



# Multi-depth soil moisture dynamics to rainfall events: An automated machine learning approach

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**Abstract.** This study proposes an integrated, event-based framework for quantifying soil moisture dynamics at multiple depths (10, 20, 30, and 40 cm) in response to rainfall events using an automated machine learning (AutoML) approach. At the observatory we record the hydrometeorological and soil moisture data at different depth below the ground surface at every 10-minute intervals. We use these datasets to capture both rapid single-peak and gradual multiple-peak soil moisture responses during diverse rainfall events.

Recognising that manual model selection and hyperparameter tuning are labour intensive and may not fully capture the complex, non-linear interactions among hydrometeorological variables. Here we propose an AutoML framework that leverages Bayesian optimisation to predict subsurface soil moisture at different depths. The model was evaluated under four temporal scenarios: S1 (March-May), S2 (March-June), S3 (March-July), and S4 (March-August), for the full dataset and rainfall-only instances, separately. This automatic selection and tuning of various regression models result in superior predictive performance as compared to benchmark algorithms. The coefficients of determination ranges from 0.88 to 0.98 and minimal root mean squared errors (1.6%–3.4%). Further, the global sensitivity analysis indicates that the atmospheric humidity and dew point strongly influence near-surface moisture. The solar radiance and evaporation drive moisture depletion, and soil temperature gradients play a critical role in the vertical profile of the soil column. These findings highlight the value of integrating advanced AutoML techniques with event-based hydrological analysis to enhance our understanding of soil moisture variability, which has significant implications for water resource management, agricultural planning, and hazard mitigation in variable climatic regimes.

## 1 Introduction

Soil moisture governs the soil-water budget and influences vegetation growth, evapotranspiration processes, infiltration, runoff, and overall water fluxes between the land and the atmosphere (Myeni et al., 2019). Given that the effects of soil moisture on plant growth, drought management, and other hydrological processes vary with depth, accurate estimation at multiple levels (10 - 40 cm) becomes essential, particularly for the root zone (Xu et al., 2021).



Traditional methods for subsurface soil moisture estimation generally rely on empirical relationships (Pan et al., 2003) and physically based land surface models, which often require extensive data inputs (Pinnington et al., 2021) and may not adequately capture the complex, non-linear interactions between soil moisture and hydrometeorological variables (Liao et al., 2024). In contrast, data-driven approaches, particularly those employing machine learning algorithms, have demonstrated improved accuracy by integrating climate and soil parameters to derive soil moisture profiles at varying depths (Tian et al., 2020). However, selecting the optimal model and fine-tuning hyperparameters remain challenging due to regional variations and the inherent complexity of soil properties and processes (Zheng et al., 2025).

Automated Machine Learning (AutoML) has emerged as a promising solution to these challenges (Tayebi Arasteh et al., 2024). This automate the tasks of data preprocessing, algorithm selection, and hyperparameter tuning, thereby minimising user intervention while achieving optimal predictive performance (Singh et al., 2024). This approach not only enhances the robustness of soil moisture predictions but also streamlines the modelling process, making it highly suitable for complex environmental datasets where traditional models often struggle (Weerts et al., 2024).

This study proposes an AutoML-SM framework customise for predicting soil moisture at multiple depths, specifically at 10 cm, 20 cm, 30 cm, and 40 cm, using a suite of hydrometeorological variables. Evaluating the global sensitivity of each input variable on soil moisture by leveraging the partial dependency plot, the dynamics between the hydrometeorological variables in modulating moisture dynamics are explained. Moreover, our approach also highlights the detailed impact of individual rainfall events and focusses on analysing rainfall occurrences. Such analysis captures the rapid and discrete changes in soil moisture induced by individual rainfall events, providing deeper insights into processes like infiltration, runoff, and evaporation that are often masked in averaged datasets. Our contributions are four folds which address the following research questions;

- What is the global sensitivity of soil moisture estimation at various depths in response to fluctuations in the input variables?
- How does the tradeoff between rainfall frequency and soil moisture estimation accuracy become evident across different soil depths?
- How does rainfall magnitude quantitatively influence soil moisture estimates across varying soil depths?
- How do small perturbations in input variables impact the accuracy of soil moisture predictions at various depths?

Overall, the proposed AutoML-SM framework not only advances the methodology for multi-depth soil moisture prediction but also contributes valuable insights into the dynamic interplay between rainfall events and soil moisture variability, thereby supporting improved water management, crop planning, and hazard mitigation strategies.





## 2 Material and methods

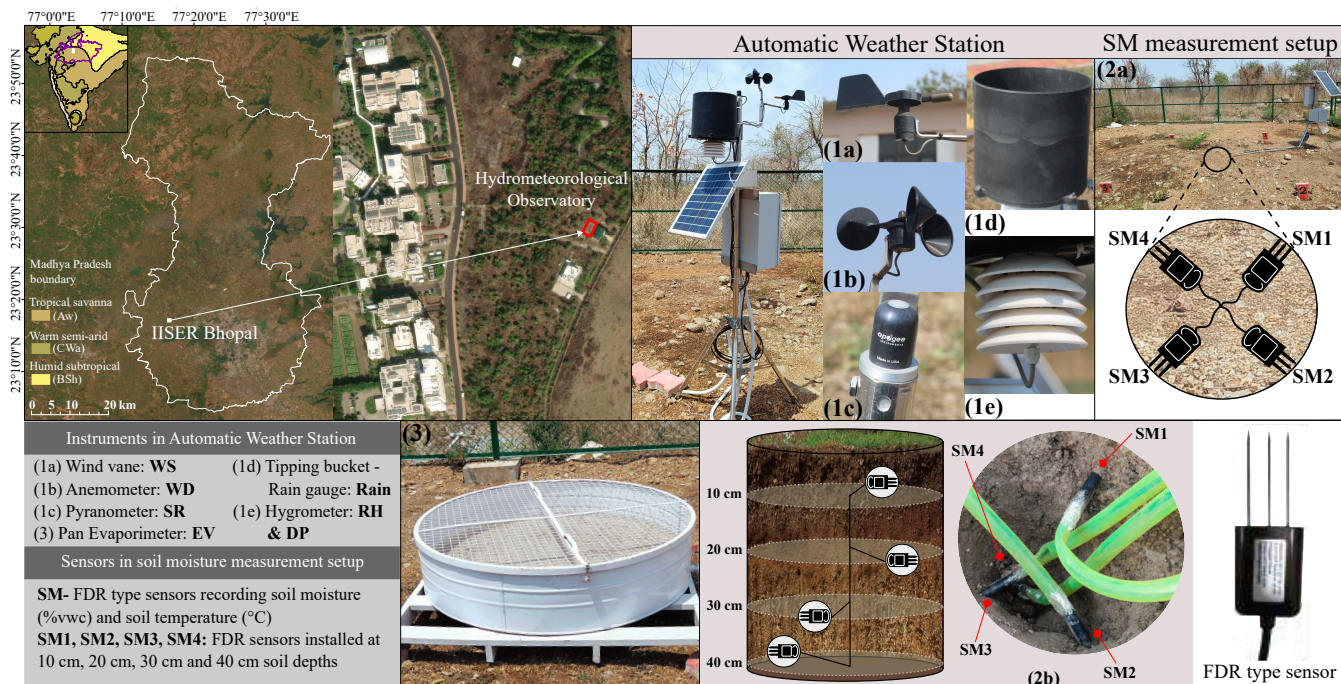
### 2.1 Experimental setup and dataset

We have setup a hydro-meteorological observatory (latitude 23.287°N and longitude 77.278°E) at the Indian Institute of Bhopal, Madhya Pradesh in Central India in February 2024. This is located in a semi-arid climatic region (ICAR-CRIDA, 2023). The dominant soil type at the observatory location is black soil which has formed due to the weathering of Deccan basalt. This soil type has a high moisture retention capacity with shrinkage characteristics in alternate wetting and drying periods. The observatory is equipped with an automatic weather station, a pan evaporimeter, and a soil moisture recorder (Figure 1). The weather station records hydrometeorological variables such as relative humidity (%), dew point (°C), and air temperature (°C) using a hygrometer, wind speed ( $\text{ms}^{-1}$ ) using an anemometer, wind direction (°) using wind vane, solar radiance ( $\text{Wattsm}^{-2}$ ) with pyranometer and rainfall (mm) with a tipping bucket rain gauge. The pan evaporimeter measures evaporation (mm), and the soil moisture recorder monitors soil moisture values (volumetric water content in %), and soil temperature (°C). Wind speed (WS) has a range of 0.5 to 67  $\text{ms}^{-1}$ , a resolution of 0.1  $\text{ms}^{-1}$ , and an accuracy  $> 0.5 \text{ ms}^{-1}$ . Wind direction (WD) covers a full 360-degree range with a resolution of 0.025 degrees and an accuracy of  $\pm 0.3\text{--}0.5\%$ . The rain gauge has a measurement capacity of 100  $\text{mmhour}^{-1}$ , resolution of 0.20 mm, with an accuracy of  $\pm 5\%$  at 25  $\text{mmhour}^{-1}$ . The Pan evaporimeter records evaporation (EV) within a range of 30 mm to 300 mm, resolution of 0.1 mm, and an accuracy of  $\pm 0.1\%$ . We installed four calibrated (both self- and cross-calibrated) Frequency Domain Reflectometry (FDR) soil moisture sensors in a dug pit at multiple depths i.e; 10, 20, 30, and 40 cm (Figure 1). The sensors were strategically placed in different orientations along the soil column under the assumption that the soil strata are homogeneous. Each sensor is capable of recording soil moisture from 0% to 100%, with a precision of  $\pm 2\%$  for moisture levels between 0-50% and  $\pm 3\%$  for levels between 50-100%. In addition, these sensors are equipped with temperature probes that record the soil temperature over a range of -40 to +60 °C.

