models were evaluated using the same six test scenes. Results are reported in RMSE, standard deviation and mean error for all six test scenes individually, as well as combined. For the combined results, the MLP-low-res model predicted TOA thermal radiance better than all other models over land, cloud and total scene. The ARTM model had the lowest RMSE for scenes over water. Individually, the MLP model had the lowest RMSE in two of the six test scenes. Except for one scene, the machine learning models produced the lowest individual total, land and cloud errors. To understand how much the predicted thermal radiances differed from the reference data, the percent prediction error was also calculated and reported in seven radiance ranges (between 1.5 and $14 W/m^2 sr \mu m$). Where the reference data were above $6 W/m^2 sr \mu m$ (apparent temperature above 271 Kelvin), most models predicted thermal radiance to within 10%.

Several possible sources of error were investigated. The first was the MERRA-2 skin temperature variable. Since skin temperature plays a significant role in sensor reaching thermal radiance, the MERRA-2 skin temperatures were evaluated using the MODIS LST and SST products. Taking the difference between MERRA-2 skin temperature and MODIS LST into account, 25% of the RMSE over land can be explained. The large variation in water temperature differences (compared to the reference data) could further explain between 5% and 23% of the error over water. Another source of error resulted from the large difference in spatial resolution between the MERRA-2 input data and the Terra/MODIS reference data. Different resampling methods were applied to the same Terra/MODIS test scene. A comparison between the down-sampled test image using

nearest neighbor and bilinear interpolation respectively resulted in an RMSE of $0.177 \text{ W/m}^2 \text{ sr } \mu\text{m}$. Another limitation of using the reanalysis data was found when predicting in-between the available MERRA-2 three hourly window. Results show that when atmospheric conditions vary faster than the three hourly MERRA-2 window, accurate predictions might not be possible. While exploring the MERRA-2 data product, the total cloud area fraction variable was noticed. However, visual inspection of this variable compared to the MODIS cloud mask and CIM model cloud predictions resulted in the variable not being used in this research. Further analysis into the differences between the MERRA-2 skin temperature and MERRA-2 skin water temperature variables lead to the discovery of inconsistencies at coastlines. Mean errors varied between -20 and +34 Kelvin near or on the coastline, and less than 0.003 Kelvin over water (not near the coast). Lastly, to confirm the importance of the MERRA-2 air temperature and relative humidity profiles, a study comparing the ARTM model with MODTRAN simulations using the built-in MODTRAN atmospheric profiles was undertaken. The results indicate that the ARTM model had a lower RMSE over all land cover types compared to the MODTRAN with built-in atmospheric profile predictions indicating that using the MERRA-2 data improves TOA prediction.

This research showed that TOA thermal infrared radiance can be estimated from MERRA-2 atmospheric data to within approximately 10% or better for typical mid-latitude scene temperatures (between 271 and 328 Kelvin). Depending on the application, and if prior knowledge of land cover type exists, either the MLP-low-res model or the ARTM should be used to estimate sensor reaching radiance. All the models could be extended to predict thermal radiance at other wavelengths if reference data is available at those thermal wavelengths.

6.1 Recommendations

To improve model performance and better understand errors associated with the models, various additional studies are recommended, namely:

- A rigorous study to validate MERRA-2 skin temperature. For this, it is suggested to repeat the studies done in Section 5.1 with a large number of test scenes for both land and water temperatures.
- Further investigation into the coastline errors could lead to better understanding of the MERRA-2 water and skin temperature variables.
- Since the largest prediction errors occur when clouds are present, a different process to infer where clouds formed could be beneficial to accurately predict TOA thermal radiance. Further investigation of other MERRA-2 variables could assist with better cloud estimation. For example, MERRA-2 collections like the Cloud Diagnostics 3D collection with variables like the *in cloud optical thickness for liquid clouds* and *cloud fraction for radiation* could be used.
- If a better cloud mask could be created, then 1) the cloud and no-cloud models, as described in Section 5.4, could be used in stead of the MLP-low-res model since they produced lower errors, and 2) the CIM could be replaced with built-in MODTRAN cloud settings for pixels where clouds are present.
- To improve the MLP-low-res model, ensembling could be used. This is a method where several neural networks are trained and then combined to produce a better result.

