Revisions of Manuscript: ESSD-2025-192

Title: Spatially adaptive estimation of multi-layer soil temperature at a daily time-step across China during 2010-2020

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Dear Reviewer,

We sincerely thank you for your thoughtful comments and constructive suggestions on our manuscript. We have carefully revised the manuscript in response to your feedback, with all changes clearly marked using track changes. In the revised manuscript and accompanying supplementary materials, modifications are highlighted in blue for ease of reference.

Below, we provide a detailed, point-by-point response to each of your comments. For clarity, your original remarks are shown in *italics*, followed by our corresponding replies. We have made every effort to address all concerns comprehensively and to improve the scientific rigor, clarity, and overall quality of the manuscript.

We sincerely appreciate the time and effort you invested in reviewing our work, and we believe the revisions have significantly improved the manuscript.

Reviewer Comment 1:

The method used many data (primarily including in-situ observations and indicator variables) to produce soil temperature. By the way, the in-situ in Figure 3 is wrongly spelled as in-suit. Since these data are with varying spatial scales, and many complicated steps are involved in this procedure to produce the Ts at different depths. I just wonder why the outputted Ts is with that good accuracy. Given than even the acknowledged MODIS LST (nearly Ts at 0 cm) is 1-2K, and it has been taken as an input in this study.

Response to Reviewer Comment 1:

We sincerely thank the reviewer for this valuable comment. The relatively high accuracy of our model can be attributed to the following three aspects:

1. Complementarity of multi-source information.

MODIS LST is only one of many predictors and not the dominant determinant. By integrating near-surface air temperature, radiation, precipitation, vegetation indices, topography, and soil texture, the model captures the key drivers of soil thermal dynamics. This multi-source data fusion enables the model to learn complex nonlinear relationships, thereby mitigating the influence of errors from any single predictor (e.g., LST).

2. Localized modeling based on the rotated quadtree.

The rotated quadtree adaptively partitions the study domain according to station density, allowing local models to better represent regional heterogeneity. This spatially adaptive approach avoids systematic bias from scale mismatch and significantly improves the model's applicability and stability across diverse regions.

3. Robust performance under different conditions.

In subsequent analyses, we compared model performance across seasons and land-use types. Results indicate that model accuracy is relatively higher in spring and autumn than in summer and winter, and is generally greater over croplands, grasslands, and barren lands compared with forests. These patterns further demonstrate that the high accuracy is reasonable and reflects the robustness of the model, rather than an artifact of overfitting.

We also appreciate the reviewer's careful note on the spelling issue in Figure 3. We have corrected "in-suit" to "in-situ" (L342–344 in the revised manuscript).

