

## Article

# Improving Atmospheric Correction Algorithms for Sea Surface Skin Temperature Retrievals from Moderate-Resolution Imaging Spectroradiometer Using Machine Learning Methods

Bingkun Luo <sup>1,2</sup> , Peter J. Minnett <sup>2,\*</sup>  and Chong Jia <sup>2</sup> 

<sup>1</sup> Harvard–Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA; bkluo@cfa.harvard.edu

<sup>2</sup> Department of Ocean Sciences, Rosenstiel School of Marine, Atmospheric, and Earth Science, University of Miami, 4600 Rickenbacker Causeway, Miami, FL 33149, USA; chong.jia@earth.miami.edu

\* Correspondence: pminnett@earth.miami.edu

**Abstract:** Satellite-retrieved sea-surface skin temperature ( $SST_{skin}$ ) is essential for many Near-Real-Time studies. This study aimed to assess the potential to improve the accuracy of satellite-based  $SST_{skin}$  retrieval in the Caribbean region by using atmospheric correction algorithms based on four readily available machine learning (ML) approaches: eXtreme Gradient Boosting (XGBoost), Support Vector Regression (SVR), Random Forest (RF), and the Artificial Neural Network (ANN). The ML models were trained on an extensive dataset comprising in situ SST measurements and atmospheric state parameters obtained from satellite products, reanalyzed datasets, research cruises, surface moorings, and drifting buoys. The benefits and shortcomings of various ML methods were assessed through comparisons with withheld in situ measurements. The results demonstrate that the ML-based algorithms achieve promising accuracy, with mean biases within 0.07 K when compared with the buoy data and ranging from  $-0.107$  K to  $0.179$  K relative to the ship-derived  $SST_{skin}$  data. Notably, both XGBoost and RF stand out for their superior correlation and efficacy in the statistical results of validation. The improved  $SST_{skin}$  derived using the ML-based algorithms could enhance our understanding of vital oceanic and atmospheric characteristics and have the potential to reduce uncertainty in oceanographic, meteorological, and climate research.

**Keywords:** sea surface skin temperature; atmospheric correction algorithms; machine learning



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## 1. Introduction

Infrared imaging radiometers onboard geostationary or polar orbiting satellites have been used to measure sea surface skin temperature ( $SST_{skin}$ ) for more than 60 years [1]. For over two decades, the Moderate-Resolution Imaging Spectroradiometer (MODIS) sensors on both the Terra and Aqua satellites have been consistently providing data with an unprecedented spectral resolution [2,3]. It is important to improve the accuracy of  $SST_{skin}$  retrievals, including in challenging situations, and to quantify its errors and uncertainties [4,5] as this facilitates the appropriate use of fields in all applications, especially in forecast model assimilation schemes.

The areas where the impact of accurate  $SST_{skin}$  fields delivered in Near-Real Time (NRT) is the greatest are weather forecasting [6] and operational oceanography [7]. The accurate forecasting of severe storms, especially landfalling Atlantic hurricanes, typhoons and cyclones in other oceans [8], and extra-tropical storms [9], requires the accurate and timely determination of the  $SST_{skin}$  around the storm and along the forecast trajectory [10–13]. A well-known example is the rapid intensification of Hurricane Katrina in the Gulf of Mexico in 2006 as it passed over the northern edge of the Loop Current, and then again over a warm eddy in the northern Gulf shortly before landfall. Providing local authorities with timely information on likely hurricane intensification or dissipation is of great value in implementing

measures to reduce injuries and the loss of lives. The recent Atlantic hurricanes have caused record property damage, disruptions to communities, and losses of lives [14,15], and these are expected to grow in future years [16]. Recent analyses have shown that the rate of peak intensification of Atlantic hurricanes has increased significantly in the last fifty years as a result of global warming [17], and the global occurrence of tropical cyclones that undergo multiple rapid intensification events has nearly doubled in the last two decades [18]. This study focuses on improving  $SST_{skin}$  retrieval in the Caribbean Sea and the surrounding region, which are vulnerable to hurricane formation and intensification, and from which we have an extensive and representative in situ SST dataset.

In this study, we applied several readily available machine learning (ML) methods capable of Near-Real-Time (NRT) application to assess the potential to improve the accuracy of atmospheric correction algorithms for MODIS  $SST_{skin}$  retrieval. This work compared the performance of the widely used existing ML algorithms with that of the NLSST (Non-Linear SST) of Walton, et al. [19], which is the basis of the standard atmospheric correction algorithm applied to cloud-free MODIS measurements [20] as a precursor to identifying where research into improvements can be focused. To achieve this goal, we need a sufficient number of factors in the training dataset used in ML to realize a statistically meaningful model. In situ oceanic and atmospheric data measured by ships, surface buoys, and drifters were used in the study to train the model and assess the accuracy of the derived  $SST_{skin}$  field. Some of the variables used in the development of the ML algorithms are from reanalysis products.

### 1.1. Atmospheric Corrections for MODIS $SST_{skin}$ Retrieval

As a prelude to the ML approaches, we first discuss the standard atmospheric correction algorithms for  $SST_{skin}$  retrieval. The  $SST_{skin}$  can be retrieved from relatively transparent “atmospheric windows” with a minimum effect caused by water vapor and other gases at wavelengths  $\sim 4 \mu\text{m}$  and  $10\text{--}13 \mu\text{m}$ . It is worth noting that a shorter wavelength window  $\sim 4 \mu\text{m}$  can only be used during nighttime due to the contamination by reflected sunlight within the atmosphere and at the surface.

According to the MODIS  $SST_{skin}$  R2019 Algorithm Theoretical Basis documents (from Goddard Space Flight Center (GSFC [21]); accessed on 21 June 2021), the existing MODIS  $SST_{skin}$  retrieval method is based on the NLSST algorithm adapted for MODIS measurements:

$$SST_{skin} = a_{ij0} + a_{ij1}BT_{11\mu\text{m}} + a_{ij2}(BT_{11\mu\text{m}} - BT_{12\mu\text{m}}) \times T_{sfc} + a_{ij3}(\sec(\theta) - 1) \times (BT_{11\mu\text{m}} - BT_{12\mu\text{m}}) + a_{ij4} \times M + a_{ij5}(\theta) + a_{ij6}(\theta)^2$$

where  $BT_{11\mu\text{m}}$  and  $BT_{12\mu\text{m}}$  indicate the brightness temperatures in the MODIS 11 and  $12 \mu\text{m}$  bands.  $M$  represents the two sides of the paddle-wheel scan mirror to correct for small differences in spectral reflectivity between the two sides.  $T_{sfc}$  is a preliminary estimation of the SST, which is reliant on two sources, SST4 (derived from measurements at  $\lambda = 3.95$  and  $4.05 \mu\text{m}$  [20]) when available for nighttime data, and otherwise, the Canadian Meteorological Center Global Foundation SST [22].  $\theta$  is the satellite zenith angle.  $a_{ij0-6}$  are coefficients derived by the regression of match-ups between the in situ and satellite measurements and vary by month in several latitude bands [20] to account for regional and seasonal variations in the properties of the atmosphere.

An example of the limitations of the NLSST algorithm to compensate for anomalous atmospheres, such as Saharan dust aerosols, is given by Luo, et al. [23], who introduced an additional index from other MODIS IR channels to provide correction to nighttime  $SST_{skin}$  retrieval in aerosol-contaminated regions, with significant improvements in accuracy. The ability to improve  $SST_{skin}$  retrievals through aerosol-containing and dry layers is important as these conditions are known to inhibit the development of Atlantic hurricanes [24]. Accurate  $SST_{skin}$  retrieval depends on a good understanding of the uncertainties caused by controlling parameters, such as aerosol distributions [25–27], dry layers [28], and air–sea temperature differences [29]. As it is not straightforward to derive explicit functional forms between satellite brightness temperature measurements and the associated surface and at-

atmospheric factors, we will apply the ML methods to attempt to improve the MODIS  $SST_{skin}$  atmospheric correction algorithms. The incorporation of multiple sources of information on atmospheric state in an algorithm optimized by ML may improve  $SST_{skin}$  retrieval.

### 1.2. Machine Learning Applications

An early application of ML to satellite oceanography was developing algorithms to estimate the air–sea exchanges of  $CO_2$  from satellite data. Given that  $CO_2$  in the atmosphere is well mixed, this problem is dominated by the variability in  $CO_2$  fugacity in the upper ocean, which is temperature-dependent. At that time, the best estimation of air–sea exchanges of  $CO_2$ , derived by Olsen, et al. [30] from the regression of ship-based measurements, was a linear expression of temperature, latitude, and longitude. However, the geographical variables could be proxies for other factors. Using an ML method, Genetic Algorithm Discovery, on measurements taken from repeated tracks around the Caribbean Sea of the Explorer of the Seas [31], Wickramaratna, et al. [32] derived sets of functions of SST and surface pressure clustered into five regions, in each of which the ML equations were more accurate than those of Olsen, Triñanes and Wanninkhof [30]. Reassuringly, the areas of the clustered algorithms fell into those of major ocean surface currents in the region.

