Reviewer 1: Comments and Suggestions

Comment 1.1

> The overall introduction & literature review is very poor and unacceptable. There is no any problem discussion or any research gap that justify the novelty and importance of the present study. How this kind of investigation was studied in the literature? Is there any similar published work? We cannot find any of these points in the manuscript.

Authors' response: We sincerely thank the reviewer for the valuable feedback. Following the suggestions, we have structured the review of existing studies to highlight the specific research gaps our study aims to address. We have also highlighted the unique contribution of this study. Given a chance to revise the manuscript, the introduction will include the following to address the reviewer's comments.

"Traditional methods such as the gravimetric technique, while accurate and low-cost, are destructive, time-consuming, and spatially limited. Indirect in-situ methods, especially Time-Domain Reflectometry (TDR), are widely used due to their precision and ease of deployment, though spatial coverage remains a constraint. Ground Penetrating Radar (GPR) offers broader spatial coverage but is less feasible due to its high cost and complexity [1]. To overcome these limitations, machine learning (ML) models emerged as powerful tools for estimating soil moisture. A comprehensive review by [2] showed that ML models like Random Forest, Neural Networks, and SVM are the most frequently applied for SM estimation, often using satellite-derived inputs. In a large-scale study using data from 1,722 ISMN stations, ensemble models such as KNR, RFR, XB achieved high predictive accuracy and outperformed individual models across climate zones [3]. However, these studies primarily focus on surface SM, with limited exploration of subsurface layers.

To estimate subsurface soil moisture (SSM), recent efforts have integrated remote sensing data with ML techniques. For example, [4] used RGB-thermal imagery and canopy characteristics to estimate SM at 10-40 cm depths in corn fields. While shallow depth predictions showed moderate accuracy ($R^2 = 0.79$), the performance declined at deeper layers ($R^2 = 0.69$). Similarly, [5] demonstrated that combining thermal and microwave retrievals in a data assimilation framework significantly improved root-zone SM estimates (R^2 increased from 0.51 to 0.73), though the approach relied on high-quality but often sparse inputs. Emerging deep learning models have further improved multi-depth SM estimation. [6] applied ANN and LSTM to predict subsurface soil moisture, achieving R^2 values of 0.80–0.98 depending on depth and model, though they used only daily-resolution data. [7] developed a dual-branch deep learning model (ALFSMP-DBCM) for alfalfa fields using half-hourly data, showing improved performance but the model is crop-specific and may not generalise well across other regions.

While these deep learning methods show promise, most models require manual tuning and are not automated, which limits their usability for broader applications. Addressing this, a recent study proposed an AutoML framework combining multi-source remote sensing, reanalysis, and field data to estimate SM at every 20 cm from 0-60 cm depth [8]. The model demonstrated moderate accuracy (R = 0.81–0.68) and still lacked performance at greater depths. In summary, although substantial progress is made using traditional, remote sensing, machine learning, and deep learning methods for soil moisture estimation, several challenges remain. These include reliance on manually designed workflows that are time-consuming, heuristic-based feature selection and hyperparameter tuning that may limit model robustness, and a narrow focus on specific crop types or short temporal datasets that fail to capture seasonal or event-driven soil moisture variability. Moreover, rainfall event-based modelling of subsurface soil moisture remains largely underexplored."

An automated machine learning (AutoML) approach, capable of integrating multiple input features and automating model selection and tuning, offers significant potential to overcome these limitations. By minimising manual effort and enhancing generalisability across soil depths, AutoML enables robust, high-resolution soil moisture predictions. Our manuscript clearly outlines how this approach stands apart from existing methods and addresses various research gaps.

Comment 1.2

> Description o the dataset is vague, basic in nature, and incomplete.

Authors' response: The current version of this manuscript provides a comprehensive and structured description of the dataset used in our study. This includes detailed information on all the hydrometeorological variables used in the study, the location and setup of the hydrometeorological observatory, and the specifications of the sensors and instruments deployed. Furthermore, we have clarified the temporal resolution of the data, as well as the approach used to segment the dataset into different scenarios for evaluating model performance. We believe this information provides a complete overview of the dataset in the context of our study objectives. However, if the reviewer think there are specific aspects that are missing or insufficiently explained, we will be happy to include any additional details as suggested to improve this section.