The instruments are synchronized to record the data at every 10 minutes interval. In this study, soil moisture data at different depths serve as the response variable, while other hydrometeorological parameters are used as input features to train the AutoML-SM model. We used six months of time-series data from March to August 2024, a period considered sufficient to capture the transition from pre-monsoon to monsoon conditions in central India (Figure 2). The Indian Summer Monsoon season extends from June to September (JJAS). To further structure the analysis, we partitioned the dataset into four scenarios: S1 (March-May), S2 (March-June), S3 (March-July), and S4 (March-August). These scenarios were devised to reflect the progressive increase in rainfall events over time, thereby enabling an evaluation of the model's performance under varying rainfall intensity and frequency.

### 2.2 Soil moisture dynamics

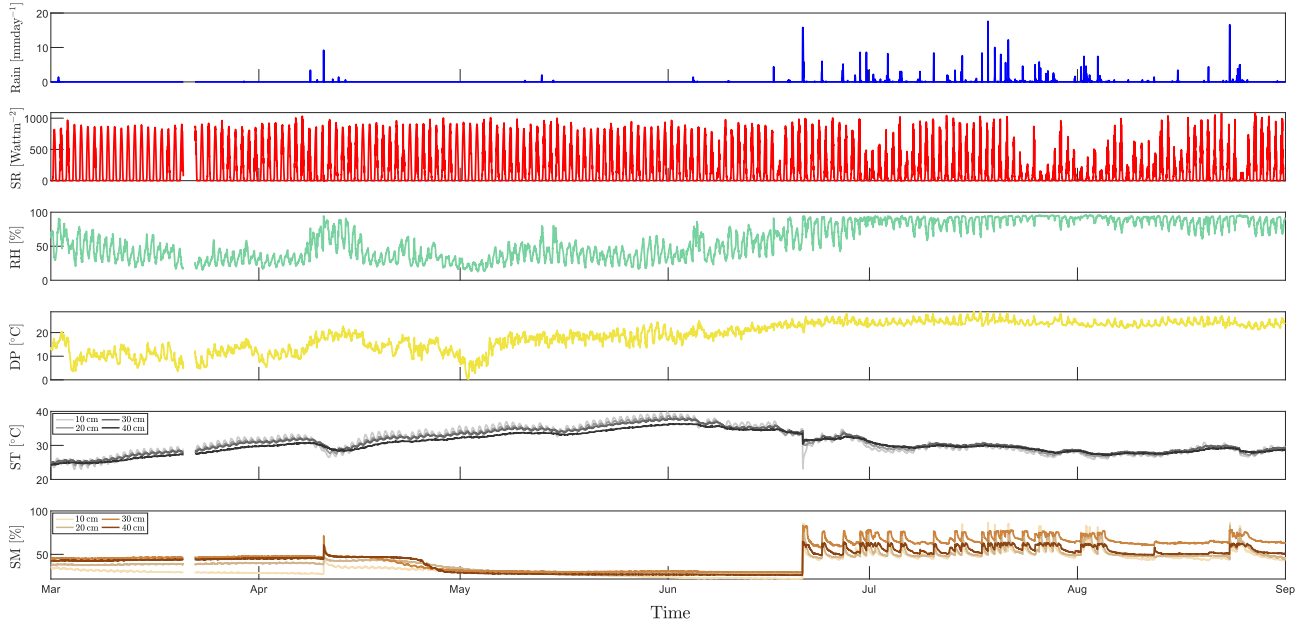
We analysed rainfall and soil moisture data recorded at the observatory to assess the dynamics of soil moisture in the study area. The objective was to critically investigate subsurface soil behaviour, particularly during the monsoon months when rainfall events are more frequent. To achieve this, we conducted a time-series analysis of soil moisture data recorded at 10-minute intervals at four distinct depths over a six-month period. Subsequently, we performed a rainfall event analysis by classifying



**Figure 1.** Hydrometeorological observatory at IISER Bhopal, Madhya Pradesh, India (Credit © Google Maps Platform). The top-left map provides a geographical reference, highlighting the observatory's location (red box) within the IISER Bhopal campus. The observatory includes (1) the Automatic Weather Station (AWS), (2) the soil moisture measurement setup, and (3) the pan evaporimeter. Instruments in the AWS (1a-1e) record various hydrometeorological parameters. Image 2a shows the sensor deployment site with a 2D schematic of sensor placement in a cross-arrangement. Image 2b (right to left) displays an FDR sensor image, an actual field deployment photograph, and a schematic representation of sensors installed at 10 cm (SM1), 20 cm (SM2), 30 cm (SM3), and 40 cm (SM4) depths.

events based on soil moisture peaks observed during periods of continuous rainfall. An event was defined as any time interval during which the cumulative rainfall exceeded 4 mm and induced a subsequent increase in soil moisture of at least  $\Delta 2$  units at the 10 cm depth (this threshold was not applied to other subsurface depths). For example, if rainfall recorded over an hour is 0.2, 0.4, 3, 2.6, 0.8, and 0.4 mm, and the corresponding soil moisture at 10 cm increases from 35 to 35.2, 38.5, 41, 42.2, and 42.3, respectively, the interval is flagged as an event. We further categorised these events into single-peak events, which exhibit one distinct rise in soil moisture, and multiple-peak events, which display two or more moisture peaks during the rainfall period.

We identified single-peak events based on the appearance of a distinct spike in soil moisture during continuous rainfall. Only events in which a significant change in soil moisture was observed at the topmost layer (10 cm depth) were selected. To ensure temporal distinction, events were classified as separate if the interval between two rainfall occurrences was five hours or more. To investigate soil behaviour across different depths during the monsoon, we calculated the cumulative rainfall associated with each event. This approach allows us to understand how rainfall intensity, duration and distribution influence moisture retention and movement across soil layers. The increase in soil moisture was quantified by subtracting the initial soil moisture value from the peak value attained during the event. Additionally, we observed extended periods of rainfall with varying intensities and minimal interruptions. If such periods triggered multiple soil moisture responses in the subsurface, particularly at the 10 cm



**Figure 2.** Time series of hydrometeorological variables, i.e., Rainfall (Rain), Solar Radiation (SR), Relative Humidity (RH), and Dew Point (DP). Soil Temperature (ST) and Soil Moisture (SM) are also shown for different subsurface depths (10 cm, 20 cm, 30 cm, and 40 cm). Data is recorded at 10-minute interval from March-Aug 2024.

depth, these occurrences were classified as multiple-peak events. To analyse these events comprehensively, we considered their entire duration, including all recorded rainfall instances at 10-minute intervals. For each instance, the change in soil moisture ( $\Delta$ ) was calculated as the difference between the soil moisture value at that timestamp and the initial moisture value for that particular depth at the start of the event.

Additionally, we applied the autocorrelation method to quantify soil moisture memory, which measures the persistence of soil moisture by evaluating the correlation between current and past values at specified time lags. The autocorrelation factor is computed using Eq. (1):

$$f = \sum \frac{(x_t - \mu)(x_{t+k} - \mu)}{\sigma^2}, \quad (1)$$

where  $x_t$  denotes the soil moisture value at time  $t$ ,  $k$  is the lag time,  $\mu$  is the mean of the soil moisture time series, and  $\sigma^2$  is its variance. Moreover, the memory timescale is determined as the time lag at which the autocorrelation factor decreases to  $1/e$  ( $\approx 0.37$ ) of its initial value ( $=1$ ) (Rahmati et al., 2024; Mujumdar et al., 2021). A higher autocorrelation thus indicates a longer soil moisture memory, reflecting prolonged retention of moisture in the soil.



### 110 2.3 Feature importance and global sensitivity

The relevance of input features is critical for improving model predictions. To identify the most and least influential factors, we performed a feature importance analysis. In this context, a higher feature score indicates a greater impact on the model's output. We employed a regression-tree ensemble approach to compute a feature score for each input variable (Singh et al., 2023). This method iteratively identifies and compensates for weaknesses in the initial decision tree, progressively strengthening the model.

115 The importance score is then evaluated using Eq. (2):

$$\Delta R = \frac{R_p - (R_{c_1} + R_{c_2})}{R_T}, \quad (2)$$

where  $\Delta R$  represents the total change in node risk normalised by  $R_T$ , the total number of branches;  $R_p$  is the risk associated with the parent node, and  $R_{c_1}$  and  $R_{c_2}$  are the risks for the child nodes.

The feature importance analysis ranks features by importance but doesn't fully capture complex, non-linear interactions among predictors. To overcome these limitations, we performed a global sensitivity analysis using Partial Dependency Plots (PDP). PDPs illustrate the marginal effect of a given input feature on the predicted response by averaging out the influence of other variables. In doing so, they reveal the overall trend, whether increasing or decreasing, of each input feature on the response variable (Singh et al., 2024; Kumar et al., 2024). The PDP for any  $T^{th}$  feature is approximated by Eq. (3):

$$f(f_T) \approx \frac{1}{N} \sum_{i=1}^N f(f_T, F - f_T), \quad (3)$$

125 where  $f(\cdot)$  denotes the mapping function and  $N$  is the total number of observations.

