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INTEGRATING LAND SURFACE TEMPERATURE (LST) IMAGES FROM THE MODERATE RESOLUTION IMAGING SPECTRORADIOMETER (MODIS) SENSOR FOR AGRICULTURAL AND HUMAN HEALTH STUDIES

by

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A dissertation submitted in partial fulfillment of the requirements for the Doctor of Philosophy Degree

State University of New York College of Environmental Science and Forestry Syracuse, New York June 2019

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TABLE OF CONTENTS

LIST OF TABLES	vii
LIST OF FIGURES	viii
ABSTRACT	X
CHAPTER 1: DISSERTATION INTRODUCTION	1
1.1 Background and Motivation	1
1.1.1 Overview of land surface temperature (LST)	1
1.1.2 The MODIS sensor and LST retrieval	2
1.1.3 Common applications of MODIS LST and topics that require additional research	n3
1.2 Research Objectives and Hypothesis	5
1.3 Intended Audience and Dissertation Outline	6
1.4 References	7
INTERPOLATION METHODS FOR MODIS 8-DAY LAND SURFACE TEMPERATURE (LST) COMPOSITES ACROSS THE CONTERMINOUS UNITE STATES	ل D 16
2.1 Introduction	17
2.2 Methods	23
2.2.1 MODIS LST data and preprocessing	23
2.2.2 Study area and test sites selection	24
2.2.3 Artificial cloud creation and empirical assessment	25
2.2.4 Assumptions and implementation of interpolation methods	27
2.2.5 Assessment of topographic, land cover, and climatic factors	30
2.3. Results and Discussion	32
2.3.1 Performance of interpolation methods under varying cloud cover and seasons	32
2.3.2 Error distribution across topographic, land cover, and climatic factors	43
2.3.3 Recommendations for Implementation	47
2.4 Conclusions	50
2.5 Supplemental Information	51
2.6 References	53

CHAPTER 3 MANUSCRIPT 2: IMPROVING CORN YIELD PREDICTION ACROSS THE US CORN BELT BY REPLACING AIR TEMPERATURE WITH DAILY MODIS	
3 1 Introduction	4
3.1.1 Traditional parameters for long term corn yield modeling and crop health assessment	5
3.1.2 Integration of satellite observations in agricultural modeling	7
3.1.3. Study objectives7	0
3.2 Methods7	1
3.2.1 Study area7	1
3.2.2 Data acquisition and preprocessing7	2
3.2.3 Computation of killing degree day metrics and univariate analysis7	4
3.2.4 Comparison of LST and Tair KDD multiple linear regression models7	7
3.3 Results	0
3.3.1 Visual correlations	0
3.3.2 Univariate comparison of derived LST and Tair KDD metrics for yield prediction8	2
3.3.3 Multivariate comparison of derived LST and Tair KDD metrics for yield prediction .8	3
3.4 Discussion	6
3.4.1 Interpretation of results and comparison to previous work	6
3.4.2 Investigating LST's ability to capture water stress and evaporative cooling: A case study comparing rainfed and irrigated counties	1
3.4.3 Exploring an alternative metric: LST – Tair difference9	3
3.4.4 Major implications and policy recommendations9	4
3.5 Conclusion	7
3.6 Supplemental Information9	8
3.6.1 Supplemental information for methods9	8
3.6.2 Supplemental information for discussion10	3
3.7 References	6

CHAPTER 4 MANUSCRIPT 3: ESTIMATING DAILY MAXIMUM HEAT INDEX ACROSS THE CONTERMINOUS UNITED STATES USING MULTISPECTRAL	
MODIS IMAGERY AND ANCILLARY SPATIAL DATA	20
4.1 Introduction	21
4.1.1 Background information	21
4.1.2 Review of previous MODIS-based air temperature and relative humidity models12	22
4.1.3 Potential benefits of remotely-sensed Heat Index (HI) estimation	24
4.1.4 Objective	27
4.2 Methodology	27
4.2.1 Study Area	27
4.2.2 Source of data, processing, and variable justification	28
4.2.3 HI model development and assessment of variable importance	34
4.3 Results and Discussion	36
4.3.1 Model selection: Assessment of performance and tradeoffs	36
4.3.2 Error assessment for the selected model14	41
4.3.3 Variable importance assessment for the selected model	17
4.3.4 Limitations and future work	50
4.4 Conclusion15	52
4.5 Supplemental Information	53
4.6 References	55
CHAPTER 5 CONCLUSIONS AND FUTURE RESEARCH	72
5.1 Conclusions	72
5.2 Limitations	74
5.3 Outlook and Future Work	75
5.4 References	77
VITA	31

LIST OF TABLES

Table 1.1:	Overview of MODIS LST products.	3
Table 2.1:	Overview of studies that interpolated invalid pixels in 8-day MODIS LST images2	0
Table 2.2:	Summary of covariates utilized for the error analysis	1
Table 2.3:	Significant coefficients from OLS regression	4
Table 2.4:	The number of sites that used each criterion to select test scenes by time of day and	
	season5	1
Table 2.5:	Standardized coefficient for full OLS regression models	2
Table 3.1:	List of additional covariates utilized for multiple regression and source7	7
Table 3.2:	Muliple regression results. Note: Coefficients are standardized	5
Table 3.3:	Regression results from previous regional corn yield models9	0
Table 3.4:	Interpolated corn developmental stage dates for US Corn Belt states9	8
Table 3.5:	The derived threshold (in °C), R ² , and RMSE (in Bu/Acre) for all tested KDD	
	periods9	9
Table 4.1:	Overview of studies that estimated daily maximum air temperature (Tmax) or relative	e
	humidity (RH) using a statstical framework	3
Table 4.2:	Overview of predictor variables	9
Table 4.3:	Overview of HI model results. Listed are the R ² , RMSE, maximum VIF, number of	
	potential observations (n), and included variables	7
Table 4.4:	The percent increase in mean square error (%IncMSE) of each variable, R^2 , and	
	RMSE for the selected HI model and comparison to similar Tmax and RH	
	models14	8
Table 4.5:	Optimal parameters selected for random forest regression15	4

LIST OF FIGURES

Figure 2.1: Footprint of the 85 101 by 101 pixel (1-km pixels) utilized study sites and
Ecoregion number25
Figure 2.2: Visual example of cloud cover simulation for selected test and center test pixel to
interpolate (Daytime LST, Site 24, Winter, 28.4% cloud cover - 20-30% category). 27
Figure 2.3: MAEs and 75th/25th percentiles by cloud cover category and season for methods
applied to daytime LST
Figure 2.4: MAEs and 75th/25th percentile by percent cloud cover category and season for
methods applied to nighttime LST34
Figure 2.5: Boxplots of absolute error between center test pixels and spatial and temporal
domain averages by cloud cover category, pooled across sites and seasons
Figure 2.6: Portion of sites for which each method performed best (Y-axis) for cloud cover
categories (X-axis) by time of day and season40
Figure 2.7: Examples of interpolation results for images following cloud mask application with
a concentration of invalid pixels around the center test cell
Figure 2.8: MAEs and 75th/25th percentiles by percent cloud cover category across all seasons
for Matlab Griddata methods applied to daytime and nighttime LST49
Figure 3.1: US Corn Belt states and 463 counties selected for the analysis
Figure 3.2: Time series of standardized corn yield and independent variables, averaged across
selected counties for each state by year
Figure 3.3: Coefficient of determination (R ²) (left) and root mean square error (RMSE) (right)
for the linear relationship between standardized corn yield and KDD (computed from
both LST and Tair) over the range of tested thresholds
Figure 3.4: Scatter plots of standardized LST KDD and Tair KDD vs. yield83
Figure 3.5: Scatter plots of standardized GDD and summer mean daily air temperature
(S_Tmean) vs. yield
Figure 3.6: Scatter plots of standardized precipitation metrics vs. yield; SPI (left), summer
precipitation (S_Precip) (right), and growing season precipitation (G_Precip)
(bottom)
Figure 3.7: Scatter plots of standardized LST and Tair KDD vs. yield for 2012 only87
Figure 3.8: Univariate model R ² for LST and Tair KDD for each state vs. mean summer Tair88
Figure 3.9: July-August daytime LST vs. maximum Tair by year for the utilized irrigated and
rainfed counties in Nebraska (NE). Created using function by Bikfalvi (2012)93
Figure 3.10: Standardized county-level CWSI vs. yield
Figure 3.11: KDD results for period from July 1st to July 31st (July only)100
Figure 3.12: KDD results for period from August 1st to August 31st (August only)100
Figure 3.13: KDD results for period from July 12th to August 31st (silking and dough with no
early buffer)101
Figure 3.14: KDD results for period from July 12th to August 20th (silking only)101

Figure 3.15: Results for traditional Tair KDD computed by summing daily KDD over the
critical development phase and an alternative Tair KDD (Tair No Cloud) computed
similar to LST KDD, by taking an average of daily KDD for cloud-free days and
multiplying by the number of days in the critical development phase
Figure 3.16: Scatter plots of standardized yield in Bu/Acre (Y-axis) vs. LST and Tair KDD in
°C (X-axis) by state103
Figure 3.17: Percent of crop area harvested that is irrigated for the 463 utilized Corn Belt
counties
Figure 3.18: July-Aug daytime LST vs. maximum Tair by year for other states than NE105
Figure 4.1: The CONUS study area and location of the 1,395 utilized Local Climatology
Dataset (LCD) stations
Figure 4.2: Estimated vs. actual HI for the selected model (Model 13)142
Figure 4.3: Histogram of residuals for the selected model (Model 13)
Figure 4.4: Residual plot (left) and corresponding box plot (right) for the selected mode
(Model 13)144
Figure 4.5: RMSE by station (in °F) for the selected model (Model 13)145
Figure 4.6: RMSE by station (in °F) for the LST only model (Model 1)
Figure 4.7: Histogram from HI observations pooled across all 1,395 stations with valid data
(n = 213, 435).
Figure 4.8: Histogram of percent impervious cover (%Imp) for all Local Climatology Dataset
(LCD) stations with valid data ($n = 1,395$)

ABSTRACT

T.J. Pede. Integrating Land Surface Temperature (LST) Images from the Moderate Resolution Imaging Spectroradiometer (MODIS) Sensor for Agricultural and Human Health Studies. 191 pages, 16 tables, 34 figures, 2019. APA (6th ed.) style guide used.

Land surface temperature (LST) images from the Moderate Resolution Imaging Spectroradiometer (MODIS) sensor have been widely utilized across scientific disciplines for a variety of purposes. The goal of this dissertation was to utilize MODIS LST for three spatial modeling applications within the conterminous United States (CONUS). These topics broadly encompassed agriculture and human health.

The first manuscript compared the performance of all methods previously used to interpolate missing values in 8-day MODIS LST images. At low cloud cover (<30%), the Spline spatial method outperformed all of the temporal and spatiotemporal methods by a wide margin, with median absolute errors (MAEs) ranging from 0.2°C-0.6°C. However, the Weiss spatiotemporal method generally performed best at greater cloud cover, with MAEs ranging from 0.3°C-1.2°C. Considering the distribution of cloud contamination and difficulty of implementing Weiss, using Spline under all conditions for simplicity would be sufficient.

The second manuscript compared the corn yield predictive capability across the US Corn Belt of a novel killing degree day metric (LST KDD), computed with daily MODIS LST, and a traditional air temperature-based metric (Tair KDD). LST KDD was capable of predicting annual corn yield with considerably less error than Tair KDD (R²/RMSE of 0.65/15.3 Bu/Acre vs. 0.56/17.2 Bu/Acre). The superior performance can be attributed to LST's ability to better reflect evaporative cooling and water stress. Moreover, these findings suggest that long-term yield projections based on Tair and precipitation alone will contain error, especially for years of extreme drought.

Finally, the third manuscript assessed the extent to which daily maximum heat index (HI) across the CONUS can be estimated by MODIS multispectral imagery in conjunction with land cover, topographic, and locational factors. The derived model was capable of estimating HI in 2012 with an acceptable level of error ($R^2 = 0.83$, RMSE = 4.4°F). LST and water vapor (WV) were, by far, the most important variables for estimation.

Expanding this analytical framework to a more extensive study area (both temporally and spatially) would further validate these findings. Moreover, identifying an appropriate interpolation and downscaling approach for daily MODIS imagery would substantially increase the utility of the corn yield and HI models.

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CHAPTER 1: DISSERTATION INTRODUCTION

1.1 Background and Motivation

1.1.1 Overview of land surface temperature (LST)

High spatial and temporal resolution datasets of temperature are a crucial requirement for numerous fields of research. Both air temperature (Tair) and land surface temperature (LST) are important input parameters for studies on urban heat islands, epidemiology, meteorology, climate change, invasive species mitigation, animal migration, crop phenology, environmental monitoring, urban forestry, hydrology, water cycling processes, and land-atmosphere energy dynamics (Ren et al., 2011; Huang et al., 2013; Xu et al., 2013; Fan et al., 2014; Metz et al., 2014; Van Nguyen et al., 2015; Ma et al., 2017). The applications are virtually limitless.

Tair is the temperature of the air near the surface of the earth and is a form of kinetic temperature, or the average translational energy of the molecules constituting the air. Typically, Tair is measured 1-2 meters above the ground by a network of weather stations. LST reflects the actual temperature of the ground's surface and is a measurement of radiant energy (i.e. an "external" manifestation of an object's energy state). Warmer objects emit more radiant energy. LST is measured by infrared thermometers and other radiometers that detect radiation in the thermal infrared portion of the electromagnetic spectrum (Lillesand et al., 2004).

More recently, global LST datasets at a high spatial and temporal resolution are available via satellite remote sensing, thanks to various earth observation missions. These include the Moderate Resolution Imaging Spectroradiometer (MODIS), Landsat, the Advanced Very High Resolution Radiometer (AVHRR), and Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) (Alferie et al., 2013; Phan and Kappas, 2018). The MODIS sensor has become the most common source for LST images due to the ideal tradeoff between its temporal (4 times daily) and spatial (1-km) resolution (Phan and Kappas, 2018).

If a researcher is interested in a large study area, satellite-derived LST is superior to readings from weather stations, which are in situ point data and do not adequately reflect spatial variability (Zeng et al., 2015). Although geostatistical methods are available for interpolation (e.g. inverse distance weighting, spline interpolation, and kriging), these can produce results with significant error due to invalid assumptions with regards to spatial averaging and the exclusion of topographic factors. This is particularly problematic in undeveloped and remote regions, which have a sparse density and uneven distribution of weather stations (Alfieri et al., 2013; Zeng et al., 2015; Xu et al., 2013; Zhang et al., 2013).

1.1.2 The MODIS sensor and LST retrieval

The MODIS constellation consists of two identical sensors, one onboard the Terra satellite and another onboard the Aqua satellite. Both visit every location on earth twice a day. Thus, there are 4 daily values for MODIS products. The sensors capture data in 36 spectral bands, ranging in wavelength from 620 nanometers to 14.28 micrometers and at varying spatial resolutions (2 bands at 250 m, 5 bands at 500 m and 29 bands at 1 km). The Terra satellite was launched in 1999 and the Aqua satellite was launched in 2002 (Justice et al., 2002). There is now nearly 20 years of data collected by the MODIS program.

MODIS sensors estimate LST from two thermal infrared bands using a split window algorithm (Alfieri et al., 2013; Xu et al., 2013). Many studies have shown that the accuracy of MODIS LST products is within 1 K in the range of 263-300 K (Wan et al., 2008). The highest temporal and spatial resolution LST products are the daily 1-km layers (MOD11A1 from Terra and MYD11A1 from Aqua). To reduce file size and minimize the number of invalid pixels resulting from cloud contamination and emissivity error, aggregated 8-day and monthly products are available. These layers are derived by taking the clear-sky 8-day (or monthly) temporal average on a pixel-by-pixel basis; clear-sky meaning the average of all valid pixels. Aggregated 6-km and 0.05° products are also available and produced by taking a spatial average of valid pixels (Justice et al., 2002). These MODIS LST products are summarized in Table 1.1.

Spatial Resolution	Temporal Resolution	Terra Product	Aqua Product
1-km	Daily	MOD11A1	MYD11A1
1-km	8-Day	MOD11A2	MYD11A2
6-km	Daily	MOD11B1	MYD11B1
0.05°	Daily	MOD11C1	MYD11C1
0.05°	Daily	MOD11C2	MYD11C2
0.05°	Monthly	MOD11C3	MYD11C3
1-km (raw swath)	Daily	MOD11_L2	MYD11_L2

Table 1.1: Overview of MODIS LST products.

1.1.3 Common applications of MODIS LST and topics that require additional research

Phan and Kappas (2018) performed a literature review to understand the global and longitudinal trends of MODIS LST applications. They determined that the three most popular uses were: 1.) drought monitoring/assessment, 2.) urban heat island (UHI) analysis, and 3.) Tair estimation. Based on their findings and a subsequent literature review, we have identified three areas in which further study could benefit researchers that require temperature information at a higher spatial resolution than provided by weather stations.

 <u>Interpolating missing LST values</u>: The main disadvantage of MODIS LST products is cloud obstruction, which results in numerous invalid pixels. Less frequently, invalid pixels can also result from emissivity error (Yu et al., 2014; Metz et al., 2014; Van Nguyen et al., 2015). To overcome this issue, studies have focused on interpolating invalid pixels to derive a spatially and temporally continuous dataset. Although several interpolation methods have been proposed for daily (Neteler, 2010; Maffei et al., 2012; Alfieri et al., 2013; Metz et al., 2014, Fan et al., 2014, Yu et al., 2015, Zeng et al., 2015, Shwetha and Kumar, 2016; Kang et al., 2018) and 8-day (Hassan et al., 2007; Hengl et al., 2012; Zhang et al. 2015; Xu and Shen, 2013, Xu et al., 2013; Zhang et al. 2013; Kilibarda et al., 2014; Weiss et al., 2014; Van Nguyen et al., 2015) LST products, there has been virtually no comparison or rigorous validation.

- 2.) Crop yield modeling: Another common application of MODIS imagery is agricultural modeling. More specifically, the Normalized Difference Vegetation Index (NDVI), Enhanced Vegetation Index (EVI), or some related near-infrared based index is used to predict early crop yield 1-2 months prior to harvest (Bolton and Friedl, 2013; Sakamoto et al., 2014; Shao et al., 2015; Wójtowicz et al., 2016). While crop canopy temperature, measured at the field level with an IR thermometer, is a widely accepted metric of crop health (DeJonge et al., 2015; Han et al., 2016; Mangus et al., 2016; Egea et al., 2017; Carroll et al., 2017), the use of MODIS LST for yield modeling has been limited, especially within the United States.
- 3.) Estimating apparent temperature: MODIS LST images are extensively utilized to monitor urban heat islands (Ngie et al., 2014; Rasul et al., 2017; Zhou et al., 2018). A subset of these studies have focused on the adverse health effects of extreme heat (Stathopolou et al., 2005; Klein Rosenthal et al., 2014; Bao et al., 2015; Ho et al., 2015; Morabito et al., 2015; Declet-Barreto et al., 2016; Lehoczky et al., 2017; Xu et al., 2017; Chen et al., 2018; Karimi et al., 2018; Méndez-Lázaro et al., 2018; Mushore et al., 2018; Song and Wu, 2018; Sun et al., 2018; Valmassoi, 2018). However, there is growing evidence to

suggest that LST is a poor indicator of both Tair (Sheng et al., 2017; Tsin et al., 2016; Xiong and Chen, 2017) and apparent temperature (Ho et al., 2016), or the human perceived temperature equivalent that reflects both heat and humidity. Various algorithms that estimate Tair from LST have been proposed (Phan and Kappas, 2018). However, research regarding the estimation of apparent temperature via remote sensing has been very limited. Moreover, heat index (HI), the apparent temperature metric used by the US National Weather Service, has yet to be estimated via remote sensing methods.

1.2 Research Objectives and Hypothesis

The overarching goal of this dissertation was to utilize MODIS LST images for three spatial modeling applications across the conterminous United States (CONUS) (discussed in section 1.1.3). These topics broadly encompassed agriculture and human health. More specifically, the first objective was (1) to compare the performance of all methods previously used to interpolate missing values in 8-day MODIS LST images. The second objective was (2) to investigate the integration of LST images for both short and long term corn yield modeling. And finally, the third objective was (3) to assess the extent to which daily maximum heat index (HI) can be estimated by a combination of MODIS multispectral imagery and auxiliary geospatial products.

Based on the objectives of this research, three hypothesis were formulated:

<u>Hypothesis 1</u>: LST interpolation methods that utilize values neighboring in both time and space (i.e. spatiotemporal) will have the greatest predictive capability for unavailable LST values.

- <u>Hypothesis 2</u>: The novel LST-based killing degree day (KDD) metric will predict annual corn yield with less error than the traditional Tair-based KDD metric.
- <u>Hypothesis 3</u>: HI can be estimated using MODIS observations and products in conjunction with ancillary land cover, topographic, and locational factors.

The CONUS was selected as an ideal study area since it encompasses a wide range of climatic and topographic conditions. Findings relevant to the entire CONUS are applicable to most other regions of the world. Furthermore, ample auxiliary spatial datasets are available for model development and validation.

1.3 Intended Audience and Dissertation Outline

Given the extensive use for MODIS LST for a variety of purposes, the intended audience of this dissertation includes academic researchers, government scientists, and industrial professionals. More specifically, findings regarding the best LST interpolation method would be of broad scientific interest and provide valuable insight to any investigator requiring a spatially and temporally continuous dataset. As LST may improve corn yield prediction, especially during unusually warm and dry growing seasons, these results could potentially benefit farmers, investors, and agricultural scientists. Finally, remotely sensed HI could be used by researchers in the areas of epidemiology, building energy demand, and environmental justice to include subregional heating trends in their analyses at a much greater spatial resolution than provided by insitu weather stations.

This dissertation is composed of 5 chapters. In Chapter 2, the performance of six MODIS LST interpolation methods are empirically compared across a range of cloud cover conditions and in different seasons. Chapter 3 investigates potential benefits of incorporating LST for predicting annual corn yield across the US Corn Belt from 2010-2016. In Chapter 4, daily maximum HI is estimated across the CONUS using MODIS multispectral imagery in conjunction with topographic, land cover, and locational factors. Conclusions and potential areas for future research are discussed in Chapter 5.

This dissertation is organized in the manuscript format. At the time of writing, Chapter 2 was published in the ISPRS Journal of Photogrammetry and Remote Sensing (Pede and Mountrakis, 2018). Chapter 3 was accepted for publication in Agricultural and Forest Meteorology (Pede et al., in press). We plan to submit Chapter 4 to Remote Sensing of Environment.

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CHAPTER 2 MANUSCRIPT 1: AN EMPIRICAL COMPARISON OF INTERPOLATION METHODS FOR MODIS 8-DAY LAND SURFACE TEMPERATURE (LST) COMPOSITES ACROSS THE CONTERMINOUS UNITED STATES

Abstract

Eight-day composite land surface temperature (LST) images from the Moderate Resolution Imaging Spectroradiometer (MODIS) sensor are extensively utilized due to their limited number of invalid pixels and smaller file size, in comparison to daily products. Remaining invalid values (the majority caused by cloud coverage), however, still pose a challenge to researchers requiring continuous datasets. Although a number of interpolation methods have been employed, validation has been limited to provide comprehensive guidance. The goal of this analysis was to compare the performance of all methods previously used for 8day MODIS LST images under a range of cloud cover conditions and in different seasons. These included two temporal interpolation methods: Linear Temporal and Harmonic Analysis of Time Series (HANTS); two spatial methods: Spline and Adaptive Window; and two spatiotemporal methods: Gradient and Weiss. The impact of topographic, land cover, and climatic factors on interpolation performance was also assessed. Methods were implemented on high quality test images with simulated cloud cover sampled from 101 by 101 pixel sites (1-km pixels) across the conterminous United States.