Comment 1.3

> The AutoML-SM bloc is unclear and it is poorly presented. The readers cannot understand how this kind of modelling farmwork can be an automated ML.

Authors' response: We acknowledge the reviewer's concern that the original description may not have sufficiently conveyed the operational workflow of our modelling framework.

To address this, we will revise and expand the current pseudocode to present a more detailed, step-by-step structure of the AutoML-SM framework. This revised pseudocode will clearly outline the key components, including data preprocessing, model selection, hyperparameter tuning using Bayesian Optimization, model evaluation, and final prediction steps. We will also present the results of each iteration performed by the model across different scenarios and soil depths to demonstrate its performance and consistency. Additionally, we will include flowchart of the methodology.

In Section 2.4 ("AutoML-SM Framework"), we will incorporate a concise yet informative explanation of Bayesian Optimization, describing how it is used to automatically explore different hyperparameters and identify optimal machine learning configurations without manual intervention. We will also include optimization curves for each soil depth (10, 20, 30, and 40 cm), showing the evolution of training loss over successive iterations of the optimization process (Figure 1) in the supplementary material. This will demonstrate how the proposed framework dynamically converges towards an optimal solution, thereby validating its automated and adaptive nature.

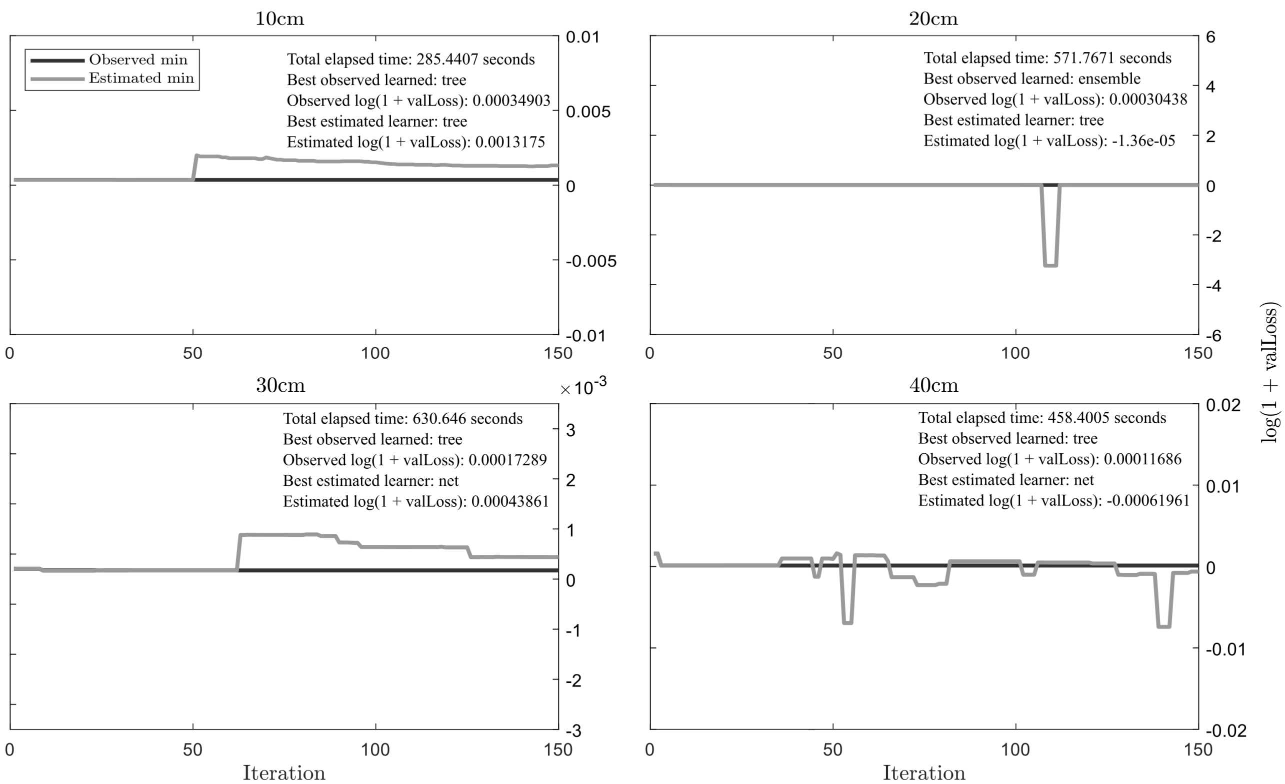

Figure 1: Optimisation curves showing the training loss during the selection of the optimal machine learning process as Bayesian Optimisation progresses for each soil depth.

