Estimation of all-sky 1km land surface temperature over the conterminous United States

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7 Abstract. Land surface temperature (LST) is a crucial parameter for hydrology, climate monitoring, and ecological and environmental research. LST products from thermal infrared (TIR) satellite data have been widely 8 used for that. However, TIR information cannot provide LST data under cloudy-sky conditions. All-sky LST can 9 be estimated from microwave measurements, but their coarse spatial resolution, narrow swaths, and short temporal 10 range make it impossible to generate a long-term, high-resolution, accurate global all-sky LST global. This study 11 12 proposes a methodology for generating the all-sky LST product by combining multiple data from Moderate 13 Resolution Imaging Spectroradiometer (MODIS), reanalysis, and ground in situ measurements using a random 14 forest. Field measurements from the AmeriFlux and Surface Radiation Budget (SURFRAD) networks were used for model training and validation. Cloudy-sky and clear-sky LST models were developed separately. To further 15 improve the accuracy of the cloudy-sky LST model, the conventional RF model was extended to incorporate 16 temporal information. The models were validated using in situ LST measurements from 2010, 2011, and 2017 17 18 that were not used for the model training. For the cloudy-sky and clear-sky models, root-mean-square-error (RMSE) = 2.767 and 2.756 K, $R^2 = 0.943$ and 0.963, and bias = -0.143 and -0.138 K, respectively. The same 19 validation samples were used to validate both the MODIS LST product under clear-sky conditions and all-sky 20 Global Land Data Assimilation System (GLDAS) LST product at 0.25° spatial resolution, with RMSE = 3.033 21

and 4.157 K, bias = -0.362 and -0.224 K, and R² = 0.904 and 0.955, respectively. Additionally, the 10-folds cross-validation results using all the training datasets further indicate the model stability. The models were applied to generate the all-sky LST product from 2000-2015 over the conterminous United States (CONUS). Our product shows similar spatial patterns to the MODIS and GLDAS LST products, but it is more accurate. Both validation and product comparisons demonstrated the robustness of our proposed models in generating the all-sky LST product.

28 K

Key words: Land surface temperature, all-sky, random forest, MODIS

29

30 **1 Introduction**

31 Land surface temperature (LST) is the skin temperature of the uppermost layer of the earth's surface. It is a 32 key parameter in land surface energy exchange and interactions between land and atmosphere. Therefore, it is a 33 crucial study factor in many scientific fields such as climate change, energy balance, hydrology, agriculture, and 34 ecology. Remote sensing data are used to obtain LST with high spatial and temporal resolution from regional to 35 global scale (Li et al. 2013; Liang 2005). In the past few decades, many LST products and algorithms based on 36 infrared satellite data have been developed, such as from the Moderate Resolution Imaging Spectroradiometer 37 (MODIS) (Ma et al. 2017; Wan and Dozier 1996) and Visible Infrared Imaging Radiometer (VIIRS) (Ma et al. 38 2018; Yu et al. 2005). However, due to the influence of clouds, LST values are valid only under clear-sky 39 conditions. Research has shown that the data loss caused by cloud contamination exceeds 50 %, and it is especially severe during the daytime (Crosson et al. 2012; Duan et al. 2017). Therefore, an appropriate method 40 41 for LST estimation under all-sky conditions should be developed.

42 Several approaches have been proposed to address the missing values in LST products resulting from cloud 43 contamination (Liang and Wang 2019; Shen et al. 2015; Zhan et al. 2013). The algorithms used for this purpose 44 can be divided into four classes: 1) temporal and spatial, 2) physically based, 3) passive microwave-data based, 45 and 4) machine learning. Among them, temporal and spatial methods use spatiotemporal information of LST, considering its temporal variation law and spatial distribution characteristics. Spatial information-based methods 46 47 establish the relationship between cloudy pixels and the nearest clear sky pixels mainly through interpolation, 48 such as kriging, spline function and inverse distance weighting (Jackson et al. 2014; Neteler 2010; Urquhart et 49 al. 2013). However, the accuracy of these methods depends on the availability of nearby clear-sky pixels, which 50 are limited in large areas of cloudy sky pixels, leading to an unsatisfactory accuracy. Temporal information-based methods including interpolation or filtering, are to obtain the missing value from the time 51 series of clear-sky LST(Pede and Mountrakis 2018; Zeng et al. 2015). Moreover, MODIS LST has four 52 53 observations from Terra and Aqua satellites, which provides the possibility to fill a gap using other clear-sky observations (Coops et al. 2007; Li et al. 2018). Some researchers combine spatial and temporal methods to 54 55 gather more information for LST reconstruction (Metz et al. 2017; Zhang et al. 2018). Although the spatial and temporal methods use the variation of LST in time and space, they are based on clear sky pixels, which results in 56 a hypothetic clear-sky LST rather than the actual cloudy-sky LST (Zeng et al. 2018). 57

58 To estimate the real LST under cloudy-sky conditions, some methods combine physical processes data (Jin 59 and Dickinson 2000; Yu et al. 2014; Zeng et al. 2018; Zhang et al. 2015). A physical algorithm based on surface 60 energy balance (SEB) was proposed by Jin and Dickinson (2000). The proposed method considered that the LST 61 under cloudy sky was affected by changing the solar radiation and downward longwave radiation. Thus, LST for 62 a cloudy pixel can be derived from a neighboring clear-pixel LST and the SEB difference between the two 63 pixels. Then the method is improved by using both temporal and spatial information from neighboring clear-pixels to estimate the cloudy LST for MODIS product (Yu et al. 2014). However, some physical 64 65 parameters required in these methods, such as wind speed and air temperature, were difficult to obtain. Then, with the emergence of advanced remote sensing products, a two-step method was proposed by using 66 67 multi-temporal LST and combined corresponding vegetation index to obtain a hypothetical LST and then correct the hypothetical LST based on SEB using solar shortwave irradiation data (Zeng et al. 2018). In addition, a scheme accounting for the solar - cloud - satellite geometry effect to estimate the LSTs of shadowed and illuminated pixels covered by clouds in the image has also been proposed (Wang et al. 2019). Moreover, a more generalized method that assimilates clear-sky LST into a surface energy balance equation has been recently proposed to estimate cloud-sky LST from MODIS and VIIRS data (Jia et al. 2021).