A subsequent study using similar techniques on the global Terra MODIS Match-Up Data Base (MUDb; [20]) “rediscovered” the formulation of the NLSST atmospheric correction algorithm [19]. When the ML technique was tasked with deriving NLSST algorithms without the  $T_{sfc}$  term, a set of regionally dependent equations and coefficients was found. The boundaries between the regions were primarily zonal, indicating dependence on the general nature of the water vapor distribution related to large-scale atmospheric circulation [33].

A cloud mask is necessary to identify and remove the cloud-contaminated pixels for MODIS  $SST_{skin}$  retrieval. Kilpatrick, et al. [34] developed an improved cloud-screening algorithm using boosted Alternating Decision trees (ADtrees). Compared to the binary tests forming the previous decision tree cloud mask, the ADtrees approach better identifies cloud types and improves the retention of SST gradients; it also provides confidence levels of the clear sky determination for each pixel.

Subsequently, RF and Cubist Decision Trees were used to represent and predict the errors and uncertainties in MODIS  $SST_{skin}$  retrieval [5]. Both the methods performed well, but the Cubist method was explored further to gain an insight into the sources of inaccuracies in retrieval, identifying seven Rule Sets with different error distributions. Each Rule Set occupied different, but overlapping volumes in the parameter space.

In addition to these early studies related to SST, different kinds of ML method have been used to derive other remote sensing products; a scalable end-to-end gradient-boosting tree (XGBoost; [35]) approach has been used to process non-linear satellite product estimations such as Chlorophyll-a [36,37], insolation at the sea surface [38], and urban heat storage [39]. The Support Vector Machine (SVM) and Artificial Neural Network (ANN) approaches were used in atmospheric correction for satellite ocean color sensors [36,40], water quality retrieval [41], and oceanic particulate organic carbon concentrations [42]. Overall, these preliminary studies demonstrate the potential of using ML to produce accurate geophysical variables and provide new insight into the errors of satellite-derived fields in different measurement conditions.

Here, our goal is to assess the ability of four ML approaches to improve on the currently used NLSST algorithms for the derivation of MODIS  $SST_{skin}$ .

## 2. Data

This study involves the joint analysis of variables derived from the measurements of satellite sensors, in situ instruments, and reanalysis data to generate a training dataset for ML development. Table 1 lists the relevant variables and data sources for this study.

**Table 1.** Relevant variables and data sources.

| Variable                                                                                                              | Satellite or Reanalysis Data                              | In Situ Source     |
|-----------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------|--------------------|
| $SST_{skin}$                                                                                                          | MODIS                                                     | M-AERI             |
| IR brightness temperatures of 11 $\mu\text{m}$ and 12 $\mu\text{m}$ bands, solar zenith angle, satellite zenith angle | MODIS                                                     |                    |
| In situ SST                                                                                                           | ---                                                       | Buoys and drifters |
| Near surface air-temperature                                                                                          | MERRA-2                                                   | M-AERI; Ship       |
| Near-surface humidity                                                                                                 | MERRA-2                                                   | Ship               |
| Near-surface winds                                                                                                    | MERRA-2                                                   | Ship               |
| First guess SST                                                                                                       | OSTIA, Canadian Meteorological Center's reanalysis of SST |                    |
| Latitude, months                                                                                                      | ---                                                       | ---                |

### 2.1. Satellite Data

The  $SST_{skin}$  data are available from MODIS starting from 2000 [20]. The newest version of MODIS  $SST_{skin}$  retrieval (R2019) generated at NASA GSFC has some significant improvements, including applying the ADtrees cloud screening algorithm [43]; newly-derived high-latitude coefficients for areas north of 60°N [44]; and nighttime dust aerosol corrections [23]. Our research uses the Level 1B brightness temperatures of the infrared Channels 20 ( $\lambda = 3.75 \mu\text{m}$ ), 29 ( $\lambda = 8.55 \mu\text{m}$ ), 31 ( $\lambda = 11.03 \mu\text{m}$ ), and 32 ( $\lambda = 12.02 \mu\text{m}$ ). The satellite data can be downloaded from different sources, primarily the NASA PO.DAAC (Physical Oceanography Distributed Active Archive Center) at the JPL (Jet Propulsion Laboratory) and the Langley Atmospheric Science Data Center.

### 2.2. In Situ Data Measurements from Ships

This study used in situ and remotely sensed data from research ships and from the Royal Caribbean Group (RCG) cruise ships. All the ships were equipped with infrared radiometers to derive the  $SST_{skin}$ . Three ships of the RCG, Celebrity Equinox, Allure of the Seas, and Adventure of the Seas, have become a major source of measurements in the Caribbean area. Figure 1 (top) illustrates the positions of the RCG ships where the  $SST_{skin}$  measurements have been included in the MODIS MUDBs.

Self-calibrating radiometers on ships facilitate the more direct evaluation of the accuracy of satellite-derived  $SST_{skin}$ . A hyperspectral interferometric ship-board radiometer, the Marine-Atmospheric Emitted Radiance Interferometer (M-AERI), is a dependable and accurate seagoing Fourier-transform infrared spectroradiometer mounted on ships to derive the spectra originating from the marine atmosphere and sea surface to derive the  $SST_{skin}$  [45] and near-surface air temperature [46]. M-AERIs include two internal black body cavities with SI-traceable calibration to provide the real-time at-sea calibration of infrared spectra.

Another important factor in  $SST_{skin}$  retrieval is the air–sea temperature difference (air–sea  $\delta T$ ), which is not explicit in the NLSST algorithms, but which can introduce large errors in  $SST_{skin}$  retrieval, as shown by Luo and Minnett [47] for GOES ABI (Geostationary Operational Environmental Satellite Advanced Baseline Imager) and by Luo, et al. [48] for Sentinel-3 SLSTR (Sea and Land Surface Temperature Radiometer). Utilizing the measurements of the emission of CO<sub>2</sub> in the M-AERI spectra produces a highly accurate retrieval of the near-surface air temperature used in the determination of air–sea  $\delta T$ , which can be used in ML model analyses.