- Lastly, the MLP-low-res model might improve with more training data (double the current training set). Thus 44 Terra/MODIS scenes and the temporarily and spatially coincident MERRA-2 scenes must be downloaded and formatted for input to the MLP-low-res model. The test set could also be expanded (or changed) to include more diverse scenes from a wider range of seasons (e.g. winter), latitude and land cover type (less scenes over desert).

Appendix A

MERRA-2 DATA

Most of the MERRA-2 collections are available from NASA’s Reverb ECHO website [31]. However, only full collections of data can be downloaded here. For more flexibility, MERRA-2 collections and single variables can be found at the Goddard Earth Sciences Data and Information Services Center (GES DISC) [32].

A complete file specification of all collections and variables with format and file organization can be found in the MERRA-2 File Specification paper produced by the Global Modeling and Assimilation Office [33].

Data is available in .nc4 format, from January 1980 to the present. All collections include the latitude and longitude data per pixel. The 3D variable collections also include the level (hPa) data to correlate the variable profile to pressure. To easily open .nc and .nc4 data files in IDL, install Coyote’s nCDF_Browser library [34]. To georegister the data in ENVI, write the downloaded variable to ENVI, and save as .img file. Update the .hdr file as per Figure A.1.

MERRA-2 collection names are in the format *freq_dims_group_HV*, for example: MER-

RA2.400.inst1_2d_asm- _Nx.20130328.nc4, where the four attributes are:

- *freq*: time-independent (cnst), instantaneous (inst F), or time-averaged (tagv F) where F indicates the frequency (1 - hourly, 3 = 3-hourly, M = Monthly mean, U = Monthly-Diurnal mean).
- *dims*: 2-dimensional or 3-dimensional fields.
- *group*: group abbreviation for the collection name.
- *HV*: horizontal (N = Native, C = Reduced, F = Reduced FV) and vertical (x = horizontal only, p = pressure-level data, v = model layer centers, e = model layer edges) grid.

The MERRA-2 data collections for both the skin temperature variables can be seen in Table A.1 and Table A.2.

```
ENVI
description = {
Create New File Result [Wed Feb 15 08:31:06 2017]}
samples = 576
lines = 361
bands = 1
header offset = 0
file type = ENVI Standard
data type = 4
interleave = bsq
sensor type = Unknown
byte order = 0
wavelength units = Unknown
map info = {Geographic Lat/Lon, 1.0000, 1.0000, -180.00, 90.00, 0.625, 0.5, WGS-84, units=Degrees}
coordinate system string = {GEOGCS["GCS WGS_1984", DATUM["D WGS_1984", SPHEROID["WGS_1984", 6378137.0, 298.257223563]]
, PRIMEM["Greenwich", 0.0], UNIT["Degree", 0.0174532925199433]]}
wavelength units = Unknown
data ignore value = -1.000000000e+000
```