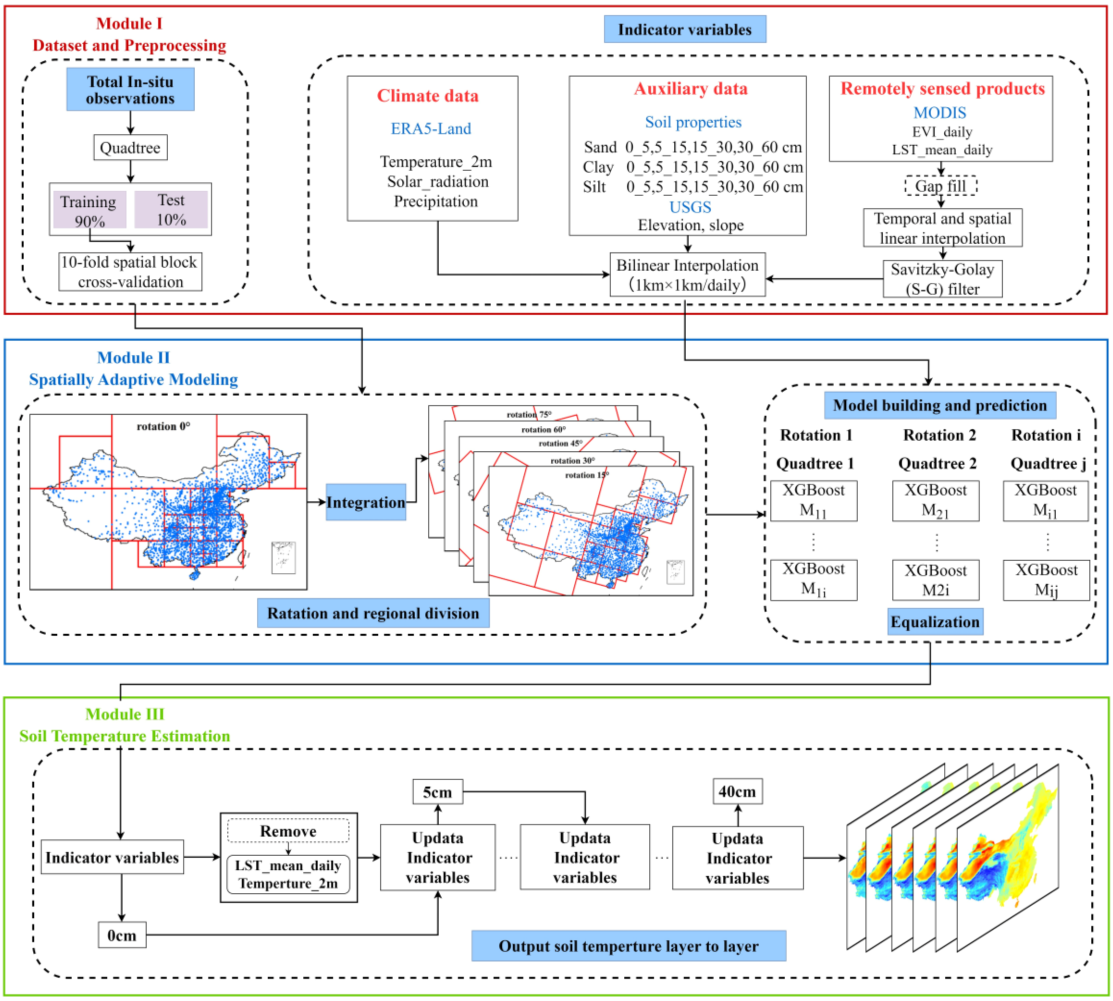

Figure 3. Workflow of the proposed method to obtain multi-layer T_s over the China.

Reviewer Comment 2:

To my knowledge, LST changed very quickly and is seriously affected by cloud. The local observation time differ across China, and most regions in the South are covered by cloud at most time. How you process these data, and whether the accuracy can be guaranteed in your study?

Response to Reviewer Comment 2:

We greatly appreciate the reviewer's attention to this issue. To address the cloud-induced data gaps and temporal mismatch in LST, we implemented the following measures:

1. Cloud-induced Data Gaps

Cloud cover, especially in southern China, is indeed a significant challenge. To mitigate this, we reconstructed missing data caused by cloud cover using spatio-temporal interpolation combined with neighboring pixel information. We then applied the Savitzky-Golay smoothing method to generate continuous daily fields, effectively reducing the data gaps caused by cloud interference.

2. Handling MODIS Daytime and Nighttime LST

We separately processed the instantaneous daytime and nighttime LST from MODIS, and calculated the mean of these two values to serve as the daily average LST input variable. Compared to instantaneous temperatures, daily mean values are less sensitive to missing data, which helps improve the stability of the data.

3. Uncertainty in Using LST as an Input Variable

We acknowledge that using mean_LST as an input variable may introduce some uncertainties, particularly in southern regions where cloud cover leads to more significant data gaps. We have discussed the limitations of this approach and future improvements in the revised discussion section of the manuscript. Despite these uncertainties, considering that mean_LST effectively captures long-term surface temperature trends at a large spatial scale, we decided to use it as a feature for modeling.

We hope these clarifications address the reviewer's concerns regarding cloud effects, temporal mismatches, and the uncertainties introduced by the use of LST as an input variable. The methods we have implemented are well thought out to ensure the accuracy and reliability of the model results.