These results provide strong evidence that spatial and spatiotemporal methods have a greater predictive capability than temporal methods, regardless of the time of day or season. This is true even under extremely high cloud cover (>80%). The Spline method performed best at low cloud cover (<30%) with median absolute errors (MAEs) ranging from 0.2°C to 0.6°C. The Weiss method generally performed best at greater cloud cover, with MAEs ranging from

16

0.3°C to 1.2°C. The regression analysis revealed spatial methods tend to perform worse in areas with steeper topographic slopes, temporal methods perform better in warmer climates, and spatiotemporal methods are influenced by both of these factors, to a lesser extent. Assessed covariates, however, explained a low portion of the overall variation in MAEs and did not appear to cause deviations from major interpolation trends at sites with extreme values. While it would be most effective to use the Weiss method for images with medium to high cloud cover, Spline could be applied under all circumstances for simplicity, considering that i) images with <30% cloud cover represent the vast majority of 8-day LST images requiring interpolation, and ii) Spline functions are readily available and easy to implement through several software packages. Applying a similar framework to interpolation methods for daily LST products would build on these findings and provide additional information to future researchers.

2.1 Introduction

Land surface temperature (LST) is the radiative skin temperature of the land surface, measured through emitted thermal infrared radiation in the direction of a given remote sensor. LST has been widely utilized across various scientific disciplines for a variety of purposes, including climatology, hydrology, metrology, land cover/land use change analysis, urban heat island monitoring, and ecosystem health assessment (Ren et al., 2011; Huang et al., 2013; Xu et al., 2013; Fan et al., 2014; Metz et al., 2014; Van Nguyen et al., 2015; Ma et al., 2017) and is a key parameter in the physics of land surface processes on regional and global scales (Shunlin Liang, 2001; Yu et al., 2014).

Traditionally, LST has been recorded by radiometers at weather stations, resulting in insitu point data. Over the past several decades, however, global LST datasets have become available via satellite remote sensing. These earth observation missions include the Moderate Resolution Imaging Spectrometer (MODIS), the Advanced Very High Resolution Radiometer (AVHRR), and Advanced Along Track Scanning Radiometer (AATSR) (Alfiere et al., 2013). If a researcher is interested in a large study area, satellite-derived LST is superior to readings from weather stations, especially in remote areas (Zeng et al., 2015). Although geostatistical methods are available for interpolation of ground observations, these can produce results with significant error due to invalid assumptions with regards to spatial averaging and the exclusion of topographic factors (Xu et al., 2013; Alfiere et al., 2013; Zhang et al., 2013; Zeng et al., 2015).

Due to an ideal tradeoff between its spatial and temporal resolution, MODIS has become the dominant satellite-based sensor for LST data (Ren et al., 2008; Zeng et al., 2016). The constellation consists of two identical sensors; one onboard the Terra satellite and another onboard the Aqua satellite. MODIS sensors estimate LST from thermal infrared bands using a split window algorithm (Li et al., 2012; Xu et al., 2013; Alfiere et al., 2013; Zeng et al., 2015). The Terra and Aqua combined sensors record the LST at each location 4 times a day at an approximately 1-km resolution; twice for the daytime temperature and twice for the nighttime temperature (Wan et al., 2008).

Daily MODIS LST images frequently contain invalid pixels as a result of cloud contamination (Yu et al., 2014; Metz et al., 2014). For cloudy regions, in particular, it is virtually impossible to accurately reconstruct a continuous time-series dataset (Van Nguyen et al., 2015). To overcome this issue, 8-day LST composites are available, which are derived from averaging all clear sky observations for a given pixel over an 8-day period. The high portion of missing pixels in daily LST images often makes it impractical for mapping purposes. Therefore, 8-day images are in many cases simpler to utilize and preferred (Hengl et al., 2012; Linghong et al., 2012). The use of 8-day images is also advantageous since it reduces storage space requirements and computation time. However, even these images can contain a large portion of invalid pixels. As there are numerous applications that require spatially and temporally continuous LST datasets (Qingbai and Yongzhi, 2004; Tomlinson et al., 2011; Linghong et al., 2012), several interpolation methods have been employed to fill gaps in composite images.

While a number of novel interpolation methods have been proposed for daily MODIS LST images (Neteler, 2010; Metz et al., 2014, Fan et al., 2014; Yu et al., 2015; Zeng et al., 2015; Shwetha et al., 2016), our work focused on methods that have been used for 8-day composite images due to their wide applicability and easier utilization, as discussed above. Invalid values for 8-day LST composites have been interpolated over a variety of study areas, varying in both spatial and temporal extents (Table 2.1). According to Metz et al. (2014), the interpolation of MODIS products can be categorized into three groups: spatial-based, temporal-based, and spatiotemporal-based. For temporal methods, invalid values are estimated on a pixel-by-pixel basis and do not consider values of geographically neighboring pixels. Spatial methods only consider the values of neighboring pixels and do not include values from different periods of time. Spatiotemporal methods consider pixels neighboring in both the temporal and spatial domain.

Study	Method	Туре	Stud Area	Temporal Extent	Spatial Extent (1,000 km ²)
Klingsiesen et al., 2010	Linear Temporal	Temporal	Australia	2000-2010	7,692
Zhang et al., 2015	Linear Temporal	Temporal	Northeast China	2001-2002	1,578
Xu et al., 2013	HANTS	Temporal	Tibetan Plateau	2003-2010	2,530
Xu and Shen, 2013	HANTS	Temporal	Yangtze River Delta Region	2005	157
Van Nguyen et al., 2015	HANTS	Temporal	Red River Delta, Vietnam	15,000	15
Linghong et al., 2012	Adaptive Window	Spatial	NE Qinghai-Tibet Plateau	2008	1,100
Zhang et al., 2013	Adaptive Window	Spatial	Jilin Province	2001-2011	187
Hengl et al., 2012	Spline	Spatial	Croatia	2008	57
Kilibarda et al., 2014	Spline	Spatial	Globe	2001-2013	Global
Hassan et al., 2007a	Gradient	Spatiotemporal	Atlantic Maritime Ecozone	2003-2005	192
Hassan et al., 2007b	Gradient	Spatiotemporal	Atlantic Maritime Ecozone	2003-2005	192
Akther and Hassan, 2011	Gradient	Spatiotemporal	Alberta, Canada	2005-2008	661
Rahman, 2011	Gradient	Spatiotemporal	Alberta, Canada	2006-2001	661
Rahaman and Hassan, 2017	Gradient	Spatiotemporal	Alberta, Canada	2001-2010	661
Weiss et al., 2014	Weiss	Spatiotemporal	Africa	2000-2012	30,370
Pigott et al., 2015	Weiss	Spatiotemporal	Africa	2000-2012	30,370
Messina et al., 2015	Weiss	Spatiotemporal	Africa-Asia-Australia	2000-2012	82,642
Weiss et al., 2015	Weiss	Spatiotemporal	Africa	2000-2012	30,370
Mylne et al., 2015	Weiss	Spatiotemporal	Africa	2000-2012	30,370
Kraemer et al., 2015	Weiss	Spatiotemporal	Pakistan	2011-2014	796
Nsoesie et al., 2016	Weiss	Spatiotemporal	Global	2000-2015	Global
Golding et al., 2017	Weiss	Spatiotemporal	Africa	2000-2015	30,370
Longbottom et al., 2017	Weiss	Spatiotemporal	Asia	2000-2014	44,580

Table 2.1: Overview of studies that interpolated invalid pixels in 8-day MODIS LST images.

In terms of temporal interpolations, the Linear Temporal approach was utilized by Klingsiesen et al. (2010) and Zhang et al. (2015). For each missing pixel, the rate of change in LST between the closest proceeding and following 8-day periods with data are determined and used to construct a linear equation. Based on the temporal distance between the period in question and the LST of the closest proceeding period with data, the linear equation can be applied to fill the missing value. A more sophisticated temporal approach is Harmonic Analysis of Time Series (HANTS). This technique was originally developed for smoothing and gapfilling Normalized Difference Vegetation Index (NDVI) images, but has been used to interpolate invalid data in both daily (Maffei et al., 2012; Affiere et al., 2013) and 8-day MODIS LST images (Xu and Shen, 2013; Xu et al., 2013; Van Nguyen et al., 2015). The algorithm uses a least squares curve fitting procedure based on harmonic components. For each harmonic, the amplitude and phase of the cosine function is determined during an iterative fitting procedure (Roerink et al., 2000).

In spatial interpolations, Linghong et al. (2012) proposed a novel method that relies on the assumption that LST is correlated with elevation. For each image, a moving window is used to interpolate invalid pixels based on the linear relationship with elevation. When a certain portion of cells within a window are valid, ordinary least squares (OLS) regression is performed, in which LST is modeled as a linear function of elevation. The LST is then interpolated based on the elevation of the center cell and the derived function. It is referred to as Adaptive Window, because this process continues after each pass until all pixels within an image are interpolated. This method was later applied by Zhang et al. (2013). Another spatial method for MODIS 8-day LST images is Spline interpolation. Three dimensional surface splines are used to interpolate a Z value (LST) for a given X and Y coordinate point. Both Hengl et al. (2012) and Kilibarda et al. (2014) used the *Close Gaps* function, available in System for Automated Geoscientific Analysis (SAGA) open source software (via the grid_tools module) for interpolation.

A simple Gradient spatiotemporal method for 8-day MODIS LST was first implemented by Hassan et al. (2007a). This technique is based on temperature differences between the LST of pixels and average LST of images. For each 8-day image, the difference between the average LST (i.e. average of all valid pixels) and each valid pixel is calculated. The average difference, or gradient, is then calculated on a pixel-by-pixel basis over a period of time. Missing values are filled by adding the average gradient of a pixel to the average LST of an 8-day image. Later studies used this approach to improve the quantification of growing degree days and surface wetness indices (Hassan et al., 2007b; Akther and Hassan, 2011; Rahman, 2011; Rahaman and Hassan, 2017)

Finally, a novel spatiotemporal approach was proposed by Weiss et al. (2014). Gaps are first filled by identifying proceeding and following calendar dates with a usable value for the gap pixel and searching outward for spatially neighboring pixels with valid values in both images. If the maximum search radius is reached without a pixel threshold being met, the search continues into calendar dates of proceeding and following years. Once the threshold is met, gap pixels are filled based on their LST from a given calendar date and the ratio of LST between images for neighboring pixels (inversely weighted by time-space distance). If all years are exhausted without the threshold being met, remaining pixels are filled using their average LST (computed across all years) and the ratio between the LST and multiyear average of valid spatially adjacent pixels within an iterative, multidirectional window. This technique, henceforth referred to as Weiss, has been extensively employed for epidemiology studies in various geographic regions (Pigott et al., 2015; Messina et al., 2015; Weiss et al., 2017; Longbottom et al., 2017).

The main limitation of studies that interpolated 8-day MODIS LST images is that assessment did not contrast an extensive number of methods and sites. There remains a need to compare the performance of methods across a variety conditions and using a common framework to assess interpolation accuracy across seasons, time of day, and site conditions. This study aimed to address this problem by empirically comparing six methods previously employed for interpolating invalid data in 8-day MODIS LST images (Linear Temporal, HANTS, Adaptive Window, Spline, Gradient, and Weiss). To the best of our knowledge, these constitute all methods that have been applied to 8-day MODIS LST. Our objectives were twofold: (1) determine which method is the best predictor of invalid 8-day LST pixels in daytime and nighttime images under a range of cloud cover and seasonality conditions and (2) assess how topographic, climatic, and land cover conditions impact their predictive power. The overarching goal was to provide an actionable guidance for scientists and practitioners with respect to the creation and usage of such datasets.

2.2 Methods

All six methods were applied to interpolate invalid data across eighty-five 101 by 101 pixel test sites (1-km pixels) sampled across the conterminous United States (CONUS); center pixels were used for assessment. Masks with varying levels of cloud cover were generated from observed imagery across sites and applied to test scenes with a high portion of valid data. Seasonality was incorporated by selecting masks and test scenes from all 4 seasons. To determine the impact of time of day, assessment was performed separately for daytime and nighttime LST images. Finally, a regression analysis was conducted to identify factors that significantly influence the predictive error of each method.

2.2.1 MODIS LST data and preprocessing

This study utilized 1-km 8-day composites from the MODIS sensor onboard the Terra satellite (MOD11A2 – version 6), which contain both daytime and nighttime LST images, as well as the corresponding Quality Assurance (QA) layers. Data from 2001 to 2016 was downloaded from the Daac2Disk tool for the CONUS, courtesy of the NASA EOSDIS Land Process Distributed Active Archive Center (LP DAAC, 2014). Tiles were mosaicked and raw

LST values were converted to °C; the original sinusoidal coordinate system was kept and all additional base layers were reprojected to match.

Ocean pixels were identified using the QA layer and excluded from interpolation and cloud mask creation. Two base layers were used for the selection of test sites: the 250-m MODIS Water Mask (MOD44W), obtained from Carroll et al. (2009), and the Level III Ecoregion shapefile, obtained from US EPA (2013).

2.2.2 Study area and test sites selection

The CONUS was identified as an ideal study area due to its wide range of topographic and climatic conditions, in addition to the availability of auxiliary data. To ensure sufficient variation in environmental conditions, one test site was selected from each of the 85 Level III Ecoregions within the CONUS. These boundaries represent areas of similar ecosystems and are delineated by the US Environmental Protection Agency on the basis of geology, landforms, vegetation, climate, land use, wildlife, and hydrology (Omernik and Griffith, 2014).

To select high quality center test pixels, the MODIS Water Mask was used to exclude pixels containing any water. Center test pixels were selected by generating random points within the minimum bounding box of their corresponding Ecoregion until a point was found that fell within the inwardly buffered region, but outside of a 1-km LST pixel containing water. Study site grids were created by extracting the 50 pixels surrounding each side the selected test pixels. As there are 46 8-day periods in a given year and 16 years of MODIS data, there were 736 101 by 101 pixel images of daytime LST, daytime QA, nighttime LST, and nighttime QA for each study site. The footprint of all 85 sites is depicted in Figure 2.1.

24



Figure 2.1: Footprint of the 85 101 by 101 pixel (1-km pixels) utilized study sites and Ecoregion number. The shape of the footprints is attributed to the MODIS sinusoidal projection. Refer to US EPA (2013) for the name corresponding to each Ecoregion number.

2.2.3 Artificial cloud creation and empirical assessment

Cloud masks were created based on the actual footprints, or patches, of cloud-contained pixels present in 8-day LST images from study sites. This replicated previously observed cloud coverage and artificially excluded LST data for interpolation. Twenty tests were performed for each site, season, and cloud cover category. It should be noted that in this case, cloud-contaminated and invalid are used interchangeably. While it is possible for invalid values to occur as a result of emissivity error, the vast majority for MODIS 8-day LST composites are derived from cloud obstruction (>99%). Seasons were defined as weather seasons (*Winter* = January, February, December; *Spring* = March, April, May; *Summer* = June, July, August; *Fall* = September, October, November) and assigned to images based on the season of the first day of
the 8-day period. Ten cloud cover categories in equal increments were utilized, ranging from (0-10%) to [90-100%). Thus, interpolation methods were assessed for daytime and nighttime images with 800 tests per site (20 tests x 10 categories x 4 season). For a given season, category, and time of day, there were 1,700 tests across all sites (20 tests x 85 sites).

Twenty masks were generated for each cloud cover category and season using imagery from study sites. Selected images contained an invalid center pixel and corresponding portion of invalid cells. Since there were an insufficient number of images meeting these criteria to utilize site-specific masks, a single set of masks was compiled from all sites. For each season and category, candidate masks were identified and sites with a potential mask were randomly selected. This avoided multiple masks coming from a single site. If there were less than 20 sites, this process was repeated for sites having multiple candidate masks until 20 were selected. This was done separately for daytime and nighttime LST to derive daytime and nighttime cloud masks. Sites containing ocean pixels were not used to derive cloud masks.

Test scenes (i.e. validation images) for seasons were identified for sites where the center pixel was high quality (QA = 00) and the portion of invalid pixels was 0%. If there were at least 20 images from 2001-2016 that met this criteria, twenty were randomly selected. If there were less than 20, images that met the criteria were kept and additional images were found where the center pixel was high quality and the portion of invalid pixels was <1%. This continued until 20 images were found, according to the criteria listed in Table 2.4 (in the Supplemental Information section, 2.5). Test scenes from the vast majority of sites were found where the center pixel was high quality. Through this process, sites were assigned 20 daytime and nighttime test scenes for all 4 seasons.

Once cloud masks and test scenes were selected, the validation process was performed. Invalid pixels were simulated by applying the 20 masks for each cloud cover category and season to each site's corresponding test scenes. Pixels in test scenes were set to invalid if the same pixel was invalid in the applied cloud mask (as depicted by Figure 2.2). The 6 interpolation methods were then implemented to predict the LST of center test pixels. To reduce the influence of outliers, performance was assessed using the median absolute difference (i.e. error) between predicted and observed LSTs across all sites for each cloud cover category and season.



Figure 2.2: Visual example of cloud cover simulation for selected test and center test pixel to interpolate (Daytime LST, Site 24, Winter, 28.4% cloud cover – 20-30% category).

2.2.4 Assumptions and implementation of interpolation methods

Linear Temporal: Following the procedure described by Klingseisen et al. (2010) and Zhang et al. (2015), the closest proceeding and following 8-day periods with valid data were identified and used to derive a linear equation to estimate the missing LST value of the test pixel. Since it is rare for a pixel to have an invalid LST value for 2 consecutive 8-day periods, most estimation was accomplished by a simple average of the two values immediately neighboring in time.

Harmonic Analysis of Time Series (HANTS): Five input parameters are required by the user for

the HANTS algorithm: the number of frequencies (NOF), high/low suppression flag (SF), valid data range (VDR), fit error tolerance (FET), and degree of over-determinedness (DOD) (Roerink et al. 2000). A value of 'Low' was used for SF, since undetected clouds result in unusually low LST values (Alfiere et al., 2013; Van Nguyen et al., 2015). A range of -50°C to 70°C was set for VDR to omit unusual temperatures for the CONUS. Values of 6°C and 7°C were used for the FET and DOD, respectively (Xu and Shen, 2013; Xu et al., 2013; Van Nguyen et al., 2015). Although some authors recommend an initial assessment to find an optimal NOF value (Xu and Shen, 2013; Van Nguyen et al., 2015), this would have been unfeasible due to the high number of sites. We used 2 to reflect annual and semiannual cycle harmonics (Xu et al., 2013). The HANTS algorithm was applied to individual years since, as noted by Maffei et al. (2012), derived coefficients can vary significantly from year-to-year. Once a cloud mask was applied to a validation image, LST values of the center pixel were compiled into a time-series. The value from the fitted curve corresponding to the 8-day period of the test image was used as the predicted value. We utilized the HANTS Matlab function created by Abouali (2012).

<u>Adaptive Window</u>: The Adaptive Window method was applied using a sliding window size of 49 by 49 pixels and 10% threshold for the portion valid pixels needed for regression (as used by both Linghong et al., 2012 and Zhang et al., 2013). A resampled and filled 1-km DEM from the NASA Shuttle Radar Topography Mission (SRTM) was employed (Jarvis et al., 2008). The layer was reprojected to the sinusoidal coordinate system (via nearest neighbor resampling) and snapped to the MODIS LST grid by taking an average of

coincident points. The MODIS Water Mask was used to identify LST pixels that were majority water to omit from validation. Once a mask was applied, images were filtered based on the QA layer (QA = 00) and histogram to eliminate unusually high and low outliers. Some checks were necessary to avoid over-filtering. There were 7 sites where QA filtering was not performed, since they had very few high quality LST readings due to the geometry of the area. QA filtering was also not performed if there were no high quality pixels in a given image.

- Spline: While previous authors have employed SAGA GIS for spline interpolation (Hengl et al., 2012; Kilibarda et al., 2014), this analysis utilized the *Griddata* function in Matlab.
 Surfaces were fit to test scenes and used to predict the value of the center test pixel.
 Biharmonic Spline was specified as the method ('v4'), since it is not based on triangulation and thus, the most sophisticated and mathematically rigorous option available.
- <u>*Gradient*</u>: Similar to HANTS, the Gradient method was implemented on an annual basis, such that all 46 8-day images in the year of a given validation image were used to calculate the average LST offsets for pixels. The average offset was calculated for center pixels following the application of the cloud mask. Averages were calculated using an entire year of data, a slight deviation from Hassan et al., (2007a), who only used 8-day images from the growing season (April 7th October 31st).
- <u>Weiss</u>: It was necessary to compile an image stack for each calendar date across all years from 2001 to 2016 (16 calendar dates for each 8-day period). Outlying LST values were initially identified and set to invalid on a pixel-by-pixel basis using their z-score (if z-score > 2.58). Mean pixel-by-pixel values were computed across all 16 years. As

implemented by Weiss et al. (2014), values of 40 and 80 were used as the minimum and maximum thresholds, respectively, along with a 3.6-km search radius (corresponding to roughly a 7 by 7 pixel window).

2.2.5 Assessment of topographic, land cover, and climatic factors

To identify potential factors that influence the performance of interpolation methods, a regression analysis was conducted between obtained errors and various topographic, land cover, and climatic variables. Based on images from selected study sites, the vast majority with cloud cover contained less than 30% (low cloud cover in 86.8% and 88.6% of daytime and nighttime images, respectively). For simplicity, median absolute errors (MAEs) for each site were computed from test results aggregated across all seasons and the first 3 cloud cover categories: (0,10%), [10,20%), and [20,30%). This resulted in sites having a single daytime/nighttime MAE for each of the 6 methods.

The source and spatial resolution of utilized covariates are summarized in Table 2.2. The strong correlation between elevation and LST is well documented (Van De Kerchove et al., 2013; Stroppiana et al., 2014; Matthew et al., 2017; Khandelwal et al., 2017). Certain interpolation methods may perform better at lower or higher elevations. Likewise, methods may perform worse if there is significant change in elevation across a study area. The relationship between LST and land cover is also well documented, with vegetative cover generally having a lower LST on average than impervious cover (Tang et al., 2011; Guo et al., 2012; Wu et al., 2013; Qiao et al., 2013; Clinton and Gong, 2013). It is important to consider the effects of land cover on the discussed methods. To date, there has been no assessment of how interpolation methods perform in different climates. If a region experiences infrequent precipitation and limited cloud coverage, temporal methods may outperform spatial and spatiotemporal methods.

Variable	Definition	Program	Spatial Resolution	Units
Elev	Average elevation	SRTM	1-km	m
Slope	Average slope	SRTM	1-km	%
PerAg	Average percent agriculture (class = 81, 82)	NLCD	30-m	%
PerDev	Average percent developed (class = 21, 22, 23, 24)	NLCD	30-m	%
PerFor	Average percent forest (class = 41, 42, 43)	NLCD	30-m	%
PerWet	Average percent wetland (class = 90, 95)	NLCD	30-m	%
PerWat	Average percent water (class = 11)	NLCD	30-m	%
Temp	Average 30-year normal mean annual air temperature	PRISM	800-m	°F
MinTemp	Average 30-year normal minimum annual air temperature	PRISM	800-m	°F
MaxTemp	Average 30-year normal maximum annual air temperature	PRISM	800-m	°F
Precip	Average 30-year normal annual precipitation	PRISM	800-m	inch

Table 2.2: Summary of covariates utilized for the error analysis.

Note: SRTM = Shuttle Radar Topography Mission (from Jarvis et al., 2008), NLCD = National Land Cover Database (2011) (from USGS, 2017, refer for class definitions), PRISM = Parameter-elevation Regressions on Independent Slopes Model (obtained from PRISM Climate Group, 2004).

In terms of data processing, covariate layers were projected to the sinusoidal coordinate system (via nearest neighbor resampling), aggregated to a 1-km cell size, and snapped to MODIS pixels. Slope was computed from the SRTM DEM and matched to the MODIS grid as well. For continuous variables, aggregation was accomplished by taking an average of coincident points. For discrete land cover variables, NCLD classes were converted to binary layers via the scheme in Table 2.2 and the percentage of each class was calculated for LST pixels. To summarize covariates as a single value for each site, a weighted (inverse distance) average was computed, giving pixels closer to the center a higher weight. This limited the influence of faraway values, since interpolation was only assessed on center pixels.