Figure A.1: MERRA-2 ENVI .hdr file format

Table A.1: MERRA-2 collection: Single-Level Diagnostics

Frequency: 1-hourly from 00:00 GMT

Spatial Grid: 2D, single-level, full horizontal resolution

Dimensions: longitude(x) = 576, latitude(y) = 361, time(t) = 24

Name	Dim	Description	Units
DISPH	tyx	zero plane displacement height	<i>m</i>
PS	tyx	surface pressure	<i>Pa</i>
QV10M	tyx	10-meter specific humidity	<i>kg kg⁻¹</i>
QV2M	tyx	2-meter specific humidity	<i>kg kg⁻¹</i>
SLP	tyx	sea level pressure	<i>Pa</i>
T10M	tyx	10-meter air temperature	<i>K</i>
T2M	tyx	2-meter air temperature	<i>K</i>
TO3	tyx	total column ozone	<i>Dobsons</i>
TOX	tyx	total column odd oxygen	<i>kg m⁻²</i>
TQI	tyx	total precipitable ice water	<i>kg m⁻²</i>
TQL	tyx	total precipitable liquid water	<i>kg m⁻²</i>
TQV	tyx	total precipitable water vapor	<i>kg m⁻²</i>
TROPPB	tyx	tropopause pressure based on blended estimate	<i>Pa</i>
TROPPT	tyx	tropopause pressure based on thermal estimate	<i>Pa</i>
TROPPV	tyx	tropopause pressure based on EPV estimate	<i>Pa</i>
TROPQ	tyx	tropopause specific humidity using blended TROPP estimate	<i>kg kg⁻¹</i>
TROPT	tyx	tropopause temperature using blended TROPP estimate	<i>K</i>
TS	tyx	surface skin temperature	K
U10M	tyx	10-meter eastward wind	<i>ms⁻¹</i>
U2M	tyx	2-meter eastward wind	<i>ms⁻¹</i>
U50M	tyx	eastward wind at 50 meters	<i>ms⁻¹</i>
V10M	tyx	10-meter northward wind	<i>ms⁻¹</i>
V2M	tyx	2-meter northward wind	<i>ms⁻¹</i>
V50M	tyx	tyx northward wind at 50 meters	<i>ms⁻¹</i>

Table A.2: MERRA-2 collection: Surface Flux Diagnostics

Frequency: 1-hourly from 00:30 GMT

Spatial Grid: 2D, single-level, full horizontal resolution

Dimensions: longitude(x) = 576, latitude(y) = 361, time(t) = 24

Name	Dim	Description	Units
BSTAR	tyx	surface bouyancy scale	m s ⁻²
CDH	tyx	surface exchange coefficient for heat	kg m ⁻² , s ⁻¹
CDM	tyx	surface exchange coefficient for momentum	kg m ⁻² , s ⁻¹
CDQ	tyx	surface exchange coefficient for moisture	kg m ⁻² , s ⁻¹
CN	tyx	surface neutral drag coefficient	1
DISPH	tyx	zero plane displacement height	m
EFLUX	tyx	total latent energy flux	W m ⁻²
EVAP	tyx	evaporation from turbulence	kg m ⁻² , s ⁻¹
FRCAN	tyx	areal fraction of anvil showers	1
FRCCN	tyx	areal fraction of convective showers	1
FRCLS	tyx	areal fraction of nonanvil large scale showers	1
FRSEAICE	tyx	ice covered fraction of tile	1
GHTSKIN	tyx	Ground heating for skin temp	W m ⁻²
HFLUX	tyx	sensible heat flux from turbulence	W m ⁻²
HLML	tyx	surface layer height	m
NIRDF	tyx	surface downwelling nearinfrared diffuse flux	W m ⁻²
NIRDR	tyx	surface downwelling nearinfrared beam flux	W m ⁻²
PBLH	tyx	planetary boundary layer height	m
PGENTOT	tyx	Total column production of precipitation	kg m ⁻² s ⁻¹
PRECANV	tyx	anvil precipitation	kg m ⁻² s ⁻¹
PRECCON	tyx	convective precipitation	kg m ⁻² s ⁻¹
PRECLSC	tyx	nonanvil large scale precipitation	kg m ⁻² s ⁻¹
PRECSNO	tyx	snowfall	kg m ⁻² s ⁻¹
PRECTOT	tyx	total precipitation from atm model physics	kg m ⁻² s ⁻¹
PRECTOTCORR	tyx	Bias corrected total precipitation	kg m ⁻² s ⁻¹
PREVTOT	tyx	Total column re-evap/subl of precipitation	kg m ⁻² s ⁻¹
QLML	tyx	surface specific humidity	1
QSH	tyx	effective surface specific humidity	kg kg ⁻¹
QSTAR	tyx	surface moisture scale	kg kg ⁻¹
RHOA	tyx	air density at surface	kg m ⁻³
RISFC	tyx	surface bulk richardson number	1
SPEED	tyx	surface wind speed	m s ⁻¹
SPEEDMAX	tyx	surface wind speed	m s ⁻¹
TAUGWX	tyx	surface eastward gravity wave stress	N m ⁻²

Table A.3: MERRA-2 collection: Surface Flux Diagnostics (continued)