Revised Text (L601-L662):

4.3 Limitations and future perspective

Despite the strong performance of our spatially adaptive T_s estimation framework, several limitations warrant acknowledgment. As shown in Figures 6 and 7, model validation at station level reveals spatial heterogeneity in prediction accuracy, with relatively lower performance observed in the YGP and the QTP regions. On the one hand, as evidenced by Figure 10, our multi-source modeling framework captures T_s variations across different elevations and geomorphic conditions more effectively than existing datasets. However, the QTP and YGP are characterized by complex terrain and high altitudes, coupled with rapidly changing climatic conditions, which significantly complicate T_s estimation. These findings align with previous studies showing that high elevations intensify the disconnect between air temperature and LST, thereby increasing the uncertainty in thermal modeling (Mo et al., 2025).

MODIS LST serves as a critical input to our modeling framework. However, as an optical remote sensing product, it is highly susceptible to cloud contamination, often resulting in data gaps. Despite the use of spatiotemporal interpolation and SG filtering, residual uncertainties persist in the reconstructed LST data. Future improvements in T_s reconstruction can be pursued along two main directions. First, more physically grounded LST reconstruction methods can be adopted, such as incorporating surface energy balance models and diurnal temperature cycle models (Hong et al., 2022; Firozjaei et al., 2024; Wang et al., 2024). These methods apply energy conservation principles to estimate T_s during periods of missing or unreliable observations, thereby providing more realistic estimates of land surface thermal conditions during periods of cloud cover. Second, integrating higher temporal resolution remote sensing observations may help overcome the limitations of MODIS. For instance, passive microwave satellite data provide all-weather observations and are less sensitive to cloud interference (Duan et al., 2017; Wu et al., 2022). In addition, next-generation geostationary satellites such as Himawari-8 offer observations at 10-minute intervals, substantially enhancing the temporal continuity and quality of surface temperature estimates (Yamamoto et al., 2022; You et al., 2024). These enhancements are expected to significantly improve the accuracy and temporal continuity of soil temperature monitoring.

Our results (Figures 8 and 9) show that model accuracy varies across different soil depths, with additional influences from season and land use. Accuracy is relatively lower at the surface (0 cm), improves at intermediate depths (5–10 cm), and then declines again at greater depths (20–40 cm). This depth-dependent pattern can be explained by the physical characteristics of soil temperature. Surface soil temperature is highly sensitive to short-term meteorological fluctuations such as radiation, precipitation, and evapotranspiration, leading to greater spatiotemporal variability and larger prediction errors. In contrast, intermediate soil layers benefit from the buffering effects of thermal diffusion and soil heat capacity, which dampen high-frequency fluctuations and stabilize the relationship between predictors and Ts, thereby improving performance at these depths. At greater depths, however, surface-level errors propagate downward through the cascading framework, resulting in reduced accuracy—particularly during summer and winter.

Seasonal changes and variations in land cover further contribute to differences in estimation accuracy. As shown in Figures 8 and 9, the model exhibits higher accuracy in spring and autumn, whereas its performance tends to decline during summer and winter. During summer, dense vegetation growth and canopy closure reduce the influence of surface–atmosphere energy exchanges on T_s, weakening the correlation between canopy temperature and subsurface T_s (Kropp et al., 2020; Cui et al., 2022). In winter, snow cover introduces a suite of confounding effects: high surface albedo reduces net radiation (Loranty et al., 2014; Li et al., 2018), while snow acts as an insulator, limiting the soil's response to cold air incursions (Zhang, 2005; Myers-Smith et al., 2015). Additionally, low temperatures lead to soil water freezing, which alters the soil's thermal conductivity and heat storage capacity. These factors, together with frequent freeze–thaw cycles, introduce complex nonlinear dynamics in T_s that increase modeling uncertainty (Li et al., 2023a; Imanian et al., 2024). While our multi-source adaptive modeling framework performs well across depths, it does not explicitly account for the physical mechanisms of vertical heat transfer. Future research could explore deep learning models that are capable of learning complex spatiotemporal features and improving the physical interpretability of T_s variations across time, space, and depth.

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Reviewer Comment 3:

On the other hand, the seemingly good accuracy is not that strange. Because the authors used the same ground measurement to validate the estimated values. Although the entire data has been divided into two sections of training and validation. They are actually homologous with the similar schemes by CMA. How about validating the estimated results with data collected from different sources.