73 Passive microwave (PMW) remote sensing data provide another approach to estimate all-sky LST retrievals 74 (Duan et al. 2017; Han et al. 2018; Zhou et al. 2015), and they are less affected by cloud contamination. However, there are also limitations in the LST retrieval from PMW measurements. For instance, PMW remote 75 76 sensing data have a coarse spatial resolution of tens of kilometers, such as the Advance Microwave Scanning 77 Radiometer-Earth Observing System (AMSR-E) with a 25 km resolution (Cavalieri 2014). Moreover, PMW data have orbit gaps to consider. In addition, the temperature obtained from PMW measurements is the subsurface 78 79 temperature, in contrast with thermal infrared (TIR) LST that provides skin temperature (De Jeu 2003; Prigent et 80 al. 1999). The accuracy of the LST retrieval from passive microwave measurements is lower than that from TIR 81 measurements by 3-5 K (Duan et al. 2017). Recently, some researchers have explored the possibility of 82 combining PMW data and reanalysis data to estimate all-sky LST (Zhang et al. 2019c; Zhang et al. 2020). In 83 contrast to PMW data, reanalyzed data is obtained by advanced land surface modeling and data assimilation 84 techniques from satellite- and in situ observations. Reanalysis data involves the continuous monitoring without 85 any gaps and can provide another possibility for all-sky LST retrieval (Long et al. 2020; Padhee and Dutta 2020; 86 Zhang et al. 2019c; Zhang et al. 2021).

Many LST estimation methods based on machine learning and deep learning have emerged (Wu et al. 2019; Zhang et al. 2020; Zhao and Duan 2020). Most of them construct a relationship between clear-sky MODIS LST and related variables and extend that relationship to all-sky conditions. However, the relationship constructed with clear-sky pixels may not apply to cloudy-sky conditions. Therefore, models that provide real cloudy-sky 91 conditions LST using in situ LST measurements are relatively reliable. One type of in situ LST is the actual LST 92 measured on the ground (Coll et al. 2005; Wan et al. 2002), which is difficult to obtain in a large area and 93 limited to homogeneous and flat surfaces. Based on thermal radiative transfer theory, LST can also be calculated 94 from the ground upwelling longwave radiation as well as emissivity and downwelling longwave radiation (Wang 95 et al. 2008). Various longwave radiation measurement sites are available in the conterminous United States 96 (CONUS), which produces sufficient representative in situ LST measurements for the training of machine 97 learning models to produce all-sky LST estimates on a national scale.

98 This study aims to estimate all-sky LST over CONUS from both MODIS/Terra (MOD) and MODIS/Aqua 99 (MYD) instantaneous clear-sky LST products and other imformation. We choose the random forest (RF) 100 algorithm to build a non-linear relationship between LST and related variables, and we developed a temporal RF 101 (T-RF) algorithm for a cloudy model, which considers the temporal variation information of LST. To accurately 102 estimate cloudy-sky LST, we incorporated several all-sky surface radiation variables and reanalysis data. The 103 surface radiation variables help capture the physical process of surface heat exchange. To enhance the model 104 performance, we constructed separate models for clear-sky conditions and cloudy-sky conditions and compared 105 the models based on two algorithms for cloudy conditions.

The remainder of this paper is organized as follows. Section 2 introduces the data sources. Section 3 describes the algorithms and the process chain in detail. Section 4 presents the results and discussion of model performance and compares it with other products. Section 5 presents the data availability. Section 6 discusses the advantages and limitations of this study, and Sect. 7 presents the conclusions.

110 2 Data

111 The data used in this study include 1) in situ LST measurements for model training and validation, 2) 112 reanalysis dataset used for the model as well as comparison, and 3) remotely sensed data as model inputs (i.e., 113 surface variables, radiation variables, and geolocation information). Table 1 summarizes the products used in this study. Each type of data (i.e., in situ measurements, remotely sensed data, and Global Land Data Assimilation
System (GLDAS) data), as well as the pre-processing steps, are described in detail in the following sections.

116 **2.1 In situ measurements**

117 To obtain the in situ LST for model training and validation, in situ longwave radiation measurements were 118 collected at two observation networks, namely AmeriFlux and Surface Radiation Budget (SURFRAD). The 119 AmeriFlux network, supported and maintained by the Lawrence Berkeley National Laboratory, was established 120 to connect research on field sites representing major climate and ecological biomes, and it has 110 current active sites (Baldocchi et al. 2001). Some sites from the AmeriFlux network have longwave radiation records. 121 122 SURFRAD networks support climate research with accurate, continuous, long-term measurements of the surface 123 radiation budget over the United States (Augustine et al. 2000; Augustine et al. 2005). Currently, seven 124 SURFRAD stations are operating in climatologically diverse regions. To reduce the uncertainties, strict quality 125 control should be conducted on all the sites. First of all, we checked the temporal continuity and removed the 126 individual sites with few and continuity records. Then, one set of site data was kept from the available nearby 127 sites to avoid the duplication and interference. Finally, we selected all sites with longwave radiation 128 measurements on CONUS from 2003 to 2017, thus including 89 sites from AmeriFlux and 7 from SURFRAD. 129 In order to verify the representativeness of the sites, we extracted the 30 m LST data of Landsat8 from 130 2016-2018 on the Google earth engine (Ermida et al. 2020). The extracted pixels were within 1 km around the 131 sites, and the standard deviation (std) value in the extracted window was calculated to represent the 132 heterogeneity. The histogram statistic of multi-year average std for each site is shown in Fig.1 (b). The result 133 shows that selected sites are highly representative, and the std of all sites is less than 3 K. Since the observation time of Landsat is during the daytime in the morning, the heterogeneity at nighttime is lower (Duan et al. 2019; 134 135 Wang and Liang 2009). However, the Aqua overpasses in afternoon, which probably increases the heterogeneity

136 (Li et al. 2014). Fig.1(a) shows the spatial distribution and std of the 96 in situ observation sites used in this137 study.