Once the covariates were determined, ordinary least-squares (OLS) regression was applied to develop a total of 12 models (a daytime and nighttime model for the 6 methods), such that each site was an observational unit, the aggregated MAE (in °C) was the dependent variable, and the covariates were the explanatory variables. To assess the relative influence of covariates, dependent and independent variables were standardized (subtracted mean and divided by standard deviation). Variation Inflation Factor (VIF) examination followed to reduce multicollinearity. OLS assumptions for uncorrelated residuals, homogenous variance, and normally distributed residuals were checked using the Durbin-Watson, White, and Kolmogorov-Smirnov tests, respectively.

2.3. Results and Discussion

2.3.1 Performance of interpolation methods under varying cloud cover and seasons

Figure 2.3 displays the median absolute error (MAE) for each method by cloud cover category and season when applied to daytime LST images. Depending on the method, season, and category, MAE values ranged from 0.27°C to 3.66°C. In general, the Spline spatial method had the lowest MAE for categories containing less than 30% cloud cover; at greater cover, the Weiss spatiotemporal method had the lowest MAE. Results were similar when interpolation methods were applied to nighttime images, only Spline had the lowest MAE up to the 40-50% cloud cover category and Weiss, Adaptive Window, or Gradient had the lowest MAE at greater cover, with relatively small separation in values (Figure 2.4).



Figure 2.3: MAEs and 75th/25th percentiles by cloud cover category and season for methods applied to daytime LST. Bins contain 1,700 samples (20 tests at 85 sites); a small portion of tests (<0.3%), especially for [90-100%), could not be completed for some spatial methods. Note: 75^{th} percentiles of 5.6°C, 10.6°C and 8.5°C not shown for last category for Spline method. Created using function by Callaghan (2014).



Figure 2.4: MAEs and 75th/25th percentile by percent cloud cover category and season for methods applied to nighttime LST. Most bins contain 1,700 samples (20 tests at 85 sites); a small portion of tests (<0.2%), especially for [90-100%), could not be completed for some spatial methods. Note: 75th percentile of 10.9 not shown for last category of spring Spline. Created using function by Callaghan (2014).

The MAE values for Spline, Adaptive Window, and Gradient were similar across seasons. Weiss exhibited minor improvement with fall and summer images, in the 0.01°C to 0.33°C range, causing it to have a lower MAE than Spline for the [20-30%) daytime summer category (by 0.03°C). The MAE for the temporal methods, however, was quite lower for summer and fall LST images compared to winter and spring images; in some cases, by almost 1°C. This is most likely due to less frequent cloud cover during these months, resulting in a greater number of values neighboring in time. While temporal MAEs for these seasons were lower, they were still greater than the MAEs of other methods, even for categories with high cloud cover. Although there were some exceptions, the best predictor for a given cloud cover category remained constant across seasons.

These findings provide strong evidence that spatial and spatiotemporal methods are capable of predicting cloud contaminated MODIS 8-day LST images with considerably less error than temporal methods. The higher predictive ability of the spatial domain may be attributed to the strong spatial dependency of LST. For variables that exhibit spatial dependency, or spatial autocorrelation, locations that are closer in space have similar values; locations further apart have less similar values (Cai and Wang, 2006). The spatial structure of LST is, in part, caused by its strong correlation with topographic and environmental factors (Neteler, 2010; Linghong et al., 2012; Zhang et al., 2013; Metz et al., 2014; Fan et al., 2014; Yu et al., 2014). These covariates also exhibit spatial autocorrelation. By only considering values neighboring in time, temporal methods omit important information related to this spatial structure of LST. Furthermore, the 8-day (instead of daily) temporal interval further reduces temporal correlations.

Prediction improved for all methods with nighttime images, but Spline, Adaptive Window, and Gradient saw the greatest improvement. As a result, Spline remained the best predictor for categories containing <50% cloud cover, with the exception of summer images (as opposed to 30% for daytime images). Adaptive Window and Gradient outperformed Weiss for some medium to high cloud cover categories as well, though the difference in MAEs was relatively small (typically <0.1°C). This improved performance may result from the more prominent spatial structure of LST at night. As authors have noted a stronger correlation between nighttime LST and elevation than daytime LST and elevation (Van De Kerchove et al., 2013; Stroppiana et al., 2014), topography and other environmental factors likely have a greater influence on nighttime LST. Although Gradient is classified as spatiotemporal, interpolated values are more reflective of the spatial domain, since the technique employs average offsets computed over time.

We expected to find a cloud cover range beyond which the temporal methods would outperform other techniques. However, with the exception of Spline for the last category [90-100%), temporal methods always produced a higher MAE. To investigate further we compared the spatial and temporal domains. Following the cloud mask application (with data pooled across seasons) it was revealed that the spatial average of remaining pixels is consistency closer to the value of the center test cell than the temporal average of the closest proceeding and following center pixels (Figure 2.5). In fact, two-sample t-tests showed that the difference between the temporal and spatial domain mean was significant for all 10 categories with both daytime and nighttime images (for $\alpha < 0.01$). Thus, LST values of the same image within a 50-km radius of an invalid cell are more predictive than LST values neighboring in time, even under high cloud cover.



Figure 2.5: Boxplots of absolute error between center test pixels and spatial and temporal domain averages by cloud cover category, pooled across sites and seasons. Outliers are not displayed. Created using function by Bikfalvi (2012).

One explanation for the poor performance of temporal methods is that a time step of 8 days is too long to solely consider values neighboring in the temporal domain. Depending on how many daily readings are used to derive clear-sky composites, the two immediately neighboring 8-day pixels could be produced from daily images captured up to 24 days apart. This has important ramifications, considering HANTS is commonly used to interpolate missing values in both 8-day and daily MODIS LST images. Although it is widely accepted that HANTS can be employed for interpolating and smoothing remotely-sensed NDVI time series datasets (Poggio et al., 2012; Michishita et al., 2014; Zhou et al., 2016; Liu et al., 2017), we caution its use for interpolating 8-day LST images. The nature of composite LST time series data is too stochastic to be represented by a trigonometric function. In fact, HANTS performed no better than the simple Linear Temporal methods.

Our finding that spatiotemporal methods did not produce considerably lower MAEs deviates from trends amongst daily interpolation methods to incorporate both the spatial and temporal domain (Neteler, 2010; Metz et al., 2014, Yu et al., 2015; Shwetha et al., 2016). As discussed, a time step of 8-days is too long for LST values neighboring in time to provide useful information for prediction. Since composites represent clear-sky readings averaged over 8-days, spatial methods to some extent already consider the temporal domain. Furthermore, unlike gaps in daily LST images, which resemble the shape of clouds, composite gaps tend to be smaller and more scattered, as they only occur when there are no readings over the 8-day period. Under low to medium cloud cover, this decreases the distance between valid and invalid pixels; under high cloud cover, this results in a wider spatial distribution of valid pixels. Using combined spatial and temporal information does, however, provide slight improvement in most cases under medium to high cloud cover (>30%).

Considering previous authors' emphasis on incorporating topographic and environmental factors to interpolate MODIS LST images, especially elevation, it was surprising that Adaptive Window did not produce lower MAEs than Spline. While it performed reasonably well and better than the temporal methods, it generally produced higher MAEs at low to medium cloud cover (<60%). A more robust regression approach may be needed to model the relationship

between elevation and LST, such as generalized least squares or autoregressive integrated moving average (ARIMA). It is also possible that for 8-day composite images, it is not necessary to consider topographic covariates.

Rather than computing the MAE from observations compiled across all sites, an alternative form of assessment is counting the number of sites for which a particular method had the lowest MAE. For the first cloud cover category (<10%), Spline performed best for the vast majority of sites (>70%) and, with the exception of daytime summer images, maintained the greatest portion at least until 30% (up to 70%) cloud cover (Figure 2.6). For daytime images, Weiss generally performed best for the greatest portion of sites at medium to high cloud cover. However, there was little separation between Weiss, Gradient, and Adaptive Window for these categories with nighttime images. This is likely due to the stronger spatial dependency of nighttime LST and improved performance of spatial methods, as discussed previously. While there is no clear indication of the most appropriate method at medium to high cloud cover for nighttime images, this assessment clearly indicates that at low cloud cover (<30%), Spline is the best interpolation method across the CONUS, regardless of the season or time of day. This is an important finding, considering that the majority of observed cloud coverage scenarios fell in this range.



Figure 2.6: Portion of sites for which each method performed best (Y-axis) for cloud cover categories (X-axis) by time of day and season.

As cloud cover was classified by the percent of obstructed pixels across the entire study area, this did not consider gap sizes surrounding center tests pixels. To further investigate the effects of gap size, we quantified the number of sites for which each method produced the lowest absolute error for low cloud cover masks (<30%) and compared this to the portion of invalid cells within a 15 by 15 pixel buffer of the center pixels. Spline produced the lowest error at the most sites for 75.0% and 75.8% of daytime and nighttime low cloud cover masks, respectively; Weiss produced the lowest error at the most sites for 19.6% and 14.2%, respectively.

Low cloud cover masks for which Weiss performed better typically had a concentration of invalid pixels around the center (Figure 2.7). In fact, the median portion of invalid pixels within the buffer when Spline performed best was 22.0% for daytime masks and 24.0% for nighttime masks, verses 38.1% and 35.4% for Weiss. The use of Weiss may be appropriate if there are extensive gaps surrounding interpolation pixels, most likely due to the iterative, multidirectional averaging windows. However, these instances are infrequent under low cloud cover, since invalid pixels tend to be scattered with 8-day composites. In addition, error improvements over Spline under these circumstances were small, with medians of 0.36°C for daytime images and 0.23°C for nighttime images.



Figure 2.7: Examples of interpolation results for images following cloud mask application with a concentration of invalid pixels around the center test cell. Refer to Figure 2.1 for location of sites.

A common concern among authors is that interpolation methods may only be applicable to clear-sky conditions, yet they are utilized to interpolate the LST of pixels obstructed by clouds (Hassan et al., 2007a; Crosson et al., 2012; Zhang et al., 2013; Xu and Shen, 2013; Metz et al., 2014; Yu et al., 2014; Zeng et al., 2015). In other words, they assume that the LST of pixels not covered by clouds can be used to predict the LST of pixels that are covered by clouds. Invalid pixels may actually have a lower temperature. In order to assess how these methods predict LST under cloud cover, it would be necessary to compare predicted values to ground-based weather stations that record LST. There are two limitations to this approach; the first is the inability to discern error caused by interpolation from error inherent in remotely sensed LST. The process of estimating LST with a space born-sensor is subject to geometric and atmospheric distortion not encountered with ground-based LST measurements (Akhoondzadeh and Saradjian, 2008). The second is a lack of weather stations that record LST. For the CONUS, there is only the Climate Reference Network (CRN), which is comprised of just 93 stations with consistent year-to-year data, does not contain readings prior to 2013, and is limited to areas dominated by forest or agriculture (US DOC, 2002).

2.3.2 Error distribution across topographic, land cover, and climatic factors

Multiple linear regression was performed to link topographic, climatic, and land cover factors with obtained errors of the assessed methods; results are displayed in Table 2.3 (for variable abbreviations see Table 2.1). Scatter plots between independent and dependent variables appeared to be linear or have a low degree of association. It was necessary to eliminate MinTemp and MaxTemp, since they had a Variance Inflation Factor of more than 10, due to their high correlation with Temp. Durbin-Watson (DW) tests revealed that autocorrelation was not a concern in any model because DW values were within the commonly accepted range of

1.5-2.5 (Alkorta et al., 2000; Zakerian and Subramaniam, 2009; Bakon and Hassan, 2013; Al-

Matari et al., 2014; Venkathaialam and Abdulwahab, 2017). Based on White tests,

heteroscedasticity was not significant in any of model (for $\alpha = 0.1$).

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Table 2.3: Significant coefficients from OLS regression. For full models, refer to Table 2.5 in the Supplmental Information section (2.5). Variable significance: $\alpha = [0.05, 0.1]$, $\alpha = [0.01, 0.05)$, ** $\alpha \leq 0.01$.

Linear Temporal		HANTS		Spline		Window		Gra	dient	Weiss	
Adj R ² : 0.411		Adj R ² : 0.4622		Adj R ² : 0.297		Adj R ² : 0.251		Adj R ² : 0.282		Adj R ² : 0.474	
<u>Term</u>	<u>Coef</u>	<u>Term</u>	<u>Coef</u>	<u>Term</u>	<u>Coef</u>	<u>Term</u>	<u>Coef</u>	<u>Term</u>	<u>Coef</u>	<u>Term</u>	<u>Coef</u>
Constant	0.000**	Constant	0.000**	Slope	0.762**	Slope	0.710**	Slope	0.447*	PerAg	0.245^
Temp	-0.733**	PerWat	-0.248^	PerFor	-0.384**	PerWat	-0.326*	PerFor	-0.312*	PerDev	-0.278^
		Temp	-0.705**			PerWet	0.436**	PerWet	0.385*	Temp	-0.469**
<u>Nighttime I</u>	Nighttime Model										
Linear Temporal											
Linear To	emporal	HAN	NTS	S	pline	Wir	ndow	Gra	dient	W	eiss
Linear To Adj R ² :	emporal : 0.505	HAN Adj R ²	NTS : 0.401	Sj Adj F	pline 8²: 0.457	Wir Adj R ²	ndow ² : 0.120	Gra Adj R	dient ² : 0.216	W Adj R	eiss ² : 0.502
Linear Te Adj R ² : <u>Term</u>	emporal : 0.505 <u>Coef</u>	HAN Adj R ² <u>Term</u>	NTS : 0.401 <u>Coef</u>	Sj Adj F <u>Term</u>	pline 8²: 0.457 <u>Coef</u>	Wir Adj R ² <u>Term</u>	ndow ² : 0.120 <u>Coef</u>	Gra Adj R <u>Term</u>	n dient ² : 0.216 <u><i>Coef</i></u>	W Adj R <u>Term</u>	Veiss ² : 0.502 <u><i>Coef</i></u>
Linear Te Adj R ² : <u>Term</u> Constant	emporal : 0.505 <u>Coef</u> 0.000**	HAN Adj R ² <u>Term</u> Constant	NTS : 0.401 <u>Coef</u> 0.000**	Sj Adj F <u>Term</u> Slope	pline & ² : 0.457 <u>Coef</u> 0.802**	Wir Adj R ³ <u>Term</u> Slope	ndow ² : 0.120 <u>Coef</u> 0.564**	Gra Adj R <u>Term</u> Temp	ndient ² : 0.216 <u>Coef</u> -0.425*	W Adj R <u>Term</u> Slope	Veiss ² : 0.502 <u>Coef</u> 0.421**
Linear Te Adj R ² : <u>Term</u> Constant Slope	emporal : 0.505 <u>Coef</u> 0.000** -0.383*	HAN Adj R ² <u>Term</u> Constant Slope	NTS : 0.401 <u>Coef</u> 0.000** -0.550**	Sj Adj F <u>Term</u> Slope PerFor	pline k ² : 0.457 <u>Coef</u> 0.802** -0.214^	Wir Adj R ³ <u>Term</u> Slope	ndow ² : 0.120 <u>Coef</u> 0.564**	Gra Adj R <u>Term</u> Temp	dient ² : 0.216 <u>Coef</u> -0.425*	W Adj R <u>Term</u> Slope Temp	7eiss ² : 0.502 <u>Coef</u> 0.421*** -0.618***
Linear Te Adj R ² : <u>Term</u> Constant Slope PerAg	emporal : 0.505 <u>Coef</u> 0.000** -0.383* 0.435**	HAN Adj R ² <u>Term</u> Constant Slope PerAg	NTS : 0.401 <u>Coef</u> 0.000** -0.550** 0.253^	Sj Adj F <u>Term</u> Slope PerFor Temp	pline 2 ² : 0.457 <u>Coef</u> 0.802** -0.214^ -0.369**	Wir Adj R [:] <u>Term</u> Slope	ndow ² : 0.120 <u><i>Coef</i></u> 0.564**	Gra Adj R <u>Term</u> Temp	dient ² : 0.216 <u><i>Coef</i></u> -0.425*	W Adj R <u>Term</u> Slope Temp	Veiss 2: 0.502 <u>Coef</u> 0.421** -0.618**
Linear To Adj R ² : <u>Term</u> Constant Slope PerAg Temp	emporal : 0.505 <u>Coef</u> 0.000** -0.383* 0.435** -0.729**	HAI Adj R ² <u>Term</u> Constant Slope PerAg Percip	NTS : 0.401 <u>Coef</u> 0.000** -0.550** 0.253^ 0.301*	SJ Adj F <u>Term</u> Slope PerFor Temp	pline R ² : 0.457 <u>Coef</u> 0.802** -0.214^ -0.369**	Wir Adj R [:] <u>Term</u> Slope	ndow ² : 0.120 <u>Coef</u> 0.564**	Gra Adj R <u>Term</u> Temp	dient ² : 0.216 <u>Coef</u> -0.425*	W Adj R <u>Term</u> Slope Temp	Veiss 2: 0.502 <u>Coef</u> 0.421** -0.618**

Most models had non-normal residuals, likely due to several positively skewed independent and dependent variables. To rectify this, any variable that significantly deviated from the normal distribution (based on the Kolmogorov-Smirnov test for $\alpha = 0.05$) was transformed via the natural log function. This included the dependent variables of daytime/nighttime Spline, Gradient, and Weiss MAE and independent variables of Elev, Slope, PerAg, PerDev, PerFor, PerWet, and PerWater. A negative reciprocal transformation was needed for daytime/nighttime Window MAE since resulting model residuals were still positively skewed when these dependent variables were initially log transformed. The negative ensured that positive and negative coefficients corresponded to direct and inverse relationships, respectively. Following variable transformation, the residuals for all models did not significantly deviate from a normal distribution (for $\alpha = 0.05$).

All models had an overall significance for $\alpha = 0.01$, with the exception of the nighttime Window model, which was significant for $\alpha = 0.05$, meaning β was significantly different than 0 for at least one variable. The daytime model explained a higher portion of variation in MAEs than the nighttime model for HANTS, Window, and Gradient. This suggests that the assessed factors have a greater influence on the predictive capability of these methods during the day. The opposite was true for other methods.

Significant variables differed by method and time of day. However, some major trends are apparent. Based on the standardized coefficient, Slope had the most influence on both daytime and nighttime MAEs for Spline and Adaptive Window. The positive value indicates that spatial methods perform better in flatter study areas. As stated previously, there is a strong correlation between LST and elevation. If there is more variation in elevation, there will also be more variation in LST. For Spline, this may cause fit surfaces to be less predictive, since there are larger discrepancies between the LST of neighboring pixels. It is also possible that for the Adaptive Window method, this increased variation causes the relationship between LST and elevation to become nonlinear and not as well captured with a linear model.

Although Spline was the best predictor for the majority of sites at low cloud cover (<30%), there was a small portion of sites for which other methods were the best. However, these anomalies appeared to be caused by unexplained variability, as opposed to outlying average slopes. The sites differed across seasons, categories, and times of day, and their average slopes were generally not above the 75th percentile. While Slope had a large, positive

standardized coefficient in the Spline and Adaptive Window models, the adjusted R²s were low, indicating a small portion of variation in MAEs was explained. There does not seem to be a threshold for Slope that at which point, other methods become more predictive than Spline at low cloud cover.

Temp had the largest influence on both daytime and nighttime MAEs for Linear Temporal and HANTS, suggesting temporal methods perform better in warmer climates. We are unable to explain this finding. Given that fewer values neighboring in time decreases the predictive capability of temporal methods, one would expect Precip to have a greater influence. However, this was only significant in the nighttime HANTs models with relatively low coefficient. Similar to Slope, the few sites where temporal methods performed best at high cloud cover was the result of unexplained variation, as opposed unusually high Temp values.

Interestingly, Temp had the largest influence on daytime and nighttime MAEs for Weiss and nighttime Gradient. Slope also had the largest influence daytime Gradient MAEs and was significant in the nighttime Weiss model. Although the standardized coefficients were comparatively smaller, spatiotemporal methods tend to perform worse in areas with steeper slopes and better in warmer climates, potentially due their utilization of both the spatial and temporal domains.

The magnitude, sign, and significance of land cover coefficients varied by model and did not have the greatest influence on any method's MAEs. The standardized coefficient for PerFor was significant and negative for the daytime and nighttime Spline models, indicating that this method may perform better in areas with greater forest cover. Researchers have found that dense forests stabilize local thermal environments, acting as a thermal buffer (Zhao et al., 2017; Lin et al., 2017). It is possible that this smaller variation in LST increases the accuracy of fit surfaces. While LST can vary across land cover categories, with the exception of forest with Spline, we did not find consistent evidence to indicate certain land cover can influence interpolation.

2.3.3 Recommendations for Implementation

Spline is the easiest method to implement, since spatial interpolation packages are available through numerous platforms, including ArcGIS, SAGA GIS, Matlab, Python, and R; Weiss is more challenging to implement. Although no external data is required, users must build an extensive LST image stack, execute iterative searches for valid pixels in both temporal and spatial domains, and perform multi-directional window averaging if the threshold for valid pixels is not initially met.

Our results indicate that it would be most effective to apply Spline for images with low cloud cover (<30%) and Weiss for images with greater cover or extensive gaps. Although there were some instances when Adaptive Window and Gradient outperformed Weiss under these circumstances, improvements were typically small (<0.1°C). Based on the data used for this analysis, the vast majority of MODIS 8-day LST composites requiring interpolation contain low cloud cover (87% and 89% for daytime and nighttime images, respectively). In fact, most (75% and 77% for daytime and nighttime images, respectively) contain <10% cloud cover, for which there was substantial separation between the predictive capability of Spline and other methods. Considering the distribution of cloud contamination and difficulty of implementing Weiss, using Spline under all conditions for simplicity would be sufficient. While it is rare (<0.5%), Linear Temporal could be employed for images with 100% cloud cover. We caution the use of Spline across areas larger than the ones we assessed (approximately 101 by 101 km). If a selected site is larger, it may be necessary to fit surfaces to sub-sections.

We employed the Biharmonic Spline option available with the *Griddata* function in Matlab. However, there are a number of other interpolation options including Linear, Nearest Neighbor, Natural Neighbor, and Cubic Spline. To further investigate the performance of these methods, a similar analysis was performed, only MAEs were computed for each category across all seasons. Biharmonic Spline did not consistently produce the lowest MAE for daytime or nighttime images. In fact, it produced a substantially greater MAE for the last category (Figure 2.8). Thus, it is not necessary to employ a particular Spline option or spatial interpolation package, as they appear to be equally effective.



Figure 2.8: MAEs and 75th/25th percentiles by percent cloud cover category across all seasons for Matlab Griddata methods applied to daytime and nighttime LST. Most bins contain 6,800 samples (20 tests at 85 sites for 4 seasons); a small portion of tests (<2.5%), especially for [90,100%), could not be completed for some methods. Note: 75th percentiles of 7.13 and 3.57 not shown for last category of daytime and nighttime Biharmonic, respectively. Created using function by Callaghan (2014).

Our analysis utilized images from the MODIS sensor onboard the Terra satellite. Images are also available from the MODIS sensor onboard the Aqua satellite. Their specifications only differ by the overpass time. Terra crosses the equator each day at approximately 10:30 AM and 10:30 PM in local solar time; Aqua crosses at 1:30 AM and 1:30 PM (Reese, 2016). Although

MAE values differed slightly between daytime and nighttime images, the performance of the methods did not substantially differ with respect to each other. As there were no major discrepancies, we would expect to derive the same findings with images from the Aqua sensor.

2.4 Conclusions

This study compared the performance of six methods previously employed to interpolate invalid pixels in 8-day MODIS LST images across various cloud cover extents and seasons. The impact of topographic, land cover, and climatic factors was also assessed. Prior to this work, there had been no empirical comparison of interpolation methods; assessment had been limited to single study area and method. Authors that utilized cloud cover simulation for validation randomly set pixels to invalid and did not consider natural cloud formations or implement a wide range of conditions. In addition, there had been no consideration of factors that may influence prediction. To the best our knowledge, this analytical framework represents the most comprehensive and rigorous assessment to date.