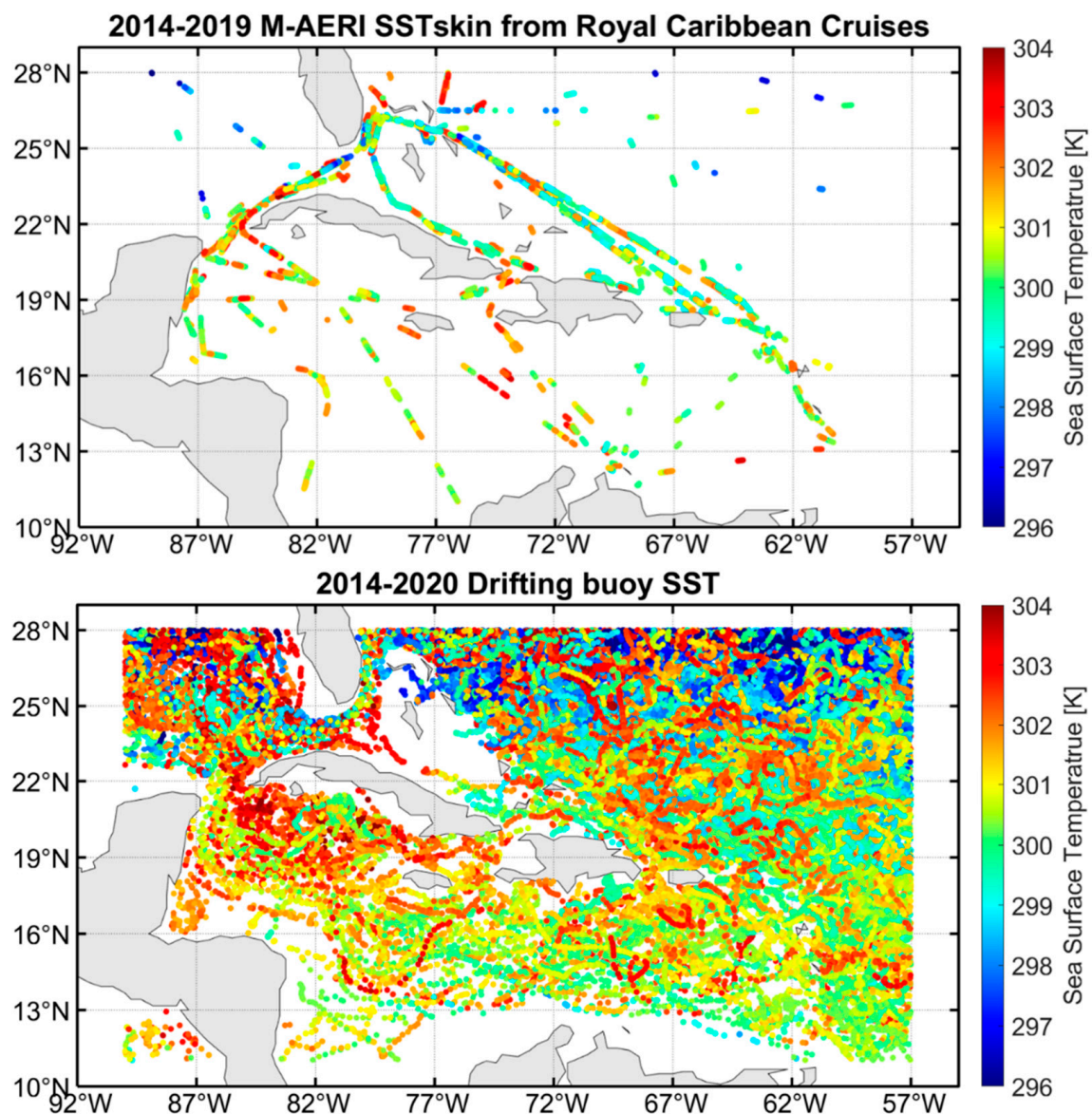


**Figure 1. (Top):** The routes of the RCG vessels equipped with M-AERIs providing the data for this investigation. The colors are the  $SST_{skin}$  derived from M-AERI measurements, as shown in the scale on the right in K. Note that the cruise ships repeat the same tracks multiple times, and so there are many more measurements than those that appear here. **(Bottom):** The drifting buoy-measured subsurface SSTs which have been matched to satellite  $SST_{skin}$  retrievals in the study region.

### 2.3. In Situ Data Measurements from Buoys

The National Oceanic and Atmospheric Administration (NOAA) took a significant step in the validation process of satellite-derived  $SST_{skin}$  products through the development of the in situ SST Quality Monitor (iQuam), which provides quality-assured data from various sources, including drifters, moored buoys, and marine vessels [49,50]. The drifters in the iQuam have a surface float and a subsurface drogue. At about 20 cm depth, the surface floats are equipped with thermometers [51,52], but it is worth mentioning that the exact thermometer depth can be influenced by surface wave conditions with potential occurrences of the float being momentarily fully immersed. The data are transmitted to land via satellite communication in NRT. The iQuam database is significant in our study because the distribution of drifters is extremely widespread, as shown in Figure 1 (bottom), for multiple years, thereby enhancing data analyses.

## 2.4. Reanalysis Fields

This study used the atmospheric state vectors from the NASA MERRA-2 (Modern-Era Retrospective Analysis for Research and Applications, Version 2) database [53]; these reanalyzed data guarantee internal consistency and present an array of geolocated and derived geophysical factors, such as wind, atmospheric temperature, and humidity recorded at 72 pressure levels (accessed on 21 June 2021). The role of the MERRA-2 repository is to furnish a detailed depiction of the atmospheric conditions at the time when both the in situ and satellite data were recorded. MERRA-2 has accurate SST values, with average differences of less than 0.1 K [54]. This, in turn, assists in the precise simulation of satellite radiometer measurements and offers inputs to the ML models.

## 3. Methods

### 3.1. Overview

Four ML methods were adopted initially to improve the atmospheric correction algorithms for MODIS  $SST_{skin}$  retrievals: eXtreme Gradient Boosting (XGBoost), Support Vector Regression (SVR), the Artificial Neural Network (ANN), and Random Forest (RF). Figure 2 shows the overall flow diagram of this study. Introductions of the four ML models are summarized here:

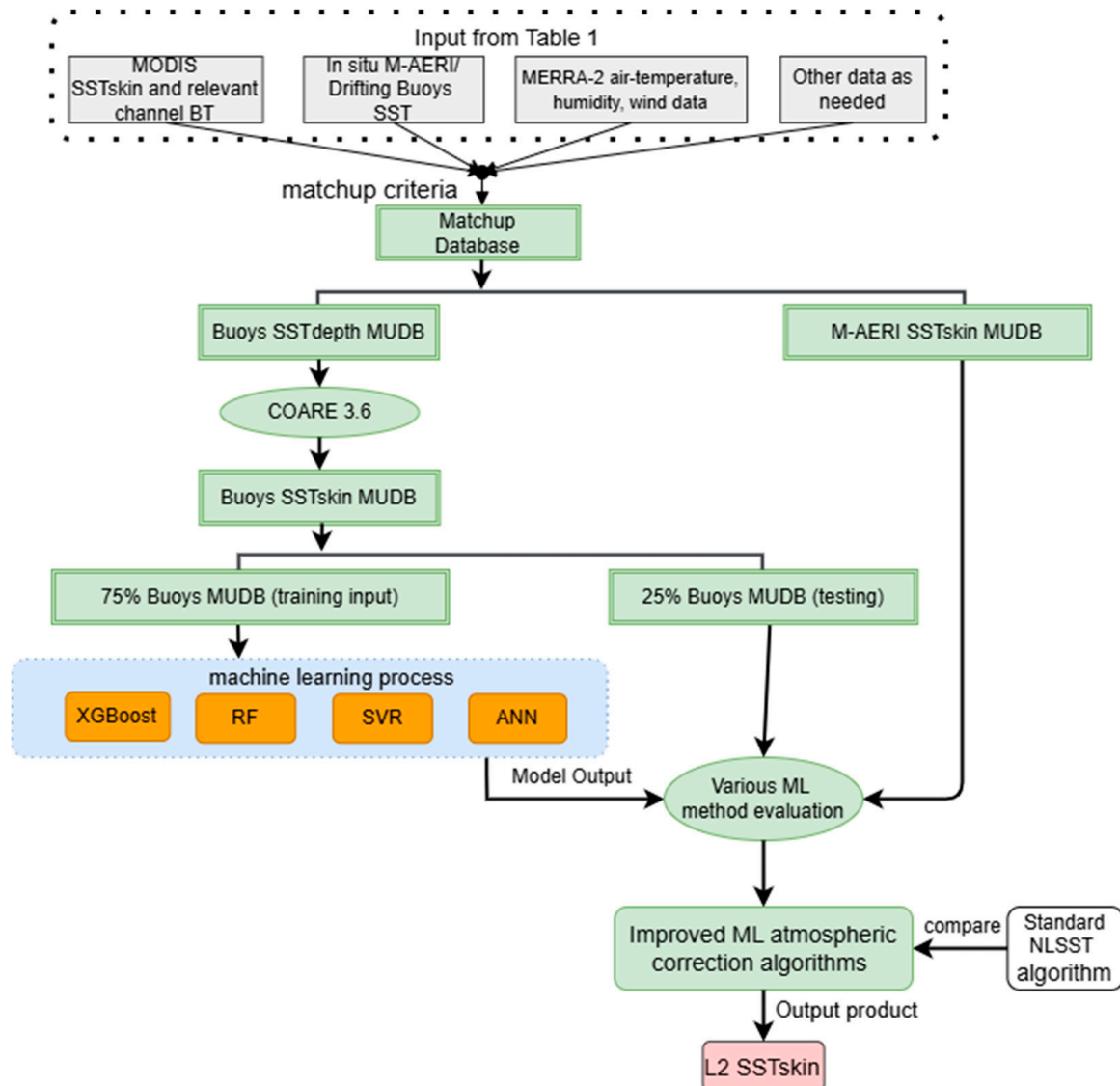


**Figure 2.** The overall framework of this study.

XGBoost stands as a contemporary variant of the gradient-boosting decision trees proposed by Chen and Guestrin [35]. XGBoost applies the entire training dataset with many regression trees rather than resampling partial samples to construct a strong predictor. The workflow of XGBoost commences with an equal weight allocation to training samples during inaugural iteration to formulate the initial tree. As the process progresses, these weights undergo adjustment, finely tuning them in accordance with the performance demonstrated by alignment with the training dataset. Subsequently, each tree assimilates a designated weight, influenced by observed fitting errors. To deduce the ultimate class allocated to an observation, the collective outputs of all trees are synthesized, with individual tree outputs being proportionally scaled by their respective weights. This methodology leverages gradient optimization to fine-tune cost functions through the least squares technique, thereby minimizing variance and precluding the possibility of overfitting.

RF constructs a forest of standard recursive partitioning trees and optimizes binary splits based on atmospheric and environmental variables by minimizing the mean squared error in the target variable at each split, thereby facilitating efficient data partitioning. Not only does this approach ensure higher predictive accuracy, as introduced by Breiman [55], but it also offers robustness against potential data fluctuations, a trait highlighted in the studies by Roy and Larocque [56]. The cumulative impact of this ensemble technique significantly mitigates the errors likely from single tree prediction, reducing variance, while maintaining a small bias, thereby promising not just an improved accuracy, but also a robust defense against overfitting issues in the data retrieval processes. Thus, the RF approach heralds a potential revolution in the fields of meteorological and marine science research, fostering enhanced accuracy and reliability in MODIS  $SST_{skin}$  retrieval accuracy assessment [5], Aerosol Optical Depth (AOD) retrieval [57], land cover [58], etc.