Name	Dim	Description	Units
TAUGWY	tyx	surface northward gravity wave stress	$N\,m^{-2}$
TAUX	tyx	eastward surface stress	$N\,m^{-2}$
TAUY	tyx	northward surface stress	$N\,m^{-2}$
TCZPBL	tyx	transcom planetary boundary layer height	m
TLML	tyx	surface air temperature	K
TSH	tyx	effective surface skin temperature	K
TSTAR	tyx	surface temperature scale	K
ULML	tyx	surface eastward wind	$m\,s^{-1}$
USTAR	tyx	surface velocity scale	$m\,s^{-1}$
VLML	tyx	surface northward wind	$m\,s^{-1}$
Z0H	tyx	surface roughness for heat	m
Z0M	tyx	surface roughness	m

Appendix B

MODEL ARCHITECTURES

B.1 Deep learning architectures

Numerous architectures were tested for the MLP-low-res model. Table B.1 displays a detailed description of some of the architectures tested. The last two models were build using only pixels with and without cloud respectively. If prior knowledge of clouds exists, then these models would better estimate TOA thermal radiance for the given cloud/cloud-free scene.

The model with the weighted temperature variables (weighted by including the skin temperatures 5 times in the training instances) performed the best overall. However, this is misleading since the test data has more cloud-free pixels than cloudy pixels. By weighting the skin temperature, more focus is placed on a cloud-free scenario.

Variables indicating land cover, season, and latitude were included in some of the MLP models. Land cover was used to simulate emissivity. The MODIS global land cover map consists of 17 land cover labels and has a spatial resolution of 0.0833 deg. Table B.2

Table B.1: Architectures tested for the MLP-low-res model with associated RMSE in $W/m^2\ sr\ \mu m$

FC layers	Variables Used	Normalization(Layers)	RMSE
20,6	T,RH,SSN,LAT,LCV	None (42)	1.41
30,20,6	T,RH,SI,LAT,LCV	One-hot (42)	2.32
30,20,6	T,RH,SI,LAT,LCV	Standardized (42)	1.59
256,512,256,128,128,64	T,RH,SI,LAT,LCV	None (42)	1.31
256,512,256,128,8	T,RH,SI,LAT,LCV	None (42)	1.29
256,512,256,128,8	T,RH	None (42)	1.27
256,512,256,128,8	T,TSH	None (42)	1.99
256,512,256,128,8	T,TSH,TS,RH,CLD	None (27)	1.27
256,512,256,128,8	T,TSH,TS,RH	Scaled RH $\times 100$ (27)	1.50
256,512,256,128,8	T,TSH,TS,RH	Log transform (27)	1.82
256,512,256,128,8	T,TSH,TS,RH	None (42)	1.30
256,512,256,128,8	T,TSH,TS,RH	None (27)	1.22
256,512,256,128,8	T,TSH,TS,RH	None (20)	1.22
256,512,256,128,8	T,TSH,TS,RH	Replaced zero values with TS (27)	1.33
256,512,256,128,8	T,TSH,TS,RH	Weight temperature $\times 5$ (27)	1.20
256,512,256,128,8	T,TSH,TS,RH	No-cloud pixels	0.71
256,512,256,128,8	T,TSH,TS,RH	Only cloud pixels	1.68

displays the labels and associated variables used for the land cover classification. The land cover classification map is generated [27] using the System for Terrestrial Ecosystem Parameterization (STEP) database as training data for the MCD12Q1 product algorithm. Results from cross-validation of the classification labels indicate an overall accuracy of 75% correctly classified. However, the range of class-specific accuracies is large according to [27]. The seasonal indicator, a discrete value from 1 to 4, was used to provide information about seasonal atmospheric trends.

Variables like the seasonal indicator, the latitude variable and the land cover variable though relevant, decreased the MLP-low-res model performance.

Table B.2: Land Cover Classification Legend

Value	Label
1	Water
2	Permanent wetlands
3	Snow and ice
4	Evergreen Needleleaf forest
5	Evergreen Broadleaf forest
6	Deciduous Broadleaf forest
7	Deciduous Needleleaf forest
8	Mixed forest
9	Woody savannas
10	Grasslands
11	Cropland/Natural vegetation mosaic
12	Savannas
13	Croplands
14	Closed shrublands
15	Open shrublands
16	Barren or sparsely vegetated
17	Urban and built-up

B.2 Data normalization techniques applied

Since the data used in the supervised learning models ranged from the continuous relative humidity variable with values between 0 and 1, the discrete variables (land cover, season, latitude) to continuous variables ranging from 180 to 330 for all temperature fields, various normalization techniques were applied and tested, namely:

- One-hot encoding (transforming categorical features into boolean vectors) was applied to the discrete variables (LCV, SI and LAT) while the temperature variables were divided by the maximum global temperature.
- Features were standardized by subtracting the mean and scaling to unit variance.