Response to Reviewer Comment 3:

We sincerely thank the reviewer for this valuable and necessary comment. In the revised manuscript, we have strengthened the validation design to address this concern by (1) implementing a spatial block cross-validation scheme and (2) incorporating independent validation against flux tower observations, thereby enhancing the independence and credibility of our evaluation.

First, we acknowledge that the CMA operational network is currently the only nationwide source of long-term (≥10 years), large-scale, and multi-layer (0–40 cm) Ts observations in China, and thus forms the most comprehensive basis for constructing a national Ts dataset. To rigorously account for the strong spatial autocorrelation of Ts

and avoid potential data leakage between training and testing subsets, we employed a spatial block cross-validation scheme rather than random splitting. Observation sites were first partitioned into rotated quadtree subregions. Within each subregion, sites were further grouped into spatial blocks by flooring their latitude and longitude values to integer degrees, such that stations sharing the same integer indices (i.e., falling within the same 1° × 1° index) were assigned to the same block. This method ensures that samples within the same spatial block are not simultaneously allocated to both the training and testing subsets, thereby preventing data leakage caused by spatial autocorrelation and providing a more reliable assessment of the model's generalization capability.
Second, to further strengthen independence, we validated the final dataset against daily Ts observations from 18 flux tower sites of the ChinaFLUX network. Measurements at 0, 5, 10, 15, 20, and 40 cm were retained for consistency. Results (Figure 5; Table S2) show that our dataset maintains high accuracy at these independent sites (R^2 = 0.85–0.90; RMSE = 3.3–4.2 K), confirming that the accuracy is robust and not merely a product of same-source validation.

Taken together, the validation results from both spatial block cross-validation and independent flux tower observations demonstrate that the spatially adaptive framework we developed achieves strong robustness, reliability, and spatial generalization ability.

Revised Text (L318-L326):
To rigorously account for the strong spatial autocorrelation of T_s and avoid potential data leakage between training and testing subsets, we employed a spatial block cross-validation scheme rather than random splitting. Specifically, within each rotated quadtree grid, observation sites were grouped into spatial blocks based on their geographic coordinates: station latitude and longitude were each divided by 1° and floored to integer values, and stations sharing the same index were assigned to the same block. This ensured that samples within the same spatial block were not simultaneously assigned to both the training and testing subsets, thereby avoiding data leakage due to spatial autocorrelation and enabling a more reliable evaluation of the model's generalization capability.

Within each spatial grid, the data were partitioned into training (90%) and testing (10%) subsets at the block level. The training subset was further subjected to 10-fold spatial block cross-validation using GridSearchCV to optimize three key hyperparameters: the number of trees (n_estimators), maximum tree depth (max_depth), and learning rate (learning_rate). Detailed parameter settings are provided in Appendix Table S1. The hyperparameter set that yielded the lowest average validation error across the ten folds was selected as optimal. The final model, retrained on the full training set with these parameters, was then evaluated on the held-out testing blocks to assess its generalization ability and examine potential overfitting within each grid.

Revised Text (L372-L381):

Furthermore, to enhance the independence of the evaluation, we validated the final dataset against daily T_s observations from 18 flux tower sites of the ChinaFLUX network. For consistency, we retained measurements only at depths of 0, 5, 10, 15, 20, and 40 cm. Metadata for these sites is provided in Table S2, and the corresponding validation results are presented in Figure 5. The evaluation shows that our dataset achieves high accuracy at these independent sites (R^2 = 0.85–0.90; RMSE = 3.3–4.2 K), further demonstrating the robustness of our approach. Taken together, the validation results from both spatial block cross-validation and flux tower observations confirm that the spatially adaptive model we developed exhibits reliable accuracy and strong spatial generalization capability.