We believe these additions will significantly improve the AutoML-SM framework, and make it more accessible to readers from both hydrological and machine learning backgrounds.

Comment 1.4

> The problem formulation seems to be standard and well known: linking an ensemble of input (relative humidity (RH), wind speed (WS), wind direction (WD), solar radiance (SR), evaporation (EV), rainfall (Rain), dew point (DP) and soil temperature at 10, 20, 30, and 40 cm depth (ST1, ST2, ST3 ST4)) to a target variable (soil moisture values at different depth). The physic phenomena behind the soil moisture variation are highly related to the weather variables especially to the rainfall, and any regression model developed based on this assumption seem to be trivial and in fact a standard problem formulation.

Authors' response: We respectfully acknowledge the reviewer's concern and would like to clarify that while the estimation of soil moisture using hydrometeorological variables may appear as a standard problem, our study introduces several novel aspects that differentiate it from conventional approaches.

First, our study is **event-based**, focusing on the detailed characterisation of single-peak and multi-peak soil moisture responses induced by rainfall events. Such an analysis is rarely emphasized in existing subsurface soil moisture studies and allow for a more intricate interpretation of soil behaviour, especially in complex soils such as black clayey soils, which exhibit unique shrink–swell and infiltration characteristics.

Second, the novelty of our study lies in the **AutoML-SM framework**, which automates model selection and hyperparameter tuning for each temporal scenario and soil depth, reducing subjectivity and bias. Additionally, we evaluate model performance across rainfall events of varying intensities to better capture soil moisture dynamics under diverse conditions.

Finally, we complement our proposed framework with **global feature sensitivity analysis** and **uncertainty analysis** to understand how individual input variables modulate soil moisture dynamics and small perturbations in input variables impact the accuracy of soil moisture predictions at various depths.

Overall, our approach introduces novel methodological and analytical contributions that advance the current state-of-the-art in subsurface soil moisture studies.

Comment 1.5

> Section results is poorly formulated and unclear. Models' evaluation ad comparison seem confusion. Necessary figures are missing, and numerical models' performances are incomplete.

Authors' response: We believe that the result section is structured in a logical and comprehensive manner. Specifically, we began with a detailed exploration of rainfall event dynamics to understand the surface to subsurface interaction of soil moisture during single and multiple peak events (subsection 3.1.1), followed by an assessment of autocorrelation and soil moisture memory to quantify moisture persistence through time-lagged correlation analysis (subsection 3.1.2).

Subsequently, we performed feature importance, global sensitivity, and feature association analysis to understand the relative contribution and interdependence of input variables in soil moisture prediction across multiple depths (subsection 3.2). This is followed by a systematic evaluation of our proposed model (AutoML-SM) across different scenarios and soil depths using various performance metrics, linear regression curve, and error histograms to visualise the predictive accuracy (subsection 3.3).

In the next section, we further analysed the model's performance during rainfall events of varying intensity- high, medium, and low (subsection 4.1). We also conducted a comparative analysis of AutoML-SM with five benchmark algorithms at each soil depth and reported the computational time of each model (subsection 4.2). To evaluate how input uncertainties propagate through the model, we performed uncertainty analysis (subsection 4.3), and assessed the robustness and generalisability of the model using random seed variation and performance tracking across multiple iterations through temporal distribution analysis (subsection 4.4). Lastly, we carried out an input ablation test to identify the minimal subset of input features necessary for near-optimal performance (subsection 4.5).

We have included relevant figures and tables reporting the performance metrics for all models considered. However, we would greatly appreciate further clarification regarding which specific figures or performance details were found to be missing or unclear. Given the opportunity to revise, we will be more than willing to incorporate any additional figures or data necessary to improve the presentation of our results.

Comment 1.6

> Models Interpretability and Explainability is completely missing. At this level of publication, the use of such techniques, i.e., SHAP and LIME is mandatory.