Errors in model estimates can be partly attributed to high correlations among input features, which may introduce uncertainty and instability (Nagar et al., 2023). To address this, we construct a feature association matrix that quantifies the inter-correlation between input features (Singh et al., 2024). The association between any two input features, denoted as  $a$  and  $b$ , is computed using Eq. (4):

$$130 P_a = \frac{\min(P_{c_1}, P_{c_2}) - (1 - P_{c_{1a}, c_{1b}} - P_{c_{2a}, c_{2b}})}{\min(P_{c_1}, P_{c_2})}, \quad (4)$$

where  $P_{c_1}$  and  $P_{c_2}$  represent the proportions of observations associated with the children nodes  $c_1$  and  $c_2$ , respectively.

### 2.4 AutoML-SM framework

An event-based study of rainfall and soil moisture dynamics is crucial for understanding the temporal and spatial variability of subsurface water content. However, traditional methods may not fully capture the complex, non-linear interactions between rainfall events and soil moisture, particularly given the high-frequency, heterogeneous nature of in-situ measurements. Therefore, to complement our event-based analysis, we developed an automated machine learning framework (the AutoML-SM model) to predict soil moisture at multiple depths using in-situ soil moisture data and various hydrometeorological variables.



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**Algorithm 1** Pseudo-code for AutoML-SM for multi-depth soil moisture estimation

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**Require:** Dataset (Input features: 11), Depths  $D = \{10, 20, 30, 40\}$  cm, and soil moisture (SM; as response variable)

**Ensure:** best\_models (Best models for each depth and condition) and best\_hyperparams (Best hyperparameters for each model)

```
1: Function AutoML-SM(data, SM)
2:   best_models  $\leftarrow \emptyset$ 
3:   best_scores  $\leftarrow \emptyset$ 
4:   (rain_data, overall_data)  $\leftarrow$  split_by_rain(data)
5:   for each  $d \in D$  do
6:     for each condition in {rain, overall} do
7:       (train_data, val_data)  $\leftarrow$  split_dataset(condition_data, 0.7)
8:       algorithms  $\leftarrow$  [FFNN, SVR, GPR, RF, Boosting EL, BDT, LR, KR]
9:       best_model  $\leftarrow$  None
10:      best_score  $\leftarrow -\infty$ 
11:      for each algorithm in algorithms do
12:        best_hyperparams  $\leftarrow$  bayesian_hyperparameter_tuning(algorithm, train_data, SM)
13:        score_sum  $\leftarrow 0$ 
14:        for each fold in cross_validation_folds(train_data, num_folds) do
15:          model  $\leftarrow$  algorithm.train(fold.train_data, SM, hyperparameters=best_hyperparams)
16:          fold_score  $\leftarrow$  algorithm.evaluate(fold.val_data, SM)
17:          score_sum  $\leftarrow$  score_sum + fold_score
18:        end for
19:        avg_score  $\leftarrow$  score_sum / num_folds
20:        if avg_score > best_score then
21:          best_score  $\leftarrow$  avg_score
22:          best_model  $\leftarrow$  model
23:        end if
24:      end for
25:      best_models[d, condition]  $\leftarrow$  best_model
26:    end for
27:  end for
28:  Return best_models
29: Function bayesian_hyperparameter_tuning(algorithm, train_data, SM)
30:   hyperparameter_space  $\leftarrow$  algorithm.get_hyperparameter_space()
31:   Define objective_function(hyperparams):
32:     model  $\leftarrow$  algorithm.train(train_data, SM, hyperparameters=hyperparams)
33:     score  $\leftarrow$  algorithm.evaluate(val_data, SM)
34:   Return score
35:   best_hyperparams  $\leftarrow$  bayesian_optimisation(objective_function, hyperparameter_space)
36:   Return best_hyperparams
37: Function bayesian_optimisation(objective_function, hyperparameter_space)
38:   best_hyperparams  $\leftarrow$  optimize(objective_function, hyperparameter_space)
39:   Return best_hyperparams
```

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This model is essential because it automates data pre-processing, model selection, and hyperparameter tuning, thereby ensuring robust and scalable predictions under varying climatic conditions. It involved training and evaluating several regression learn-





ers, including gaussian process regression, support vector regression, ensemble learning, kernel regression, decision tree, linear regression and feed-forward neural network (FFNN) (Singh et al., 2024; Singh and Gaurav, 2023; Singh et al., 2022, 2021; Turon et al., 2023; Eldeeb and Elshaw, 2024). The model used 11 hydrometeorological parameters, 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) as the input features and soil moisture values at each depth as the target variables. The data was preprocessed by standardising the input features and the response variable by using z-scores to ensure consistent scaling. The total number of observations used to train and test the proposed framework count to 12998 for S1, 17313 for S2, 21777 for S3, and 26241 for S4 scenario, respectively. Further, the data was split into training (70%) and testing (30%) subsets. The training data was then used to build the predictive model, which facilitates the automated selection and optimisation of regression algorithms. Additionally, this model encompasses use of Bayesian optimisation for hyperparameter tuning of various regression algorithms, automating both algorithm selection and fine-tuning. This minimises computational cost and ensures the model with the best predictive performance and lowest error is chosen (Singh et al., 2024). A pseudo-code for the proposed framework is illustrated in Algorithm 1.

### 3 Results

#### 3.1 Soil moisture dynamics

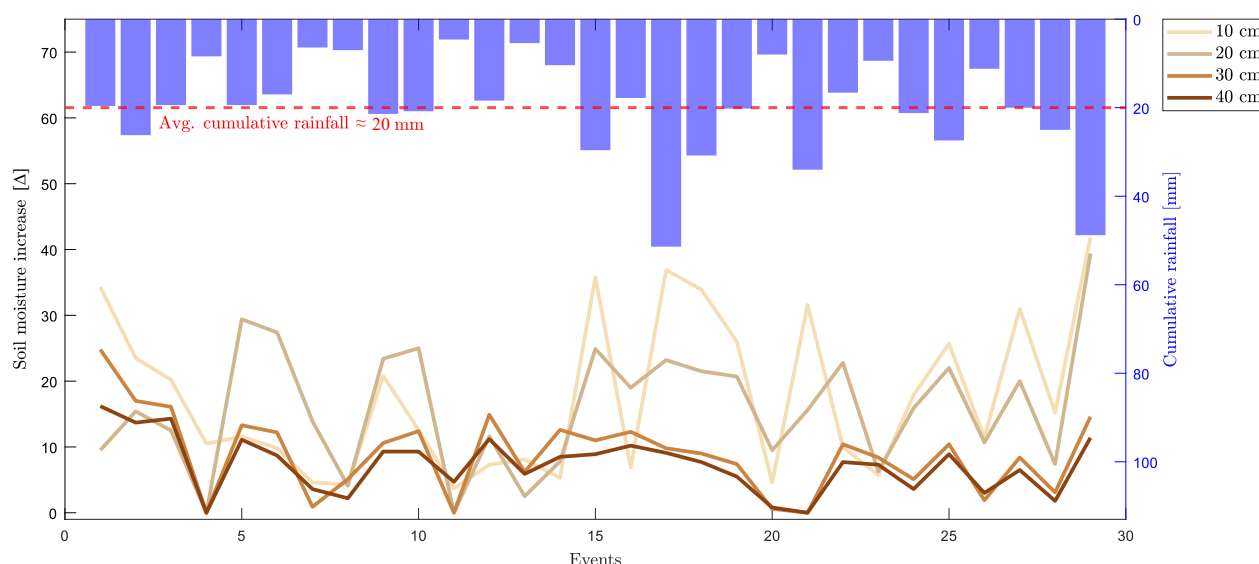
##### 3.1.1 Rainfall event analysis

###### – Single peak events

We identify a total of 29 events in which continuous rainfall initiates a single soil moisture peak at different soil depths (Figure 3). The blue bars represent cumulative rainfall for each event, with an average rainfall threshold  $\approx 20$  mm marked by a red dashed line. The soil moisture change ( $\Delta$ ) observed in multiple layers range as follows:  $3.5 < 10 \text{ cm} < 42$ ,  $0 < 20 \text{ cm} < 39.5$ ,  $0 < 30 \text{ cm} < 25$  and  $0 < 40 \text{ cm} < 16.3$ . In total, 13 events exceed the cumulative rainfall threshold. The response stimulated by rainfall in these events clearly highlights a rapid increase in soil moisture levels, especially at 10 and 20 cm depth, as soon as cumulative rainfall exceeds the threshold. However, this rise is followed by the sudden drop of 10-30 units at the top depth for the events that fall below the threshold. The topmost depth consistently exhibits the highest moisture response, followed by progressively dampened responses at deeper layers. This trend highlights the greater sensitivity of the surface soil to rainfall and suggests slower infiltration or restricted percolation into deeper layers due to soil properties.