138 The ground-based LST at the in situ observation sites was retrieved from the surface upwelling and 139 atmospheric downwelling longwave radiation using the Stefan–Boltzmann law:

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$$T_{S} = \left(\frac{F_{up-(1-\varepsilon)F_{dn}}}{\sigma\varepsilon}\right)^{\frac{1}{4}} , \qquad (1)$$

141 where T_s is the LST, F_{up} is the longwave upwelling radiation, F_{dn} is the longwave downward fluxes, σ is the 142 land surface of broad-band emissivity, and ε is the Stefan–Boltzmann's constant (5.67×10⁻⁸ Wm⁻² K⁻⁴). The 143 surface broadband emissivity of the flux towers was obtained from the broad band emissivity (BBE) product 144 referred to in Sect. 2.2.



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Fig. 1. (a) Spatial distribution of selected sites in the study area. SURFRAD network is shown with circles while AmeriFlux network is shown with triangles. The std value of each site is represented by different colors. Land use cover types for 2011 (background colored shading) are from a MODIS land use cover product at a 500 m spatial resolution. (b) The histogram of multi-year average values of standard deviation for each site is shown.

150 2.2 Remotely sensed data

The remotely sensed data used in this study are summarized in Table 1. The MODIS LST products (i.e., MOD11L2 and MYD11L2) in Collection 6, are at a 1 km spatial resolution. They can provide instant LSTs in daytime and nighttime from different satellite viewing times, retrieved by the generalized split-window (GSW) method (Wan and Li 1997). Pixels with quality control (QC) flags of clouds were identified as cloudy pixels, and 155 clear-sky LST was used to compare them with the clear-sky LST estimates. The MOD03 and MYD03 products with 1 km resolution represent the geolocation products, and they provide the solar zenith angle (SZA), solar 156 157 azimuth angle (SAA), viewing zenith angle (VZA), viewing azimuth angle (VAA), and surface elevation 158 variables. The relative azimuth angle was calculated from SAA and VAA. The geolocation products were also 159 utilized to match pairs between in situ longwave radiation measurements and satellite LST. Furthermore, the 160 MODIS land cover product (MCD12Q1) provides land cover types once a year with a 500 m resolution. The 161 daily MODIS snow cover data (MOD10A1 and MYD11A1) in Collection 5 was utilized to identify snowy 162 conditions at a 500 m resolution. They were not upscaled to 1 km to better represent the surface condition of the 163 site.

164 Five products from the Global LAnd Surface Satellite (GLASS) suite were used (Liang et al. 2020), 165 including BBE, surface longwave net radiation (LWNR), downward shortwave radiation (DSR), surface 166 broadband albedo (albedo), and leaf area index (LAI). The BBE product (GLASS03A01) was derived from 167 Advanced Very High Resolution Radiometer (AVHRR) and MODIS optical data using newly developed 168 algorithms (Cheng et al. 2016; Cheng et al. 2014). BBE was used to calculate the in situ LST. For the GLASS 169 LWNR (GLASS06M01), a new parameterized scheme was proposed to calculate instant downward longwave 170 radiation (LWDN) based on MODIS data (Cheng et al. 2017; Yang and Cheng 2020). As for the LWDN under 171 cloudy condition, Yang and Cheng (2020) discussed the algorithm for estimating LWDN from the derived active 172 and passive cloud property parameters, such as cloud thickness, cloud-base temperature. For that, the LWDN 173 variable in the LWNR product was used. The DSR product (GLASS05B01) provided daily DSR values 174 produced using MODIS data based on a look-up table from radiative transfer models established with and without clouds (Zhang et al. 2019b). The GLASS albedo was produced using MODIS and AVHRR data from a 175 176 direct-estimation algorithm (Liu et al. 2013; Qu et al. 2014). The GLASS LAI product was produced using the MOD09A1 product by the general regression neural network method (Xiao et al. 2014; Xiao et al. 2016). The
GLASS products mentioned above have the same spatial resolution of 1 km, except for DSR with 0.05°.

179 The temporal resolution of these products is eight days (use 8 d to represent the eight days in the following), 180 except for DSR (daily) and the LWDN (instant). All of them are global land surface products for all-sky 181 conditions. To obtain daily values of each 8 d variable (i.e., BBE, Albedo, LAI), interpolation methods were 182 utilized for each product. As for BBE and Albedo, the nearest neighbour interpolation method was used, as these 183 two variables are nearly invariant within eight days. However, there may be snowy days leading to a mutation. 184 Therefore, we identified the BBE value of snowy days as 0.985 according to the snow cover product. If it is not 185 snowy, but the BBE value is 0.985, it will be replaced by the nearest value. The BBE data with good quality 186 (QC=0) was used. As for LAI, the linear interpolation method was used to obtain daily LAI, which would 187 represent the trend of LAI.

188 The rationale for choosing the variables in these products are given in Sect. 3.



Table 1. Summary of remotely sensed data used in this study.

Variables	Product	Resolution (spatial/temp oral)
Land surface temperature (LST)	MOD11L2, MYD11L2	1 km/instant
View angle, solar angle, and height	MOD03, MYD03	1 km/instant
Snow cover	MOD10A1, MYD11A1	500 m/daily
Land cover (LAC)	MCD12Q1	500 m
Broadband Emissivity (BBE)	GLASS03A01	1 km/8 d
Downward longwave radiation (LWDN)	GLASS06M01	1 km/instant
Downward Shortwave Radiation (DSR)	GLASS05B01	0.05°/daily
Surface Broadband Albedo (Albedo)	GLASS02A06	1 km/8 d
Leaf area index (LAI)	GLASS01A01	1 km/8 d

190 **2.3 GLDAS LST data**

191 The GLDAS data represent global reanalysis data containing a series of land surface states and flux. It

192 incorporates both ground- and space-based observation systems to constrain the modeled land surface states and

193 flux (Rodell et al. 2004). There are four different models, namely MOSAIC, NOAH, CLM, and VIC, to simulate

the hydrological fields of GLDAS for different products. In this study, the instantaneous LST was used in the GLDAS NOAH dataset with 0.25° spatial resolution at a 3-h time scale. GLDAS LST was temporally interpolated to the value at the MODIS observation time via a cubic spline interpolation and resampled to 1 km using the nearest neighbour method.