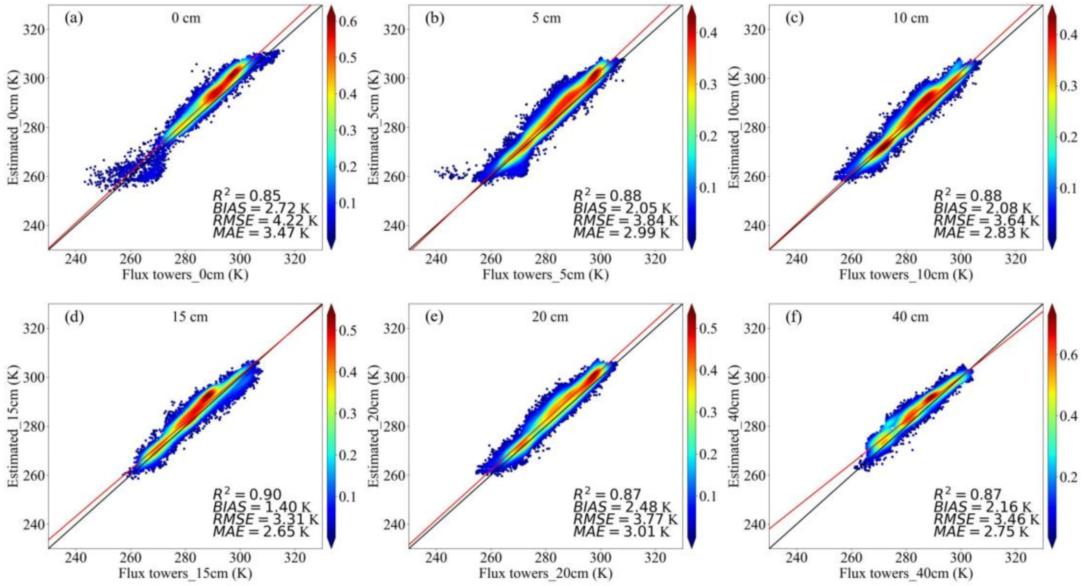

Figure 5. Density scatter plots comparing estimated daily T_s with flux tower observations at different depths

Table.S2 Metadata of daily T_s observations from flux towers used for validation.

Site	Ecosystem	Depth (cm)	Time series
Baotianman Forest Station	Forest	0,5,20	2010-2014
Changling Rice Paddy Station	Cropland	5,10,20	2018-2020
Daan Cropland Station	Cropland	0,5,10,15,20	2017-2020
Damao Grassland Station	Grassland	0,5,10,15,20,40	2017-2020
Danzhou Rubber Plantation Station	Forest	5,10,20	2010
Haibei Alpine Meadow Station	Grassland	5,10,15,20,40	2015-2020
Haibei Shrubland Station	Grassland	0,5,20,40	2016-2018
Huzhong Boreal Forest Station	Forest	5,10,20	2014-2018
Jinzhou Cropland Station	Cropland	5,10,15,20,40	2011-2014
Lijiang Alpine Meadow Station	Grassland	5,10,15,20,40	2013-2020
Maoershan Forest Station	Forest	5	2016-2018
Panjin Reed Wetland Station	Wetland	10,20,40	2018-2020

Qianyanzhou Plantation Forest Station	Forest	5,10,20	2011-2015
Ruoergai Alpine Wetland Station	Wetland	0,5,10,20	2013-2020
Sanjiangyuan Alpine Grassland Station	Grassland	0,5,15	2013-2015
Taoyuan Cropland Station	Cropland	5,10,15,20,40	2010-2014
Xishuangbanna Rubber Plantation Station	Forest	0,5,20	2010-2014
Yuanjiang Dry-Hot Valley Savanna Station	Grassland	5,10,20,40	2013-2015

Reviewer Comment 4:

The authors used on XGBoost, why not try other machine learning algorithms. It is not sure that XGBoost perform best. Maybe a balance of multiple algorithms is more convincible.

Response to Reviewer Comment 4:

We thank the reviewer for this valuable comment. We agree that other machine learning approaches (e.g., RF, GBDT, LSTM) could in principle be applied to soil temperature estimation. However, the main innovation of our study lies not in algorithm comparison, but in the spatially adaptive modeling framework (rotated quadtree + local modeling + layer-wise cascading), which addresses the challenges posed by spatial non-stationarity and uneven observation distribution in nationwide *Ts* estimation.