- In models with relative humidity and temperature fields only, the relative humidity variable was scaled ($\times 100$).
- Non-linear (log) transformation of the temperature variables were applied.
- Data points where the air temperature was zero (due to no data at that altitude), were replaced by the skin temperature value for that pixel.

Various combinations of the listed normalization techniques were tested to optimize the final models. However, none of the listed techniques improved the MLP-low-res model performance.

Appendix C

MODTRAN Tape5 file

Figure C.1 is an example of one tape5 radiosonde file used as input to MODTRAN for the CIM model.

		Number of Atmospheric layers										Skin temperature (Kelvin)				1-albedo		
User-defined profile	TS	7	2	2	-1	2	2	2	2	2	2	2	1	1	0	277.233	0.03	
	F	0F	0	0	0.00000	0	0	0	F	F	F	0.000	0.000	0.000	0.000	0.000	0.738	
		1	2	0	3	0	0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.738	
Altitude profile (km)	40	0	0															
	0.738	9.000e+02	2.772e+02	2.632e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	0.935	8.750e+02	2.731e+02	2.591e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	1.138	8.500e+02	2.739e+02	2.565e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	1.347	8.250e+02	2.726e+02	2.567e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	1.562	8.000e+02	2.709e+02	2.566e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	1.784	7.750e+02	2.694e+02	2.547e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	2.014	7.500e+02	2.680e+02	2.496e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	2.251	7.250e+02	2.670e+02	2.543e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	2.497	7.000e+02	2.661e+02	2.578e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	3.015	6.500e+02	2.634e+02	2.572e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
	3.576	6.000e+02	2.594e+02	2.548e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	4.185	5.500e+02	2.554e+02	2.535e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	4.852	5.000e+02	2.516e+02	2.510e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	5.590	4.500e+02	2.484e+02	2.484e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	6.414	4.000e+02	2.434e+02	2.434e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	7.349	3.500e+02	2.367e+02	2.367e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	8.428	3.000e+02	2.289e+02	2.289e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	9.704	2.500e+02	2.196e+02	2.196e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	11.266	2.000e+02	2.066e+02	2.066e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	13.280	1.500e+02	2.077e+02	2.017e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	16.118	1.000e+02	2.074e+02	1.917e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	18.615	7.000e+01	2.053e+02	1.893e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	20.970	5.000e+01	2.057e+02	1.876e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	22.532	4.000e+01	2.060e+02	1.864e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	24.546	3.000e+01	2.078e+02	1.850e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	27.384	2.000e+01	2.152e+02	1.831e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	32.236	1.000e+01	2.347e+02	1.788e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	34.733	7.000e+00	2.449e+02	1.763e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
	37.088	5.000e+00	2.561e+02	1.743e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00
38.650	4.000e+00	2.634e+02	1.717e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
40.664	3.000e+00	2.681e+02	1.707e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
43.502	2.000e+00	2.654e+02	1.699e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
48.354	1.000e+00	2.623e+02	1.689e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
50.851	7.000e-01	2.586e+02	1.676e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
53.206	5.000e-01	2.530e+02	1.655e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
54.768	4.000e-01	2.501e+02	1.643e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
56.782	3.000e-01	2.476e+02	1.629e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
70.000	2.200e-02	2.476e+02	1.629e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
85.000	5.300e-03	2.476e+02	1.629e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
100.000	0.600e-03	2.476e+02	1.629e+02	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
		705.000	0.738	180.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	
		1	0	91	0													
		60.000	240.625	0.000	0.000	3.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	
		10.550	11.525	0.025	0.025RM	MR A												
		0																

Figure C.1: Example of a MODTRAN tape5 file for the CIM model

Appendix D

PYTHON CODE

The code to create, save and use the MLP and CNN models are available below. The Keras library in Python was used to create the models.