There is strong evidence that the predictive capability of spatial and spatiotemporal methods is superior to temporal methods, even at very high cloud cover. This was the case for both daytime and nighttime LST and across all seasons. Based on the regression analysis, spatial methods appear to be most influenced by topography, such that areas with steeper slopes have higher MAEs. Temporal methods are most influenced by mean annual temperature, with warmer areas having lower MAEs. Due to their consideration of both domains, these factors also influence spatiotemporal methods, but to a lesser extent. With the exception of forest for Spline, land cover did not influence prediction. Although several factors were significant, the assessed covariates explained a relatively low portion of variation in MAE values and did not

cause a departure from our major findings at sites with extreme values. Based on the distribution of cloud contamination, ease of Spline's implementation, and its improved predicative capability over other methods under low cloud cover (<30%), we conclude that the use of Spline under all circumstances is sufficient.

While it would be challenging to perform a comprehensive assessment of daily interpolation methods, given the wide range and complexity of proposed methods, a similar framework could be employed to compare some of the more commonly utilized approaches. Although spatial methods were found to work best for 8-day composites, the temporal domain may prove to be more useful at a smaller time step. This analysis could also be expanded to additional sensors that capture thermal infrared radiation, such as AVHRR and AATSR, or study areas beyond the CONUS. Findings from daily images, alternative sensors, and locations beyond the CONUS would provide valuable information to future researchers.

2.5 Supplemental Information

Table 2.4: The number of sites that used each criterion to select test scenes by time of day and season. Note: HQ means center pixel is high quality; % refers to the portion of invalid pixels within a test scene. Sites are counted if at least one test scene for the season was selected using the less strict criteria.

Ī	Daytime Val	idation Ima	ges	Nighttime Validation Images						
Criteria	Winter	Spring	Summer	Fall	Criteria	Winter	Spring	Summer	Fall	
HQ & 0%	35	67	69	70	HQ & 0%	47	71	71	71	
HQ & <1%	33	10	8	9	HQ & <1%	23	7	8	8	
HQ & <2%	0	0	0	0	HQ & <2%	5	1	0	0	
HQ & <3%	1	0	2	0	HQ & <3%	0	0	0	0	
0%	9	6	6	6	0%	8	6	6	6	
<1%	6	2	0	0	<1%	0	0	0	0	
<2%	1	0	0	0	<2%	1	0	0	0	
<3%	0	0	0	0	<3%	0	0	0	0	

Table 2.5: Standardized coefficient for full OLS regression models.
 Variable significance:
 $\alpha = [0.05, 0.1], *\alpha = [0.01, 0.05), **\alpha \le 0.01.$

Daytime run woulds												
	Lin. Temp.		HANTS		Spline		Window		Gradient		Weiss	
	Adj R ² : 0.411		Adj R ² : 0.4622 Adj R ² : 0.297		Adj R ² : 0.251		Adj R ² : 0.282		Adj R ² : 0.474			
<u>Term</u>	<u>Coef</u>	<u>Sig</u>	<u>Coef</u>	<u>Sig</u>	<u>Coef</u>	Sig	<u>Coef</u>	<u>Sig</u>	<u>Coef</u>	<u>Sig</u>	<u>Coef</u>	<u>Sig</u>
Constant	0.000	**	0.000	**	0.000		0.000		0.000		0.000	
Elev	0.073		0.163		-0.066		-0.064		0.291		0.156	
Slope	-0.178		-0.250		0.762	**	0.710	**	0.447	*	0.239	
PerAg	0.098		0.022		-0.002		0.244		0.092		0.245	^
PerDev	-0.028		-0.020		0.018		-0.018		0.163		-0.278	^
PerFor	-0.091		0.031		-0.384	**	-0.216		-0.312	*	-0.176	
PerWat	-0.042		-0.248	^	0.049		-0.326	*	-0.094		0.061	
PerWet	0.022		0.091		0.136		0.436	**	0.385	*	0.093	
Percip	0.093		-0.018		-0.023		-0.141		-0.051		0.080	
Temp	-0.733	**	-0.705	**	-0.091		-0.112		-0.223		-0.469	**

Davtime Full Models

Nighttime Full Models

Nighttime Full Models												
	Lin. Temp.		HANTS		Spline		Window		Gradient		Weiss	
	Adj R ² : 0.505		Adj R ² : 0.401		Adj R ² : 0.457		Adj R ² : 0.120		Adj R ² : 0.216		Adj R ² : 0.502	
<u>Term</u> Constant	<u>Coef</u> 0.000	<u>Sig</u> **	<u>Coef</u> 0.000	<u>Sig</u> **	<u>Coef</u> 0.000	<u>Sig</u>	<u>Coef</u> 0.000	<u>Sig</u>	<u>Coef</u> 0.000	<u>Sig</u>	<u>Coef</u> 0.000	<u>Sig</u>
Elev	-0.073		0.193		-0.230		-0.110		-0.079		-0.135	
Slope	-0.383	*	-0.550	**	0.802	**	0.564	**	0.307		0.421	**
PerAg	0.435	**	0.253	۸	-0.023		0.101		0.006		0.146	
PerDev	-0.129		-0.138		0.063		0.016		-0.091		-0.163	
PerFor	0.146		0.065		-0.214	۸	-0.226		-0.143		-0.198	
PerWat	-0.102		0.052		0.127		-0.185		-0.043		0.069	
PerWet	-0.106		-0.108		0.197		0.231		0.198		0.065	
Percip	0.185		0.301	*	0.040		0.037		0.043		0.212	
Temp	-0.729	**	-0.575	**	-0.369	**	-0.225		-0.425	*	-0.618	**

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CHAPTER 3 MANUSCRIPT 2: IMPROVING CORN YIELD PREDICTION ACROSS THE US CORN BELT BY REPLACING AIR TEMPERATURE WITH DAILY MODIS LAND SURFACE TEMPERATURE

Abstract

While canopy temperature has been extensively utilized for field-level crop health assessment, the application of satellite-based land surface temperature (LST) images for corn vield modeling has been limited. Furthermore, long term vield projections in the context of climate change have primarily employed air temperature (Tair) and precipitation, which may inadequately reflect crop stress. This study assessed potential benefits of satellite-derived LST for predicting annual corn yield across the US Corn Belt from 2010-2016. A novel killing degree day metric (LST KDD) was computed with daily LST images from the Moderate Resolution Imaging Spectroradiometer (MODIS) sensor and compared to the typically used Tairbased metric (Tair KDD). Our findings provide strong evidence that LST KDD is capable of predicting annual corn yield with less error than Tair KDD ($R^2/RMSE$ of 0.65/15.3 Bu/Acre vs. 0.56/17.2 Bu/Acre). Even while adjusting for seasonal temperature and precipitation parameters, the R² and RMSE of the LST model were approximately 9% higher and 2.0 Bu/Acre lower than the Tair model, respectively. The superior performance of LST can be attributed to its ability to better incorporate evaporative cooling and water stress. We conclude that MODIS LST can improve yield forecasts several months prior to harvest, especially during extremely warm and dry growing seasons. Furthermore, the superior performance of LST over Tair and precipitation models suggest that subsequent long term yield projections should consider additional factors indicative of water stress.

3.1 Introduction

3.1.1 Traditional parameters for long term corn yield modeling and crop health assessment

Corn (i.e. *Zea mays*) production represents a large portion of both the US and global economy and is vital to the world's food supply. Recent studies have indicated that corn yield may decrease in future years as a result of anthropogenic climate change (Lobell et al., 2011; Butler and Huybers, 2013; Hawkins et al., 2013; Moore and Lobell, 2015). In order to assess food availability in the coming decades, it is crucial to understand climatic effects on corn production.

In an effort to assess future supply, a growing body of work has examined the effects of climate and meteorological parameters on corn yield at a regional scale, namely average air temperature (Tair) and total precipitation through the growing season. Corn yield was found to increase with greater seasonal temperatures up to certain threshold (~29-32°C) and decrease at greater temperatures (Schlenker and Roberts, 2009; Hawkins et al., 2013; Troy et al, 2015), though a strictly negative response was reported in France (Ceglar et al., 2016) and a non-significant, positive response was reported in Pakistan (Ali et al., 2017). Most studies that compared trends in temperature and yield over time (i.e. the OLS slope) found an inverse relationship (Lobell and Anser, 2003; Lobell and Field, 2007; Kucharik and Serbin, 2008; Moore and Lobell, 2015). However, a positive relationship has been reported in China (Zhang et al., 2015). A subset of studies focused on yield loss due to heat stress by using the killing degree days (KDD) is derived similar to the more common growing degree day (GDD) metric, but quantifies the extent to which maximum Tair exceeds a threshold for optimal growing conditions (typically 28-30°C for corn). Multiple authors determined that

corn had a positive correlation with GDD and negative correlation with KDD (Butler and Huybers, 2013; Shaw et al., 2014; Butler and Huybers, 2015).

Findings regarding the impact of rainfall are less consistent. On a global scale, trends in growing season precipitation exhibit little to no association with trends in corn yield (Lobell and Anser, 2003; Lobell and Field, 2007). For rainfed counties in the US, a non-linear threshold-type response has been reported (Schlenker and Roberts, 2009; Troy et al., 2015), as well a positive response in Wisconsin (Kucharik and Serbin, 2008) and France (Ceglar et al., 2016). Others have found drought frequency or severity, quantified as Standardized Precipitation Index (SPI), to explain a significant portion of variation in corn yield (Zipper et al., 2016; Lu et al., 2017; Mathieu and Aires, 2018). If considered, the relationship between precipitation and corn yield is limited for irrigated counties (Troy et al., 2015; Cater et al., 2016; Zipper et al., 2016), suggesting that the important factor is not necessarily rainfall, but soil moisture.

The extent to which yield loss is derived from heat stress versus water stress is fairly ambiguous, as extreme temperatures can be associated with droughts (Lockart et al. 2009; Hirschi et al. 2011; Mueller and Seneviratne 2012; Shaw et al., 2014). In addition, Anderson et al. (2015) determined that the sensitivity of corn yield to high temperatures is dependent on water availability. This interaction is confirmed by those who have noted a weaker relationship with growing season temperatures in irrigated districts (Shaw et al., 2014; Troy et al., 2015) and regions experiencing increased precipitation (Schlenker and Roberts, 2009; Leng, 2017a). Rainfall may be an inadequate proxy for soil moisture, especially in areas with deep root zones, such as the US Midwest (Fawcett, 2013; Ransom, 2013). The actual amount of water available to crops (or lack thereof) can depend on a range of factors related to soil and hydrological characteristics, including soil water holding capacity, soil quality and type, rooting depth, water

table depth, and land use/land cover (Hund et al., 2009; Hamilton et al., 2015; Licht et al., 2018). Thus, any regional attempt to model corn yield should reflect water availability, as opposed to simply Tair and precipitation.

Canopy temperature is widely accepted as an indicator of field-level crop water stress, since plants close their stomata under water constraints to reduce evapotranspiration and subsequent water loss; this process increases leaf temperatures. When leaf stomata are open, water evaporates and cools the leaf (i.e. evaporative cooing) (DeJonge et al., 2015; Han et al., 2016; Mangus et al., 2016; Egea et al., 2017; Carroll et al., 2017). Idso et al (1981) and Jackson (1981) first developed the Crop Water Stress Index (CWSI) to compare canopy temperatures against a non-water stressed (minimum) and water-stressed (maximum) baseline. Numerous follow-up analyses have applied this metric to a variety of crops, often in the context of irrigation scheduling; nearly all measured canopy temperature using a hand-held infrared (IR) thermometer or camera (Taghvaeian et al., 2012; Durigon and de Jong van Lier, 2013; Taghvaeian et al., 2014; DeJonge et al., 2015; Mangus et al., 2016; Carroll et al., 2017).

3.1.2 Integration of satellite observations in agricultural modeling

Over the past several decades, global land surface temperature (LST) datasets have become available via satellite remote sensing. These earth observation missions include the Moderate Resolution Imaging Spectroradiometer (MODIS), the Advanced Very High Resolution Radiometer (AVHRR), and Advanced Along Track Scanning Radiometer (AATSR) (Alfieri et al., 2013). Due to its superior spatial, spectral, and temporal resolution, MODIS has become the predominant satellite-based sensor for agricultural studies (Ren et al., 2008; Becker-Reshef et al., 2010; Bolton and Friedl et al., 2013; Zeng et al., 2016; Song et al., 2017). The majority of analyses that utilize satellite imagery for agriculture modeling do not consider LST and employ Normalized Difference Vegetation Index (NDVI), Enhanced Vegetation Index (EVI), or some other index based on the visible and near-infrared portion of the electromagnetic spectrum (Ren et al., 2008; Becker-Reshef et al., 2010; Sakamoto et al., 2014; Bolton and Friedl, 2013; Shao et al., 2015; Wojtowicz et al., 2016). Other authors have used MODIS Gross Primary Productivity (GPP) to develop a production efficiency model (PEM) or light use efficiency model (LEM) for corn yield prediction (Xin et al., 2013; Xin et al., 2015; Yuan et al., 2016). This approach is based on the assumption that crop yields under non-stressed conditions linearly correlate with the amount of absorbed photosynthetically active radiation. While PEMs have been found to adequately predict annual corn yield in the US Midwest (Xin et al., 2013), they do not incorporate LST, as MODIS GPP is derived from visible, near-infrared, and mid-infrared bands.

The limitation of near-infrared vegetation metrics is that their utility for long term agricultural projection is limited. NDVI primarily reflects the leaf structure and greenness of vegetation (Gammon et al., 1995; Ji and Peters, 2004), which are difficult to predict into the future (Ji and Peters, 2004). Moreover, they do not provide information on the underlying drivers of crop health or growing conditions. LST, however, is more indicative of external controls, such as the surface-energy balance, Tair, and soil moisture. In contrast to NDVI, it is possible to forecast these drivers using a combination of geophysical principals and output from climate change models (Houle, 2012; Cuxart et al., 2015; Diallo et al., 2017).

For regional drought assessment, recent studies computed a modified CWSI or similar LST-based water index, such as Temperature Difference Vegetation Index (TDVI), using 8-day and monthly MODIS composites. In this case, the minimum and maximum baselines are

alternatively estimated using Normalized Difference Vegetation Index (NDVI) (Khomarudin and Sofan, 2010; Son et al., 2012; Leroux et al., 2016; Bai et al., 2017), Enhanced Vegetation index (EVI) (Holzman et al., 2014; Holzman and Rivas, 2016; Chen et al., 2017; Swain et al., 2017), or Leaf Area Index (LAI) (Dhorde and Patel, 2016). Authors commonly found a strong relationship when these indices were compared to NDVI (Khomarudin and Sofan, 2010), in-situ measurements of soil moisture (Bai et al., 2017), in-situ precipitation (Liang et al., 2014; Bai et al., 2017; Swain et al., 2017), or microwave-based precipitation grids (Son et al., 2012; Chen et al., 2017). Holzman and Rivas (2016) cumulated TDVI over the growing season for an agricultural district of Argentine Pampas, Argentina and found an R² of 0.61 with corn yield. LST-based water indices, however, are more suited for heterogeneous landscapes with sparse farmland, which have a range of vegetative conditions to compute the minimum and maximum baselines, and would be less applicable to a homogeneous region dominated by agriculture, such as the US Corn Belt. Furthermore, defining the baselines can be an arbitrary, cumbersome process that requires LST/NDVI readings across a variety of vegetative environments (DeJong et al., 2015; Bai et al., 2017).

Only three studies have related MODIS LST to corn yield in the US. Johnson (2014; 2016) did this on an image-by-image basis using 8-day composites over the course of the growing season. They found that daytime and nighttime LST peaked in August and had relatively low correlations with yield ($\rho = -0.58/-0.62$ and $\rho = -0.29/-0.32$, respectively). Heft-Neal et al. (2017) substituted daytime LST for average maximum Tair in an existing climate-response model for corn yield and derived comparable results for the US and improved results for Africa, as a result of sparse weather stations. In all three cases, the authors employed 8-day

or monthly composites, which smooth out daily extreme temperatures and do not reflect conditions within critical crop developmental stages.

3.1.3 Study objectives

There is much evidence to suggest agricultural modeling can be improved by the utilization of daily MODIS LST. However, applications to corn yield have been fairly limited. While authors used LST to estimate Tair and increase the spatial resolution of in-situ GDD (Neteler, 2010; Zhang et al., 2013; Zorer et al., 2013; Alemu and Henebry, 2016), agricultural LST metrics that evaluate the impact of high temperatures (i.e. KDD) have yet to be computed directly from LST. Results from this analysis were intended to contribute to two areas of agricultural modeling.

The first is short term, within-season yield prediction (i.e. forecasting yield several months prior to harvest). From an operational perspective, LST could potentially be capable of measuring evaporative cooling across a large region similar to an infrared thermometer at the field-level. Considering canopy temperature's reflection of both heat and water stress, KDD derived from LST may offer significant improvements in regional corn monitoring, yet require relatively simple computations.

The second area is long term, multi-decadal corn yield projection in the context of climate change. Comparing the predictive power of LST and Tair could benefit subsequent climate-yield models, which to date have predominately relied on Tair and precipitation. While LST is not an output of climate models and cannot be directly used for projection, improvements with LST over traditional meteorological factors would suggest that soil and hydrological characteristics indicative of water availability should additionally be considered. A complete

understanding of the controls on corn yield requires information regarding both heat and water stress, which are likely better captured by LST.

In this study, we focused on county-level corn yield across the US Corn Belt from 2010-2016. The overarching goal was to assess the utility of accumulated degree day metrics derived from satellite-based LST. Our specific objectives were twofold: (i) compare the corn yield predictive capability of KDD derived from Tair and daily MODIS LST and (ii) determine if any improvements remained while controlling for meteorological variables commonly utilized for regional agricultural modeling (i.e. GDD, growing season air temperature and precipitation, and drought indices).

3.2 Methods

3.2.1 Study area

The US Corn Belt was identified as the study area since it produces nearly three-quarters of the nation's corn (73.3% in 2016 – USDA, 2018a) and represents a fairly homogeneous, agriculturally dominated landscape (Loveland et al., 1995). The Corn Belt geographic boundaries followed the definition by Green et al. (2018), which is based on a spatiotemporal analysis of land-use patterns and includes 8 states: Illinois (IL), Indiana (IN), Iowa (IA), Minnesota (MN), Nebraska (NE), Ohio (OH), South Dakota (SD), and Wisconsin (WI). Figure 3.1 depicts the counties that were utilized for the analysis; refer to Section 3.2.2 for selection criteria.



Figure 3.1: US Corn Belt states and 463 counties selected for the analysis.

As annual NASS Crop Data Layers (CDLs) were only available since 2010 at the time of writing, it was necessary to limit the study period to 7 years from 2010 to 2016. This timeframe encompasses a diverse range of growing conditions, including 2012, which was an unusually warm and dry year, resulting in widespread corn yield losses (Yu et al., 2014; Wang et al., 2016; Lu et al., 2017), as well as 2014 and 2016, which produced higher yields due to preferable temperature and precipitation levels. While long term increases in yield are evident over decades due to continued improvements in breeding and cultivation methods, a span of only 7 years is not extensive enough to reflect an upward trend.

3.2.2 Data acquisition and preprocessing

This analysis employed MODIS daily daytime 1-km LST (MYD11A1 – version 6) (Wan, 2015); images from the Aqua satellite were selected over Terra because of their ~1:00 PM overpass time for the Corn Belt (vs. 10:00 AM), which is closer to solar noon and consistent with

other field-based studies that used canopy temperature to evaluate crop stress (Taghvaeian et al., 2012; Taghvaeian et al., 2014; DeJonge et al., 2015; Han et al., 2016; Mangus et al., 2016; Carroll et al., 2017; Egea et al., 2017). MODIS data from 2010-2016 for the Corn Belt was downloaded in the Albers Equal Area – WGS 1984 datum/coordinate system courtesy of the USGS Application for Extracting and Exploring Analysis Ready Samples (AppEEARS) (USGS, 2018).

Daily 4-km meteorological information was obtained from the Parameter Elevation Regression on Independent Slopes (PRISM) (PRISM Climate Group, 2004). The use of this (Schlenker and Roberts, 2009; Heft-Neal et al., 2017, Lu et al., 2017) or other gridded climate datasets (Lobell and Anser, 2003; Lobell and Field, 2007; Kucharik and Serbin, 2008; Lobell et al., 2011; Hawkins et al., 2013; Troy et al., 2015, Ceglar et al., 2016; Leng, 2017a) is common for regional corn yield modeling. The PRISM variables used for this analysis are daily mean air temperature (Tmean), maximum air temperature (Tmax), minimum air temperature (Tmin), and total precipitation (Precip). Historical monthly precipitation was also used to compute SPI.

County-level annual corn yield (in bushels per acre, Bu/Acre) from 2010-2016 was derived from NASS surveys (from Quick Stats 2.0, USDA, 2018b). The *Counties Cartographic Boundary Shapefile* (1:500,000 scale) defined the boundary and location of counties (US Census Bureau, 2015). Annual NASS Crop Data Layers (CDLs) were also used to isolate majority corn MODIS pixels. Starting in 2010, CDLs provide crop-specific land cover classification at a 30-m resolution for the entire CONUS (USDA, 2018c). For each year, the reprojected CDL was used to calculate the percent corn for each 1-km MODIS pixel; those that were >75% were defined as majority corn. Similar crop masks from CDLs were developed for previous agriculture analyses that employed MODIS images (Bolton and Friedl, 2013; Johnson, 2014; Johnson, 2016). Counties were deemed to have sufficient data on the basis of having yield data and at least one majority corn pixel each year during the 7-year study period. This filtering process resulted in a total of 463 counties for the analysis (depicted in Figure 3.1). The county boundary layer was reprojected to the datum/coordinate system of the MODIS grids and daily daytime LST values were summarized for each county by taking an average of contained, cloud-free majority corn pixels. To further reduce mixed pixel error, averages were weighted using percent corn, such that pixels with a greater portion of corn land cover were assigned a higher weight. If a county contained no cloud free pixels for a given day, it was assigned a value of "No Data".

The county boundary layer was then reprojected to match the PRISM datum/coordinate system and daily Tmean, Tmax, Tmin, and Precip values were summarized by taking an average of coincident points. PRISM averages were not filtered or weighted by percent corn due the higher than MODIS LST spatial resolution of 4-km and fact that pixels are interpolated from insitu weather stations and do not reflect direct readings. For SPI calculations, monthly PRISM values from 1895 to 2016 were also averaged for counties.

3.2.3 Computation of killing degree day metrics and univariate analysis

A univariate comparison was initially performed to directly compare LST and Tair corn yield prediction. The traditional killing-degree day metric, subsequently referred to as Tair KDD, was computed from daily Tmax by accumulating values above a specified temperature threshold through the critical developmental period of the corn growing season:

$$Tair \ KDD = \sum_{d=1}^{d=n} KDD_d \qquad KDD_d = \begin{cases} 0 & if \ Tmax < Tair \ Thresh \\ Tmax - Air \ Thresh \ if \ Tmax > Tair \ Thresh \end{cases}$$

Where KDD_d is the KDD computed for a single day, Tmax is the daily maximum temperature, Tair Thresh is the threshold for Tair KDD (29.8°C), and d = 1 through n corresponds to the start and end of the critical development phase.

Butler and Huybers (2015) determined that corn yield in the US is most affected by extreme temperatures during the early grain filling phase (silking and dough stages). The utilized critical development period for which KDDs were accumulated was defined as July and August, since this approximately corresponds to the start and end of the silking and dough phases for the Corn Belt, respectively (see Table 3.4 in the Supplemental Information, section 3.6.1). Different temporal periods for accumulating KDD were tested, but produced similar results. For more details refer to the Supplemental Information for Methods, section 3.6.1.