The ANN was devised as a network of interconnected artificial neurons assembled in a layered configuration [59]. Neurons in the input layer represent the various input variables that describe atmospheric conditions, radiative transfer properties, and other relevant parameters. For  $SST_{skin}$  retrieval, these neurons include the parameters listed in Table 1. At its core, an ANN encompasses a minimum of three tiers, the input layer, an intermediary or hidden layer, and the output layer, each being a nexus of intricately interconnected neurons. This multi-layered structure facilitates complex computational operations, enabling sophisticated analyses and predictions. Gross, et al. [60] used the ANN method to retrieve chlorophyll pigments from SeaWiFS (Sea-viewing Wide Field-of-view Sensor) ocean color measurements; they showed the advantages of the ANN in performing the bio-optical inversion, non-linear complexity, and noise filtering compared to those of the classical polynomial inverse methods.

SVR functions as a supervised learning algorithm grounded in kernel-based principles, which are used to transform input data into a higher-dimensional space to handle the non-linear relationships and complexities for  $SST_{skin}$  retrieval. Initially, the training dataset undergoes a transformation, projected into a higher-dimensional space via a kernel function. The optimization process then focuses on identifying the ideal hyperplane that aligns well with the training dataset, as described by Drucker, et al. [61]. Mountrakis, et al. [62] discussed the applications of SVR in remote sensing, showing it can provide a non-linear fitting ability between input variables and the target variable. Su, et al. [63] studied Subsurface Temperature Anomalies (STAs) in the Indian Ocean, utilizing SVR to analyze a compilation of satellite-derived data, including SST, sea surface elevation, and salinity. This analysis underscored the proficiency of SVR in delineating deeper oceanic thermal configurations and enhancing the precision of STA estimation. Furthermore, SVR has exhibited a remarkable aptitude in data categorization and regression analysis, coupled with an adeptness in pattern recognition, and thus its main contribution here is to identify the regions where atmospheric anomalies introduce large inaccuracies in  $SST_{skin}$  retrieval, and consequently require a different set of algorithms.

### 3.2. Match-Up Process

A comprehensive MUDB has been developed to facilitate the comparison between the MODIS  $SST_{skin}$  fields and the iQuam in situ measurements and the M-AERI data. The term ‘match-up’ in this context refers to a data vector comprising both in situ and satellite-derived variables, including attributes such as brightness temperatures from various MODIS infrared bands, captured as a  $5 \times 5$  pixel array centered on each match-up location. Moreover, it incorporates other supplementary data, including preliminary SST estimates, in situ SST, meteorological variables, latitude and longitude, satellite zenith angle, and time stamps. Each MUDB record comprises 145 variables.

These match-ups are also synchronized between the satellite and in situ data within a 30 min window and within a geographical radius of 10 km [20,64]. In this study, we utilized data records extracted from the SST MUDB for the MODIS onboard NASA’s Aqua satellite. We conducted a rigorous filtration process for MODIS Aqua match-up, selectively incorporating the MODIS data that met quality levels of 0, 1, or 2. Quality level 0 data are of the best quality, being confidently cloud-free with a satellite zenith angle of  $<55^\circ$ ; quality level 1 data are also confidently cloud-free, but have satellite zenith angles  $>55^\circ$ . Quality level 3 data are also likely to be good, but with a risk of some degradation; they were included in this study to explore the ability of the ML algorithms to deal with less-than-perfect data. Removing the data from this study with quality level 3 prevented potential inaccuracies arising from significant cloud interference or other underlying factors that could compromise analyses. Despite the broad geographical scope encompassed by these match-ups, our study predominantly focused on the Caribbean area, a decision driven by the abundance of available M-AERI measurements in that region (Figure 1).

### 3.3. Machine Learning Model Setup

In this research, the configuration and validation of the model were conducted using the Scikit-learn library (v0.24) in Python (v3.9). We used the grid search methodology facilitating the comprehensive exploration of potential parameter values for a chosen estimator. This process, fundamental to the identification of optimal parameters, operates on the principles of a cross-validation system, meticulously examining every possible combination of parameters within this framework. Our strategy used the k-fold method, a robust approach that segments the entire sample pool into k equally sized subsets, commonly referred to as ‘folds’. This procedure fosters a learning environment where the predictive function is cultivated utilizing data from  $k - 1$  folds, reserving the remaining fold exclusively for testing purposes. We used  $k = 4$  to balance computational efficiency and analytical accuracy.

Data collected between 2014 and 2020 within the region from  $11^\circ\text{N}$  to  $28^\circ\text{N}$  latitude and  $57^\circ\text{W}$  to  $90^\circ\text{W}$  longitude were selected, covering the Caribbean area. Using iQuam as the in situ data source, a total of 123,612 samples were available after filtering. Of these, 75% were used as the training set, and the remaining 25% (30,903 samples) were allocated to the testing set.

To assess the accuracy of each ML model, several parameters were calculated, including the mean differences between the ML-predicted SST and the in situ measured SST, median, standard deviation (STD), robust standard deviation (RSD), and runtime to validate the model’s performance. STD serves as an indicator of the model’s statistical dispersion, reflecting the deviation between the predicted and actual values. RSD is less sensitive to outliers. Smaller STD and RSD values signify a smaller deviation, indicating the higher capability of the model. The runtime parameter was analyzed to determine the ML models’ computational costs.

Aiming to enhance the atmospheric correction algorithms for MODIS  $SST_{skin}$  retrievals using ML, the partition of training and test datasets aids in constructing robust ML models trained with a substantial number of samples to recognize complex patterns and correlations.

#### 4. Results

It is widely acknowledged that the  $SST_{skin}$  is generally cooler than the water beneath the thermal skin layer, a phenomenon resulting from upward heat flux from the ocean to the atmosphere caused by a combination of factors, including net longwave radiation and sensible and latent heat fluxes at the air–sea interface. The characterization of the upper-ocean vertical temperature structure has been outlined by the Science Team of the Group for High-Resolution Sea Surface Temperature (GHRST) using schematic profiles [4].

To facilitate the more accurate representation of the  $SST_{skin}$ , it becomes necessary to adapt buoy measurements, which are typically obtained approximately 0.2 m beneath the surface [51,52], to align with the  $SST_{skin}$ . This represents the temperature of the thermally conductive skin layer, typically ranging between 10  $\mu\text{m}$  and 100  $\mu\text{m}$  in thickness, and which is approximated by the measurements of infrared radiometers. The previous studies have addressed this discrepancy by applying a fixed adjustment of  $-0.17\text{ K}$  to buoy SST measurements to approximate the  $SST_{skin}$  [5,65,66], representing the global mean skin–subsurface temperature difference. However, such static corrections can introduce systematic biases, particularly when training ML models, as they fail to account for the dynamic variability in cool skin and diurnal heating effects due to changes in the environmental conditions, such as wind speed, solar radiation, and surface fluxes. Accurately modeling the cool skin and warm layer (diurnal heating) effects presents a significant challenge, prompting numerous refinements to the existing parameterizations and models [25,29,67–69]. In this study, we use the Coupled Ocean Atmosphere Response Experiment (COARE; Fairall, et al. [70]) model to more accurately account for both the cool skin and diurnal warming effects in buoy SST measurement. The COARE model dynamically corrects these processes by incorporating meteorological and oceanographic variables, such as air–sea fluxes, solar radiation, and wind speed, allowing for the more accurate estimation of the  $SST_{skin}$ . By applying these corrections, we generate a more accurate in situ  $SST_{skin}$  dataset, which serves as a reliable basis for training and validating ML models.

We compared the ML models' performance against that of the currently implemented NLSST atmospheric correction algorithm to establish any improvements.

##### 4.1. Comparison with iQuam

In Figure 3, the scatter plots illustrate the correlation between the NLSST-retrieved  $SST_{skin}$  and the ML predictions and the in situ measured SST from iQuam, converted to  $SST_{skin}$  using the COARE model, in which the dashed line represents one-to-one agreement, indicating a perfect match between the predictions and the observations. The outputs from RF show the best correspondence with the in situ SSTs, having a linear regression equation of  $y = 1.00x + 0.03$ . In comparison, the slopes for XGBoost and ANN are approximately equal to 0.99, whereas it is 0.95 for the SVR method. The central panels of Figure 3 show histograms of the ML-derived  $SST_{skin}$  and the iQuam SST data, providing a visualization of the frequency of occurrence of different temperatures. The ML models were found to surpass the conventional NLSST algorithm in multiple metrics. Specifically, NLSST presented a mean bias of  $-0.319\text{ K}$  and an STD of  $0.547\text{ K}$ . When focusing on mean bias as a performance indicator, the XGBoost model demonstrated superior accuracy, recording a negligible mean bias of  $0.0012\text{ K}$ . This was followed by RF ( $-0.0103\text{ K}$ ), SVR ( $0.0133\text{ K}$ ), and the ANN ( $-0.0762\text{ K}$ ) in this respective order. In relation to STD and RSD, a consistent performance was shown among XGBoost, RF, and the ANN. The ANN displayed the lowest STD of  $0.243\text{ K}$ , with those of RF and XGBoost at  $0.247\text{ K}$  and  $0.252\text{ K}$ , respectively. However, SVR was slightly inferior, with the highest ML STD of  $0.341\text{ K}$ . The distribution of SST predicted by the ANN best fits that of iQuam SST.