###### – Multiple peak events

We classify three distinct multiple peak events with different durations and intensities of rainfall. The first event shows high-intensity rainfall occurring over a short duration of 4 hours and 20 minutes (Figure 4). This event records a maximum rainfall of 15.8 mm in an instantaneous time interval. During this high-intensity, short-duration rainfall event, a substantial downpour of approximately 15 mm triggers a sharp rise in soil moisture, particularly at the 10 cm depth,

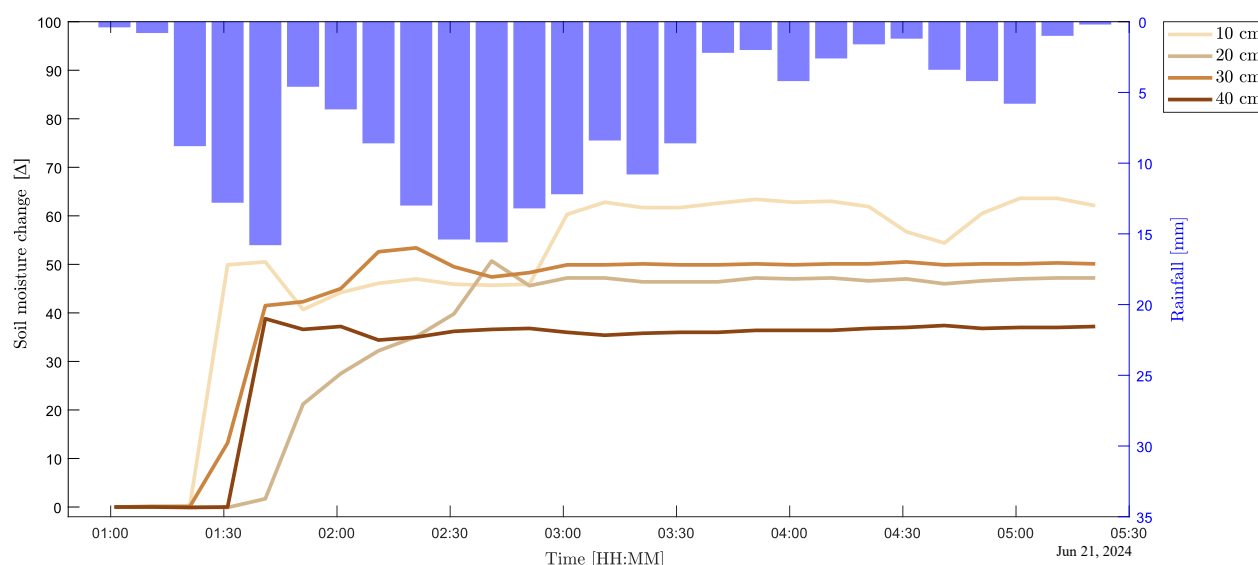


**Figure 3.** Soil moisture change in rainfall events initiating a single peak response at all depths. The red dotted line shows the average cumulative rainfall of all 29 events.

which exhibits the most pronounced change, reaching around 50 units. The response at deeper layers is delayed, with moisture changes at 20 cm and 30 cm occurring approximately 60 minutes and 30 minutes later, respectively. Notably, the magnitude of change is higher at 30 cm ( $\approx 53$  units) compared to 20 cm ( $\approx 50$  units), indicating a slower infiltration rate, causing moisture to accumulate more gradually in the subsurface layers. At 40 cm depth, response to the initial rainfall is observed, with soil moisture increasing by about 39 units. As rainfall intensity once again exceeds 15 mm, the surface layer (10 cm) experiences another peak, with moisture levels rising by approximately 63 units from pre-event conditions. However, despite continued rainfall, soil moisture at the deeper layers remains relatively stable, suggesting that these layers reached saturation. In the later part of the event (post-04:00 AM), minor fluctuations are observed at 10 cm, emphasising the sensitivity of the topmost layer to even slight variations in rainfall.

The second event exhibits medium-intensity rainfall occurring over a long duration of 7 hours (Figure 5). This event records a maximum rainfall of 5.8 mm in a single logging interval. During this event, soil moisture changes at multiple depths as precipitation reaches 5.8 mm (primary peak). The most prominent increase occurs at 10 cm, peaking at 29 units about 30 minutes after the maximum rainfall. Moisture levels start declining once rainfall intensity drops below 0.1 mm/min. At 20 cm, the response is quicker, occurring just 10 minutes after peak rainfall, but with a lower magnitude ( $\approx 19$  units) than the surface layer. The moisture change (6 units) is observed at 30 cm, while the 40 cm depth shows only a minimal increase ( $\approx 2$  units) after 20 minutes. The 10 cm layer, being more exposed to evaporation, can experience an initial delay in moisture retention as some water moves downward before equilibrium is reached. Once the infiltration front saturates lower layers, the moisture percent increase at the top layers. However, this may also be due to preferential

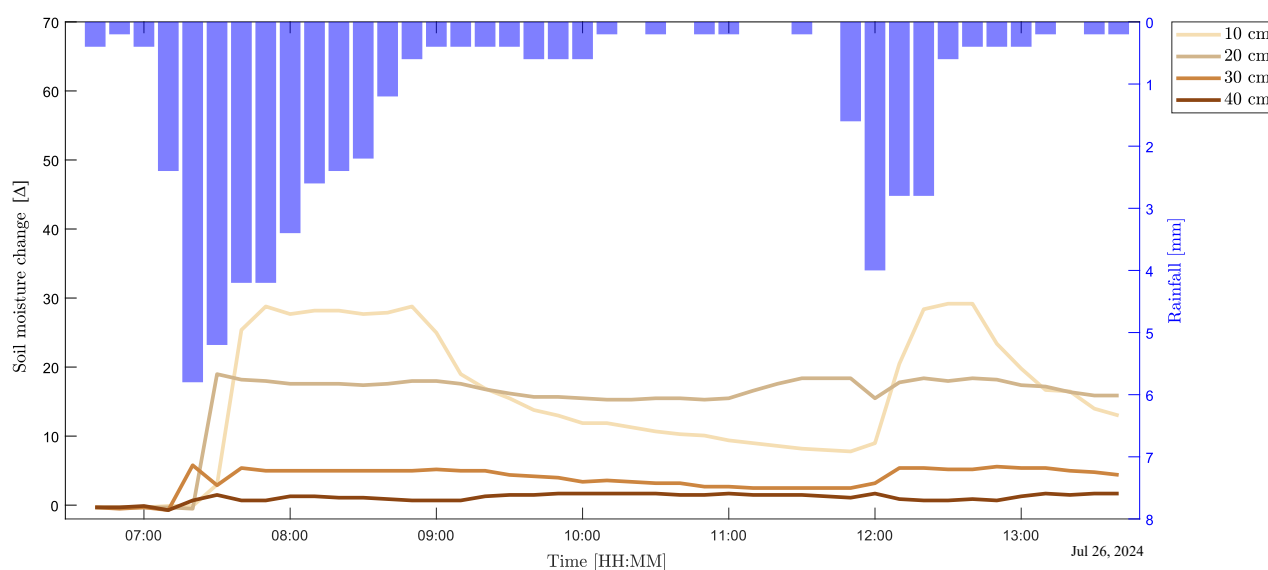




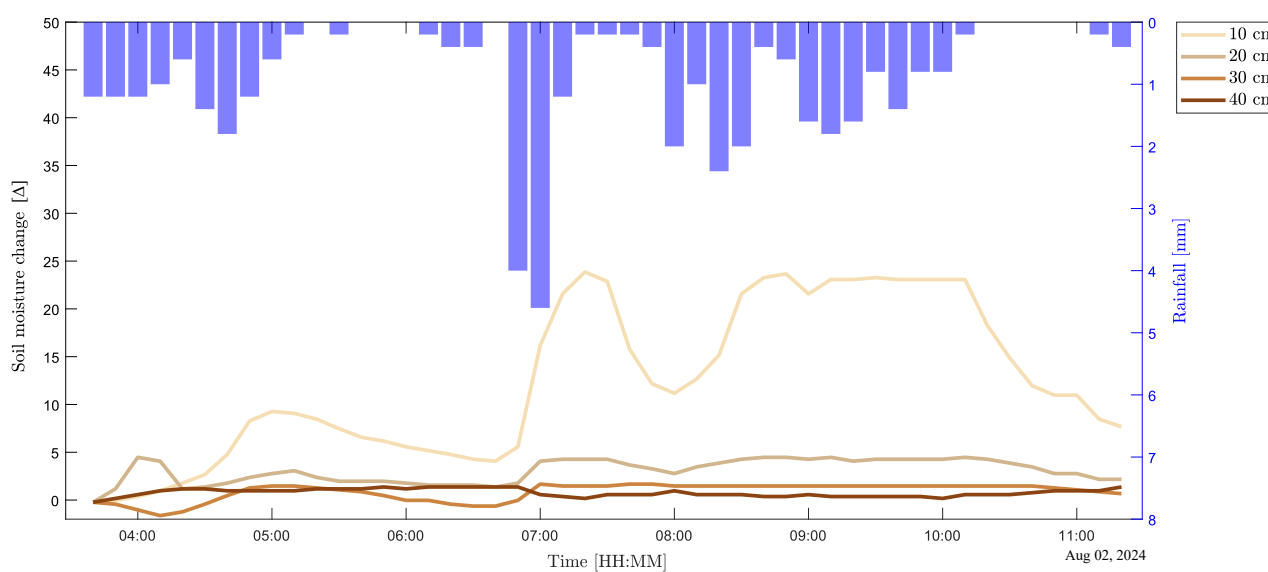
**Figure 4.** Soil moisture response at multiple soil depths in the high-intensity, short-duration type multiple peak event.

flow paths or macro pores present in the soil matrix. During the secondary peak of rainfall (4 mm), the 10 cm layer exhibits another sharp rise of 29 units relative to pre-event levels. However, following the primary peak, moisture initially drops by 20 units before increasing by 9 units in the secondary peak. At 20 cm, moisture declines gradually from the primary peak, showing only a slight increase with the secondary peak. A similar minor rise occurs at 30 cm, while changes at 40 cm remain minimal which indicates that much of the rainwater had already infiltrated or redistributed within the soil during the primary peak.