198 **3. Methods**

The overall framework of the process developed in this study is shown in Fig. 2. First, parts of the samples were compiled for model training and validation, and the remaining samples were used as an independent dataset for the model evaluation. Subsequently, the mean decrease impurity (MDI) method was used to remove the redundant variables. After the variables were determined, grid research was combined with random search to determine the parameters of the final model. The RF and T-RF are described in Sect. 3.2.







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Fig. 2. Flowchart of the process to estimate all-sky LST from MODIS data.

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207 **3.1. Temporal RF model**

208 RF is a machine learning method proposed by Breiman (2001) and has been widely used for regression and 209 classification (Belgiu and Drăguț 2016; Gibson et al. 2020; Kuter 2021; Pelletier et al. 2016). In regression tasks, 210 the RF method is outstanding in constructing complex nonlinear relationships between predictor and response 211 variables for a large dataset (Hutengs and Vohland 2016). The RF method has the characteristics of randomness 212 in the selection of samples and attributes. This counterintuitive strategy leads to better performance compared to 213 several other machine learning methods and is robust against overfitting (Liaw and Wiener 2002).

214 RF is an ensemble algorithm that consists of multiple decision trees (Breiman 2001). In a random forest, 215 each decision tree grows on a bootstrap sample of the training data. A decision tree is a tree-like model with 216 multiple nodes. The dataset is segmented at each node using a random subset of predictors through information 217 gain, Gini index or other methods to construct the splitting rules. Besides, the number of predictors is limited for 218 a split, which can reduce the computational complexity of the algorithm and the correlation among the trees. The 219 split process of RF introduces randomness that contributes to a less variable and more reliable result (Hutengs 220 and Vohland 2016). Generally, the spilt process is repeated recursively on each subset until the node contains 221 similar samples, or the splitting no longer improve the predictions The final result is obtained from all decision 222 trees by voting (in case of classification) or averaging (in case of regression) (Pelletier et al. 2016). In this study, 223 model training and predictions were undertaken using the scikit-learn package in Python (Pedregosa et al. 2011). 224 RF method is widely used in remote sensing (Belgiu and Drăgut 2016). However, it is common to input 225 several independent variables and not consider temporal information. Recent studies have combined

spatiotemporal information with RF in other fields (Wei et al. 2019; Wei et al. 2020). As LST varies considerably over time, many studies have utilized temporal information to reconstruct or estimate LST under cloudy conditions (Kilibarda et al. 2014). We combined the time-weighted LST information with the RF model, thus creating the T-RF model to estimate cloudy LST. Therefore, the T-RF model considers not only the

information of multiple variables but also the LST in the time dimension. The temporal characteristic Pt in eachpixel can be expressed as

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$$Pt = \frac{\sum_{l=1}^{L} \frac{1}{dt_l^2} P_l}{\sum_{l=1}^{L} \frac{1}{dt_l^2}}$$

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In the equation, dt_l represents the temporal distance, and L represents the prior or later l days for the same pixel, P_l represents the LST on *l* day. Considering the variation of LST, the available observations at almost the same time within 8 days were used.

(2)

237 **3.2 Model training**

All clear-sky and cloudy-sky samples from 2003 to 2009 and 2012–2016 were compiled. Usually, in RF algorithm, approximately two-thirds of the samples are used for model training and the remaining are for model validation (Breiman 2001). The other samples from the other three years (2010, 2011, and 2017) were used as independent datasets for validation.

242 We initially selected the following variables: DSR, LWDN, LAI, SZA, VZA, RAA, surface elevation 243 (Height), GLDAS LST (GLST) and broadband albedo that contains black-sky albedo and white-sky albedo in 244 the three bands of shortwave (B-SH, W-SH), visible (B-VIS, W-VIS), and near infrared (B-NIR, W-NIR). LST 245 was determined by the difference between incident and outgoing energy in the process of surface energy 246 exchange. According to Eq. (1), longwave radiation is essential in this process. Meanwhile, DSR can reflect the 247 significant changes in solar radiation caused by clouds that influence LST to a certain extent. Thus, LWDN and 248 DSR were used to reflect the contributions of long and shortwave radiation to LST. In addition, the LAI and 249 broadband albedo were used to represent surface conditions such as vegetation coverage, soil moisture, and land 250 cover type, which also influence LST. In addition, the prediction of LST at a finer resolution is influenced by 251 geographical and topographical parameters including surface elevation, and the view and relative angle of the

satellite and the sun (Zhao et al. 2019). All abovementioned variables were at high resolution for all-sky
conditions. Moreover, the reanalysis data were available in all-sky conditions but with coarse resolution. The
LST of the GLDAS was also utilized as an input variable.

255 To prevent the model from being too complex thus leading to overfitting, the model was further adjusted by 256 selecting the most important variables and adjusting the parameters. The mean decrease in impurity (MDI) was 257 widely used in tree models as a variable importance measure because of its high efficiency and stability (Han et al. 2016; Louppe et al. 2013). The MDI index shows the total decrease in node impurities from splitting on the 258 259 variable, averaged over all trees; and it reflects the contribution of the parameters to the model. In this study, we 260 used the MDI method to filter the variables. MDI was used separately for the clear and cloudy-sky condition 261 samples, and some variables with low contributions were removed. The MDI results of the cloudy-sky and 262 clear-sky models are shown in Fig. 3. The results indicate that GLST, temporal characteristic P, and radiation 263 data are the main contributors to the models. However, the variables with low MDI values did not indicate an 264 insufficient correlation with LST. This may have been caused by a higher correlation with the variables at the 265 ranking top, which is also a characteristic of the MDI method. We eliminated the variables with an MDI value of 266 less than 1 %. The variables ranked in the last four were eliminated. There were no obvious changes in the model 267 accuracy after feature selection, which demonstrates that the eliminated variables were redundant for the model 268 construction. After feature selection, the LST estimation can be expressed as: LST = f (GLST, P, LWDN, DSR, 269 B-VIS, LAI, height, B-NIR, DOY, SZA, B-SH, RAA, and VZA). The temporal characteristic P was only used in 270 the cloudy-sky model.



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Fig. 3 MDI results of cloudy-sky and clear-sky models.