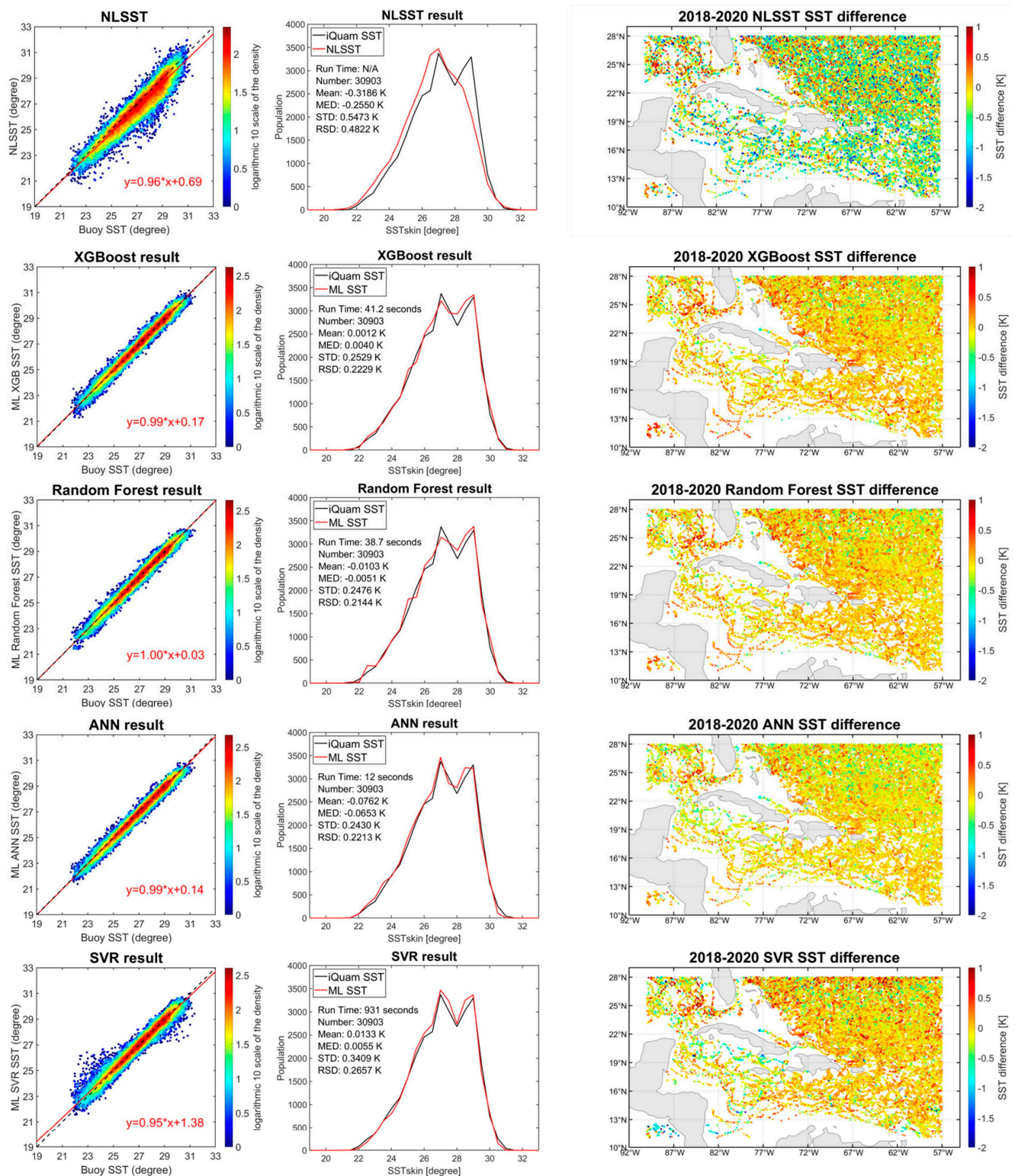


**Figure 3.** Diagnostic plots illustrating the performance of the standard NLSST atmospheric correction in the study area with the  $SST_{skin}$  derived from the ML approaches. The buoy SSTs have been adjusted to the  $SST_{skin}$  using the COARE model. **Left** column: scatter plots of the predicted and buoy  $SST_{skin}$ ; the dashed line is a one-to-one correspondence, while the red line represents the linear least-squares fit. **Center** column: histograms of the predicted  $SST_{skin}$  and those from iQuam. **Right** column: maps of the disparities between the predicted  $SST_{skin}$  and those from iQuam using a color-coded scheme to show the magnitudes in degrees, given on the right.

An additional aspect of the evaluation was the computational efficiency of these ML models. In the dataset comprising 30,903 match-ups, the ANN delivered results in only 12 s. XGBoost and RF demonstrated comparable computational efficiency, taking around 40 s to process the same dataset. SVR fell behind significantly, taking 931 s due to its high computational complexity when dealing with large datasets. XGBoost, RF, and the ANN can handle high-dimensional feature spaces efficiently through their network topology; geospatial variables, such as longitude, latitude, and various atmospheric parameters, can be easily accommodated. The traditional non-linear relationships between these factors are optimized by using XGBoost's and RF's decision trees and the ANN's activation functions and multiple layers, while SVR requires calculating the distances in this feature space and uses different kernel functions, which can be computationally intensive. Furthermore, XGBoost, RF, and the ANN are parallelized across multiple CPU cores, making them highly efficient for analyzing big datasets. SVR has a computational complexity ranging from  $O(N^2)$  to  $O(N^3)$ , depending on the choice of kernel and other settings, and this complexity makes SVR less efficient for large-scale problems. To sum up, among the ML algorithms, XGBoost and RF appear to offer the most reliable and efficient approaches for improving the accuracy of MODIS  $SST_{skin}$  retrieval, outperforming both the ANN and SVR.

The right column of Figure 3 shows maps of the discrepancies between NLSST retrieval and the ML predictions and the in situ SST measurements after correction for the warm layer and cools skin effects; the color bars illustrate the temperature differences in Kelvin. The ML models yielded more-accurate spatial distribution patterns with respect to iQuam SST than those from the NLSST. However, notable discrepancies were observed in the SVR model's predictions. Specifically, SVR tended to underestimate the SST in the southwestern regions, while overestimating in the northern parts of the study area. One of the intricacies of using SVR is its reliance on kernel functions to model the non-linear relationships in data. Selecting and fine-tuning the appropriate kernel for SVR is challenging, especially when dealing with high-dimensional geospatial datasets.

Figure 4 shows the discrepancies between NLSST retrievals and the ML predictions and the buoy-derived  $SST_{skin}$  values varying with various environmental factors, including wind speed, 2 m air temperature, geographic latitude, in situ  $SST_{skin}$  values, the month, and specific humidity. Each subplot includes error bars to highlight the variability in temperature differences, while the dots signify the mean discrepancy associated with each parameter. Grey histograms depict the data distributions in the parameters.

The vertical gradients of the SST in the near-surface ocean layer are controlled by multiple factors, including solar radiation absorption, the vertical diffusion of heat, and mixing due to wind turbulence [29,67,71]. We used the OSTIA surface temperature,  $T_{sfc}$ , as the initial guess of the SST. This was then used as the input for the ML models and in the NLSST algorithm. As shown in Figure 4A, the observational SST data and the ML model-predicted SST showed a good agreement with 10 m wind speeds (U10) ranging from 3 m/s to 8 m/s, where the U10 values were concentrated, having a minimal bias below 0.1 K. At very low wind speeds, both the SVR and NLSST exhibited pronounced inaccuracies. For  $U10 > 10$  m/s, there is a larger bias in the predicted  $SST_{skin}$ , especially for the SVR method. Ideally, all ML algorithms should not exhibit a large bias at high wind speeds because the  $SST_{skin}$  relationship with subsurface temperature shows very little variation due to wind-driven turbulence mixing. In high-dimensional spaces, especially when the sample size is small, the risk of overfitting is high. Therefore, SVR's performance might be affected more in such conditions without proper regularization.

The effect of surface air temperature on these ML schemes is shown in Figure 4B. The temperature difference between the  $SST_{skin}$  and the overlying air influences the effect of the atmosphere on the propagation of the sea surface emission to satellite height [72–74]. Within the air temperature range from 24 to 29 °C, the  $SST_{skin}$  simulated by the ML models is close to the observed values. However, the deviations for SVR become distinct at air temperatures below 22 °C or above 30 °C, with an average bias up to 2 K.