A novel killing degree day metric, subsequently referred to as LST KDD, was computed through a similar process, only it was necessary to account for "No Data" values resulting from cloud coverage. Rather than accumulating all values above a temperature threshold, KDDs were calculated for cloud-free days by subtracting the temperature threshold from LST (negative differences were set to 0) and taking an average (as opposed to the summation). The average was then multiplied by the number of days in the critical development phase:

$$LST \ KDD = \overline{KDD_d} \ *N \qquad KDD_d = \begin{cases} 0 & if \ LST < LST \ Thresh \\ LST - LST \ Thresh \ if \ LST > LST \ Thresh \end{cases}$$

Where KDD_d is the KDD computed for a single cloud-free day, N is the number of days in the critical development phase, and LST Thresh is the threshold for LST KDD (23.7°C). This omitted days with invalid data and avoided an unrepresentative number of 0's by assuming cloud-obstructed days had an LST below the threshold. Invalid values were fairly uncommon

and on average only represented 23.4% of days through July and August for the selected counties. To assure this assumption did not produce biased results, Tair KDD was alternatively computed using a similar approach (averaging cloud-free daily KDD); nearly identical results were obtained (see Figure 3.15 in the Supplemental Information for Methods, section 3.6.1).

Yield predictive capabilities were compared on the basis of the resulting coefficient of determination (R²) and root mean square error (RMSE) when corn yield was modeled via ordinary least squares (OLS) as a linear function of (i) Tair KDD and (ii) LST KDD. Observations were pooled across counties and years, resulting in 3,241 observations (463 counties X 7 years). Heft-Neal et al. (2017), Troy et al. (2015), and Schlenker and Roberts (2009) utilized this data-pooling approach as well. Similar to Butler and Huybers (2013; 2015), yield and KDD were standardized on a county-by-county basis prior to fitting to control for regional effects, such as climate, soils, cultivars, or growing practices. For both variables, a 7year average was calculated for each county. That average was then subtracted from each county's 7 observations. For example, Adam County, IL's LST KDD for 2010 was 332.1°C and the 7-year average was 313.6°C. Thus, the standardized LST KDD in 2010 was 18.5°C. In this way, greater than average observations had a positive value; less than the average observations had a negative value. Studies that encompassed a longer time frame (i.e. 30+ years) standardized variables with a linear trend to reflect increases in yield due to technological improvements and climate change (Lobell et al., 2011; Shaw et al., 2014; Zipper et al., 2016; Zhang et al., 2015; Ceglar et al., 2016; Wang et al., 2016; Leng, 2017a; Leng, 2017b; Lu et al., 2017; Mathieu and Aires, 2018). In this case, however, a simple multiyear average was sufficient due to the short 7year period, for which changes in technology and climate were negligible.

While authors have employed 29°C as the threshold for Tair KDD (Butler and Huybers, 2013; Shaw et al., 2014; Butler and Huybers, 2015), there is no information available on the ideal LST range for corn. To identify a threshold, LST KDD was iteratively calculated with candidate values from 10°C to 40°C in 0.1°C increments. The optimal threshold was selected as the value that produced the highest R² and lowest the RMSE when standardized yield was modeled as a linear function of standardized KDD (via OLS regression). For consistency, this process was repeated to identify a threshold for Tair KDD.

3.2.4 Comparison of LST and Tair KDD multiple linear regression models

Following fitting single variable regression models, a multiple regression analysis was performed to determine if improvements in the predictive capability of LST KDD remained while controlling for factors traditionally used for corn yield modeling. The assessed covariates are listed in Table 3.1.

Variable	Definition	Source
GDD	Growing degree days	PRISM
S_Tmean	Summer mean daily air temperature	PRISM
G_Precip	Growing season total precipitation	PRISM
S_Precip	Summer total precipitation	PRISM
SPI	August 3-month standardized precipitation index	PRISM

Table 3.1: List of additional covariates utilized for multiple regression and source.

For simplicity, authors have defined the corn growing season as the summer months of June, July, and August (Lobell and Anser, 2003; Lobell and Field, 2007; Kucharik and Serbin, 2008; Leng, 2017a) or longer period from late Spring to mid Fall to encompass planting and harvesting (Schlenker and Roberts, 2009; Hawkins et al., 2013; Zhang et al., 2015). For the

CONUS, annual average state-level planting and harvest dates specified by *NASS Crop Status Reports* have been used as well (Butler and Huybers, 2013; Shaw et al., 2014; Butler and Huybers, 2015; Troy et al., 2015). We defined the growing season from May 1st to October 31st, which approximately corresponds to typical planting and harvesting dates for Corn Belt states (see Table 3.4 in Supplemental Information for Methods, section 3.6.1).

GDD is usually included in multiple regression models with KDD to explain yield variability in cooler years with few extreme heat events (Butler and Huybers, 2013; Shaw et al., 2014; Butler and Huybers, 2015), but has also been used in the absence of KDD (Anandhi, 2016; Angel et al., 2017). GDD was quantified by accumulating daily mean temperatures within an ideal range over the course of the growing season, similar to Butler and Huybers (2013; 2015). In this case, the upper and lower bounds were defined as 29°C and 9°C, respectively.

Tmean, averaged over the summer (Lobell and Anser, 2003; Lobell and Field, 2007; Kucharik and Serbin, 2008; Leng, 2017a) or entire growing season (Lobell et al., 2011; Hawkins et al., 2013; Moore and Lobell, 2015; Troy et al., 2015; Zhang et al., 2015; Ceglar et al., 2016; Wang et al., 2016; Ali et al., 2017), has been extensively utilized to model corn yield. We only considered average summer mean Tair (S_Tmean), since average growing season mean Tair would have been highly correlated with GDD. For each county, annual S_Tmean was calculated as the average of county mean daily temperatures from PRISM through June, July, and August.

Summer precipitation (Lobell and Anser, 2003; Lobel1 and Field, 2007; Kucharik and Serbin, 2008; Schlenker and Roberts, 2009) or growing season precipitation (Lobell et al., 2011; Hawkins et al., 2013; Moore and Lobell, 2015; Troy et al., 2015; Zhang et al., 2015; Ceglar et al., 2016; Wang et al., 2016; Ali et al., 2017) is also commonly used to model corn yield. Both were calculated by accumulating daily PRISM precipitation over the corresponding period (June

1st to August 31st for summer; May 1st to October 31st for growing season). Others have used the more mathematically rigorous metric, SPI, which can be interpreted as the number of standard deviations by which observed precipitation deviates from a long term mean (typically 100+ years) (Keyantash, 2018). CONUS corn yield has been found to be most sensitive to a short window SPI (1-3 months) during the summer (Lu et al., 2017; Mathieu and Aires, 2018). We, therefore, considered 3-month SPI, since this encompasses June, July, and August, and followed Lu et al.'s (2017) approach of using monthly historical PRISM data from 1895-2016 and fitting a gamma distribution.

Variables were also standardized for the multiple regression analysis on a county-bycounty basis as the difference from the 7-year average, with the exception of SPI since it is already standardized. Two linear models for corn yield were fit via an OLS regression: (i) a Tair model, which included Tair KDD and the 5 additional variables and (ii) and a LST model, which included LST KDD and the 5 additional variables. OLS is a common approach for modeling regional corn yield (Lobell and Anser, 2003; Lobell and Field, 2007; Kucharik and Serbin, 2008; Butler and Huybers, 2013; Shaw et al., 2014; Butler and Huybers, 2015; Ali et al., 2017). To assess their relative influence on yield, variables were again standardized by subtracting the mean and dividing by the standard deviation. Variation Inflation Factor (VIF) examination followed to reduce the effects of multicollinearity. Similar to the univariate analysis, multiple regression models were compared on the basis of their adjusted R² and RMSE.

3.3 Results

3.3.1 Visual correlations

Figure 3.2 displays the annual averages of standardized variables for each state. With the exception of MN, corn yield was lowest in 2012 and greatest in 2014, 2015, or 2016, depending on the state. While they varied in magnitude, the series for LST and Tair KDD followed a similar pattern, having the greatest values in 2012 and lowest values after 2013. Precipitation metrics showed a significant decrease in rainfall for 2012.



Figure 3.2: Time series of standardized corn yield and predictor variables, averaged across selected counties for each state by year. Refer to Table 3.1 for variable definitions.

3.3.2 Univariate comparison of derived LST and Tair KDD metrics for yield prediction

The R² and RMSE between standardized corn yield and Tair KDD peaked at 0.56 and 17.2 Bu/Acre, respectively, with a corresponding temperature threshold of 29.8°C. LST KDD peaked at a lower threshold (23.7°C) with a higher R² of 0.65 and lower RMSE of 15.3 Bu/Acre (Figure 3.3). Thus, LST KDD served as a better predictor of corn yield from 2010-2016, as it explained approximately 10% more of the variation and produced estimates with a smaller standard deviation of error (by ~2 Bu/Acre). Note that RMSE values are in standardized yield (i.e. difference from the 7-year mean). For reference, the average annual yield across counties was 161.3 Bu/Acre (max = 206.2 Bu/Acre, min = 72.5 Bu/Acre).



Figure 3.3: Coefficient of determination (\mathbb{R}^2) (left) and root mean square error (RMSE) (right) for the linear relationship between standardized corn yield and KDD (computed from both LST and Tair) over the range of tested thresholds.

Scatter plots between yield and LST/Tair KDD using their respective thresholds are depicted by Figure 3.4. Both had a strong linear trend, but LST KDD exhibited less scatter, especially in 2012, the drought year. Even on a year by year basis, LST KDD appeared to better capture the negative relationship with yield.



Figure 3.4: Scatter plots of standardized LST KDD and Tair KDD vs. yield.

3.3.3 Multivariate comparison of derived LST and Tair KDD metrics for yield prediction

Additional air temperature covariates:

S_Tmean had a negative relationship with yield, but captured less variability than the KDD metrics. GDD had virtually no correlation with yield (Figure 3.5).



Figure 3.5: Scatter plots of standardized GDD and summer mean daily air temperature (S_Tmean) vs. yield.

Additional precipitation covariates:

All 3 of the precipitation metrics exhibited a threshold-type response with corn yield. S_Precip had the greatest R^2 and lowest RMSE when fit with a parabolic function (Figure 3.6).



Figure 3.6: Scatter plots of standardized precipitation metrics vs. yield; SPI (left), summer precipitation (S_Precip) (right), and growing season precipitation (G_Precip) (bottom).

LST and Tair KDD multiple regression models:

Multiple linear regression was performed to compare the corn yield predictive power of LST and Tair KDD while controlling for commonly utilized meteorological variables. As the three precipitation metrics were highly correlated with VIFs over 10, we eliminated SPI and G_Precip and kept S_Precip since it had the greatest R² and lowest RMSE with yield of the three. Although the VIF for S_Tmean was below 10, it had a response similar to GDD and was removed to avoid redundancy. Regression results are listed in Table 3.2.

LST KDD Model				Taiı
Adj. $R^2 = 0.72$	RMSE =	13.8		Adj. $R^2 =$
Term	Coeff	VIF		Term
Intercept	0.0000	-		Intercept
LST KDD	-0.9417	2.45		Tair KDD
GDD	0.1732	1.15		GDD
S_Precip ²	-0.1286	1.28		S_Precip ²
S_Precip	-0.2067	2.1		S_Precip

Tair KDD Model

Adj. $R^2 = 0.63$	RMSE = 15.8		
Term	Coeff	VIF	
Intercept	0.0000	-	
Tair KDD	-0.7854	2.25	
GDD	0.1709	1.18	
S_Precip ²	-0.2179	1.19	
S_Precip	-0.0849	1.95	

The LST KDD model had a higher adjusted R^2 (by ~9%) and lower RMSE (by ~2.0 Bu/Acre). The standardized coefficient for LST and Tair was roughly 4-times larger in magnitude than the coefficients for other covariates, indicating that they, by far, had the greatest influence on yield from 2010-2016 across the Corn Belt.

3.4 Discussion

3.4.1 Interpretation of results and comparison to previous work

The R² and RMSE of Tair and LST KDD remained flat for low thresholds, since these values were less than the maximum temperature for nearly all days. These lower thresholds essentially subtract a constant value from each year's KDD, which does not change the variability in KDD among years. Only at higher thresholds does KDD vary among years. The optimal R² and RMSE for Tair KDD occurred near the commonly used threshold of 29 °C (Butler and Huybers, 2013; 2015), which is based on previous field-level analyses that compared yield and growth rates across a range of simulated heat conditions. Our findings indicate that this value is also applicable to regional, county-level data. The highest R² for LST was found at 23.7°C, but there was no peak as there was for Tair KDD. In fact, alternatively using 0°C for the threshold derived a comparable R^2 of 0.65 and RMSE of 15.4 Bu/Acre. This suggests that there is not an optimal LST level for corn; a higher LST during July and August across the Corn Belt corresponds to lower yield. This may not, however, be true for other regions with significantly cooler or warmer climates. As the utilized threshold for LST KDD had little effect on results, this metric is essentially a clear sky average of LST multiplied by a constant (the number of days during the critical development period).

The higher R^2 and lower RMSE for both the univariate and multiple linear LST models provide strong evidence that KDD computed from MODIS LST is a superior predictor of corn yield than KDD derived from Tair. In fact, the univariate LST KDD model outperformed the multiple linear Tair KDD model ($R^2/RMSE$ of 0.65/15.3 Bu/Acre vs. 0.63/15.8 Bu/Acre). Thus, LST alone can provide a better estimate of yield than Tair and precipitation combined.

Improvements over Tair were especially apparent in 2012, highlighting LST's ability to reflect water stress. By limiting the univariate regression to observations from 2012, the $R^2/RMSE$ for LST KDD was 0.61/18.8 Bu/Acre, in comparison to Tair KDD's $R^2/RMSE$ of 0.39/23.6 Bu/Acre (Figure 3.7). 2012 observations in both scatter plots show considerable separation from other years, but LST KDD does a better job of capturing the linear trend. The two metrics performed worse when 2012 observations were excluded (LST KDD $R^2/RMSE = 0.41/14.3 \text{ Bu/Acre}$; Tair KDD $R^2/RMSE = 0.28/15.9 \text{ Bu/Acre}$).



Figure 3.7: Scatter plots of standardized LST and Tair KDD vs. yield for 2012 only.

Univariate results were similar when fit to state-level data (see Figure 3.16 in the Supplemental Information for Discussion, section 3.6.2). Tair KDD did, however, perform slightly better for WI (R²/RMSE of 0.52/15.2 Bu/Acre vs. 0.56/14.5 Bu/Acre). Both LST and Tair KDD poorly predicted corn yield for MN, possibly due to the cooler climate. In comparison to other states, MN experienced fewer extreme temperatures and lower KDDs from 2010-2016. As a result, LST/Tair KDD and yield remained relatively stable over the study period. When multiple linear models were fit to just MN data, GDD had a larger standardized coefficient (LST KDD Model: GDD β = 0.60, KDD β = -0.69; Tair KDD Model: GDD β = 0.72 and KDD β = -0.79), indicating yield is more influenced by temperatures within an ideal growing range than extreme heat. Furthermore, the adjusted R²s of the multiple linear models were substantially higher than the univariate models (0.59 for LST, 0.50 for Tair). When comparing all states, there was a slight, positive trend between the 7-year mean summer Tair and R², suggesting KDD is more predictive of yield in warmer climates (Figure 3.8). NE deviates from this trend, possibly due to the higher portion of irrigated crop area, further investigated in Section 3.4.2.



Figure 3.8: Univariate model R² for LST and Tair KDD for each state vs. mean summer Tair.

In agreement with Butler and Huybers (2013), Shaw et al. (2014), and Butler and Huybers (2015), we found a negative correlation with yield for both LST and Tair KDD. Note that our study differs from these as it employed remotely sensed LST to derive KDD, as opposed to Tair. Surprisingly though, the relationship we found for GDD with yield was slightly negative. This is most likely due to the influence of 2012 data, which contained lower yields but higher GDDs induced by warmer temperatures. A similar relationship with yield occurred for mean summer air temperature (S_Tmean). The coefficient for GDD did become positive in both multiple linear regression models, which accounted for extreme temperatures with KDD.

Similar to Schlenker and Roberts (2009) and Troy et al. (2015), corn yield exhibited a threshold-type response to precipitation metrics; the relationship was weaker than temperaturebased metrics, as reported by Lobell and Field (2007) and Hawkins et al. (2013). In fact, the R²s were fairly low, supporting the notion that precipitation measured across a network of weather stations inadequately reflects crop water availability. We did not expect summer precipitation to be a better predictor of corn yield than August SPI, especially considering the severity for the 2012 drought. This inconsistency from Mathieu and Aires (2018), who found SPI to be a better predictor than total precipitation, could be due to the smaller geographic and temporal extent of our analysis.

Since the multiple linear LST and Tair KDD models exhibited only marginal improvement over univariate models (a ~7% increase in R² and ~1.5 Bu/Acre decrease in RMSE), KDD alone can explain the vast majority of inter-annual variation in corn yield from 2010-2016. Even while adjusting for commonly utilized meteorological factors, the R² and RMSE of the multiple linear LST KDD model remained ~9% higher and ~2.0 Bu/Acre lower than the Tair KDD model. Thus, improvements from the utilization of LST cannot be accounted for by the inclusion of additional meteorological parameters.

The multiple linear LST KDD model compared favorably to previous regional models of corn yield (Table 3.3). It should be noted that several of these studies incorporated a numerical time variable (i.e. year), which to some extent obscures the amount of variation actually explained by climate factors, since the upward yield trend is so strong. As shown by Shaw et al. (2014), including a time parameter can substantially improve the model R^2 (from 0.30/0.44 to 0.71). When our multiple linear LST model is fit on a county-by-county basis, the average R^2 was 0.68 (0.63 for Tair KDD), even without a time variable. While some caution is advised with

interpreting direct comparisons, as these analyses utilized different regression approaches, study

areas, and explanatory variables, this indicates that our model performed reasonably well,

especially when considering the limited temporal extent.

Table 3.3: Regression results from previous regional corn yield models. NOTE: FE = Fixed
Effect; OLS = Ordinary Least Squares, FGLS = Feasible Generalized Least Squares, Precip =
Precipitation, Tmean = mean air temperature, Tmax = maximum air temperature, Tmax =
maximum air temperature, Tmin = minimum air temperature.

Study	Spatial Extent	Temporal Extent	Method	Covariates	\mathbb{R}^2
Heft-Neal et al., 2017	US, Africa	2003-2014	Fixed Effect	Season LST, Season Precip, Time FE, County FE	0.73
Shaw et al., 2014	US (100 Counties)	1981-2011	OLS	GDD, KDD, Time	0.30-0.71
Schlenker and Roberts, 2009	US W. of 100 deg	1950-2005	Fixed Effect	Summer Tair, Summer Precip, Time, Counte FE	0.77
Lobell and Field, 2007	Global	1961-2002	OLS	Summer Tmax, Summer Tmin, Summer Precip	0.47
Butler and Huybers, 2015	US	1981-2008	OLS - Bootsrapping	GDD, KDD, Time	0.69
Zipper et al., 2016	US	1958-2007	OLS	SPI	0.09-0.20
Lobell and Anser, 2003	US	1982-1998	OLS	Simmer Tair, Summer Precip, Summer Solar Radiation	0.25
Kucharik and Serbin, 2008	Wisconsin	1950-2006	OLS	Summer Tair, Summer Precip	0.13-0.40
Ali et al., 2017	Pakistan	1989-2015	OLS and FGLS	Season Tmax, Season Tmin, Season Precip, Season Humidity, Season Sunshine, Time	0.29

To further compare our findings to previous work (Johnson, 2014; Johnson, 2016; Heft-Neal et al., 2017), we investigated the extent to which alternatively using 8-day images affected the portion of yield variability explained by LST KDD. This, however, produced similar results to daily images ($R^2 = 0.62$, RMSE = 15.9 Bu/Acre). Since yield is a single response value summarized for the entire growing season, the loss of daily variation inherent in aggregated 8day composites does not significantly impact the predictive capability. We also recomputed LST KDD using the entire growing season (May 1st to October 31st). This resulted in a much lower R^2 and higher RMSE of 0.48/18.6 Bu/Acre for LST KDD and 0.50/18.2 Bu/Acre for Tair KDD. It is possible that Heft-Neal et al.'s (2017) finding of LST and Tair comparably predicting yield may have been due to their use of values over a greater extent of the growing season. Moreover, the improved performance of LST mainly pertains to the time phase associated with critical development phase of corn (silking through dough stages).

3.4.2 Investigating LST's ability to capture water stress and evaporative cooling: A case study comparing rainfed and irrigated counties

One explanation for improved yield estimation with LST is its superior ability to reflect water stress and evaporative cooling. To test this theory, we compared the performance of LST and Tair KDD for irrigated and rainfed counties. Assuming irrigated counties are not subject to water deprivation, examining them separate from rainfed counties would isolate heat stress from water stress. Counties were classified as irrigated if >70% of the total crop area harvested was irrigated and rainfed if <30% was irrigated (based on the 2012 US Census of Agriculture). Note that the majority of irrigated counties within the Corn Belt are located in NE (see Figure 3.17 in the Supplemental Information, section 3.6.2).

Both KDD metrics produced a lower R^2 and RMSE when fit to irrigated counties (LST KDD $R^2 = 0.25$, RMSE = 9.8 Bu/Acre; Tair KDD: $R^2 = 0.23$, RMSE = 9.9 Bu/Acre), consistent with previous findings that corn yield exhibits a weaker relationship with Tair in irrigated areas (Shaw et al., 2014; Troy et al., 2015; Cater et al., 2016). The surprisingly lower RMSE than the LST and Tair models that used all counties is due to fewer degrees of freedom (105 vs. 3,241), since only a small subset of counties are irrigated (15 out of 463). With similar R^2 and RSME values, LST and Tair appear to equally reflect heat stress. When fit to rainfed counties, however, LST KDD outperformed Tair KDD by a wider margin ($R^2/RMSE$ of 0.68/15.2 Bu/Acre vs. 0.60/17.1 Bu/Acre), especially in 2012 ($R^2/RMSE$ of 0.71/16.4 Bu/Acre vs. 0.55/20.3 Bu/Acre).

While both metrics similarly measure heat stress, LST is particularly advantageous for capturing water stress, most notably during droughts.

NE makes an interesting case to examine LST's ability to measure evaporative cooling, since there are a comparable number of irrigated (n = 15) and rainfed (n = 25) counties. At the field level, one would expect healthy crops, with sufficient water, to have a lower canopy temperature than Tair. As water becomes limited, evapotranspiration decreases and canopy temperature approaches Tair; in extreme cases, canopy temperature can exceed Tair (Singh and Kanemasu, 1982; Fukuoka et al., 2003; Webber et al., 2017). Authors have noticed significantly lower canopy temperatures for irrigated crops in comparison to nearby rainfed ones (Gardner et al., 1981; Cavero et al., 2009; Vadivambal and Jayas, 2011; Carroll et al., 2017).

For each NE county, the average maximum Tair and daytime LST was taken across cloud-free days through July and August from 2010 to 2016. As irrigated counties were not subjected to water depravation, evapotranspiration levels remained stable and the median LST stayed well below the median Tair, even in 2012. For rainfed counties, however, there was a sharp increase in median LST for 2012, due to decreased evapotranspiration and increased water stress (Figure 3.9). Thus, LST is not simply lower than Tair by a constant factor, the difference appears to be dependent on water availability and indicative of yield loss; yields for NE irrigated counties in 2012 (184.9 Bu/Acre) were roughly 2X greater than yields for rainfed counties (96.8 Bu/Acre). Moreover, this demonstrates that MODIS LST can measure regional evaporative cooling across the Corn Belt, similar to an IR thermometer at the field level.



Figure 3.9: July-August daytime LST vs. maximum Tair by year for the utilized irrigated and rainfed counties in Nebraska (NE). Created using function by Bikfalvi (2012).

Although it is not possible to compare temperatures of irrigated and rainfed temperatures outside of NE, a similar phenomenon is observed for rainfed counties in other states (see Figure 3.18 in the Supplemental Information for Discussion, section 3.6.2). There was generally a sharp increase in LST for 2012, causing the difference with maximum Tair to become positive or close to 0; for other years, the difference was negative.

3.4.3 *Exploring an alternative metric: LST – Tair difference*

Prior field-level studies focused on irrigation optimization computed CWSI as the difference between maximum canopy temperature and maximum Tair, relative to the vapor pressure deficit. We considered LST and Tair separately since their difference is dependent on humidity and our study area encompassed several states with varying atmospheric moisture levels. In addition, our primary focus was on crop stress measured by KDD. For a follow-up analysis, an analogous county-level metric was calculated by using maximum daily vapor pressure deficit (VPDmax) from PRISM. For each county, valid daily LST readings were

subtracted by the corresponding maximum Tair and divided by VPDmax. An average was then taken through July and August.