Authors' response:

We thank the reviewer for this valuable suggestion. We agree that model's interpretability and explainability are critical and to address this, we will incorporate SHAP (SHapley Additive exPlanations) and LIME (Local Interpretable Model-agnostic Explanations) techniques in our analysis.

SHAP (SHapley Additive exPlanations) quantifies the contribution of each feature to the model's prediction by comparing outputs with and without the feature. Specifically, it evaluates the difference in the model's prediction when a feature is included versus excluded and computes the Shapley value as a weighted average of these differences across all possible feature combinations. As an additive feature attribution method, the sum of all feature contributions closely approximates the model's original output. In our study, we will utilise the Tree SHAP implementation from the SHAP Python library [9] to efficiently compute Shapley values for tree-based models. To derive global feature importance, we will calculate the mean absolute Shapley values for each input variable, identifying those with the highest overall influence on soil moisture predictions [10]. We present the results using the same temporal dataset employed in our study, illustrated through a SHAP summary (Bee swarm) plot in Figure 2. Upon revision, we will extend this analysis using the expanded dataset and include the updated results in the revised manuscript.

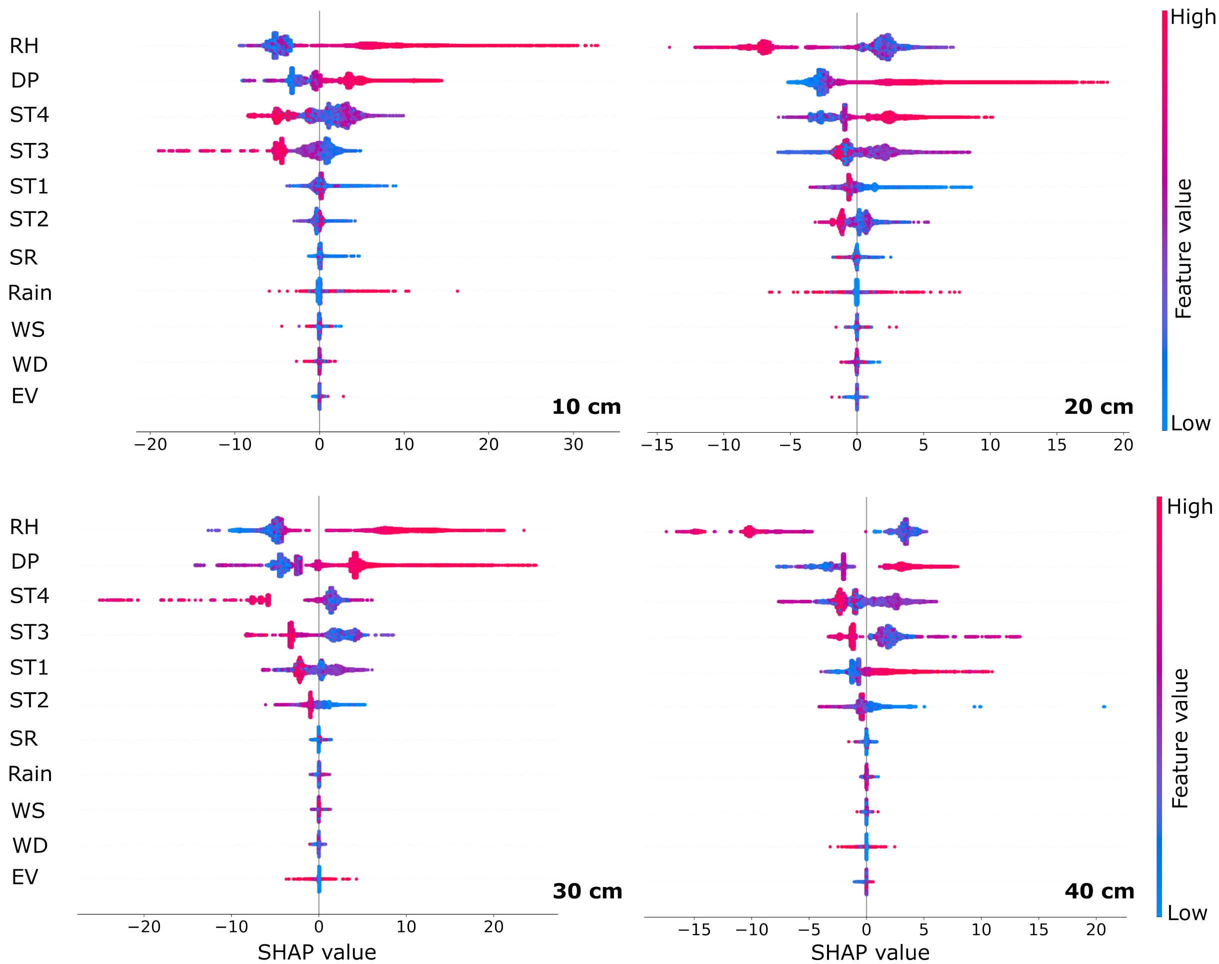

Figure 2: SHAP summary (Bee swarm) plot showing Shapley values for all the input features. In this plot, the features are arranged in decreasing order of importance in each subplot, highlighting the key drivers of soil moisture estimation across different depths.

To incorporate LIME (Local Interpretable Model-agnostic Explanations) in our study, we will first identify representative rainfall events across different temporal scenarios. For each selected event, we will extract corresponding feature vectors and apply LIME to generate locally interpretable surrogate models, typically linear regressions that approximate the AutoML model's behaviour in the vicinity of each prediction. These surrogate models will help isolate the contribution of individual input features to specific model outputs at different depths.

These additions will significantly enhance the transparency and interpretability of our AutoML-SM framework. By integrating both global (SHAP) and local (LIME) explanation techniques, we aim to strengthen the scientific robustness and practical applicability of our findings.