D.1 Multi Layer Perceptron code

```
import pandas
import math
import csv
import numpy as np
import scipy.io
import matplotlib.pyplot as plt
from numpy import inf
from keras.models import Sequential, model_from_json
from keras.layers import Dense, Dropout
```

```
from keras.optimizers import SGD,Nadam, Adam
from keras.callbacks import EarlyStopping
from sklearn.preprocessing import StandardScaler
from keras.layers.normalization import BatchNormalization
```

```
# IMPORT DATA
```

```
# load dataset - train
```

```
rd = open("C:/Users/garny/Documents/RIT/IDL/DL_project/
Train_images/train_20170119.csv")
csv_reader = csv.reader(rd)
data = list(csv_reader)
data = np.asarray(data)
data = data.astype(float)
```

```
# load dataset - test
```

```
rd = open("C:/Users/garny/Documents/RIT/IDL/DL_project/
Test_images/test_20170119.csv")
csv_reader = csv.reader(rd)
data_test = list(csv_reader)
data_test = np.asarray(data_test)
data_test = data_test.astype(float)
```

```
# FORMAT DATA
```

```
# format training set and labels

train1 = data[0:27,:]
train2 = data[27:29,:]
train3 = data[29:56,:]

train = np.concatenate((train1,train2,train2,train2,
train2,train2,train3),axis=0)

train[train == -inf] = 0
train = np.nan_to_num(train)
labels = data[57,:]

X = train.T
Y = labels.T

# format test set and labels

test1 = data_test[0:27,:]
test2 = data_test[27:29,:]
test3 = data_test[29:56,:]

test = np.concatenate((test1,test2,test2,test2,test2,
test2,test3),axis=0)

test[test == -inf] = 0
test = np.nan_to_num(test)
labels_test = data_test[57,:]
```

```
X_test = test.T
Y_test = labels_test.T

# CREATE AND FIT MODEL

# create model
model = Sequential()
model.add(Dense(512, input_dim=X.shape[1], init='glorot_normal',
    , activation='relu'))
model.add(Dense(512, init='glorot_normal', activation='relu'))
model.add(Dense(256, init='glorot_normal', activation='relu'))
model.add(Dense(128, init='glorot_normal', activation='relu'))
model.add(Dense(8, init='glorot_normal', activation='relu'))
model.add(Dense(1, init='glorot_normal'))

# compile model
model.compile(loss='mean_squared_error', optimizer='adam')

# Fit the model with validation set
loss_list = []
valloss_list = []

es = EarlyStopping(monitor='val_loss',patience=4,verbose=0,
mode='auto')
```



```

for _ in range(4):

    history = model.fit(X, Y, validation_split=0.1,
        nb_epoch=500, batch_size=100, verbose=2, callbacks=[es])
    model.optimizer.lr.set_value(np.float32(
        model.optimizer.lr.get_value()/10.0))
    loss_list.extend(history.history['loss'])
    valloss_list.extend(history.history['val_loss'])

# EVALUATE MODEL

# evaluate the model
scores =model.evaluate(X, Y)
print(" Training : %.2f MSE and %.2f RMSE" %
    (model.metrics_names[0], scores, math.sqrt(scores)))

# test the model
scores = model.evaluate(X_test, Y_test)
print(" Test data : %.2f MSE and %.2f RMSE" %
    (model.metrics_names[0], scores, math.sqrt(scores)))

# plot history for loss
plt.plot(loss_list)
plt.plot(valloss_list)

```

```
plt.title('model_loss')
plt.ylabel('mean_square_error_(loss)')
plt.xlabel('epoch')
plt.legend(['train', 'validation'], loc='upper_left')
plt.show()
```