The third event shows its likeness to the second, lasting for a long duration of 7 hours and 40 minutes, although with low-intensity rainfall persisting throughout the event (Figure 6). This event records a maximum rainfall of 4.6 mm in a single logging interval. In this low-intensity, long-duration event, three distinct sets of rainfall instances lead to noticeable soil moisture peaks. Following the first peak of rainfall (1.8 mm), moisture at 10 cm depth increased by 9.5 units, occurring 20 minutes after the peak and 80 minutes after the event began. At 20 cm, moisture initially rises by  $\approx 3$  units at the event's onset but declines rapidly, later showing a slight increase of ( $\approx 2$  units) after the first peak. Changes at 30 and 40 cm depths are minimal. During the second peak of rainfall (4.6 mm), the 10 cm layer exhibits a significant rise of 24 units from pre-event levels and 20 units from just before the peak. At 20 and 30 cm, minor increases of 2.5 and 2 units, respectively, are observed, while the lowest depth shows no significant response. The final peak (2.4 mm) has its primary effect on the 10 cm layer, where moisture increases by 24 units from pre-event conditions and 12 units just before this set of rainfall, with stable moisture levels throughout this period. However, it declines once rainfall ceases. Other depths show no significant fluctuations during the third peak.



**Figure 5.** Soil moisture response at multiple soil depths in the medium-intensity, long-duration type multiple peak event.



**Figure 6.** Soil moisture response at multiple soil depths in the low-intensity, long-duration type multiple peak event.



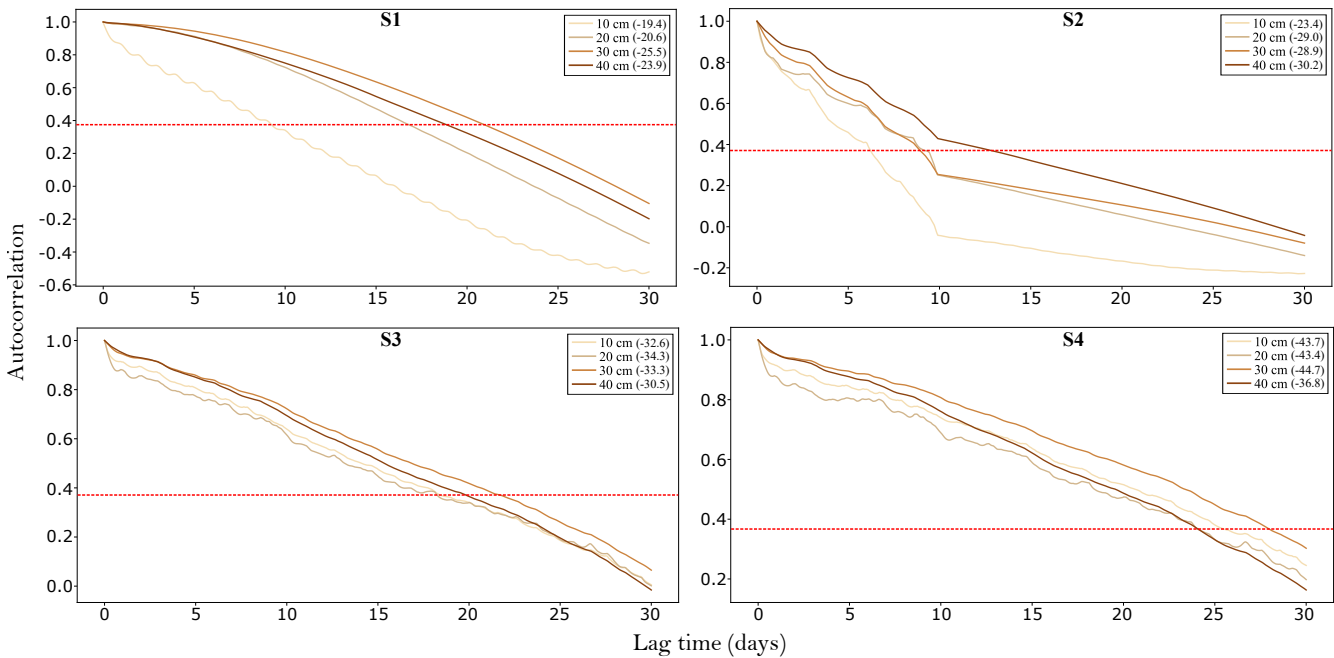
### 3.1.2 Autocorrelation and Soil moisture memory

The autocorrelation versus lag time curves (Figure 7) illustrate soil moisture memory across multiple depths under different conditions. The red dotted line marks the threshold value ( $\approx 0.37$ ) for autocorrelation. The lag time at which the autocorrelation drops below this threshold represents soil moisture memory, indicating how long past moisture conditions continue to influence current values. In S1, the soil moisture at a depth of 10 cm retains influence for approximately 9 days before dropping below the threshold. Similarly, for depths of 20 cm, 30 cm, and 40 cm, the corresponding lag times are around 17, 21, and 19 days, respectively. This pattern is further supported by the slope of the curves, which indicates the rate of moisture loss, with more negative slopes reflecting a slower decline in autocorrelation and longer memory (30 cm (-25.5) > 40 cm (-23.9) > 20 cm (-20.6) > 10 cm (-19.4)). Thus, shallower depths exhibit shorter soil moisture memory, whereas deeper layers retain moisture for extended periods, with the 30 cm depth demonstrating the greatest retention.

In S2, the lag time for each depth decreases compared to S1. For 10 cm, it reduces to  $\approx 7$  days while 20 cm and 30 cm declines to  $\approx 9$  days. 40 cm depth also show a reduction in lag time ( $\approx 13$  days). The slope of each curve also follows a similar trend: 40 cm (-30.2) > 20 cm (-29.0) > 30 cm (-28.9) > 10 cm (-23.4). The possible explanation for this observation is that S2 constitutes data from March to June, which marks the transition into the monsoon season, bringing irregular but intense rainfall. This combination of high pre-monsoon evaporation and early rainfall events may cause frequent moisture variations because, in the peak summer months, the soil is drier due to limited availability of water, and moisture loss occurs primarily through evaporation or evapotranspiration while at the onset of monsoon, drainage flux increases which is a faster process leading to a shorter soil moisture memory (Rahmati et al., 2024; McColl et al., 2017a, b). This also justifies the longer soil moisture memory in S1 due to the inclusion of dry months (March-May).

In S3, the lag time for 10 and 20 cm increases to approximately 18 days each, while 30 cm and 40 cm extend to around 22 and 20 days, respectively. The slope values follow the order: 20 cm (-34.3) > 30 cm (-33.3) > 10 cm (-32.6) > 40 cm (-30.5). In this scenario, the slope values do not align with the soil moisture memory effect. This can be attributed to the changing trends of the autocorrelation curves for 10, 20, and 40 cm depth past the threshold line. The 20 cm depth has the most negative slope yet a shorter lag time than 30 cm, implying its being influenced by rapid infiltration, drainage, and increased interaction with the atmospheric conditions, leading to fluctuating moisture availability. However, its decline is more gradual compared to other depths. Conversely, 40 cm depth has the least negative slope but a longer lag time than the shallower depths, suggesting that its loss rate is relatively steady but it retains moisture for a longer period, likely due to reduced evaporation and slower percolation at greater depths.

In S4, the lag time increases further, with 10 cm and 30 cm reaching about 25 and 28 days, respectively, while 20 cm and 40 cm show a similar duration of  $\approx 24$  days. The slope values range from 30 cm (-44.7) > 10 cm (-43.7) > 20 cm (-43.4) > 40 cm (-36.8). Since this scenario includes peak monsoon months, frequent and intense rainfall events lead to soil saturation, reducing the rate of moisture loss. As a result, the soil retains moisture for an extended period across all depths, with higher water availability minimising the impact of evaporation and drainage contributing to the increased lag time observed.



**Figure 7.** Autocorrelation - lag time curves of soil moisture at different depths (10 cm, 20 cm, 30 cm, and 40 cm) for scenarios S1, S2, S3, and S4. The red dotted line indicates the threshold value ( $\approx 0.37$ ) for autocorrelation used to estimate soil moisture memory. Slope values (in parentheses) represent the rate of decline in autocorrelation at each depth.