273 Several important RF parameters also required adjustments. Accordingly, n estimators, max depth, max 274 feature, and min sample leaf of the RF model were adjusted after the feature selection. N estimator is the RF 275 frame parameter that determines the maximum number of trees. Max depth, max feature, and min sample leaf 276 limit the maximum number of the depth and features in the tree structure, and the minimum number of samples 277 required to split an internal node, respectively (Pelletier et al. 2016). We used grid search combined with a 278 random search to determine the parameters. The grid search performs multiple cross-validations for each 279 parameter combination within a certain range according to the accuracy of the model, and it selects the 280 parameter combination with the highest average score as the best parameter. This method can provide accurate 281 parameter optimization results, but the efficiency is significantly low for large datasets. Therefore, we firstly used 282 random search to obtain a set of parameters, which were used as a reference for the setting of grid search, and then 283 obtained the optimal parameters through the grid search. After tuning, the model parameters were set as follows: 284 n estimators = 420, max depth = 43, max feature = 9, min samples leaf = 1.

285 **3.3 Evaluation approaches**

Both independent validation with samples from three years (2010, 2011, and 2017) and 10-fold cross-validation (CV) were used for the model validation. In the process of 10-fold CV, the training dataset was divided into ten folds. Among them, nine folds were utilized to train the model, and one was used for model validation. This process was repeated 10 times until all 10 folds were used for the independent validation. The above validation methods were also used to examine the sensitivity of the models. In addition, we evaluated the

model performance on individual sites, seasons, and land cover types. Lastly, we applied the final models to the
CONUS for 2010 and 2011. The generated LST product was compared with the corresponding MODIS LST and
GLDAS LST.

4. Results analysis

295 **4.1 Model training and validation**

296 Figure 4 shows the density scatterplots of the training results using data from 2003 to 2009 and 2012–2016. 297 For the cloudy-sky and clear-sky models, the root-mean-square-error (RMSE) = 2.536 and 2.354 K, $R^2 = 0.952$ 298 and 0.973, bias = -0.005 and 0.005 K, respectively. The training results indicate that both models performed 299 well. The clear-sky model presented a slightly better accuracy than the cloudy one in the model training. The 300 validation results using data from 2010, 2011, and 2017 are shown in Fig. 5. The two models have comparable 301 accuracy, with RMSE = 2.767 and 2.756 K, $R^2 = 0.943$ and 0.963, and bias = -0.143 and -0.138 K, respectively. 302 The training and individual validation results suggest that both fitting models had no obvious overfitting and can robustly estimate LST. The 10-CV results, shown in Fig. 6, can further verify the stability of the model 303 304 performance. According to the training and 10-CV results, the clear-sky model presents slightly higher accuracy, 305 which is comparable to the validation results. Therefore, the obtained difference was probably caused by the 306 different datasets used. In general, auxiliary products present larger uncertainty under cloudy sky conditions. The 307 proposed T-RF method for the cloudy-sky model effectively provided an accuracy comparable with the clear-sky 308 model. Overall, the accuracy of the model indicates the feasibility of the proposed methods for estimating all-sky 309 LST.







Fig. 5. Density scatterplots of model validation for (a) cloudy-sky and (b) clear-sky models



Fig. 6. Density scatterplots of sample-based cross-validation results for (a) cloudy-sky and (b) clear-sky models.

318 As shown in Table 3, we further derived the statistics from the individual validation datasets for the different overpass-time observations and different satellites for the cloudy-sky and clear-sky models separately. 319 320 The left table shows the accuracy of the two models during daytime and nighttime, respectively. The results 321 indicate that the accuracy of nighttime is higher than daytime in both models. In the daytime, the in situ LST 322 measurements may suffer from the influence of solar radiation, which brings uncertainty. During the daytime, 323 the spatial thermal heterogeneity of the land surface is relatively high, and the TIR directional anisotropy is 324 higher and more complicated (Cao et al. 2019; Lagouarde et al. 2012; Xu et al. 2019). In addition, the LST value 325 during daytime is relatively high than at nighttime, which can result in a higher RMSE value. The higher 326 accuracy at nighttime than at daytime has also occurred in the validation of other LST products (Duan et al. 327 2018; Shwetha and Kumar 2016; Wang and Liang 2009). For the cloudy-sky model, the accuracy of MOD is 328 higher than that of MYD, with respective RMSE values of 2.71 and 2.82 K. For the clear-sky model, the RMSE 329 is similar, but the bias of MYD is -0.27 K, which is larger than that of the MOD (0.01 K). Both models show the 330 relatively higher accuracy of MOD. This probably occurs due to the earlier observation time of MOD at which the 331 spatial thermal heterogeneity of the land surface is generally lower than that in the afternoon when MYD 332 overpasses.

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Table 3. Individual validation of the models at

		R ²	RMSE (K)	Bias (K)	Ν			R ²	RMSE (K)	Bias (K)	B 35	dayti
Cloudy	Daytime	0.94	3.09	0.15	32025	Cloudy	MOD	0.94	2.71	-0.13	30724	
	Nighttime	0.94	2.40	-0.44	31574		MYD	0.94	2.82	-0.15	32875	me
Clear	Daytime	0.94	3.02	0.13	32793	Clear	MOD	0.96	2.76	0.01	2837387	and
	Nighttime	0.92	2.41	-0.44	28702		MYD	0.96	2.75	-0.27	32717	night

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time (left), and of MOD and MYD (right).

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341 In generating of the product, we established two models using the T-RF or RF method for the cloudy-sky 342 models. The same cloudy-sky datasets were used for comparison. The training and validation results for the 343 T-RF and RF methods are shown in Table 4. The results show that the T-RF algorithm performs slightly better 344 than the traditional RF in terms of both the training and validation results. The error histograms of the models 345 and MODIS LST against in situ LSTs using independent validation datasets are shown in Fig. 7. The error 346 distribution of the T-RF cloudy-sky model (Fig. 7a) performed slightly better than that of the RF-based cloudy-sky model (Fig. 7b) with mean values of -0.14 and -0.19 K and std values of 2.76 K and 2.90 K, 347 respectively. Although the accuracy between the two models is less than 0.2 K, it is the average error of all 348 stations. The results obtained from the clear sky models (Fig. 7c) outperformed MODIS LST (Fig. 7d), with 349 350 mean values of - 0.14 and - 0.36 K, and std values of 2.75 and 3.01 K, respectively.