D.2 Convolutional Neural Network code

```
import pandas
import math
import csv
import numpy as np
import matplotlib.pyplot as plt
from keras.models import Sequential
from keras.layers import Dense, Dropout, Activation, Flatten
from keras.layers import Convolution2D, MaxPooling2D,
AveragePooling2D
from keras.optimizers import Adam
from keras.utils import np_utils
from keras.callbacks import EarlyStopping
from keras.layers.normalization import BatchNormalization

# load dataset - train
filter_size = 9
rd = open("C:/Users/garny/Documents/RIT/IDL/DL_project/
```

```
Train_images/train_CNN_image.csv")
csv_reader = csv.reader(rd)
train = list(csv_reader)
train = np.asarray(train)
train = np.float32(train)

C = (56, filter_size, -1, filter_size)
train = np.reshape(train, C)
train = np.rollaxis(train, 2, 1)
train = np.rollaxis(train, 1)
train = np.rollaxis(train, 2, 1)
X = np.rollaxis(train, 3, 2)

# load dataset - train labels
rd = open("C:/Users/garny/Documents/RIT/IDL/DL_project/
Train_images/train_labels_CNN_image.csv")
csv_reader = csv.reader(rd)
labels = list(csv_reader)
labels = np.asarray(labels)
Y = np.float32(labels)

# load dataset - test
rd = open("C:/Users/garny/Documents/RIT/IDL/DL_project/
Test_images/test_CNN_image.csv")
```

```

csv_reader = csv.reader(rd)
test = list(csv_reader)
test = np.asarray(test)
test = np.float32(test)

C = (56, filter_size, -1, filter_size)
test = np.reshape(test, C)
test = np.rollaxis(test, 2, 1)
test = np.rollaxis(test, 1)
test = np.rollaxis(test, 2, 1)
X_test = np.rollaxis(test, 3, 2)

# load dataset - test labels
rd = open("C:/Users/garny/Documents/RIT/IDL/DL_project/
Test_images/test_labels_CNN_image.csv")
csv_reader = csv.reader(rd)
labels_test = list(csv_reader)
labels_test = np.asarray(labels_test)
Y_test = np.float32(labels_test)

#TRAIN MODEL

model = Sequential()

```

```

model.add(Convolution2D(64, 3, 3, border_mode='same',
input_shape=X.shape[1:], activation='relu'))
model.add(AveragePooling2D(pool_size=(2, 2)))
model.add(BatchNormalization())
model.add(Dropout(0.2))
model.add(Convolution2D(32, 3, 3, border_mode='same',
, activation='relu'))
model.add(AveragePooling2D(pool_size=(2, 2)))
model.add(Flatten())
model.add(Dense(1, init='glorot_normal'))
model.compile(loss='mean_squared_error', optimizer='adam')

# Fit the model
loss_list = []
valloss_list = []

es = EarlyStopping(monitor='val_loss', patience=4, verbose=0
, mode='auto')

for _ in range(3):

    history = model.fit(X, Y, validation_split=0.1,
    nb_epoch=50, batch_size=100, verbose=2, callbacks=[es])
    model.optimizer.lr.set_value(np.float32

```

```

(model.optimizer.lr.get_value()/10.0))
loss_list.extend(history.history['loss'])
valloss_list.extend(history.history['val_loss'])

# EVALUATE MODEL

# evaluate the model
scores =model.evaluate(X, Y)
print("_Training_ %s: _%.2f_MSE_and_%.2f_RMSE" %
(model.metrics_names[0], scores, math.sqrt(scores)))

# test the model
scores = model.evaluate(X_test, Y_test)
print("_Test_data: _%.2f_MSE_and_%.2f_RMSE" %
(model.metrics_names[0], scores, math.sqrt(scores)))

```

D.3 Running and saving models

```

from keras.models import Sequential, model_from_json

# serialize model to JSON
model_json = model.to_json()
with open("C:/Users/garny/Documents/RIT/Python/
modelRMSE_1_20.json", "w")
    as json_file: json_file.write(model_json)

```

```
# serialize weights to HDF5
model.save_weights("C:/Users/garny/Documents/RIT/
Python/model_1_20.h5")
print("Saved_model_to_disk")

# load json and create model
json_file = open('C:/Users/garny/Documents/RIT/
Python/modelRMSE_1_23.json', 'r')
loaded_model_json = json_file.read()
json_file.close()
loaded_model = model_from_json(loaded_model_json)
# load weights into new model
loaded_model.load_weights("C:/Users/garny/Documents
/RIT/Python/model_1_23.h5")
print("Loaded_model_from_disk")
```

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