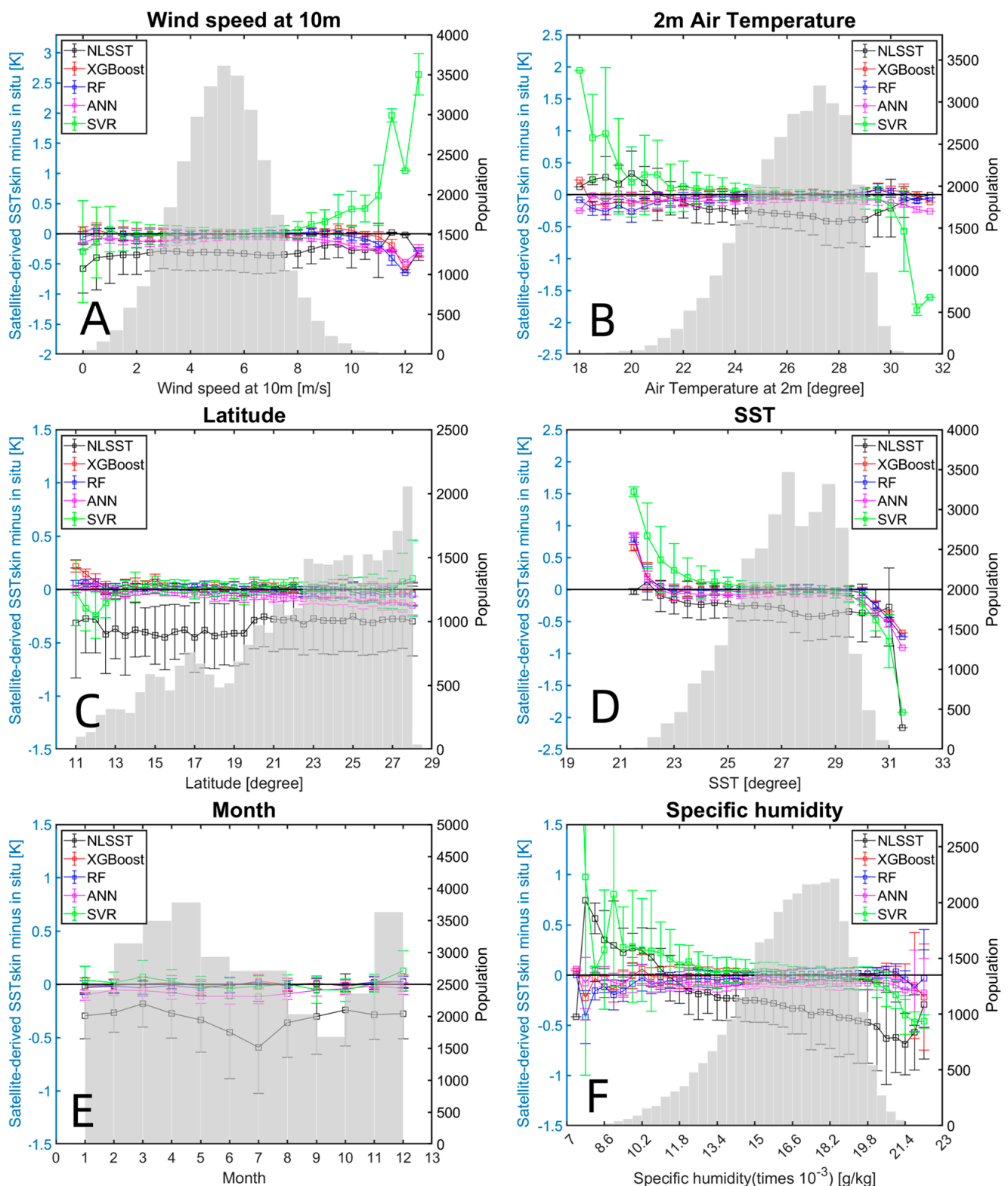


**Figure 4.** The discrepancies between the ML and NLSST outputs and the buoy-determined  $SST_{skin}$  influenced by various environmental parameters: wind speed (A), air temperature at 2 m above sea level (B), geographic latitude (C),  $SST_{skin}$  (D), the month (E), and specific humidity at 2 m (F). Each subplot includes error bars, denoting the STD in the temperature differences, with a dot representing the mean discrepancy. The grey histograms illustrate the data distribution of parameters on the x-axis.

The coefficients used in the NLSST algorithm are dependent upon both the latitude and the month [21]. The latitude- and month-based variations in the NLSST-derived  $SST_{skin}$  discrepancies are apparent in Figure 4C,E. The SVR ML model displays a negative bias reaching up to 0.25 K, while the other ML models exhibit a positive bias for latitudes below 13°N. The scarcity of buoy measurements south of 13°N, as depicted in Figure 1 (bottom), results in inadequate training data for the ML algorithms, contributing to such large biases. No significant seasonal impact was found on the different ML models, but the NLSST shows a pronounced bias during summer. Furthermore, between 11°N and 20°N, the NLSST reveals a significant bias of −0.5 K, which indicates that the coefficients or the formulation of the NLSST algorithm derived at this latitude range for the entire range of longitudes require further refinement and optimization for this region, particularly in summer.

Figure 4D illustrates the biases across different SST values. All the ML models exhibit pronounced positive biases for colder SSTs and negative biases under warmer SSTs, with a paucity of input training the data for these conditions. It is essential to understand that an abundant dataset is important for ML models to reduce the risk of overfitting and to enable the successful identification and depiction of the underlying patterns and tendencies within the data. These, in turn, enhance the robustness of ML algorithms and the accuracy of the derived  $SST_{skin}$ .

Water vapor has a profound impact on the atmospheric absorption and emission of infrared radiation. Consequently, fluctuations in specific humidity directly alter the atmospheric transmittance of radiation originating from the sea surface [75], leading to potential inaccuracies in the satellite-derived  $SST_{skin}$  [27,28,76,77]. As depicted in Figure 4F, a distinct trend of SST biases relative to specific humidity emerges for the NLSST; as specific humidity increases, the bias becomes increasingly negative. Regarding the ML models, all exhibit negative biases when the specific humidity exceeds 20 g/kg, but this is found in a small proportion of the conditions represented in the MUDBs. To address this issue, a more-extensive atmospheric dataset to capture a wider range of environmental conditions is needed.

The patterns of the  $SST_{skin}$  biases presented in Figure 3 (right) do not reveal temporal changes. Figure 5 presents Hovmöller diagrams that outline both the temporal and spatial evolution of  $SST_{skin}$  biases using the NLSST and the four ML algorithms. Such visualization aids in understanding spatio-temporal variations and identifying patterns. There is a significant data gap between July 2019 and January 2020 resulting from a lack of available in situ SST measurements from iQuam. Prominent negative biases in the NLSST retrievals in the study area from July to October are apparent.

From the Hovmöller diagrams, substantial seasonal fluctuations, especially in July each year, and notable latitudinal variations are found in the  $SST_{skin}$  biases for all the ML models used. Despite the presence of large and negative biases at the lower latitudes, the ML models demonstrated a superior performance compared to that of the  $SST_{skin}$  derived from the standard NLSST algorithm. Specifically, the XGBoost and RF models exhibited enhanced robustness to noise, a characteristic of their ensemble nature, which aggregates predictions from multiple trees, thereby reducing the risk of overfitting and noise sensitivity.