352

Table 4 Training and validation results of T-RF and RF methods for the cloudy-sky model.



353 Fig. 7. Error histograms of (a) T-RF cloudy-sky model, (b) RF cloudy-sky model, (c) clear-sky model, and (d) MODIS clear sky LST

354 against independent in situ LSTs.

355

356 **4.2 Model performance at individual sites**

357 Figure 8 shows the spatial distributions and histograms of the RMSE calculated by individual validation 358 results of the cloudy-sky model, clear-sky model, and corresponding MODIS clear-sky LST. The background 359 color represents the elevation data from GMTED2010. For the cloudy model (Fig. 8a), the RMSE values of all 360 individual sites ranged from 1.67 to 3.89 K. According to the corresponding histograms, over 70 % of the 361 stations have RMSE values smaller than 3 K. However, it has a relatively lower accuracy on the complicated 362 terrain in the western part of the CONUS. In regions with relatively high elevations, complex atmospheric 363 conditions affect the estimation of surface parameters. In addition, complex topography increases TIR directional 364 anisotropy (Cao et al. 2021; Jiao et al. 2019), leading to more uncertainty in estimating LST. This phenomenon 365 also exists in MODIS LST products (Fig. 8e) and other research (Zhao et al. 2020). For the clear-sky models, the 366 results of RMSE values and MODIS LST were 1.62-4.32 K and 1.66-4.88 K, respectively. The accuracy of the 367 clear-sky and cloudy-sky models are comparable, and the RMSE values of over 60 % of the sites are below 3 K. 368 Nevertheless, the RMSE value of a few sites exceeds 4 K. The relatively higher RMSE may be caused by a 369 higher LST value under clear-sky conditions. In contrast to cloudy-sky model, temporal information is not used 370 in the clear-sky model. Moreover, few sites with large errors appear in the center of the CONUS only in the 371 clear-sky model. These errors likely occurred because parts of the in situ measurements were affected by the 372 solar radiation under clear-sky conditions. Solar radiation also increases the LST heterogeneity and TIR 373 directional anisotropy, resulting in differences between in situ and MODIS pixel-scale LST (Cao et al. 2019; 374 Wang and Liang 2009). Overall, the accuracy of individual sites of the cloudy-sky model and clear-sky models 375 were generally similar, and the accuracy of the clear-sky model was comparable to MODIS LST.

376



377

Fig. 8. RMSE spatial distributions (left) and histograms (right) of (a, b) cloudy-sky model, (c,d) clear-sky model, and (e, f) MODIS
clear-sky LST. The spatial distribution figures are based on the DEM background. The red lines in the histograms represent 25 %, 50 %, and
75 % of the sites.

381 **4.3 Model performance in seasons and land cover types**

Figure 9 shows the validation statistics of the proposed models for each season. The RMSE results (Fig. 9a) show the comparable accuracy of the cloudy-sky and clear-sky models, and both models show relatively high uncertainty in spring and summer. The reason for that may be that these seasons represent the growing and peak seasons of vegetation, which can affect the LST values. The R² values (Fig. 9b) of the cloudy-sky model are lower in spring and summer, and the R² values of the clear-sky model are all higher than those of the cloudy-sky 387 model. The absolute bias values in summer and winter are relatively high (Fig. 9c). However, the biases in all 388 seasons are not large, and the maximum absolute value is below 0.3 K. In general, seasonal differences in the 389 accuracy of the models exist, but they are not significant.



392 393

394 Table 5 lists the validation results of the cloudy-sky and clear-sky models for different land cover types. 395 Among all land cover types, forest presented the highest accuracy, and the RMSE values in both models were 396 less than 2.5 K. The accuracies of shrublands and grasslands were slightly lower than those of other vegetation 397 types. Except for barren and snow/ice, the other land cover types presented similar validation results. The reason 398 for the relatively poor performance of barren and snow/ice may be the high albedo and low specific heat capacity 399 in these areas. For the barren land, there are significant biases with -0.56 K and -0.26 K under the cloudy-sky 400 and clear sky models, respectively. The LST may be underestimated due to the overestimation of emissivity on 401 barren land (Duan et al. 2019; Zhang et al. 2019a). Otherwise, there is a limited amount of available snowy 402 observations in CONUS, affecting the model stability under snowy conditions. The poor accuracy of the LST on 403 snow/ice and barren surface is also reflected in other study (Williamson et al. 2017; Zhang et al. 2019a; Zhang et 404 al. 2021). In general, there were no significant differences between the results for different land cover types. In 405 the proposed models, the differences between the maximum and minimum RMSE values were less than 2 K, 406 which is consistent with the results obtained in other study (Yoo et al. 2020).

	(Cloudy-sky	model	С	lear-sky mo	odel
Land cover	RMS	Bia	ł	RMS	Bias	R
types	E (K)	s (K)	2	E (K)	(K)	2
Forest	2.27	-0.	С	2.29	-0.1	0
		08	.94		8	.96
Shrubland	3.35	-0.	С	2.58	0.04	0
		14	.94			.98
Savannas	2.91	-0.	С	2.59	0.07	0
		07	.94			.94
Grassland	3.15	-0.	С	2.80	-0.2	0
		27	.94		7	.96
Wetlands	2.51	-0.	С	2.25	-0.2	0
		15	.92		5	.98
Croplands	2.57	-0.	С	2.99	-0.1	0
		09	.96		9	.96
Urban	2.83	-0.	С	3.39	-0.1	0
		54	.94		8	.94
Barren	3.24	-0.	С	3.71	-0.2	0
		56	.92		6	.85
Snow/ice	3.46	0.1	С	3.87	0.88	0
		4	.83			.85

Table 5 Validation results of cloudy-sky and clear-sky models for different land cover types.