County-level CWSI exhibited a linear, negative relationship with corn yield from 2010-2016, but performed relatively poorly in comparison to LST and Tair KDD ($R^2 = 0.41$, RMSE = 20.0 Bu/Acre) (Figure 3.10). As traditional CWSI uses canopy temperature and Tair both recorded at the same location, values interpolated from a nearby weather station may inadequately reflect the actual temperature conditions of corn fields. At the field level, Tair is traditionally used as a baseline to compare canopy temperature against. A multiyear mean may serve as a better baseline at the regional, county-level.



Figure 3.10: Standardized county-level CWSI vs. yield.

3.4.4 Major implications and policy recommendations

An array of short term, early yield forecasting models exist (estimate yield several months prior to harvest), many of which employ NDVI-based vegetation indices (Bolton and Friedl, 2013; Sakamoto et al., 2014; Shao et al., 2015; Wójtowicz et al., 2016). The use of MODIS LST, however, has been limited. The findings in this paper stress the need for future

models to incorporate satellite-derived LST, especially values from the silking and dough development stages. As the LST KDD threshold had little impact on yield prediction and 8-day images produced comparable results, using a simple average of valid composite LST through July and August would suffice.

While corn yield is highly dependent on water availability, in-situ soil moisture measurements at metrological stations are limited and provide a poor spatial coverage (Liang et al., 2014; Escorihuela and Quintana-Seguí, 2016; Bai et al., 2017). This issue is further complicated by the high spatial and temporal variability of soil moisture induced by a range of factors, including topography, rainfall, groundwater level, and soil type (Holzman and Rives, 2016). In addition, station measurements are typically taken at depths of 5-50 cm, which may not reflect conditions at the actual root depth of corn (Fawcett, 2013; Ransom, 2013; Ford et al., 2015). Obtaining field measurements can be costly, time consuming, and intrusive (Jackson et al., 1981; Veysi et al., 2017).

MODIS LST can provide an effective means to assess regional water stress across the US Corn Belt, especially in extremely dry years. Considering the frequency and severity of droughts are expected to intensify in the coming decades (Strzepek et al., 2010), this information will become increasingly important for agricultural monitoring. As the USGS Appears platform now allows users to download MODIS products in a custom datum/coordinate system and spatial extent, the USDA or a state agricultural department can easily employ our analytical framework. A similar model could provide within-season forecasts of yield deviation from a 5-10 year mean based on average July and August LST. Estimates would be available 1-2 months prior to harvest and 6-7 months before the release of NASS yield reports. Our results indicate that such a

model would be more predictive of yield loss due to water stress than existing Tair and precipitation datasets.

Attempts to utilize climate change models for long term future yield projection have relied heavily on predicted changes in Tair and precipitation (Kucharik and Serbin, 2008; Kang et al., 2009; Schlenker and Roberts, 2009; Schlenker and Lobell, 2010; Hawkins et al., 2013 Leng, 2017b). As the improved predictive capability of LST can be attributed to its reflection of evaporative cooling and water stress, the use of Tair and precipitation alone have limitations when employed within statistical models. While LST is not an output from climate models and cannot be directly used for long term corn yield projections, the result from this study suggest that in order to obtain a more complete understanding of the conditions affecting crop growth, prospective models should additionally incorporate variables indicative of water availability. If these are not considered, estimates will contain substantial error in unusually warm and dry growing seasons (such as 2012). Further work is needed to understand how soil moisture at root depth can be modeled as a function of soil conditions and rainfall across different periods of the year. Moreover, MODIS LST can be used as an indicator to help identify potential soil and hydrological characteristics pertinent to yield estimation.

It is important to note that our models were developed via ordinary least squares (OLS) regression. As this method is quite limited, our results only pertain to the US Corn Belt. While more robust regression approaches are available, our intention was not to propose a finalized yield model, but demonstrate the benefits of incorporating LST for yield prediction. Moreover, results pertaining to the Corn Belt have important global food supply implications, as this region produces 73.3% of US Corn and 24.4% of global corn (USDA, 2018a; USDA, 2019).

3.5 Conclusion

This study investigated the utility of satellite-derived LST for estimating annual corn yield across the US Corn Belt. Our analysis indicates that LST KDD is a better predictor of yield than the common Tair KDD. Even while controlling for metrological variables commonly used for agricultural modeling, the LST KDD model's R² and RMSE remained approximately 9% higher and 2.0 Bu/Acre lower, respectively, than the Tair KDD model. In fact, the univariate LST KDD estimates exceeded the multiple linear Tair KDD estimates (R²/RMSE of 0.65/15.3 Bu/Acre vs. 0.63/15.8 Bu/Acre), suggesting LST alone is a better predictor of corn yield than Tair and precipitation combined. While both metrics equally captured heat stress, improvements with LST are likely due to its ability to reflect water stress and evaporative cooling considering that: (i) LST KDD outperformed Tair KDD by a much wider margin in 2012, a year of severe drought (R²/RMSE of 0.61/18.8 Bu/Acre vs. 0.39/23.6 Bu/Acre) and (ii) relative year-to-year increases in LST for rainfed counties in Nebraska corresponded more to yield loss than neighboring irrigated counties.

Prior to this analysis, the use of MODIS images for corn yield modeling had primarily involved the near-infrared portion of the electromagnetic spectrum; applications of LST had been limited, especially within the US. The proposed KDD metric is conceptually simple and offers considerable improvements in yield prediction over Tair KDD. While crop health and water availability have traditionally been evaluated at the field-level with an IR thermometer, it was demonstrated that this can be achieved at a regional scale with satellite-based LST. Considering the difficulty of obtaining soil moisture data, MODIS LST would be especially advantageous for within-season early yield forecasts during extremely warm and dry growing seasons.
In the context of climate change, the improved predictive capability of LST indicates that Tair and precipitation alone provide an insufficient representation of water stress. While LST is not an output of climate models and cannot be directly used to predict future corn yield, subsequent attempts to project yield over several decades should consider a more holistic set of parameters indicative of water availability. If these factors are ignored, estimates may contain substantial error for years with severe drought.

3.6 Supplemental Information

3.6.1 Supplemental information for methods

Dates for corn planting, harvesting, silking, and dough stages were obtained from *National Agricultural Statistics Survey (NASS) Crop Progress Reports* (USDA, 2018d). These weekly reports list the percent of corn acreage by state that has reached each development stage. Assumed dates were derived by linearly interpolating the dates immediately preceding and following 50%. For instance, if the percent of acres planted for IL was 38% on May 1st and 56% on May 8th, the interpolated date was May 6th. For simplicity, 2011-2015 averages were used for the entire 7-year study period (Table 3.4).

State	Planted	Harvested	Silking	Dough	Dented
IL	5/6	10/8	7/12	8/3	8/21
IN	5/12	10/20	7/17	8/10	8/28
IA	5/7	10/18	7/19	8/12	8/27
MN	5/10	10/19	7/22	8/15	8/31
NE	5/6	10/21	7/18	8/9	8/26
OH	5/14	10/28	7/21	8/13	9/2
SD	5/10	10/20	7/24	8/14	9/1
WI	5/16	10/29	7/26	8/20	9/6

Table 3.4: Interpolated corn developmental stage dates for US Corn Belt states. Source: USDA(2018d).

While there was some variation, setting the growing season period from May 1st to October 31st encompassed all of the states' planting and harvesting dates. According to Butler and Huybers (2015), corn is most sensitive to KDD during the early grain filling stages. Based on the available stages in *NASS Crop Progress Reports*, this was assumed to be the start of the silking phase to the end of the dough phase (i.e. start of the dented phase). Based on the 2011-2015 average dates by state (Table 3.4), we accumulated KDD values from July 1st to August 31st. Since there is some year-to-year variation, this allowed roughly a 1 week buffer for states/years with an early start to the silking stage. This period also produced the highest R² and lowest RMSE for both LST and Tair KDD (Table 3.5). The other tested periods included the months of July and August, separately (Figure 3.11 and Figure 3.12), July 12th through August 31st (silking through dough without an early buffer) (Figure 3.13), and July 12th through August 20th (silking only) (Figure 3.14).

	LS	Г KDD		Tai	r KDD		
<u>Period</u>	<u>Threshold</u>	$\underline{R^2}$	<u>RMSE</u>	<u>Threshold</u>	$\underline{R^2}$	<u>RMSE</u>	
7/1 to 8/31	23.7	0.65	15.3	29.8	0.56	17.2	
7/1 to 7/31	25.4	0.58	16.8	29.8	0.53	17.7	
8/1 to 8/31	23.8	0.56	17.2	30.3	0.38	20.3	
7/12 to 8/31	22.0	0.63	15.7	29.8	0.49	18.4	
7/12 to 8/20	24.9	0.59	16.6	30.6	0.45	19.1	

Table 3.5: The derived threshold (in $^{\circ}$ C), R², and RMSE (in Bu/Acre) for all tested KDD periods.



Figure 3.11: KDD results for period from July 1st to July 31st (July only) - Coefficient of determination (R2) (left) and root mean square error (RMSE) (right) for the linear relationship between standardized corn yield and KDD (computed from both LST and Tair) over the range of tested thresholds.



Figure 3.12: KDD results for period from August 1st to August 31st (August only) - Coefficient of determination (R2) (left) and root mean square error (RMSE) (right) for the linear relationship between standardized corn yield and KDD (computed from both LST and Tair) over the range of tested thresholds.



Figure 3.13: KDD results for period from July 12th to August 31st (silking and dough with no early buffer) - Coefficient of determination (R2) (left) and root mean square error (RMSE) (right) for the linear relationship between standardized corn yield and KDD (computed from both LST and Tair) over the range of tested thresholds.



Figure 3.14: KDD results for period from July 12th to August 20th (silking only) - Coefficient of determination (R2) (left) and root mean square error (RMSE) (right) for the linear relationship between standardized corn yield and KDD (computed from both LST and Tair) over the range of tested thresholds.



Figure 3.15: Results for traditional Tair KDD computed by summing daily KDD over the critical development phase and an alternative Tair KDD (Tair No Cloud) computed similar to LST KDD, by taking an average of daily KDD for cloud-free days and multiplying by the number of days in the critical development phase - Coefficient of determination (R^2) (left) and root mean square error (RMSE) (right) for the linear relationship between standardized corn yield and KDD over the range of tested thresholds.



Figure 3.16: Scatter plots of standardized yield in Bu/Acre (Y-axis) vs. LST and Tair KDD in °C (X-axis) by state



Figure 3.17: Percent of crop area harvested that is irrigated for the 463 utilized Corn Belt counties. Source: 2012 US Census of Agriculture.

With some exception, Corn Belt states experienced a sharp increase in LST for 2012, causing the difference with maximum Tair to become positive or close to 0; for other years, the difference was negative (Figure 3.18). IW may have had a larger relative LST in 2013 since it, in comparison to other states, received little summer precipitation. As previously discussed, yield in MN was less impacted by the stressful growing conditions of 2012 due to the cooler climate. In fact, MN experienced the lowest yield in 2013 and 2014 when the difference between LST and Tair was close to 0. It is likely that LST was greater than maximum Tair for all years in SD since it is the driest state of the Corn Belt and, consequentially, had the lowest yields from 2010-2016.



Figure 3.18: July-Aug daytime LST vs. maximum Tair by year for other states than NE. Created using function by Bikfalvi (2012).

We expected drier states to have further separation between LST and maximum Tair than humid states when water is not limited. As dry air can hold more water, greater evapotranspiration occurs resulting in cooler canopy temperatures (relative to Tair) (Wanjura and Upchurch, 1997; Renata, 2013). Surprisingly, IL and IA had larger separation between LST and Tmax during wet years (2010 and 2016) than SD. This inconsistency could have been caused by several factors, including error inherent in aggregate county-level agricultural data and remotely sensed images. While this was unexpected, the follow-up analysis highlights LST's superior ability to reflect evaporative cooling and water stress at a regional scale.

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CHAPTER 4 MANUSCRIPT 3: ESTIMATING DAILY MAXIMUM HEAT INDEX ACROSS THE CONTERMINOUS UNITED STATES USING MULTISPECTRAL MODIS IMAGERY AND ANCILLARY SPATIAL DATA

Abstract

Satellite-derived land surface temperature (LST) is widely utilized to study urban heat islands in the context of human health and thermal exposure. However, there is growing evidence to suggest that LST may be a poor indicator of apparent temperature, or the humanperceived equivalent temperature that reflects both heat and humidity. Moreover, heat index (HI), the apparent temperature metric used by the US National Weather Service, has yet to be computed at an increased spatial resolution than available with weather stations via remote sensing methods. The goal of this study was to: 1) assess the extent to which HI can be estimated by a combination of multispectral imagery from the Moderate Resolution Imaging Spectroradiometer (MODIS) sensor and ancillary geospatial products and 2) determine which factors are most important for estimation. Specifically, daily maximum 1-km HI from May through September of 2012 was modeled across the conterminous US as a function of MODIS LST, water vapor (WV), and near-infrared indices, in addition to static land cover, topographic, and locational factors.

The derived model was capable of estimating HI within a reasonable level of error ($R^2 = 0.83$, RMSE = 4.4°F). LST and WV were, by far, the most important factors for estimation. The incorporation of all other parameters only marginally improved model performance (R^2 : +0.14, RMSE: -1.5°F). We hope that future researchers in the areas of epidemiology, building energy demand, and environmental justice can use this analytical framework to incorporate HI into their analyses at a much greater spatial resolution than provided by in-situ weather stations. Further

work to interpolate cloud-contaminated satellite observations and downscale estimates to a 60-m resolution would considerably increase the utility of this HI product.

4.1 Introduction

4.1.1 Background information

Heat waves refer to a prolonged period of abnormally hot weather and induce numerous adverse effects, including heat-related illness, increased energy use, and ecosystem degradation (Imhoff et al., 2010; Li and Bou-Zied, 2013; Kravchenko et al., 2013; Wu and Ren, 2018). In fact, on an average annual basis, extreme heat is the deadliest natural disaster in the US, killing ~600 people per year (CDC, 2013). Projections indicate that heat waves will become more frequent, more severe, and longer lasting in the US (Meehl, 2004).

The negative impacts of extreme temperature are amplified in cities due to the Urban Heat Island (UHI) effect (Li and Bou-Zied, 2013). This term refers to the phenomenon in which developed areas are significantly warmer than surrounding rural areas due to human activity and less vegetative cover (Tang et al., 2011; Li et al., 2014). Considering 80.7% of the US population resides in urbanized areas (US Census, 2010), spatially explicit temperature information will become increasingly important.

Satellite-derived land surface temperature (LST) images are widely utilized to examine UHIs due to their increased spatial specificity in comparison to in-situ weather station observations (Gallo et al., 1995; Ngie et al., 2014; Rasul et al., 2017; Wu and Ren, 2018; Zhou et al., 2018). Moderate Resolution Imaging Spectroradiometer (MODIS) LST images are commonly employed for this purpose, since the sensor has a very high temporal resolution (4 measurements daily), a medium spatial resolution (1-km), global coverage, and free availability (Ngie et al., 2014; Rasul et al., 2017; Zhou et al., 2018). Many UHI studies that employ satellite LST focus on thermal-comfort and human health (Stathopolou et al., 2005; Klein Rosenthal et al., 2014; Bao et al., 2015; Ho et al., 2015; Morabito et al., 2015; Declet-Barreto et al., 2016; Lehoczky et al., 2017; Xu et al., 2017; Chen et al., 2018; Karimi et al., 2018; Méndez-Lázaro et al., 2018; Mushore et al., 2018; Song and Wu, 2018; Sun et al., 2018; Valmassoi, 2018). However, there is growing evidence to suggest that LST alone is a poor indicator of air temperature (Ho et al., 2016; Tsin et al., 2016; Sheng et al., 2017; Xiong and Chen, 2017). In addition, heat-related illness and mortality are more related to apparent temperature, or the perceived temperature that reflects both heat and humidity, than air temperature (Kim et al., 2006; Chung et al., 2009; Zhang et al., 2014; Heo and Bell, 2018). Further adding to the complexity is the fact that humidity tends to vary over urban landscapes due to changes in evaporation rates across land cover types (Yang et al., 2017; Lokoshchenko, 2017; Hoa et al., 2018). Thus, satellite-based UHI studies could benefit by incorporating additional spatial information that captures the combined effects of air temperature and humidity.

4.1.2 Review of previous MODIS-based air temperature and relative humidity models

Numerous researchers have employed MODIS LST to estimate near surface air temperature (Tair) (i.e. the air temperature 1-2 m above the ground) (Phan and Kappas, 2018). According to Zaksek and Schroedter-Homscheidt (2009), these methods can be grouped into 3 categories: 1.) Statistical, 2.) Temperature Vegetation Index (TVX), and 3.) Energy balance. This portion of the literature review focuses on studies that estimated daily maximum air temperature (Tmax) using a statistical framework (Table 4.1), meaning Tair models consisting of one or more independent variables were empirically estimated with weather station observations. The TVX and energy balance methods are not considered, since these are inapplicable to urbanized areas and require site-specific assumptions (Yoo et al., 2018). Studies have commonly found that daily Tmax can be estimated with a reasonable level of error ($R^2 > 0.75$, RMSE <

4.5°F).

Table 4.1: Overview of studies that estimated daily maximum air temperature (Tmax) or relative humidity (RH) using a statistical framework

Tmax Studies	Predictor Variables	Method	Location	\mathbb{R}^2	RMSE/MAE
Zhang et al., 2011	LST (Ad, An), Elev. (by land cover)	LR	China	0.87	-
Emamifar et al., 2013	LST (Td), JD, SR	Regression Tree	Khuzestan province	0.84-0.92	-
Kim and Han, 2013	LST (Td), NWDI	S-LR	South Korea	0.82	5.2°F
Lin et al. 2013	LST (Ad), WV (Ad), NDVI, EVI, SA, Elev, Lat, Lon	S-LR	East Africa	0.79	3.4°F
Recondo et al., 2013	LST (Td), NDVI, Elev, JD	Robust Reg.	Spain	0.89	4.7°F
Rhee and Im, 2014	LST (Ad, An) - Diurnal Curve - (by land cover)	Sin Curve Fit	South Korea	0.64-0.87	-
Xu et al., 2014	LST (Ad), NDVI, NDWI, Lat, Lon, Dist. ocean, Elev, albedo, and SR	Random Forest	British Columbia	0.74	3.6°F
Zeng et al., 2015b	LST (Td, Tn), Elev (by land cover)	LR	US Corn Belt	0.76-0.83	4.0-4.1°F
Noi et al., 2016	LST (Ad, An, Td, Tn), NDVI, Elev, Lon, Lat, Day Length, JD, VA	LR	North Vietnam	0.93	2.6°F
Rosenfield et al., 2017	LST (An), NDVI, Population Density, Dist. water, %Road, %Open, Elev, Slope, Aspect	Linear FE	Israel	0.9	3.4°F
Shi et al., 2017	LST (Td), NDVI	LR	Yangtze River Delta	0.85-0.90	-
Didari and Zand-Parsa, 2018	LST (Ad, Td), NDVI, Elev, Lat	S-LR	Iran	0.93	4.7°F
Yoo et al., 2018	LST (Ad, An, Td, Tn), Elev, aspect, SR, NDVI, Lat, Lon, %Impervious	Random Forest	Los Angeles/Seoul	0.77-0.85	2.2-3.1°F
Zhang et al., 2018	LST (Ad, An, Td, Tn), Elev	LR	Tibetan Plateau	-	9.5-13.5°F
Phan et al., 2019	LST (Ad, An, Td, Tn)	LR	NW Vietnam	0.74-0.94	2.0-3.4°F

RH Studies	Predictor Variables	Method	Location	R2	RMSE/MAE
Peng et al., 2006	AT (Ad), AM (Ad), NDVI	QR	Peninsular Malaysia	0.90-0.99	-
Sofan et al., 2010	WV (Ad),	LR	Java Island	0.71-0.85	-
Adab et al., 2013	WV (Ad), Elev	PR	Zarin Gol Valley	-	5.80%
Lin et al., 2013	AT (Ad), AM (Ad), NDVI	LR	East Africa	0.17-0.39	-
Recondo et al., 2013	LST (Td), NDVI, JD, Elev	Robust Reg.	Spain	0.40-0.51	-
Ho et al., 2016*	LST (Landsat), WV (Td), NDWI, Dist. ocean, SR, Sky View Factor	Random Forest	Greater Toronto	0.87	9.0°F
Li and Zha, 2018	Red, Green, Blue reflectance (MODIS), EVI, Land cover (MODIS - categorical), Dist. water, Dist. road, Dist city, Elev Nighttime lights	Random Forest	China	0.7	-

Note: Ad, An, Td, Tn refer to Aqua Day, Aqua Night, Terra Day, and Terra Night, respectively, NDVI = Normalize Difference Vegetation Index, EVI = Enhanced Vegetation Index, NDWI = Normalize Difference Water Index, AT = Atmospheric Temperature (MOD07/MYD07), AM = Atmospheric Moisture (MOD07/MYD07), JD = Julian Day, SR = Solar Radiation, VA = View Angle, SA = Solar Angle, (by land cover) indicates separate models were fit for each land cover type, LR, S-LR, PR, FE, and QR = linear, stepwise linear, polynomial, fixed effects, and quadratic regression, respectively, *denotes Ho et al. (2016) estimated HUMIDEX.

Estimating relative humidity (RH), or the amount of water vapor in air as a percentage of

the amount needed for saturation, from MODIS imagery is far less common. Researchers

typically estimate daily mean RH, though models have been derived for daily

minimum/maximum RH (Recondo et al., 2013), 8-day mean RH (Peng et al., 2006), and summer

mean RH (Li and Zha, 2018). While several of the studies listed in Table 4.1 used LST or atmospheric temperature (AT, from MYD07/MOD07), all but Li and Zha (2018) used some form of MODIS moisture product, such as near-infrared (NIR) water vapor (WV, from MOD05/MYD05) or atmospheric moisture (AM, from MOD07/MYD07). In terms of the derived R² and RMSE, results for RH are much less consistent than daily Tmax (Table 4.1).

Recondo et al. (2013) was the only author to derive models for both Tmax and RH, which could theoretically have been used to derive apparent temperature. The study performed by Ho et al. (2016) is most relevant to this analysis, as they estimated HUMEDIX, a Canadian measurement of apparent temperature, using a combination of Landsat LST, MODIS WV, and auxiliary data related to urbanization level.

4.1.3 Potential benefits of remotely-sensed Heat Index (HI) estimation

Heat Index (HI) is the standard apparent temperature metric used by the US National Weather Service (NWS) and based on extensive biometeorology studies (Steadman, 1979; Rothsfuz, 1990). HI is computed as a 2nd order polynomial function of Tair and RH (NWS, 2014). The NWS advises caution with HIs above 80°F, as prolonged exposure or physical activity can lead to heat exhaustion. Sunstroke is possible for HIs above 90°F and highly likely for HIs above 105°F (NWS, 2019).

A spatially explicit HI product derived from satellite imagery would allow for the study of variation in heating trends and thermal exposure across metropolitan and rural areas at a much higher spatial resolution than provided by in-situ weather stations. We have identified three areas of research that could significantly benefit from this new information:

124

Heat-related illness: Identifying vulnerable populations:

A major concern related to climate change is increased illness and mortality due to more frequent heat waves (Hajat et al., 2010; Kravchenko et al., 2013; Kristic et al., 2017). Medical studies focused on the adverse health effects of extreme temperatures are traditionally performed using a combination of mortality data and weather station observations (Wang et al., 2018).