### 3.2 Feature importance, global sensitivity, and association

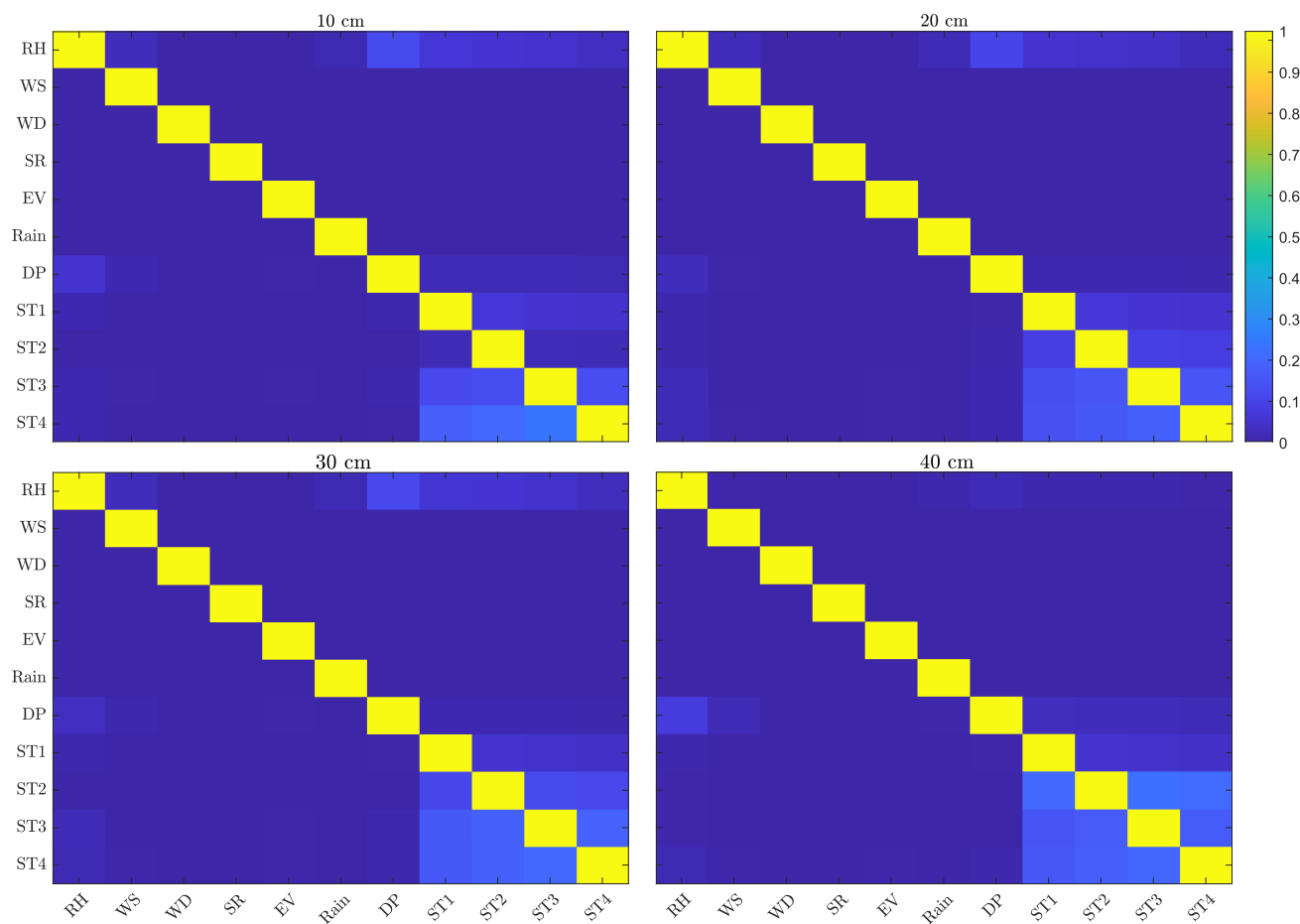
The radar plot shows the importance score of each input feature in soil moisture variability across multiple soil layers in different scenarios (Figure 8). RH shows a higher importance score, particularly at depths of 10 and 30 cm for S3 and S4, indicating its strong influence on surface and shallow soil moisture with increasing rainfall instances. WS and WD exhibit minimal importance, suggesting that these factors play a negligible role in determining soil moisture variability. SR demonstrates moderate importance, particularly for the top depth in S3 and S4. This is expected, as solar radiation directly affects surface evaporation and soil temperature, thereby influencing near-surface moisture levels. Subsurface depths of 20 and 40 cm depth also show a considerable influence of SR in S4. EV is a crucial factor for soil moisture variability, particularly at depths of 10 and 20 cm in S1 and S2, where it reflects the interaction between surface water loss and soil water content. The role of EV increases at 10 cm for S3 and decreases for S4, whereas it shows a slight increase at 20 cm for S4. This may be because of more rainfall instances in S4, affecting overall evaporation in monsoon months. However, for deeper layers (30 and 40 cm), EV remains mostly similar in the two scenarios. RAIN emerges as one of the most significant features across all scenarios, especially at 10 cm, highlighting its direct role in replenishing soil moisture near the surface. From S1 to S4, the importance of RAIN progresses at all depths except for 30 cm, where it remains mostly constant. This can be attributed to frequent rainfall events in the latter scenarios, with high infiltration playing a critical role in moisture variability at deeper layers. DP also holds notable



**Figure 8.** Feature importance score of each hydrometeorological predictor at multiple soil depths for scenarios S1, S2, S3, and S4.

importance across all scenarios, prominently at 10 and 30 cm in S2 and at 20 cm in S3. However, the importance value at all depths is slightly reduced in S4. Among soil temperature variables, ST1 is important in affecting soil moisture variation in all the scenarios across all depths. ST2 shows a high value at 20 cm and 30 cm for S3 and S2, respectively, whereas ST3 shows notable importance at 20 cm and 40 cm in S2 and moderate importance at 30 cm in S3 and S4. ST4 highlights relatively higher importance across all depths in S1, which reduces to minimal value in further scenarios.

We also performed the global feature sensitivity analysis to evaluate the impact of each input feature on soil moisture prediction at multiple soil depths using the Partial Dependency Plot (PDP) and Individual Conditional Expectation (ICE) curves (Figures 10 and 11). RH and DP show a strong positive trend across all the soil depths. When RH exceeds 80%, and DP surpasses 20°C, the peaks align closely with increased soil moisture levels as higher humidity and dew point temperature result in greater soil moisture retention. WS has a minor influence on soil moisture variation. At shallower depths (10 cm and 20 cm), soil moisture increases when WS ranges between  $\approx 0-5 \text{ ms}^{-1}$  but declines beyond  $6 \text{ ms}^{-1}$ . In deeper layers (30 cm and 40 cm), no clear trend is observed for  $WS \approx 0-3 \text{ ms}^{-1}$ , though a slight decrease occurs at higher wind speeds. Despite these