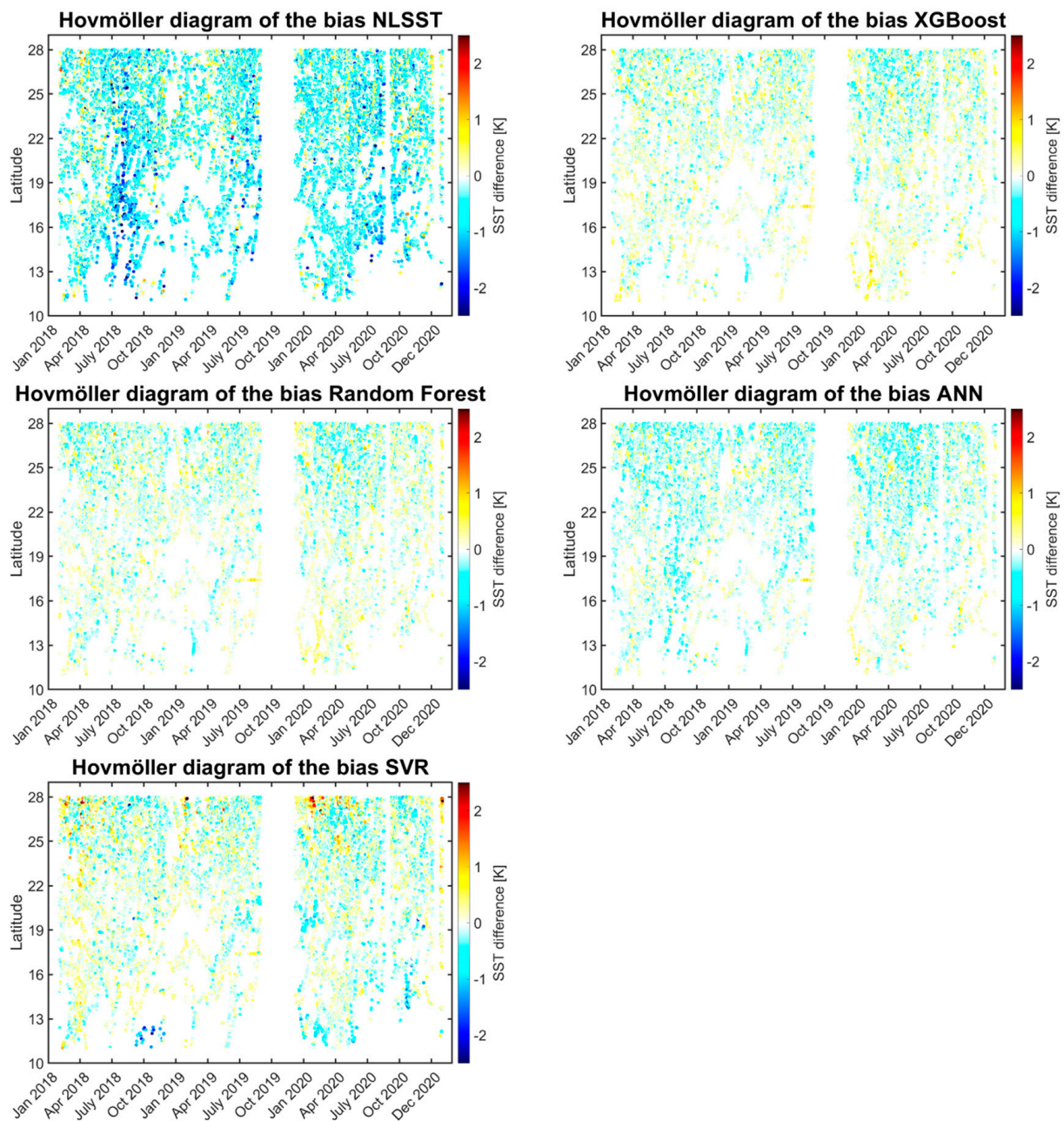


**Figure 5.** Hovmöller diagrams show the time and latitude evolutions of the biases from NLSST retrievals and four ML predictions compared with iQuam SSTs for 2018 to 2020. Since the in-situ data from July 2019 to Jan 2020 were not available, a gap exists between them. The color indicates SST difference in K, according to the scale on the right.

#### 4.2. Comparisons with M-AERI $SST_{skin}$

To further assess each ML method's ability to predict accurate  $SST_{skin}$ , the  $SST_{skin}$  data derived from the M-AERIs mounted on ships were utilized as the reference. This approach is well established, with several published studies using the M-AERI  $SST_{skin}$  to assess the accuracy of retrievals from MODIS [20], GOES-ABI [47], and Sentinel-3 SLSTR [48], and also from the MERRA-2 and ERA-5 fields [54,78]. The ML-derived  $SST_{skin}$  was also compared with the current NLSST retrieved  $SST_{skin}$  [79] using the MUDBs to quantify accuracy improvements and to understand under which conditions improvements are minimal or absent, and thus direct further algorithm development.

Figure 6 includes scatter plots, histograms, and maps of differences of the NLSST retrievals and the four ML predictions against M-AERI  $SST_{skin}$  in the Caribbean region. Figure 6 has the same structure as Figure 3, but using  $SST_{skin}$  derived from M-AERIs mounted on ships to assess the performance of the NLSST  $SST_{skin}$  and ML algorithms. Such ship-based, self-calibrating radiometers provide data for a like-with-like  $SST_{skin}$  comparison, thereby avoiding the need for corrections of the diurnal heating and thermal skin layer effects.

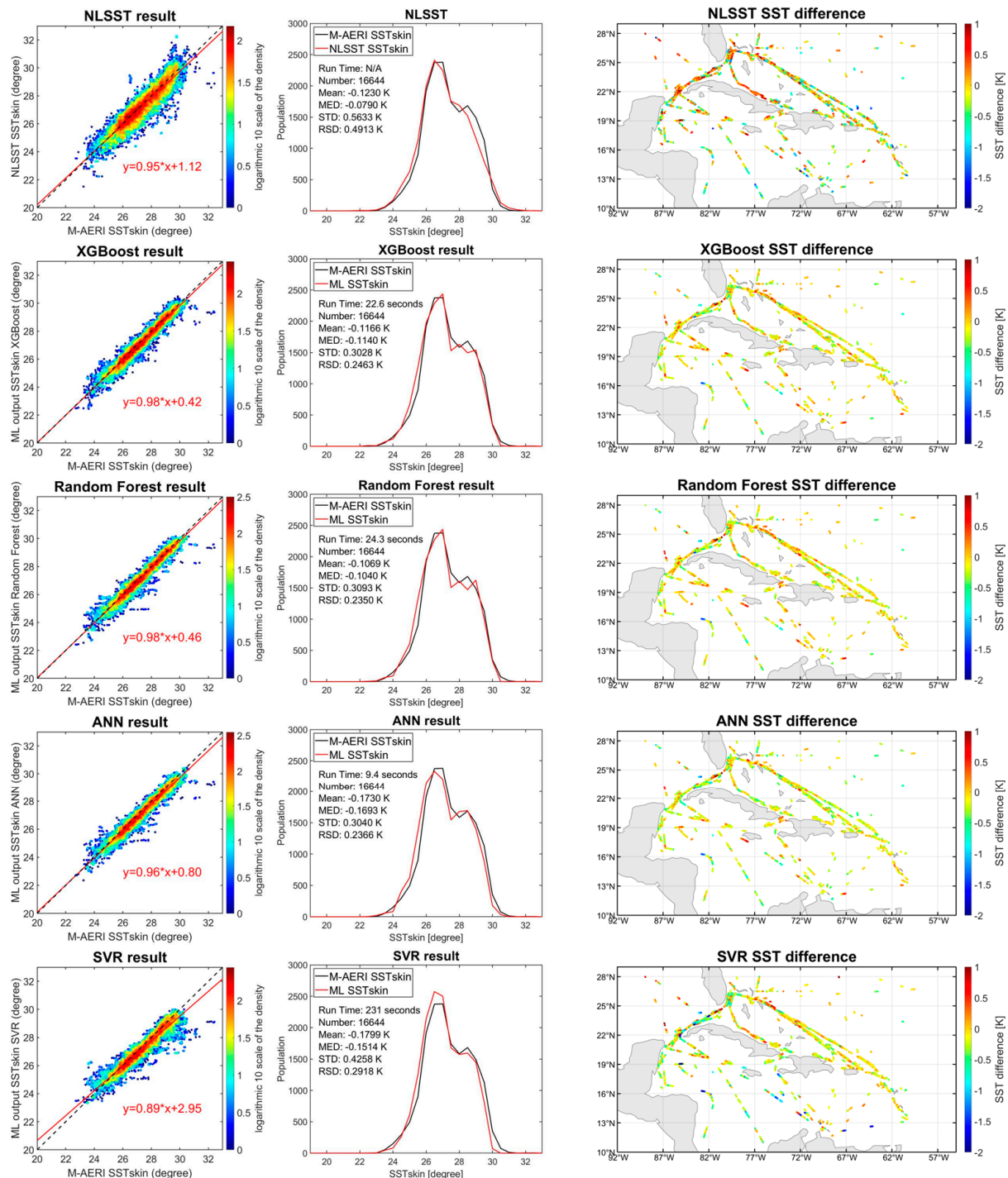


Figure 6. Like Figure 3, but utilizes the  $SST_{skin}$  values derived from the M-AERIs mounted on ships as comparisons for the assessment of the NLSST retrievals and ML prediction errors.

The left panel of Figure 6 presents scatter plots showing the correlation between NLSST retrieval and the ML predictions and the  $SST_{skin}$  derived by using the ship-mounted M-AERIs. The dashed line indicates an ideal one-to-one correspondence, the central panel histograms show the distribution of both the satellite- and M-AERI-derived  $SST_{skin}$  data. The NLSST algorithm exhibits an average discrepancy of  $-0.123$  K, with an STD of  $0.563$  K. The ML models present varying performance metrics. Specifically, the XGBoost and RF models produce mean biases of  $-0.117$  K and  $-0.107$  K, with STDs of  $0.303$  K and  $0.309$  K, respectively. However, larger mean discrepancies of  $-0.173$  K and  $-0.180$  K are found in the ANN and SVR results. Notably, the SVR model demonstrates the highest STD of the ML results at  $0.426$  K. The right panel provides a visualization of the spatial distribution of temperature differences between the satellite-derived  $SST_{skin}$  and the M-AERI data; the NLSST and SVR models  $SST_{skin}$  values show pronounced discrepancies from the M-AERI data in specific regions. Such significant biases contribute to larger STDs, emphasizing the need for the refinement in those methods. Overall, validation with the M-AERI data demonstrates the potential of using ML approaches to produce accurate atmospheric corrections for  $SST_{skin}$  retrieval and gain new insight into the source of inaccuracies in the MODIS-derived  $SST_{skin}$  fields under different conditions.