Comment 1.7

> The study focuses exclusively on black soil, which has unique characteristics, including high moisture retention capacity and shrinkage behaviour in alternate wetting and drying cycles. However, this is not adequately discussed when analysing infiltration or moisture dynamics.

Authors' response: We sincerely thank the reviewer for this thoughtful and important observation. We agree that the unique physical characteristics of black soil, particularly its high clay content play a critical role in governing infiltration dynamics and subsurface moisture behaviour, and this demands a critical explanation.

The black soil exhibit high water retention capacity but low permeability, resulting in reduced infiltration rates. Their shrink–swell behaviour under wetting and drying cycles leads to deep and wide cracks, which can influence preferential flow pathways and soil moisture redistribution after rainfall events. Moreover, their high bulk density and fine texture further contribute to delayed and prolonged moisture responses, particularly under intense or prolonged rainfall conditions.

In the revised manuscript, we will expand subsection 3.1.1 (Rainfall event analysis) to explicitly discuss how these physical properties influence the observed single-peak and multiple-peak soil moisture responses. We will correlate event-based infiltration behaviour with known characteristics of black soils, highlighting how soil structure, texture, and moisture retention capacity govern subsurface moisture variations under different rainfall regimes.

Additionally, to address the generalisability of our model both temporally and spatially, we will be extending this study on two additional sites in Africa: Kalipululira and Chipata. The data is accessible to us through Zambia metrological department. Kalipululira is located in the hot semi-arid steppe climate (BSh), and the Chipata in a tropical savannah climate (Aw). Both locations are characterised by red to brown clay-loamy soils. For the reviewer's reference, time series of soil moisture at multiple depths (10 cm, 20 cm, 30 cm, and 40 cm) for Chipata is shown in Figure 3. This will allow us to conduct a comparative assessment of model performance and soil moisture responses across different soil types, providing a better evaluation of our framework's adaptability beyond black soils.