In addition to being exposed to higher temperatures due to their location within a metropolitan area (i.e. the UHI effect), certain populations are at a greater risk of heat-related illness due to underlying demographic and socioeconomic factors. Vulnerable individuals are most commonly defined as elderly, very young, low income/unemployed, or low educational attainment. Thus, a growing number of studies have derived a heat vulnerability index for different metropolitan regions using a combination of satellite LST and Census data (Klein Rosenthal et al., 2014; Bao et al., 2015; Ho et al., 2015; Morabito et al., 2015; Declet-Barreto et al., 2016; Chen et al., 2018; Karimi et al., 2018; Méndez-Lázaro et al., 2018; Sun et al., 2018). These indices identify warmer than average neighborhoods that contain a high portion of vulnerable residents. In comparison to LST, remotely-sensed HI would better reflect the actual heat stress experienced by different neighborhoods.

Building energy use: Forecasting peak electrical demand and assessing grid vulnerability:

Building energy demand for cooling purposes is expected to increase in the coming decades as a result of anthropogenic climate change (Ning Lu et al., 2010; Schaffer et al., 2012; Affhammer and Mansur, 2016; Lim and Yun, 2017). This will lead to greater electrical grid vulnerability and more frequent power transformer failures (Schaffer et al., 2012). Cooling-degree days (CDD) are a temperature based metric traditionally used to quantify the energy needed to cool a building. However, a growing number of studies have employed a more holistic

125

set of weather-related parameters, including humidity, precipitation, and wind speed (Sailor, 2001; Frazeli et al., 2016; Affhammer and Mansur, 2016; Ortiz et al., 2018). HI could serve as a better predictor of cooling energy demand than air temperature since it combines humidity and temperature (Ortiz et al., 2018). Remotely-sensed HI would enable planners to examine the weather-related drivers of cooling energy demand at a high resolution and better prepare for peak electricity demand during heat waves.

Environmental justice: Quantifying thermal inequalities:

Disparities in heat-related mortality rates amongst race and socioeconomic classes are well documented (Yardley et al., 2011; Kravchenko et al., 2013; Gronlund 2014). Limited access to air conditioning makes lower income individuals especially vulnerable to the adverse health effects induced by heat waves (Curriero et al., 2002; O'Neil et al., 2005; Hajat et al., 2010; Yardley et al., 2011). Moreover, lower socioeconomic and minority groups are more likely to live in warmer neighborhoods with greater exposure to heat stress (Harlan et al., 2006; Kravchenko et al., 2013).

Several recent studies have used satellite LST to compute warming disparities across metropolitan areas and align this information with demographic data (Mitchel et al., 2014; Mitchel and Chakraborty, 2015; Li et al., 2016; Tang et al., 2017; Ahmed, 2018; Mithcel et al., 2018). Building off this work, remotely-sensed HI could be used in conjunction with existing weather-based epidemiology models (Perry et al., 2011; Na et al., 2013; Kovach et al., 2016) to examine how, during heat waves, the risk of heat-related illness varies across neighborhoods and relates to socioeconomic factors.

4.1.4 Objective

While researchers have used satellite images to predict high-to-moderate spatial resolution Tair and RH, with the exception of Ho et al. (2016), none have directly computed an index related to apparent temperature. Furthermore, HI, the metric used by meteorologists, policy makers, and health professionals in the US, has yet to be derived via remote seasoning techniques.

The goal of this analysis was twofold: (1) to determine the extent to which HI can be estimated using a combination of static and dynamic satellite and geospatial products and (2) assess which factors are most important for estimation. Specifically, daily maximum 1-km HI was modeled across the CONUS for 2012 using MODIS LST, WV, and near-infrared (NIR) indices, as well as land cover, topographic, and locational factors.

4.2 Methodology

4.2.1 Study Area

The CONUS was identified as an ideal study area due to its wide range of topographic and climatic conditions, in addition to the availability of auxiliary data (Figure 4.1). The timeframe for this analysis was defined by the 5 month period from May 1st to September 30th of 2012. These months capture the warmest part of the year and provide a several-week buffer for late/early extreme temperatures. In addition, 2012 was an unusually hot year in which most of the CONUS was adversely affected by prolonged and excessive heat waves (Rippey, 2012). However, there were also some cooler periods, resulting in a broad and normally distributed range in HI values (min = 34.2° F, max = 129.1° F, median = 84.7° F) (see Figure 4.7 in the Supplemental Information, section 4.5).



Figure 4.1: The CONUS study area and location of the 1,395 utilized Local Climatology Dataset (LCD) stations. The station grouping scheme used for the modified 10-fold cross-validation (discussed in Section 4.2.3) is displayed as well.

4.2.2 Source of data, processing, and variable justification

Response variable: Daily Heat Index (HI) from weather stations:

Daily HI was available through the US Local Climatology Dataset (LCD). This dataset consists of hourly meteorology parameters, including Tair and RH (NOAA, 2019). Similar to Ho et al. (2016), Zhang et al. (2014), and Hass et al., (2016), daily HI was calculated at the time of maximum Tair to reflect the apparent temperature during the hottest part of the day. The polynomial formula for computing HI is described by NWS (2014). Adjustments are made if the HI is less than 80°F or for unusually high/low RH and Tair values. Figure 4.1 shows the location of the 1,395 CONUS stations with valid data for 2012. Valid refers to having hourly observations from 11:00 AM to 6:00 PM (local time) for at least 145 days (95%) from May 1st to September 31st.

Predictor variables:

Independent variables used for HI estimation are summarized in Table 4.2 and described below in greater detail. The MODIS sensor was the source for daily satellite imagery, including LST, WV, red, NIR, and mid-infrared (MIR) products. Other static variables were employed as well. Land cover information was obtained from the 2011 National Land Cover Dataset (NLCD); topographic factors were derived from the Shuttle Radar Topography Mission (SRTM). **Table 4.2:** Overview of predictor variables.

Variable	Definition	Туре	Res. (m)	Source
LST _{AD}	Afternoon (Aqua daytime) LST	Daily	1,000	MYD11A1
LST _{TD}	Morning (Terra daytime) LST	Daily	1,000	MOD11A1
WV _{AD}	Afternoon (Aqua daytime) NIR water vapor (WV)	Daily	1,000	MYD05
WV _{TD}	Morning (Terra daytime) NIR WV	Daily	1,000	MOD05
ΔLST_M	Delta Morning LST: Difference between afternoon and morning LST	Daily	1,000	MYD/MOD11A1
ΔLST_N	Delta Night LST: Difference between afternoon and nighttime LST	Daily	1,000	MOD11A1
ΔLST_{DB}	Delta Day Before LST: Difference between afternoon LST and afternoon LST from the day before.	Daily	1,000	MOD11A1
ΔWV_M	Delta Morning WV: Difference between afternoon and morning WV	Daily	1,000	MYD/MOD05
ΔWV_{DB}	Delta Day Before WV: Difference between afternoon WV and afternoon WV from the day before	Daily	1,000	MYD05
NDVI	Normalized Difference Vegetation Index: (NIR – Red)/(NIR + Red)	Daily	500	MYD09GA
NDWI	Normalized Difference Water Index: (NIR – MIR)/(NIR + MIR)	Daily	500	MYD09GA
%Imp	Percent impervious cover (NLCD classes 21-24)	Static	30	NLCD
%Ag	Percent agriculture cover (NLCD classes 81-82)	Static	30	NLCD
%For	Percent forest cover (NLCD 41-43)	Static	30	NLCD
Elev	Elevation (m)	Static	90	SRTM
Slope	Slope (as percent)	Static	90	SRTM
Lat	Latitude (in decimal degrees - NAD83)	Static	-	-
DC	Distance to nearest coast (includes ocean and great lakes)	Static	-	USGS (2014)

Note: Res. = Original resolution of the source data, NIR = near-infrared reflectance (Band 2), Red = red reflectance (Band 1) MIR = mid-infrared reflectance (Band 7), NLCD = 2011 National Land Cover Database, SRTM = Shuttle Radar Topography Mission

Land surface temperature (LST): LST is the most widely utilized variable for estimating Tmax and has also been used to estimate RH (Table 4.1). Daily, 1-km daytime LST from the Aqua satellite was employed (MYD11A1) (Wan et al., 2015), since Aqua's daytime overpass is closer to solar noon than Terra's (~1:00 PM vs. ~10:00 AM for the CONUS). While some have used atmospheric temperature (AT) from MODIS Atmospheric Profile products (MOD07/MYD07) to estimate RH (Peng et al., 2006; Lin et al., 2013), we used LST, since it was shown to be closer to radiant ground temperatures (Wang et al., 2008). LST from Terra (MOD11A1) was also used to assess potential benefits alternatively using morning observations.

<u>Water vapor (WV)</u>: With the exception of Li and Zha (2018) WV or AM was used by all studies that estimated RH and Lin et al. (2012) to estimate Tmax (see Table 4.1). Daily, 1-km NIR WV from the Aqua satellite was available through the MODIS Total Precipitable Water product (MYD05) (MODIS Atmospheric Science team, 2014). While some have used atmospheric moisture from the MODIS Atmospheric Profile products (MOD07/MYD07) (Peng et al., 2006; Lin et al., 2013), we used WV from MYD05, since it was shown to be closer to ground-level humidity (Wong et al., 2015). WV from Terra (MOD05) was also used to assess potential benefits of alternatively using morning observations.

<u> $\Delta LST(s)$ </u>: To account for temperature trends over the course of a given day, the difference (or Δ) between afternoon LST and morning (Terra day, MOD11A1), night (Aqua night, MYD11A1), and day before LST (Aqua day-1, MYD11A1) was included. Several authors have used both day and night LST images for Tmax estimation (Zhang et al., 2011; Zeng et al., 2015b; Noi et al., 2016; Rosenfield et al., 2017; Yoo et al., 2018; Zhang et al., 2018; Phan et al., 2019); others have additionally included Terra observations (Noi et al., 2016; Didari and Zand-Parsa, 2018; Yoo et al., 2018; Zhang et al., 2018; Zhang et al., 2018; Zhang et al., 2014).

Although some have compared different day/night and Aqua/Terra combinations, findings regarding the best group of predictors are inconsistent (Zhang et al., 2011; Zeng et al., 2015b; Phan et al., 2019). Yoo et al. (2018) noted that LST from the day before was critical for estimating Tmax.

<u>AWV(s)</u>: Similar to LST, the difference between afternoon and morning (Terra day, MOD05) and day before WV (Aqua day-1, MYD05) was used to account for humidity trends over the course of a day. Note: Nighttime WV is not available, since this product is based on NIR bands. <u>Normalized Difference Vegetation Index (NDVI)</u>: To account for differences in vegetative cover and evaporation rates across study areas, several authors have included Normalized Difference Vegetation Index (NDVI) or the similar Enhanced Vegetation Index (EVI) for Tmax and RH estimation (Peng et al., 2006; Lin et al. 2012; Lin et al., 2013; Recondo et al., 2013; Xu et al., 2014; Shi et al., 2017; Li and Zha, 2018). Daily NDVI was computed with the red and NIR bands (1 and 2, respectively) from the 0.5-km Aqua reflectance product (MYD09GA, E. Vermorte, 2015).

<u>Normalized Difference Water Index (NDWI)</u>: Authors also used Normalized Difference Water Index (NDWI) for estimating Tmax and RH, as it tends to be more related to plant water content than NDVI (Kim and Han, 2013; Xu et al., 2014; Ho et al., 2016). We computed daily NDWI with the NIR and MIR bands (2 and 7, respectively) from the 0.5-km Aqua reflectance product (MYD09GA).

<u>*Percent land cover*</u>: As Tair and RH are highly dependent on land cover, authors have included percent land cover variables in their models or proximity to certain urban features, such as roads or city centers (Rosenfeld et al., 2017; Li and Zha, 2018; Yoo et al., 2018). Some fit separate models for each land cover type (Zhang et al., 2011; Rhee and Im, 2014; Zeng et al., 2015b). To

131

account for varying land cover, percent impervious (%Imp), forest (%For), and agriculture (%Ag) were computed with the 2011 NLCD (USGS, 2017). These cover types are the most commonly considered for Tmax and RH estimation (Zhang et al., 2011; Rhee and Im, 2014; Zeng et al., 2015b).

Additional topographic and locational factors: As Tmax and RH vary with respect to elevation, many authors utilized elevation from a digital elevation model (DEM) for estimation (Zhang et al., 2011; Adab et al., 2013; Recondo et al., 2013; Zeng et al., 2015b; Noi et al., 2016; Rosenfeld et al., 2017; Didari and Zand-Parsa, 2018; Li and Zha, 2018; Yoo et al., 2018; Zhang et al., 2018). Some additionally considered slope (Rosenfeld et al., 2017). To reflect the effects of topography, we incorporated elevation and slope from the SRTM DEM (Kautz, 2017). Similar to Lin et al. (2012), Lin et al., (2013), Xu et al. (2014), Noi et al. (2016), Didari and Zand-Parsa, 2018, and Yoo et al. (2018), latitude (Lat) was used to adjust for warmer temperatures closer to the equator. Corresponding to Xu et al. (2014), Ho et al. (2016), Rosenfield et al. (2017), and Li and Zha (2018), distance to nearest coast (DC) was also included to account for greater humidity closer to large bodies of water. We used USGS's (2014) definition for the CONUS coast, which includes the shorelines of the Great Lakes and oceans. To assign a higher weight to closer stations, natural log of distance was taken.

Variables omitted: While some authors included solar radiation, solar angle, solar declination, day length, or Julian day to avoid seasonal bias (Lin et al. 2012; Emamifar et al., 2013; Recondo et al., 2013; Xu et al., 2014; Noi et al., 2016; Yoo et al., 2018; Ho et al., 2016), this was not necessary for our HI product, since it was only derived for the hottest portion of the year (May through September). Other uncommon variables that were not used include MODIS Red, Green, and Blue reflectance (Li and Zha, 2018), aspect (Rosenfeld et al., 2017; Yoo et al., 2018), sensor

view angle (Noi et al., 2016), surface albedo (Xu et al., 2014), Sky View Factor (Ho et al., 2016), population density (Rosenfeld et al., 2017), and nighttime lights (Li and Zha, 2018). Geoprocessing and grid alignment:

The MODIS 1-km LST grid defined the spatial reference for the HI model. All other variables were resampled to match (via bilinear interpolation). After the independent variables were aligned, values for pixels that contained a LCD station were extracted. To account for registration issues, a weighted spatial average of valid values was taken using a 3 by 3 window around each station. Invalid values within the window were ignored. However, if the center pixel was invalid, the average was set to invalid. This was done for LST, WV, all Δ parameters, Lat, Elev, and Slope. To reflect a larger area of environmental conditions and the landscape around each station, NDVI, NDWI, and land cover variables were calculated with 5 by 5 unweighted average of valid values. The unweighted average assigned equal weights to all values within a ~25-km² area around each station. This approach was based on authors who employed the TVX method with a sliding window size of 5-7 pixels (Zhu et al., 2013; Kitsara et al., 2018; Misslin et al., 2018). As with the 3 by 3 window, an average was taken only if the center pixel was valid; invalid pixels were not used to compute the average.

Observations were then pooled across stations and days (1,395 stations X 153 days = 213,435 observations). Each station had 153 different values for daily variables, which in some cases were invalid due to cloud cover or emissivity error. For static values, stations were assigned the same value for each day.
4.2.3 HI model development and assessment of variable importance

Due to the large number of observations and nonlinearity of the HI equation, Random Forest (RF) regression was identified as the most appropriate method for model development. RF is a nonparametric machine learning technique that uses a set of regression trees, each trained with a subset of training data, with a random subset of available predictors used to split the data into each node of each tree. To reach a final estimate, outputs from all trees are aggregated with an average (Ho et al., 2016; Yoo et al., 2018). Refer to Breiman (2001) for further details.

Due to its flexibility in areas with complicated and heterogeneous landscapes (Noi et al., 2017; Yoo et al., 2018), RF regression has been extensively used to estimate Tair (Xu et al., 2014; Meyer et al., 2016; Noi et al., 2017; Sanikahni et al., 2018; Yoo et al., 2018; Zhu et al., 2019), RH (Li and Zha, 2018), and HUMIDEX (Ho et al., 2016) from MODIS products. Several authors have found RF to serve as a better predictor of Tair than ordinary least squares (OLS) regression (Xu et al., 2014; Meyer et al., 2016; Noi et al., 2016; Noi et al., 2017) and other machine learning techniques (Zhu et al., 2019).

Model performance was assessed on the basis of the resulting coefficient of determination (R²) and root mean square error (RMSE). To avoid using observations from the same station for both training and validation, a modified 10-fold cross-validation approach was employed, such that stations were randomly assigned to 10 groups (see Figure 4.1). When a group was used for validation, the other 9 groups were used for training. Multicollinearity was evaluated with variable inflation factors (VIFs). The optimal parameters for RF regression were identified by iteratively testing values and finding the combination that produced the lowest mean square error (MSE). These parameters included the learn rate, maximum number of splits, and minimum number of leafs.

To evaluate relative improvements in HI estimation from adding additional parameters, a series of simple to complex models were developed. Starting with LST, variables were included in order of highest expected importance to least, based on previous findings for Tmax, RH, and HUMIDEX models (Lin et al., 2012; Kim and Han, 2013; Recondo et al., 2013; Ho et al., 2016; Noi et al., 2016; Didari and Zand-Parsa, 2018; Li and Zha, 2018; Yoo et al., 2018). NIR indices (NDVI and NDWI) were added last, since these variables were the most data-intensive to derive and may already be captured by land cover. To ensure an unbiased comparison, the same 52,464 observations were used to train and validate each model. These represent instances in which all MODIS parameters were valid. The best model was selected on having an ideal tradeoff between performance and loss of observations. "Best", in this context, refers to the most ideal model across a restrictive set of predictor variables (described in Table 4.2) and does not imply that all possible parameters or combination of parameters were tested. Once the best model was selected, variable importance was further evaluated using the percent increase in mean square error (%IncMSE), similar to Xu et al. (2014), Ho et al. (2016), Didari and Zand-Parsa (2018), Li and Zha (2018), and Yoo et al. (2018). This metric quantifies the relative increase in model error when each variable is removed. Model error for the %IncMSE was again computed with the modified 10-fold cross-validation approach.

4.3 Results and Discussion

4.3.1 Model selection: Assessment of performance and tradeoffs

To assess the utility of LST for estimating HI and improvements derived from incorporating additional variables, 14 models were fit via RF regression. The results are summarized in Table 4.3. For consistency, the models were all trained and validated with the same 52,464 observations, which had valid values for all MODIS-derived variables. Further information on the optimal RF parameters is available in Table 4.5 in the Supplemental Information, section 4.5.

Table 4.3: Overview of HI model results. Listed are the R^2 , RMSE, maximum VIF, number of potential observations (n), and included variables. While the total number of potential variables is listed, each model was trained and validated with the same 52,464 observations. Refer to Table 4.2 for variable definitions. The total number of potential observations was 213,435.

Model	\mathbb{R}^2	RMSE (°F)	VIF _{max}	n	LSTAD	LST _{TD}	WVAD	WVTD	ΔLST_M	ΔLST _N	ALSTDB	ΔWV_{M}	ΔWV _{DB}	%Imp	%For	%Ag	Elev	Slope	DC	Lat	NDVI	NDWI
1	0.34	8.4	1.0	117,269	Х																	
2	0.70	5.7	1.0	117,237	Х		х															
3	0.71	5.6	1.0	120,086		х		х														
4	0.75	5.1	1.3	94,932	Х		х		Х			Х										
5	0.78	4.8	4.5	82,109	Х		х			Х												
6	0.74	5.3	1.2	76,594	Х		х				Х		Х									
7	0.80	4.6	6.0	52,483	Х		х		Х	Х	Х	Х	Х									
8	0.79	4.7	1.8	94,932	Х		х		Х			Х		Х	Х	Х						
9	0.81	4.5	4.9	82,109	Х		х			Х				Х	Х	Х						
10	0.81	4.5	1.9	94,932	Х		х		Х			Х		Х	Х	Х	Х	Х	Х	Х		
11	0.82	4.4	5.5	82,109	Х		х			Х				Х	Х	Х	Х	Х	Х	Х		
12	0.84	4.1	8.8	82,080	Х		х			Х				Х	х	Х	Х	х	Х	Х	Х	Х
13	0.83	4.3	3.4	94,891	Х		х		Х			Х		Х	Х	Х	Х	Х	Х	Х		Х
14	0.84	4.1	5.7	81,097	Х		Х			Х				Х	Х	Х	Х	Х	Х	Х		Х

<u>Model 1 - LST</u>: The relatively low R^2 and high RMSE of Model 1 suggests that LST alone is a poor predictor of HI. Although this model was the least restrictive, in terms of the total number of potential observations, it captured only 34% of the variation in HI.

<u>Model 2 - Addition of WV</u>: Incorporating WV considerably improved HI estimation, increasing the R² by 0.36 and decreasing the RMSE by 2.7°F. Thus, utilizing WV as an independent variable is critical for HI model performance. Virtually no observations were lost by including WV. In nearly all instances, when afternoon LST was valid, so was afternoon WV.

<u>Model 3 - Replacement of Afternoon with Morning LST and WV</u>: A morning model was assessed to determine the extent to which morning LST and WV can substitute invalid afternoon values (Model 3). Using morning observations produced nearly identical results to the afternoon model (Model 2). In fact, the morning model performed slightly better. The similar performance is due to the high correlation between morning and afternoon LST/WV (LST $R^2 = 0.82$, WV $R^2 =$ 0.88). Thus, morning LST and WV derived from the Terra sensor can be substituted for invalid afternoon values from the Aqua sensor. Doing so increases the number of potential observations from 117,237 to 143,643. Note that the total number of potential observations was 213,435.

Given the wide swath width of the MODIS sensor (2,330 km), the local solar time across a given scene can vary by 2-3 hours. The similar performance of the Morning and Afternoon models also suggests that it is not necessary to account for within-scene differences in solar angle, as observations several hours apart appear to be equally effective at estimating HI.

Previous researchers have compared the daily Tmax predictive capability of LST collected from the Aqua and Terra sensors. Zeng et al. (2015b) and Didari and Zand-Parsa (2018) similarly found Terra LST to perform slightly better than Aqua LST; Zhang et al. (2018) found no significant difference.

Models 4-7 - Addition of ΔLST and ΔWV: Models with ΔLST and ΔWV (difference from afternoon value) were used to determine the extent to which including temperature and humidity trends over different parts of the day can improve HI estimation. Incorporating Δ parameters increased model performance (R²: +0.04-0.10, RMSE: -0.4-1.09°F). Of all the models with a single Δ LST/WV, Δnight performed best (Model 5), followed by Δmorning (Model 4), and Δday-before (Model 6). This is consistent with studies that found nightime LST to be a better predictor of Tmax than daytime LST (Zhang et al., 2011; Zeng et al., 2015b; Zhang et al., 2018; Phan et al., 2019). Note that the Δnight model does not contain a ΔWV parameter since only daytime MODIS WV products are available. The fact that the Δday-before model did not perform best was surprising, as Yoo et al. (2018) determined that LST from the day before was crucial for estimating daily Tmax. Including all of the Δ parameters in a single model (Model 7) resulted in little improvement over the Δnight model and a significant loss of data. Furthermore, the VIF was >5.

There is a tradeoff between performance and loss of data with the Δ night and Δ morning models. While the Δ night model performed marginally better than the Δ morning model, it resulted a greater loss of data (n = 82,109 vs. n = 94,932). As there was no clear "best option", subsequent model development proceeded with the inclusion of both.

<u>Models 8-11 - Addition of land cover, topographic, and locational factors</u>: Adding land cover variables yielded a marginal improvement in HI estimation for both the Δ morning and Δ night models (Models 8 and 9) (R²: +0.03-0.04, RMSE: -0.4°F). The further inclusion of topographic and locational factors resulted in only a small improvement (Models 10 and 11) (R²: +0.01-0.02, RMSE: -0.1-0.2°F). The addition of land cover, topographic, and location factors improved the Δ morning model to a greater extent, albeit with a small difference. <u>Models 12-13 - Addition of NIR indices</u>: When NDVI and NDWI were used in the same model (Model 12), their resulting VIFs were >5. To reduce multicollinearity, only NDWI was used in subsequent models, since it had a higher bivariate R² with HI. Including NDWI yielded minor model improvement for both the Δ morning (Model 13; R²: 0.02 RMSE: -0.3°F) and Δ night (Model 13; R²: 0.02 RMSE: -0.2°F) models. One possible reason for the unsubstantial change was that NIR indices were, to some extent, already reflected with the land cover variables. Suggestions for implementation and model selection for this analysis:

These results provide strong evidence that LST alone is a poor predictor of HI. Adding WV resulted in the most significant improvement in model performance. Including all of the other parameters only increased the R² by 0.14 and decreased the RMSE by 1.5°F. While HI estimation can be enhanced by incorporating these factors, using just afternoon LST and WV for a simplified model may be sufficient, depending on the accuracy required for a given application. Missing afternoon observations from the Aqua sensor could also be substituted for morning observations from the Terra sensor to reduce the frequency of invalid data.