Figure 7 displays the discrepancies between NLSST retrievals and the ML predictions and the M-AERI-determined  $SST_{skin}$  under various environmental factors, similar to Figure 4. The satellite-derived  $SST_{skin}$  data align favorably at U10 spanning from  $3$  to  $8$  m/s or at surface air temperature between  $24$  and  $29$  °C, maintaining a small bias below  $0.2$  K. In extreme conditions, such as strong wind speeds and high air temperatures, there are pronounced inaccuracies in both the SVR and NLSST outputs. Ideally, all the  $SST_{skin}$  values should exhibit negligible wind speed and air temperature dependences; however, the performance of SVR is highly impacted at air temperatures poorly represented in the data. As shown in Figure 7C, the influence of latitude on the NLSST algorithm and the ML models is evident; the SVR and the NLSST display a discernible negative bias of up to  $-0.75$  K south of  $15^{\circ}$ N, likely due to the sparsity of M-AERI data, as illustrated in Figure 1. The lack of comprehensive data lowers the ML models' training efficacy. Note that the behavior at latitudes south of  $15^{\circ}$ N is more extreme than when validating that of the NLSST and ML outputs with the iQuam in situ SST. The deviations in all the ML models increasing with the rise in  $SST_{skin}$ , as shown in Figure 7D, is primarily attributed to the lack of sufficient training data at a warmer  $SST_{skin}$ . As the ML models heavily rely on the patterns present in the training data, the dataset we used for model training has more  $SST_{skin}$  values in the range of  $24$  °C to  $30$  °C compared to those at a warmer  $SST_{skin}$ , which limits the ability of the ML models to accurately learn and predict patterns when  $SST_{skin} > 31$  °C. The monthly variations shown in Figure 7E indicate a larger training dataset is needed, especially for the SVR algorithm for summertime conditions. The ML models display significant variance at low humidity and high temperatures, underscoring potential data inadequacies for those specific conditions.

Considering that the M-AERIs provide  $SST_{skin}$  data, there is a need to improve the subsurface-temperature-to- $SST_{skin}$  conversion when using the iQuam SST from drifting buoy measurements taken at depth to derive the coefficients for the NLSST algorithm. There is also a need for better optimization for regional applications.

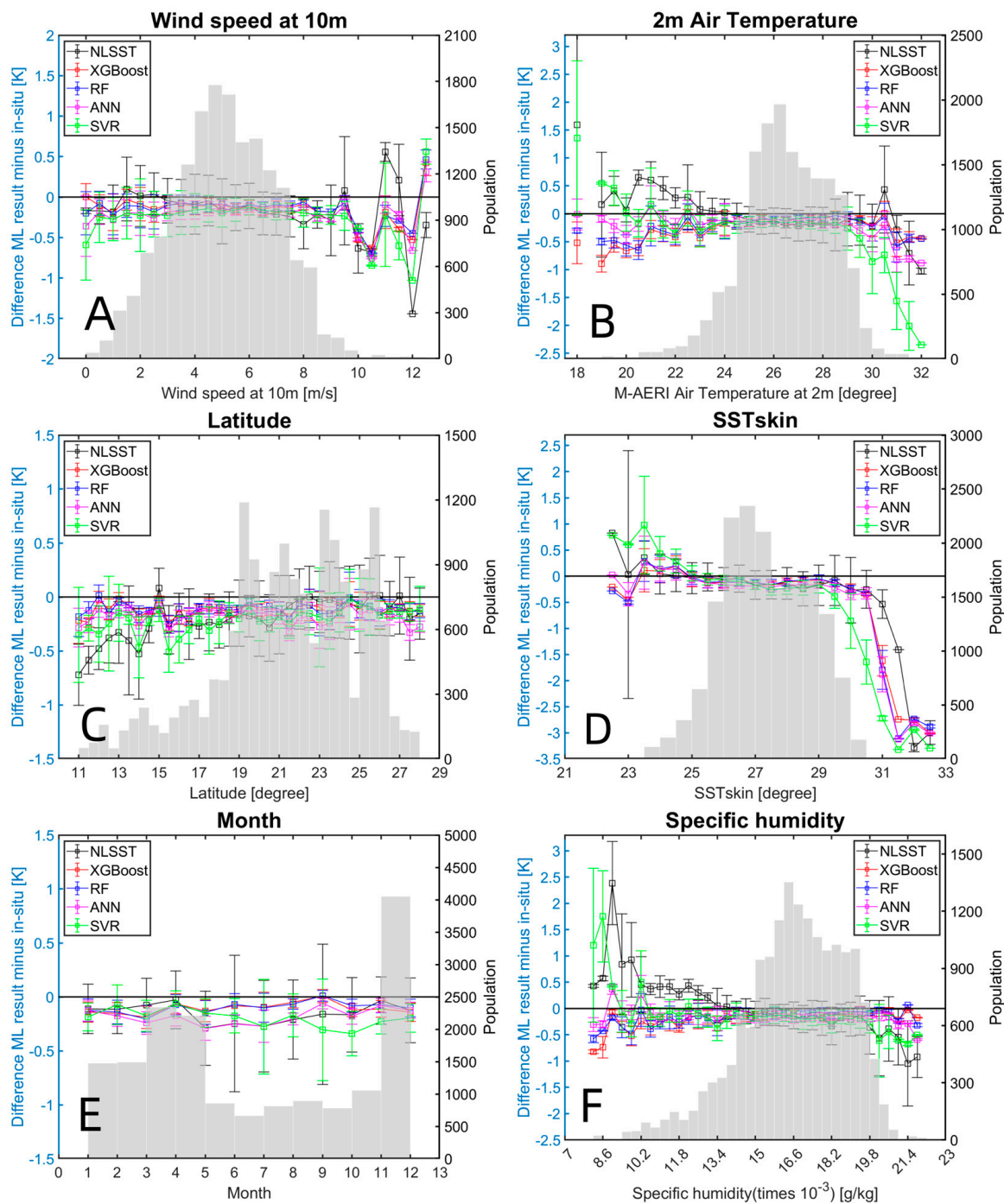


**Figure 7.** As Figure 4, but for NLSST and ML  $SST_{skin}$  values compared with M-AERI  $SST_{skin}$  data.

## 5. Summary

This paper reports the application of four ML models, XGBoost, RF, the ANN, and SVR, in enhancing the accuracy of  $SST_{skin}$  retrieval from the MODIS onboard NASA Aqua satellite. Research demonstrates the ML methods compared well with the conventional NLSST algorithm in retrieving  $SST_{skin}$  in the Caribbean region. The ML models were trained using an extensive MUDb containing both satellite and in situ measurements and related meteorological variables. The NLSST algorithm coefficients were derived from very large datasets in latitude bands that span the entire range of longitudes. The NLSST  $SST_{skin}$  values were taken from NASA data servers. The primary sources of validation data for the NLSST- and ML-derived SSTs were iQuam and M-AERI datasets. When the outputs from

the various models were assessed against M-AERI  $SST_{skin}$ , XGBoost and RF demonstrated a superior performance, while SVR fell behind due to issues, including overfitting and higher computational requirements. Some factors, such as wind speed, surface air temperature, latitude, and specific humidity, were found to influence the accuracy of the ML models'  $SST_{skin}$  predictions. There were larger discrepancies in the ML models' retrievals under conditions, which were often associated with sparse training data.

The ML models, especially XGBoost, provides a promising avenue for improving the accuracy and robustness of  $SST_{skin}$  retrieval, with mean differences of  $-0.001$  K compared with iQuam SST and  $-0.117$  K compared with M-AERI  $SST_{skin}$ , suggesting potential benefits over the current NLSST algorithm. Overall, this research advocates for the further investigation of ML models to refine the atmospheric correction processes for  $SST_{skin}$ ; this research also emphasizes the need for more comprehensive datasets by sampling the global range of marine conditions and meticulous validation to ensure the optimal performance of the NLSST algorithm and ML models and the confident assessment of the accuracies of the derived  $SST_{skin}$  values on a global basis.

Future work should focus on reducing the discrepancies observed, particularly in regions or temperature ranges that challenge the current atmospheric correction algorithms, including high latitudes [76,77], equatorial and tropical conditions with a high water vapor content, aerosol-burdened atmospheres, and coastal regions influence by terrestrial atmospheres. The focus of the research reported here was primarily in the Caribbean region; this was a choice driven by the abundant in situ data available in this area. As we continue to gather more data for training and validating these algorithms, we plan to broaden the scope of our study to encompass larger geographical regions. Moreover, applying the ML techniques to data from newer satellite sensors, such as the VIIRS on the Suomi-NPP, and subsequent NOAA satellites [80], and the SLSTR onboard the Copernicus Sentinel-3 satellites [48], should be explored.

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**Data Availability Statement:** The MUDB databases used here are accessible through the SeaBASS validation system at the NASA Ocean Biology Distributed Active Archive Center (OB.DAAC). <https://seabass.gsfc.nasa.gov/archive/SSTVAL> (accessed on 21 June 2021).

**Conflicts of Interest:** The authors declare no conflicts of interest.

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