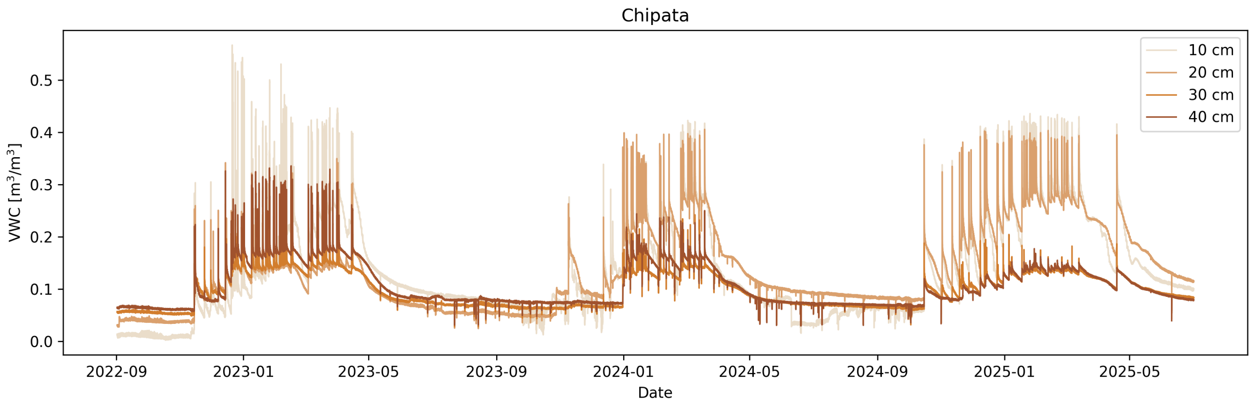

Figure 3: Time-series showing soil moisture variation across multiple soil depths (10 cm, 20 cm, 30 cm and 40 cm) at Chipata in Africa.

Comment 1.8

> There is no any discussion and comparison of the results with previous published paers.

Authors' response: We thank the reviewer for this useful feedback. We agree that discussing and comparing our results with previous studies is essential to highlight the relevance of our work. In the revised manuscript, we will incorporate a detailed comparison of our model's performance with those reported in relevant published studies, especially focusing on similar soil moisture prediction tasks. This will help to better contextualize the significance of our findings and demonstrate the effectiveness of the proposed approach.

References

[1] Pariva Dobriyal, Ashi Qureshi, Ruchi Badola, and Syed Ainul Hussain. A review of the methods available for estimating soil moisture and its implications for water resource management. *Journal of Hydrology*, 458:110–117, 2012.

[2] Abhilash Singh, Kumar Gaurav, Gaurav Kailash Sonkar, and Cheng-Chi Lee. Strategies to measure soil moisture using traditional methods, automated sensors, remote sensing, and machine learning techniques: review, bibliometric analysis, applications, research findings, and future directions. *Ieee Access*, 11:13605–13635, 2023.

[3] Qianqian Han, Yijian Zeng, Lijie Zhang, Calimanut-Ionut Cira, Egor Prikaziuk, Ting Duan, Chao Wang, Brigitta Szabó, Salvatore Manfreda, Ruodan Zhuang, et al. Ensemble of optimised machine learning algorithms for predicting surface soil moisture content at global scale. *Geoscientific Model Development Discussions*, 2023:1–40, 2023.

[4] Milad Vahidi, Sanaz Shafian, and William Hunter Frame. Depth-specific soil moisture esti-

mation in vegetated corn fields using a canopy-informed model: A fusion of rgb-thermal drone data and machine learning. *Agricultural Water Management*, 307:109213, 2025.

[5] Fuqin Li, Wade T Crow, and William P Kustas. Towards the estimation root-zone soil moisture via the simultaneous assimilation of thermal and microwave soil moisture retrievals. *Advances in Water Resources*, 33(2):201–214, 2010.

[6] Heechan Han, Changhyun Choi, Jongsung Kim, Ryan R Morrison, Jaewon Jung, and Hung Soo Kim. Multiple-depth soil moisture estimates using artificial neural network and long short-term memory models. *Water*, 13(18):2584, 2021.

[7] Rui Liu, Lifeng Lu, Yongqi Ge, Liguo Dong, and Juan Zhou. An approach for multi-depth soil moisture prediction in alfalfa based on a dual-branch combined model. *Computers and Electronics in Agriculture*, 222:109038, 2024.

[8] Shenglin Li, Yang Han, Caixia Li, and Jinglei Wang. A novel framework for multi-layer soil moisture estimation with high spatio-temporal resolution based on data fusion and automated machine learning. *Agricultural Water Management*, 306:109173, 2024.

[9] Scott M Lundberg, Gabriel G Erion, and Su-In Lee. Consistent individualized feature attribution for tree ensembles. *arXiv preprint arXiv:1802.03888*, 2018.

[10] Christoph Molnar. *Interpretable machine learning*. Lulu. com, 2020.