A major disadvantage of using multiple Δ parameters is the loss of usable observations, especially since Model 7 performed only slightly better than the Δ night model. Thus, we recommend that researchers use either Δ morning LST/WV or Δ night LST variables. Adding land cover, topography, locational, and NIR factors resulted in a marginal improvement in HI estimation. Considering the extensive data processing required to incorporate daily NDWI and NDVI, these variables can potentially be omitted.

It is important to note that if the primary goal is HI estimation, multicollinearity would not necessarily be an issue. In fact, several researches developed Tmax models that utilized multiple LST products with a high degree of correlation (Noi et al., 2016; Didari and Zand-Parsa,

2018; Yoo et al., 2018; Zhang et al., 2018; Phan et al., 2019). However, Model 13 was selected as the best model for subsequent error and variable importance assessment, since it had a maximum VIF smaller than 5 and provided a good trade-off between performance and loss of observations. In this context, "best" refers to the most ideal across all 14 models that were tested. The results discussed in the following sections (4.3.2 and 4.3.3) were derived from retraining and validating this model with all 94,891 observations available for regression.

4.3.2 Error assessment for the selected model

When the selected model (Model 13) was retrained and validated using all available 94,891 observations via the modified 10-fold cross validation approach, the resulting R^2 and RMSE was 0.83 and 4.4°F, respectively; the maximum VIF was 3.1. Figure 4.2 shows the estimated versus actual HI values; there is a strong degree of linear association between the two. For extreme HI (<50°F and >110°F), there were some instances of over and under estimation, most likely due to the limited number of observations available for model development in this range. However, the vast majority of observations follow the one-to-one relationship.



Figure 4.2: Estimated vs. actual HI for the selected model (Model 13). Note: this plot shows the 94,891 observations that were used to train and validate the model.

Based on the R², Model 13 compared favorably to previous Tmax models and outperformed most RH models (see Table 4.1). The RMSE was actually lower than the RMSE for Ho et al.'s (2016) HUMIDEX model (9°F). While some caution is advised when interpreting direct comparisons, as these analyses utilized different dependent variables and study areas, this indicates that our HI model performed reasonably well, especially when considering that it was validated across a wide range of conditions over the entire CONUS.

Model residuals were normally distributed, indicating that there was no bias towards over or under estimation (Figure 4.3). Note that residuals were derived with estimates from the modified 10-fold cross validation approach. The maximum and minimum residuals were $40.7^{\circ}F$ and $-24.3^{\circ}F$, respectively. However, the vast majority (77.6%) were within +/-5°F; <0.1% were outside of +/-20°F. These unusually high residuals did not appear to be concentrated among a small group of stations, as no station had more than 2. In fact, only 8 stations had more than 1. In addition, they did not appear to be caused by abnormal HI or predictor values. While the model performed very poorly for these observations, they represented a negligible portion of the data (n = 45) and are not a cause of major concern.



Figure 4.3: Histogram of residuals for the selected model (Model 13).

The residual plot indicated that model error was homogenous (Figure 4.4). There did not appear to be greater error for higher or lower HI.



Figure 4.4: Residual plot (left) and corresponding box plot (right) for the selected mode (Model 13). Note: x-axis for the boxplot lists the midpoint for each estimated HI range.

Most station-specific RMSEs were $<5^{\circ}F(73.5\%)$. There were no major spatial trends to station error across the CONUS (i.e. increasing error north to south, east to west, or closer to the coast) (Figure 4.5). However, several stations with a RMSE $>10^{\circ}F$ were concentrated in Southern Coastal California. This may be due to the region's later peak in maximum annual temperatures, which occurs in mid-September (NOAA, 2019). Hoshimoto et al. (2008) produced a vapor pressure deficit model from MODIS data and similarly found that area of the CONUS to have a high prediction error.



Figure 4.5: RMSE by station (in °F) for the selected model (Model 13).

When comparing the RMSE map of the selected model (Model 13) to the RMSE map of the LST only model (Model 1), it is evident that including additional factors improved HI estimation across the CONUS (Figure 4.6). The improved performance was most apparent for stations along the eastern coast of the US (south of Pennsylvania) and Gulf of Mexico. This was expected though, as these areas are hotter and more humid than the rest of the CONUS. Interestingly, the LST only model performed better in the western portion of states bisected by the 100° Meridian, especially Texas, likely due to the dyer climate. While this analysis did not consider Longitude, subsequent models may benefit by incorporating it to account for dyer conditions west for the 100° Meridian. Moreover, it appears that including additional variables to account for atmospheric moisture, land cover, and topography is most important for hot and humid regions of the CONUS.



Figure 4.6: RMSE by station (in °F) for the LST only model (Model 1).

Much of the justification for this study focused on metropolitan areas, since urban areas encompass >80% of the US population, exacerbate heat waves, and have sharp changes in temperature over relatively short distances due to the UHI effect (making spatially explicit temperature datasets especially important). However, the model could be applied to rural locations as well. HI estimates would be of great use to rural communities, since weather stations in these areas are highly sparse. Furthermore, the model could be used to better examine the impact of heat stress on ecosystems. Understanding and predicting biological responses to extreme heating events is critical for effective ecosystem modeling (Jentsch et al., 2007; Smale and Wernberg, 2013). These HI estimates offer complementary insight to climatic pressures exhibited on terrestrial ecosystems, thus leading to improved modeling opportunities. Another point to make with respect to the RF modeling capabilities is that when Model 13 was alternatively fit with an OLS regression, results were close to those derived from RF ($R^2 = 0.79$ vs. 0.83, RMSE = 4.9°F vs. 4.4°F). This is consistent with Meyer et al. (2016), who found only a slight improvement of RF over OLS regression when modeling Tair. Thus, the use of OLS may be sufficient for HI prediction.

4.3.3 Variable importance assessment for the selected model

The percent increase in mean square error (%IncMSE) was used to further assess the importance of variables included in the selected model (Model 13) (Table 4.4, first column). LST and WV were, by far, the most important variables for HI estimation. This corresponds to previous authors who determined that these factors had the highest variable importance in their respective Tmax (Ki et al., 2012; Lin et al., 2012; Xu et al., 2014; Recondo et al., 2013; Noi et al., 2016; Yoo et al., 2018), RH (Lin et al., 2013; Recondo et al., 2013), and HUMIDEX (Ho et al., 2016) model. The %IncMSE for LST was about 2/3rds larger than the %IncMSE for WV. However, the inclusion of both LST and WV is essential, as model error roughly doubled when either was removed (2.3X greater for LST, 1.8X greater for WV).

_	HI	Tmax	RH		
\mathbf{R}^2	0.83	0.83	0.74		
RMSE (°F)	4.4	4.3	7.4		
<u>%IncMSE</u>					
LST	126.3	172.9	73.1		
ΔLST	11.7	12.9	6.2		
WV	76.0	32.8	44.8		
ΔWV	11.1	9.1	2.1		
%Imp	2.0	3.1	4.1		
%For	0.9	1.7	1.1		
%Ag	0.0	0.0	1.0		
Elev	8.6	8.9	25.7		
Slope	0.7	1.1	0.0		
DC	0.0	0.0	0.0		
Lat	0.2	0.5	0.0		
NDWI	13.3	13.4	7.3		

Table 4.4: The percent increase in mean square error (%IncMSE) of each variable, R^2 , and RMSE for the selected HI model and comparison to similar Tmax and RH models.

NDWI had the next highest importance score, with a %IncMSE just above Δ LST and Δ WV. Authors have similarly found NIR indices to be the second most important factor behind LST and/or WV (Kim and Han, 2013; Lin et al., 2012; Xu et al., 2014; Recondo et al., 2013; Li and Zha, 2018; Yoo et al., 2018); others have found them to have little to no influence on estimation (Lin et al., 2013; Ho et al., 2016; Noi et al., 2016; Didari and Zand-Parsa, 2018). Considering the number of Tmax models that included multiple LST predictors (Zhang et al., 2011; Zeng et al., 2015b; Noi et al., 2016; Rosenfield et al., 2017; Didari and Zand-Parsa, 2018; Yoo et al., 2018; Zhang et al., 2018; Phan et al., 2019), it was surprising to find that Δ LST and Δ WV did not have a higher %IncMSE.

With the exception of elevation (Elev) and percent impervious (%Imp), removing land cover, topographic, and locational factors resulted in virtually no increase in model error. In

prior work, these variables were commonly found to have moderate to low importance scores (Lin et al., 2012; Kim and Han, 2013; Recondo et al., 2013; Xu et al., 2014; Ho et al., 2016; Noi et al., 2016; Li and Zha, 2018; Yoo et al., 2018). Percent impervious (%Imp) was the most important land cover variable, perhaps due to differences in temperature and humidity across urbanization levels (Yang et al., 2017; Lokoshchenko, 2017; Hoa et al., 2018). However, the importance score for all land cover variables was relatively low. In contrast to authors that used a smaller study area (Xu et al., 2014; Ho et al., 2016; Rosenfield et al., 2017; Li and Zha, 2018), distance to nearest coast (DC) did not appear to have any influence on estimation at a continental scale.

In general, quantifying %IncMSE for predictors produced results that were consistent with section 4.3.1. The most important factors were LST and WV, Δ parameters and NDWI were moderately important, and land cover, topographic, and locational factors had little to no impact on HI estimation.

To further compare our results to previous studies, maximum air temperature (Tmax) and relative humidity (RH) models were fit with the same parameters via RF regression (Table 4.4, last two columns). Consistent with Recondo et al. (2013), the RH model performed worse than the Tmax model. As expected, LST was the most important variable in the Tmax model. However, WV had the second highest factor, suggesting that the incorporation of WV is critical for Tmax estimation. This is a significant finding, as only Lin et al. (2012) included WV in their Tmax model. A major distinction between HI and Tmax is that WV had a much larger importance factor for HI. When WV was removed from the Tmax model, the estimation error increased by only 33%. When WV was removed from the HI model, however, the error nearly

doubled. In fact, WV was just as important for HI estimation as it was for RH. Thus, failing to include WV will result in model estimates that poorly reflect apparent temperature.

4.3.4 Limitations and future work

It is important to note several limitations and topics for future research that would build off our preliminary findings. As mentioned by Lin et al. (2012), weather stations are not randomly distributed and tend to spatially correlate with population. There was, however, a nice spread of both urban and rural stations across the CONUS (see Figure 4.1). Most had 10-35% impervious cover and there was decent representation for all levels from 0-100% (see Figure 4.7 in the Supplemental Information, section 4.5). While there was some bias, the large number of utilized stations (n = 1,395) encompassed a wide range of conditions for model development.

To minimize the amount of invalid data, we chose to incorporate all valid MODIS observations. Some researchers alternatively limited their Tmax model to high quality observations (Zhang et al., 2011; Zeng et al., 2015b; Shi et al., 2017; Didari and Zand-Parsa, 2018; Zhang et al., 2018; Phan et al., 2019). Considering MODIS data are available back to 2002, subsequent HI models could be developed with 15+ years of data. The greater number of observations would allow for more stringent data filtering. Furthermore, the longer timespan would encompass more extreme HI observations (<50°F and >110°F), which were fairly limited with data from just one year. While in comparison to other years from 2002-2018, 2012 encompassed the most HI values >110°F, incorporating additional years would provide a wider range of observations for robust model development.

In its current state, our model can only produce HI estimates with cloud-free observations. There are several daily LST interpolation methods that can be used to derive a temporally and spatially continuous dataset (Neteler, 2010; Maffei et al., 2012; Alfieri et al.,

2013; Metz et al., 2014, Fan et al., 2014, Yu et al., 2015, Zeng et al., 2015a, Shwetha and Kumar, 2016; Kang et al., 2018); one of which was specifically designed for CONUS urban areas (Li et al., 2018). To our knowledge, however, no such method exists for WV or NWDI. An interpolation approach for LST, WV, and NDWI that is applicable to the entire CONUS could be used to produce a gap-free HI product.

Our HI model is also limited by its 1-km spatial resolution. While this scale is sufficient to examine sub-regional heating trends, aligning HI estimates with socioeconomic data at the Census block-group level may be challenging. Bindhu et al. (2013) proposed a disaggregation method to downscale MODIS LST to match the 60-m resolution of Landsat's thermal band. As Ren et al. (2015) demonstrated how WV could be derived from Landsat 8, it may be possible to downscale MODIS WV and NDWI as well. While applying interpolation and downscaling methods to the entire CONUS would be data-intensive, a gap-free, daily 60-m HI product could be highly beneficial to future researchers.

It is possible to indirectly estimate surface humidity based on the difference in daily minimum and maximum air temperature (Kimball et al., 1997). However, this approach requires site specific calibration that would be difficult to apply at the continental scale used for this study (Eccel, 2012). Nevertheless, given the limited number of weather stations that record RH, there remains some potential to increase HI data available for model development, assuming a set of calibration parameters for the entire CONUS were identified. For instance, the Global Historic Climatology Network contains over 10,000 stations for the CONUS (vs. the ~1,400 LCD stations used for this study) and records daily minimum and maximum air temperature (but not RH).

4.4 Conclusion

This analysis aimed to estimate daily maximum 1-km HI across the CONUS using MODIS multispectral products in conjunction with ancillary spatial datasets and determine which factors were most important for estimation. We produced a model that was capable of estimating HI with an acceptable level of error ($R^2 = 0.83$, RMSE = 4.4°F). Stations with a relatively high level of error were concentrated in Southern Coastal California, perhaps due to the late peak in maximum summer temperatures. However, the vast majority of observations were estimated within 5°F. LST and WV were, by far, the most important variables for HI estimation. Moreover, the use of LST alone poorly reflects apparent temperature. The incorporation of additional NIR indices, land cover, topographic, and locational factors only resulted in a marginal improvement in model performance (R^2 : +0.14, RMSE: -1.5°F). Applying a simplified model that includes just LST and WV may be sufficient, depending on the required accuracy.

Prior to this analysis, research regarding satellite-based apparent temperature indices had been limited. In comparison to previous Tmax and RH models, our derived HI product is unique in that it was produced at a continual scale and is applicable across a wide range of conditions. We hope that researchers in multiple study areas, for example in epidemiology, building energy demand, and environmental justice, can use this analytical framework to assess sub-regional heating patterns at much greater spatial resolution than previously possible. Further work to interpolate cloud-contaminated values and downscale estimates to a 60-m resolution would considerably increase the utility of this HI product.

4.5 Supplemental Information



Figure 4.7: Histogram from HI observations pooled across all 1,395 stations with valid data (n = 213,435).

Table 4.5: Optimal parameters selected for Random Forest regression. These include the learn rate, minimum number of leafs (Min Leafs), maximum number of splits (Max Splits), and corresponding mean square error (MSE) for the selected best set of parameters. Note: HI, Tmax, and RH refer to values for the selected model (Model 13), which was trained and validated with all available 94,891 observations.

	1	I	I	I
Model	Learn Rate	Min Leafs	Max Splits	MSE
Model 1	0.10	16	16	71.0
Model 2	0.10	8	16	32.5
Model 3	0.10	32	16	32.2
Model 4	0.10	32	16	27.7
Model 5	0.10	8	16	24.1
Model 6	0.10	32	32	28.6
Model 7	0.10	16	128	21.4
Model 8	0.10	32	32	21.5
Model 9	0.10	8	32	18.7
Model 10	0.10	32	128	19.9
Model 11	0.15	32	16	19.0
Model 12	0.10	32	32	16.4
Model 13	0.10	32	64	17.7
Model 14	0.10	32	128	17.0
HI	0.15	16	64	18.9
Tmax	0.10	16	128	18.4
RH	0.10	16	64	55.0



Figure 4.8: Histogram of percent impervious cover (%Imp) for all Local Climatology Dataset (LCD) stations with valid data (n = 1,395).

4.6 References

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CHAPTER 5 CONCLUSIONS AND FUTURE RESEARCH

5.1 Conclusions

This dissertation applied land surface temperature (LST) images from the Moderate Resolution Imaging Spectroradiometer (MODIS) sensor for three spatial modeling applications across the conterminous United States (CONUS). These topics broadly encompassed agriculture and human health. More specifically, the predictive performance of six interpolation methods for 8-day LST composites were compared, potential benefits of integrating LST for corn yield modeling were assessed, and finally, daily maximum HI was estimated across the CONUS using MODIS multispectral imagery in conjunction with topographic, land cover, and locational factors. Recalling the three hypotheses formulated in Chapter 1, the conclusions are as follows: **Hypothesis 1: LST interpolation methods that utilize values neighboring in both time and space (i.e. spatiotemporal) will have the greatest predictive capability for unavailable LST values.**

At low cloud cover (<30%), the Spline spatial method actually outperformed all of the temporal and spatiotemporal methods by a wide margin, with median absolute errors (MAEs) ranging from 0.2°C to 0.6°C. However, the Weiss spatiotemporal method generally performed best at greater cloud cover, with MAEs ranging from 0.3°C to 1.2°C. Thus, this hypothesis was partially correct. The superior performance of Spline at low cloud cover is significant, considering that the vast majority of MODIS 8-day LST composites requiring interpolation contain low cloud cover (87% and 89% for daytime and nighttime images, respectively). Moreover, considering the distribution of cloud contamination and difficulty of implementing Weiss, using Spline under all conditions for simplicity would be sufficient.

Hypothesis 2: The novel killing degree day metric (LST KDD) will predict annual corn vield with less error than the traditional air temperature based metric (Tair KDD).

The results from Chapter 3 provide strong evidence that LST KDD is capable of estimating annual corn yield with less error than Tair KDD (R²/RMSE of 0.65/15.3 Bu/Acre vs. 0.56/17.2 Bu/Acre). Even while adjusting for seasonal temperature and precipitation parameters, the R² and RMSE of the LST model were approximately 9% higher and 2.0 Bu/Acre lower than the Tair model, respectively. We conclude that satellite-based LST offers an effective means to provide yield forecasts several months prior to harvest for the US Corn Belt, especially during extremely warm and dry growing seasons. Furthermore, long term future yield projections should consider factors indicative of water availability. If these are ignored, yield estimates could contain substantial error for years such as 2012 (a drought year).

Hypothesis 3: HI can be estimated using MODIS observations and products in conjunction with ancillary land cover, topographic, and locational factors.

The derived model was capable of estimating HI within an acceptable level of error ($R^2 = 0.83$, RMSE = 4.4°F). LST and water vapor (WV) were, by far, the most important factors for estimation. Moreover, the use of LST alone poorly reflects apparent temperature. The incorporation of all other parameters only marginally improved model performance (R^2 : +0.14, RMSE: -1.5°F). Therefore, applying a simplified model that includes just LST and WV may be sufficient, depending on the required accuracy.

5.2 Limitations

It is important to note several limitations for this dissertation that stem from the utilized study area and error inherent in remotely sensed data. Given the moderate spatial resolution of MODIS LST, accounting for sub-pixel temperature variation is challenging. From a development and applicability standpoint, both the corn yield and HI models were limited by their observational scale (1-km). For the corn yield model, a single LST value was used to summarize pixels containing a mix of corn and other land cover types. For the HI model, values were assigned to weather stations based on the pixel they were contained. A given station's observations may not pertain to the entire pixel. Moreover, derived HI estimates may not be directly applicable to locational information less than 1-km² in size (i.e. geocoded addresses, Census block-groups, etc).

The process of estimating LST with a satellite-based sensor is subject to geometric and atmospheric distortion. While the MODIS geolocation algorithm is intended to minimize geometric error, minor off-nadir and along-track distortion is induced by a tilt in the mirror coordinate system and uncertainty in spacecraft altitude estimates (Nisihama et al., 2000; Nisihama et al., 2002). Likewise, the split window algorithm is an effective means to reduce atmospheric distortion, but emissivity error can still result from undetected clouds and heterogeneous pixels (Zhengming and Dozier, 1996; Ghent et al., 2019). Nevertheless, MODIS LST has been extensively utilized by numerous studies ranging in scale from sub-city to global (Phan and Kappas, 2018).

The three analyses that comprised this dissertation were performed within the CONUS, due to the wide range of climatic and topographic conditions, as well as the availability of auxiliary data. This study area did omit some environmental conditions though. There are

174

regions with extreme climates for which these findings would not be applicable, such as savannah, tropical rain forests, and arctic ecosystems. However, it would be impossible to consider all conditions found globally in a single study area. Overall, while there were some limitations related to the use for MODIS LST and study area, they by no means invalidate the major findings of this work.

5.3 Outlook and Future Work

Considering that the study area for this dissertation was limited to the CONUS, the next logical step for future research would be applying the utilized spatial models to other parts of the world. The only input other than MODIS data required for the six 8-day LST interpolation methods is a digital elevation model (DEM), which is globally available via the Shuttle Radar Topography Mission (Kautz, 2017). Thus, the analytical framework used in Chapter 2 could easily be expanded to regions beyond the CONUS. As the Food and Agricultural Organization of the United Nations (FAO) provides national-level corn yield estimates (FAO, 2019), an analysis similar to the one performed in Chapter 3 could help determine the extent to which MODIS LST can improve global yield prediction. If land cover variables are excluded (as the National Land Cover Dataset is only available for the US), the HI model from Chapter 4 could be applied to any location in the world.

This analysis could also be expanded in time. Including additional years is especially pertinent to the HI model, as it was only trained with observations from 2012. While this timeframe encompassed an adequate distribution in HI for an initial assessment, there were few extreme observations ($<50^{\circ}$ F and $>110^{\circ}$ F). Incorporating additional years would provide more data in this range for model training. The timeframe for Chapter 3 was limited due to the

175

availability of the US Department of Agriculture National Agricultural Statics Survey (NASS) Crop Data Layers (CDLs). Since writing that manuscript, CDL layers have become available for 2008, 2009, 2017, and 2018 and could be incorporated into a follow-up study.

Chapter 2 provided a comprehensive comparison of interpolation methods for 8-day LST images. However, several methods have been proposed for daily LST (Neteler, 2010; Maffei et al., 2012; Alfieri et al., 2013; Metz et al., 2014, Fan et al., 2014, Yu et al., 2015, Zeng et al., 2015, Shwetha and Kumar, 2016; Kang et al., 2018). While 8-day composites are often sufficient (see Table 2.1) many of these studies could be enhanced by the utilization of daily LST. The analytical framework from Chapter 2 could be expanded to identify the most appropriate daily LST interpolation technique for different conditions. Interpolation methods for MODIS Normalize Difference Vegetation Index (NDVI) have been proposed as well (Zhou et al., 2012; Spruce et al., 2016; Liu et al., 2017). To our knowledge, however, no such methods exist for WV or Normalized Difference Water Index (NDWI). If an appropriate method (or set of methods) for daily LST, WV, and NDWI were identified, it would allow for a spatially and temporally continuous HI product.

It is important to note that this dissertation focused on MODIS LST. A growing trend among remote sensing studies is fusing imagery from multiple sensors (Scheunders et al., 2018). Landsat has been used to downscale MODIS LST and NDVI to a 60-m and 30-m spatial resolution, respectively (Roy et al., 2008; Bindhu et al. 2013; Wu et al., 2015). Downscaling LST to 60-m would allow for field-level agricultural modeling, though yield data at this scale is difficult to obtain. Additionally downscaling WV and NDWI to 60-m would enable the HI model to better assess variation in heating at the Census block-group level.

176

In summary, expanding the analytical framework used for this dissertation to a more extensive study area (both temporally and spatially) would further validate the conclusions discussed above. Moreover, identifying an appropriate interpolation and downscaling approach for daily MODIS imagery would substantially increase the utility of the corn yield and HI models.

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