409

410 **4.4 Spatial pattern and temporal variability analysis**

The proposed T-RF model was used for cloudy pixels. However, for a small part of the pixels, there were no available clear-sky pixels. According to the rough statistics of the training and validation datasets, less than 5 % of them did not have a match for clear-sky LST. Therefore, the traditional RF method was supplemented with T-RF for a small number of cloudy pixels. The comparison of two cloudy models is further described in the Sect. 5. Figure 10 shows the MOD daytime LST images (a–d), corresponding estimated all-sky LST images (e–h), and

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GLDAS LST images (i–l) at 93, 180, 276, and 360 Julian days in 2010. It is clear that the original MODIS LSTs show different extents of missing areas caused by cloud contamination, whereas the estimated LSTs present spatially continuous results. For the same day, the three products show a similar spatial pattern on clear sky conditions. The spatial distribution follows a latitudinal gradient with relatively low values in higher latitude areas caused by the change in solar radiation. In the summer and autumn, the eastern area has relatively high LST values than the western area due to the forest and cropland in the eastern area, which mitigates the effects of solar heating (Li et al. 2018). In addition, all of them show the same seasonal LST dynamics.



423

424 Fig. 10. (a-d) Original Terra MODIS LST daytime LST images, (d-h) estimated LST images, and (i-l) their corresponding GLDAS LST

425

images on four different days in 2010 (93, 180, 276, 360 Julian days).





Fig. 11. Density scatterplots of (a) GLDAS LST, (b) clear-sky MODIS LST, (c) Stefan-Boltzmann derived LST and (d) estimated
 all-sky LST from independent validation dataset.

448 Fig. 12 shows a temporal comparison among the estimated LST, in situ LST, and MODIS LST over six 449 sites from different regions in 2010. The observation time of the data is the same as that of the daytime MOD LST. The black and red lines represent the in situ LST and estimated all-sky LST, respectively. The 450 451 corresponding MODIS LST under clear-sky conditions is shown as a blue circle. The temporal variability of the 452 six sites indicates that the estimated LST sufficiently captured seasonal and daily changes, with an accuracy 453 comparable to the MODIS LST. It should be noted that there were days when high LSTs sharply dropped, and 454 the estimated LST can capture such low values, as shown in Fig. 11.a (DOY 330). Because the variables used are 455 instantaneous or daily, the proposed method performs better than traditional methods, such as temporal 456 interpolation, for capturing extreme and sudden weather conditions (Metz et al. 2014). In addition, all estimated 457 LST time series presented excellent temporal consistency with the in situ LSTs at different sites, at RMSE ≤ 3.27 458 K, bias < 1.24 K, and R² > 0.96.



459

Fig. 12. Time series for in situ LST, estimated all-sky LST, and clear sky MODIS LST in 2010 six sites at different regions. The latitude and longitude of the sites are: (a) 48.30783° , -105.1017° ; (b) 35.93109° , -84.33242° ; (c) 36.62373° , -116.01947° ; (d) 38.7441° , -92.2° ; (e) 36.6358° , -99.5975° ; (f) -34.3349° , 106.7442° . The altitudes are 634, 381, 1004, 239, 647, and 1596 m, respectively. The statistical metrics of estimated LST and MODIS LST against in situ LST are displayed in red and blue, respectively.

464 **5 Discussion**

In this study, all-sky LST was estimated using the T-RF and RF models by constructing a non-linear 465 466 relationship between the reanalysis data, radiation variables, land surface characteristics variables, and in situ 467 LSTs. The accuracy of the estimated all-sky LST is acceptable. There was no significant difference between the 468 validation results of the clear-sky (RMSE = 2.756 K) and cloudy-sky (RMSE = 2.767 K) models, and the clear 469 sky estimations are comparable to the corresponding MODIS LST products on a temporal and spatial scale, 470 showing high consistency. In addition, there were no obvious differences in the accuracy of the models for Terra 471 and Aqua MODIS observations during the daytime or nighttime, which demonstrates the stability of the model at 472 different observation times.

473 Estimating LST from the in situ measurements has advantages, but there are two issues to discuss. First, 474 there is the issue of site representativeness. There may be some inhomogeneous sites so that the 'point' 475 measurements may not be able to represent the entire pixel. We initially selected the sites and the std of the 476 selected sites were below 3 K. Through experiments, we found that removing the selected sites with larger std 477 (above 2K) has basically no effect on the overall accuracy of the model, showing in the table 6. The reason may 478 be that the number of samples with the std of site larger than 2 K is very small compared to total samples. When 479 the sites were kept only with std below 1 K, the accuracies were slightly improved by 0.208 K and 0.161 K for 480 clear-sky model and cloudy-sky model, respectively. In addition, we further examined the relationship between 481 the heterogeneity of selected sites and estimation accuracy shown in Fig.13. There was no significant correlation 482 between estimation accuracy and the site heterogeneity under both clear-sky conditions (R = 0.366) and 483 cloudy-sky conditions (R = 0.206). This illustrated that the heterogeneities of the selected sites in this study had 484 no significant impact on the model construction.





486 487

Fig.13. The relationship between site accuracy and site STD under (a) clear-sky condition and (b) cloudy-sky condition. Table 6 The accuracy of different independent datasets selected based on the std value of sites

	Clear	sky	Cloudy sky		
Range of std (K)	RMSE (K)	Ν	RMSE (K)	Ν	
0-1	2.525	38801	2.602	40186	
0-2	2.733	58863	2.761	60123	
0-3	2.756	61495	2.767	63599	

489 As initially clarified in Cao et al. (2019), the thermal radiation directionality (TRD) leads to the definition 490 differences of MODIS LST and in situ LST extracted from pyrgeometer measurement. The in situ LST 491 measurement (i.e., the reference of our RF LST product) is close to hemispherical LST, while MODIS LST is a 492 directional LST. Since we used the in situ LST to construct the model, there may be differences between our 493 product and MODIS LST. Thus, we made a further comparison. Figure 14 shows the spatial distribution and 494 corresponding histogram of the estimated LST bias against MODIS LST from 2010 to 2011. The bias statistics 495 are mean = 0.80 K, std = 1.28 K. The overall results are relatively consistent, but there are differences in the 496 western CONUS. The differences probably come from the relatively high heterogeneity (Xu et al. 2019) and 497 thermal radiation directionality (TRD) effect (Cao et al. 2019), which is more pronounced in complex terrains. 498 Many studies have reported the large differences of LST under different view angles (Cao et al. 2021; Hu et al. 2016). MODIS LST is observed from 0° ups to > 60° , while the proposed LST retrieval from in situ LST. 499 500 The difference of view angles may lead to the difference between the estimated LST and MODIS LST. 501 Meanwhile, we have compared the error distribution via the VZA of the estimated LST and MODIS LST, using 502 the separated validation dataset. The error distribution is shown in Fig.15. The error of the estimated LST is 503 relatively stable with the change of VZA. However, as for MODIS LST, with the increase of VZA, the part 504 where the density points gather gradually deviates from 0. TRD is a complicated process and is not the research 505 content of this study, therefore, we did not discuss it further. From the above comparison, difference exists 506 between the estimated LST and MODIS LST. Theoretically and in practice, in contrast to MODIS LST, our 507 proposed LST is less affected by the observation angle.