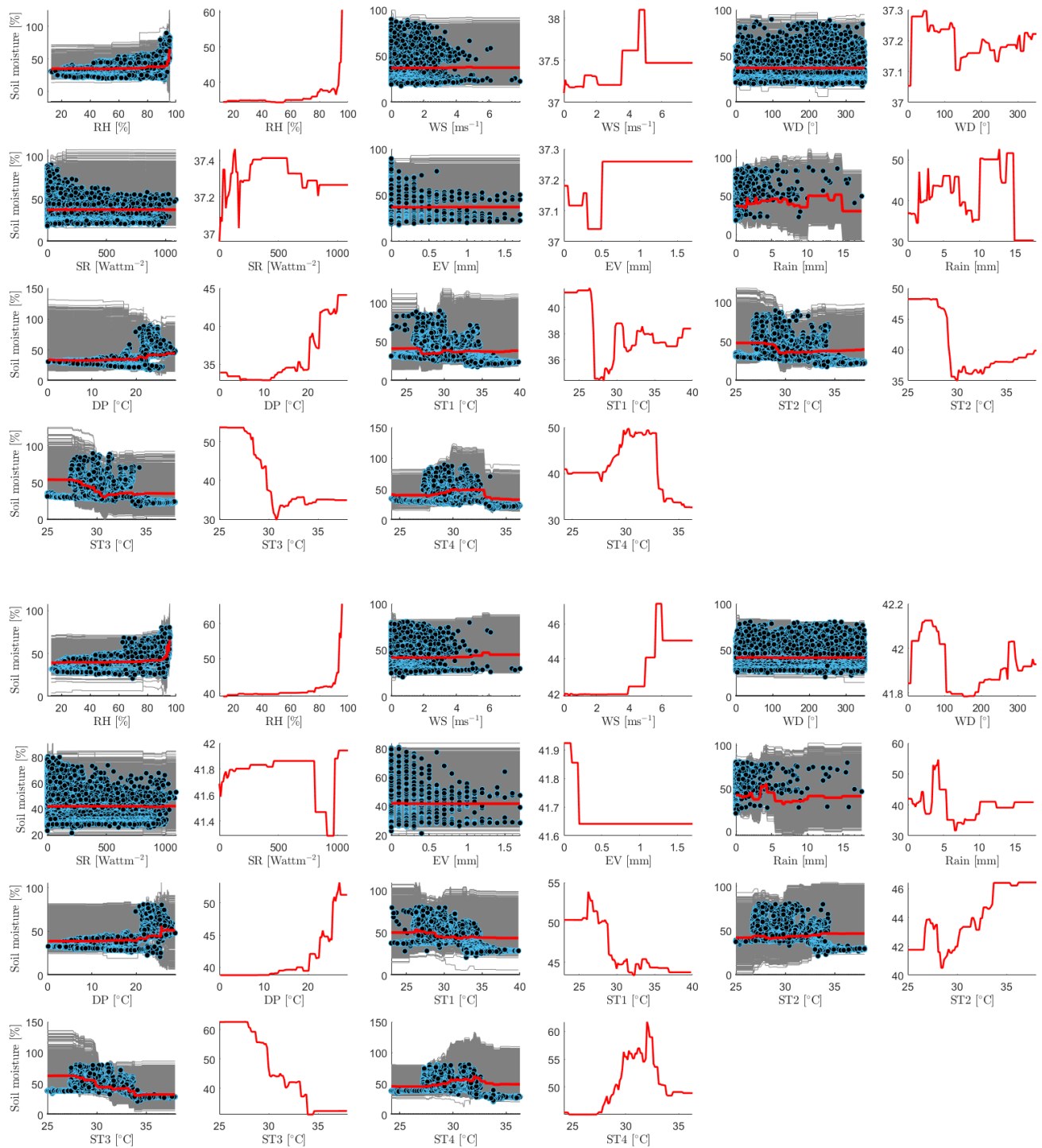


**Figure 9.** Feature association estimates for different soil depths.

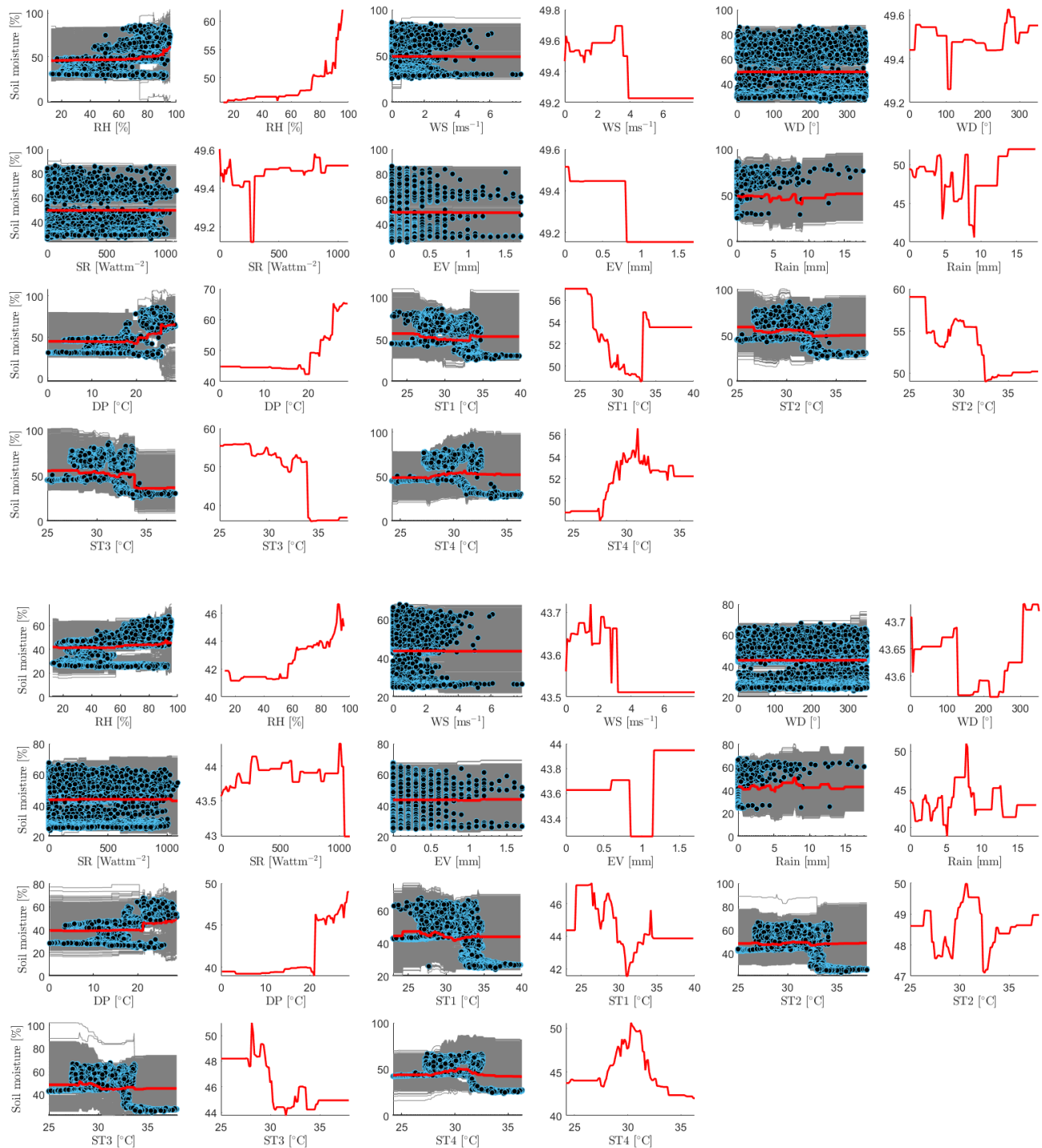
small fluctuations, the results suggest that increased wind speed contributes to soil moisture reduction. No strong correlation is evident between soil moisture and WD as it shows undulating behavior across all the soil depths within a minimal moisture range with no significant trend.

SR exhibits fluctuating trends across different depths. At shallower depths, soil moisture increases when SR is below 500  $\text{Wattsm}^{-2}$  but declines as SR rises further. At 30 cm, no clear impact is observed, while at 40 cm, minor variations occur between 0–1000  $\text{Wattsm}^{-2}$ , followed by a sharp decrease. This behavior suggests that high solar radiance results in the gradual drying of soil moisture, especially at shallower depths. EV shows a negative correlation with soil moisture at all depths, with an initial decline followed by a static trend. As EV increases from 0 to 0.5 mm at 10 cm, 0 to 0.2 m at 20 cm, 0 to 0.8 mm at 30 cm, and 0 to 1.2 at 40 cm, soil moisture decreases overall with small variations in between, which further stabilizes at higher evaporation values. This trend indicates that soil moisture depletion is most pronounced at lower evaporation rates, after which the system reaches a state of equilibrium where further increases in evaporation do not significantly impact soil





**Figure 10.** Global feature sensitivity analysis for hydrometeorological predictors using partial dependency plot (red line) and individual conditional expectation curve (gray lines) for 10 cm (top panel) and 20 cm (bottom panel) soil depth.



**Figure 11.** Global feature sensitivity analysis for hydrometeorological predictors using partial dependency plot (red line) and individual conditional expectation curve (gray lines) for 30 cm (top panel) and 40 cm (bottom panel) soil depth.



moisture. This could be because once a critical threshold of moisture depletion is reached, the remaining soil water is either  
280 more tightly bound within the soil matrix or evaporation is limited by other factors such as reduced surface water availability  
or increased resistance to moisture loss. Rain exhibits a positive undulating impact on soil moisture, with higher rainfall values  
leading to a rise in soil moisture levels. Trends at all the depths also show several small peaks in between where moisture  
increases or decreases. These observed fluctuations suggest intermittent wetting and drying cycles, likely influenced by short-  
term rainfall events or other transient hydrological processes such as infiltration and redistribution. The range of soil moisture  
285 variability corresponding to Rain reduces progressively from shallow to deeper soil layers ( 25% at 10 and 20 cm; 13% at 30  
and 40 cm). This trend implies that surface layers are more responsive to rainfall, while deeper soil layers act as a moisture  
buffer, dampening the effects of surface hydrological changes. This may be due to factors such as reduced permeability, slower  
infiltration rates, or greater retention capacity.

ST1 initially exhibits a negative correlation with soil moisture across all depths, indicating that rising soil temperature gen-  
290 erally leads to moisture loss. However, beyond a certain temperature threshold, a slight positive trend emerges at some depths.  
At 10 cm, soil moisture decreases as ST1 increases from 20°C to 28°C but shows a minor increase afterward with small fluc-  
tuations. At 20 cm, the correlation remains strongly negative throughout, suggesting consistent drying with rising temperature.  
At 30 cm, soil moisture declines until ST1 reaches 33°C, after which a slight recovery is observed. The deepest soil layer  
(40 cm) displays an undulating negative trend in soil moisture up to ST1, reaching 31°C, followed by a gradual increase. ST2  
295 exhibits a trend similar to ST1 at 10 cm, where soil moisture declines as ST2 increases from 25°C to 30°C, followed by a  
gradual rise. At 20 cm, ST2 exhibits an oscillating pattern with an overall positive influence on soil moisture, while at 30 cm,  
the trend remains undulating but with a predominantly negative impact. At 40 cm, ST2 demonstrates fluctuations without any  
clear positive or negative correlation with soil moisture. ST3 follows a similar trend at 10 cm as ST1 and ST2, where soil  
moisture initially decreases until ST3 reaches 31°C, after which a slight increase is observed. At 20 cm, ST3 exhibits a strong  
300 negative correlation with soil moisture. At 30 cm, soil moisture generally declines with some fluctuations until ST3 reaches  
34°C, after which it drops sharply. At 40 cm, soil moisture shows a brief increase between 25°C and 30°C but predominantly  
follows a negative trend beyond this point, with minor undulations. ST4 exhibits two distinct trends across all depths: an initial  
increase in soil moisture up to 33°C at shallower depths and up to 31°C at deeper depths, followed by a sharp decline at all  
depths except at 30 cm, where soil moisture shows only a slight reduction.