We selected XGBoost because it offers clear advantages over alternative methods for large-scale mapping:

1. Compared to RF

XGBoost converges faster, is more memory-efficient, and yields lighter prediction models;

2.**Compared to traditional GBDT:**

XGBoost incorporates parallelization, sparse-aware processing, and cache optimization, leading to much higher efficiency on large datasets;

3. Compared to LSTM and deep learning models:

XGBoost has lower computational complexity, less dependence on GPUs, and runs efficiently on CPUs, making it more practical for nationwide, daily, decade-long mapping tasks.

Therefore, in the revised manuscript, we emphasized the novelty of the spatially adaptive framework and cited relevant literature to highlight the widespread use of XGBoost in large-scale mapping. The focus of this work is the framework itself rather than a benchmarking exercise among algorithms. For details, please refer to the revised manuscript.

Revised Text (L303-L317):

We adopted the XGBoost (Extreme Gradient Boosting) algorithm as the core regression model for T_s estimation due to its strong predictive performance, computational efficiency, and scalability across large environmental datasets. XGBoost builds an ensemble of regression trees in a stage-wise boosting process, where each tree is trained to minimize the residuals from the previous iteration, leading to a robust and optimized model (Chen and Guestrin, 2016). A key strength of XGBoost is its ability to handle heterogeneous and high-dimensional predictor sets, which are common in geoscience applications involving complex terrain, land cover variability, and climatic gradients. Recent studies have demonstrated its effectiveness in similar domains, including land surface temperature reconstruction (Li et al., 2024), multi-layer soil moisture estimation (Karthikeyan and Mishra, 2021), drought event attribution (Wang et al., 2025), and crop yield prediction (Li et al., 2023). Given these proven strengths and the spatially nonstationary characteristics of T_s in our study area, XGBoost was selected to train localized prediction models within spatial subregions.

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Reviewer Comment 5:

Like many other overabundant pure machine learning articles, the present study lacks of innovation, but eligible as a data description paper. Reanalysis data such as ERA5-Land also have Ts at multiple layers, except for the finer spatial resolution (they can also do that if they want), what are the advantages of your data? Why do you think a *user should consider your data?*

Response to Reviewer Comment 5:
We sincerely thank the reviewer for raising the important issue of innovation. The novelty of this study lies in two main aspects: methodology and data products.

1. On the methodological side, the core improvements include:
(1) A rotated quadtree–based local modeling framework, which effectively addresses the challenges of spatial non-stationarity and uneven station distribution in nationwide soil temperature estimation;

(2) A layer-wise cascading prediction strategy, which takes the estimated shallow-layer temperature as input for deeper layers, explicitly incorporating the continuity of soil heat conduction and thereby improving both the accuracy and consistency of multi-depth soil temperature estimation.

2. On the data-product side, our dataset offers several distinct advantages over existing reanalysis products (e.g., ERA5-Land, GLDAS):
(1) Higher spatial resolution — ERA5-Land provides a resolution of ~9 km, while our dataset achieves 1 km daily resolution, making it more suitable for agricultural and regional ecosystem applications.

(2) Finer vertical structure — reanalysis products (e.g., ERA5-Land) generally provide soil temperature at relatively broad layers (e.g., 0–7 cm, 7–28 cm, 28–100 cm, 100–289 cm), whereas our dataset delivers a more detailed profile at 0, 5, 10, 15, 20, and 40 cm, which better captures near-surface soil thermal dynamics critical for agriculture and ecosystem studies.

(3) Extensibility — The proposed spatially adaptive framework is modular and scalable, allowing the dataset to be readily extended both backward and forward in time as long as in-situ observations and corresponding environmental predictors are available. We are currently extending the dataset to cover 2001–2009 and plan to provide continuous annual updates in the future, with all versions to be openly released through the National Tibetan Plateau Data Center.

(4) Uniqueness — to the best of our knowledge, this is currently the only nationwide T_s dataset that combines high spatial resolution, multi-layer vertical profiles, and long-term temporal coverage.

In summary, this study not only introduces a new spatially adaptive modeling framework, but also delivers a nationwide T_s dataset that is unique in its resolution, depth coverage, and temporal span. We believe this dataset will provide significant value for agricultural production, ecosystem modeling, carbon budget assessments, and climate change research, and will serve a broad scientific and applied user community.