508

Fig. 14. Spatial patterns of statistical metrics of (a) bias between the estimated LST and MODIS LST under clear sky conditions, and
 corresponding frequency distribution histograms (b) from 2010 to 2011.



512 Fig.15.The error distributions of the estimated LST (a) and MODIS LST (b) against in situ LST from the separated validation dataset 513 Compared with previous research, the method proposed in this paper has certain advantages. First, the 514 variables used in this paper are all from optical remote sensing and reanalysis products, which are all-sky data 515 and worldwide. Thus, it provides a possibility to expand the proposed method to other regions. In contrast to the 516 PMW data, the data used avoided dealing with the uncertainty caused by different sampling depths and swath gaps. Meanwhile, the data used has a continuous and long sequence, which can be used to produce long-term 517 518 continuous all-weather LST products. Second, the model is trained with real in situ LSTs instead of clear-sky 519 MODIS LSTs for both clear-sky and cloudy-sky conditions, thus avoiding obtaining the hypothetic cloudy LST. 520 Meanwhile, using the in situ LSTs reduced the uncertainty caused by different view angles. Third, with the 521 development of advanced remote sensing data, the method proposed in this paper uses sufficient radiation

variables including LDWN and DSR with high resolution, which considered the LST under the cloudy sky, and was affected by changing the solar radiation and downward longwave radiation. Furthermore, the proposed method has high efficiency. Once the models are trained, they can be easily used for generating long time series all-sky LST products. The generated product can be used for agricultural drought monitoring, climate change analysis, and also as input to estimate other parameters, such as air temperature, soil moisture, etc.

However, the method also has limitations. Although the highest possible amount of representative ground stations in the long-term sequence was selected and an independent dataset was used for validation, it was still difficult to quantitatively evaluate the areas without in situ observations. In addition, on the surface types of ice, snow, and barren, as well as areas with high thermal heterogeneity, the accuracy was relatively low, which is a difficulty also faced by other methods. In the future, the effects of surface terrain and spatial information should be considered, and deep learning should be incorporated to explore a more adaptive model using the information provided by remote sensing observations and data products, such as geostationary satellite sensors.

6. Conclusions

535 We aimed to estimate LST under all-sky conditions from different product data and other auxiliary 536 information. To achieve this, sufficient variables from optical remote sensing and reanalysis data were used, 537 including radiation variables, land surface characteristics variables, and geographical and topographical 538 parameters. All variables were available under all-sky conditions and contributed to the estimation of LST after 539 feature optimization. To further improve the model performance under cloudy-sky conditions, temporal 540 information was introduced in the RF model. This procedure was applied for instantaneous observations from 541 both MOD and MYD sensors to obtain daily LST at daytime and nighttime. The major conclusions are shown as 542 follows.

543 (1) For the cloudy-sky and clear-sky models, the validation results of the proposed models presented high 544 accuracy, with RMSE = 2.767 and 2.756 K; $R^2 = 0.943$ and 0.963; bias = -0.143 and -0.138 K, respectively.

545 The T-RF method used for the cloudy-sky model presented a slightly higher accuracy than the traditional RF 546 method (RMSE = 2.914 K, bias = -0.191 K, R² = 0.937). There were no significant differences in the accuracy 547 between clear-sky and cloudy-sky estimations. The 10-cross validation results (RMSE=2.616 K, and 2.474 K) 548 indicate that the constructed models have a robust performance.

(2) The accuracies of individual sites from the separated dataset are 1.67 K–3.89 K under cloudy sky conditions. In contrast, those under clear-sky condition are 1.62 K–4.32 K, which is comparable to MODIS LST. The sites in the western part of CONUS have relatively lower accuracy, especially in mountainous areas. Besides, in contrast to MODIS LST, the estimated LST in this study is less affected by the directionality effect.

(3) In terms of temporal variability, the estimated LSTs were highly consistent with in situ LST and comparable with MODIS LST. The performance of the proposed method was excellent for daily LST estimation since daily LST variation and extreme events were captured. In terms of the spatial distribution, the estimated LSTs have the similar patterns with MODIS LST and effectively fill the data gaps. Besides, the estimated LSTs have more spatial details than GLDAS LST under all-sky conditions. The estimated LST (RMSE =2.870 K) has higher accuracy than GLDAS LST (RMSE = 4.157 K), Stefan-Boltzmann derived LST (RMSE = 4.128 K) and MODIS LST (RMSE = 3.033 K).

Thermal infrared sensors are unable to provide LST data under cloudy conditions. High-accuracy all-sky LSTs with 1 km resolution are in high demand. The proposed methodology is a feasible way to predict LST at high spatial and temporal resolution under all-sky conditions at all land cover types during daytime and nighttime. It provides a new framework and advances capabilities for reconstructing other sensors and other regions using local data. This capability will be beneficial for land surface monitoring and ecological dynamics. However, this method does not consider spatial information. Future development should focus on using deep learning methods that consider both temporal and spatial information.

567 **Author contribution**

568 Shunlin Liang and Bing Li designed the research and developed the methodology; Yan Chen and Tianchen

569 Liang collected the data. Bing Li and Xiaobang Liu processed satellite images; Bing Li wrote the manuscript;

570 Shunlin Liang, Han Ma and all other authors revised the manuscript.

571 **Competing interests**

572 The authors declare that they have no conflict.

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