305 Finally, we computed feature association estimates at each soil depth to examine correlations among the input variables.  
Highly correlated features can introduce redundancy, leading to model instability and increased computational inefficiency.  
The yellow diagonal blocks signify perfect self-correlation (value = 1), while the varying off-diagonal colors represent different  
degrees of association between predictors. Our findings indicate that there are no significant correlations among the input  
features (Figure 9). However, slight correlations ( $\approx 0.1$ -0.25) are observed between ST1, ST2, ST3, ST4 and between RH and  
310 DP. Since both humidity and dew point measure atmospheric moisture, their relationship is expected. Similarly, soil temperature  
at different depths shows weak associations due to heat transfer processes within the soil profile. Thus, the overall weak  
associations among the input features support the inclusion of all predictors in the model without necessitating the exclusion  
of any single feature.



### 3.3 AutoML-SM performance

315 We used an AutoML-SM model to predict soil moisture at multiple subsurface depths for four scenarios. S1 included 9099 training samples and 3899 testing samples, while S2, S3, and S4 had 12119, 15244, and 18369 training samples and 5194, 6533, and 7874 testing samples, respectively. The model performed exceptionally well at all depths in all four scenarios as shown in Table 1, with accuracy assessed using the coefficient of determination ( $R^2$ ) and root mean squared error (RMSE). At 10 cm depth, the model achieved  $R^2 \sim 0.97$ – $0.986$  with  $RMSE \leq 0.016$  across all scenarios. Performance at 20 cm remained  
320 high ( $R^2 \sim 0.97$ – $0.99$ ) in S1–S3 but dropped slightly in S4 ( $R^2 = 0.88$ ), with RMSE ranging from 0.0029 to 0.034. Predictions at 30 cm showed  $R^2 \sim 0.98$ – $0.997$  and  $RMSE \leq 0.021$ , while the 40 cm depth maintained strong accuracy ( $R^2 \sim 0.96$ – $0.99$ ,  $RMSE \leq 0.022$ ) across all scenarios.

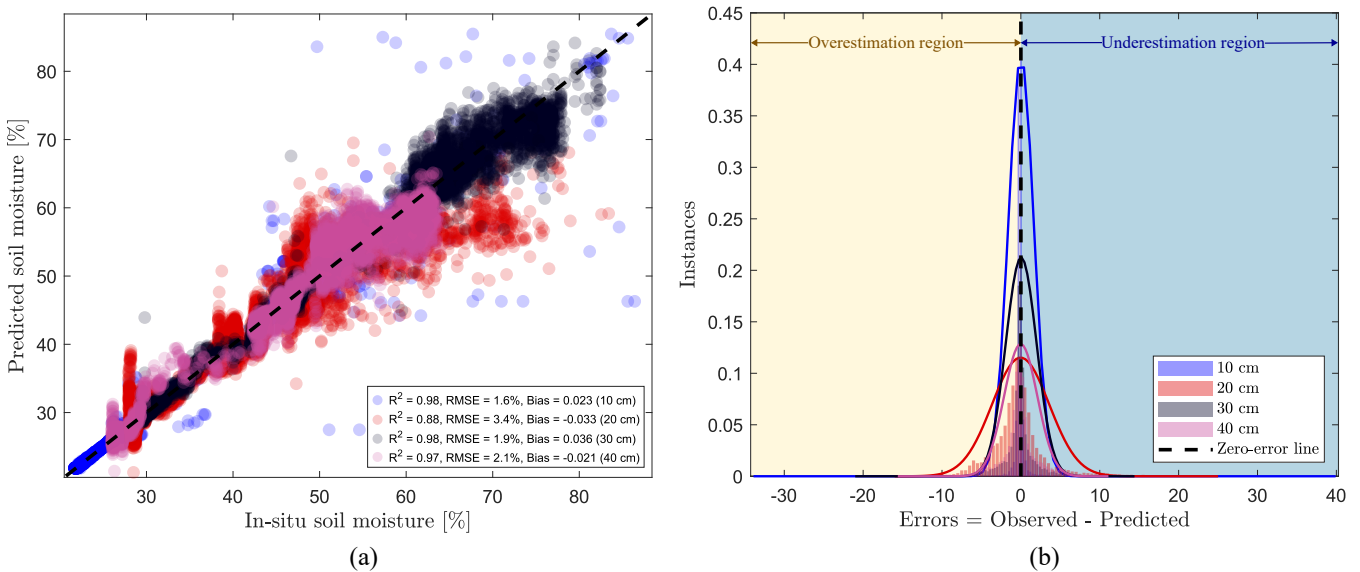
We intricately analysed in-situ data to examine soil moisture response to different rainfall events, as rainfall is the primary driver of soil moisture dynamics. To assess its impact on soil moisture prediction, we tested the AutoML-SM model using a  
325 dataset containing only rainfall instances. S1 included 27 training samples, accounting for about 0.3% of the total training data, and 16 testing samples, which is approximately 0.4% of the overall testing data. S2 had 136 training (1.1%) and 70 testing samples (1.4%). S3 comprised 458 training (3%) and 201 testing samples (3.1%), while S4 used 729 training (4%) and 283 testing samples (3.6%). At 10 cm depth, the model achieves  $R^2$  values of 0.913 (S1) and 0.966 (S2), but accuracy declines in S3 (0.886) and S4 (0.783). RMSE follows a similar trend, increasing from 0.034 in S1, 0.036 in S2, 0.042, and 0.067 in S3 and S4,  
330 respectively. At 20 cm depth,  $R^2$  remains high in S1 (1.00) and S2 (0.956) but decreases in S3 (0.86) and S4 (0.76). RMSE is lowest in S1 (0.0016) and rises progressively in S2 (0.034), S3 (0.041), and S4 (0.044). Deeper layers (30 cm and 40 cm) show a different pattern in S4, where accuracy improves. 30 cm depth, exhibit high  $R^2$  values in S1 (0.999) and S2 (0.936), with a relatively low  $R^2 = 0.864$  (S3), and further increased  $R^2 = 0.91$  in S4. Similarly, at 40 cm depth,  $R^2$  is 0.907 (S1), increases in S2 (0.97), declines in S3 (0.839), and slightly improves in S4 (0.883). Overall, we can infer that at shallower depths (10  
335 cm and 20 cm), accuracy is highest in smaller datasets (S1 and S2) but declines in larger datasets (S3 and S4), indicating that increased rainfall instances may introduce variability, reducing predictive performance. In contrast, deeper layers (30 cm and 40 cm) show an opposite trend, where accuracy improves in S4, suggesting that incorporating more rainfall instances enhances predictions at greater depths.

To better visualise the model's predictive accuracy, we constructed a scatter plot between observed and predicted soil mois-  
340 ture for the S4 scenarios across all the depths (Figure 12 (a)). The 10 cm depth (in blue) shows that the data points are tightly clustered around the 1:1 line, suggesting high model accuracy. It achieves an  $R^2 = 0.98$ , indicating well-aligned observed and predicted values, the RMSE of 1.6%, and a small positive Bias of 0.023, which reflects minimal error. The 20 cm depth (in red), shows wider spread scatter points compared to the top layer, highlighting increased prediction uncertainty. Therefore, it produced the  $R^2$  of 0.88, implying a weaker correlation, RMSE of 3.4%, and a negative Bias of -0.033 suggesting a slight  
345 underestimation at this depth. The 30 cm depth (in green) shows that the scatter points are again closely aligned with the 1:1 line, similar to the 10 cm depth. The  $R^2$  value of 0.98, RMSE of 1.9%, and the Bias of 0.036 indicate accurate predictions with minimal errors. The 40 cm depth (in black) shows that data points remain well aligned with the 1:1 line, though with a slightly



| Depth | Scenarios | Rainfall instances |            | Testing (only Rainfall) |        | Testing (overall) |        |
|-------|-----------|--------------------|------------|-------------------------|--------|-------------------|--------|
|       |           | Train              | Test       | $R^2$                   | RMSE   | $R^2$             | RMSE   |
| 10 cm | S1        | 27 (0.3%)          | 16 (0.4%)  | 0.913                   | 0.034  | 0.97              | 0.0058 |
|       | S2        | 136 (1.1%)         | 70 (1.4%)  | 0.966                   | 0.036  | 0.986             | 0.0085 |
|       | S3        | 458 (3%)           | 201 (3.1%) | 0.886                   | 0.042  | 0.981             | 0.015  |
|       | S4        | 729 (4%)           | 283 (3.6%) | 0.783                   | 0.067  | 0.981             | 0.016  |
| 20 cm | S1        | 27                 | 16         | 1.00                    | 0.0016 | 0.997             | 0.0029 |
|       | S2        | 136                | 70         | 0.956                   | 0.034  | 0.99              | 0.0075 |
|       | S3        | 458                | 201        | 0.861                   | 0.041  | 0.972             | 0.016  |
|       | S4        | 729                | 283        | 0.764                   | 0.044  | 0.883             | 0.034  |
| 30 cm | S1        | 27                 | 16         | 0.999                   | 0.005  | 0.997             | 0.0039 |
|       | S2        | 136                | 70         | 0.936                   | 0.049  | 0.992             | 0.0099 |
|       | S3        | 458                | 201        | 0.864                   | 0.047  | 0.981             | 0.021  |
|       | S4        | 729                | 283        | 0.91                    | 0.036  | 0.985             | 0.019  |
| 40 cm | S1        | 27                 | 16         | 0.907                   | 0.041  | 0.99              | 0.0084 |
|       | S2        | 136                | 70         | 0.97                    | 0.026  | 0.996             | 0.0067 |
|       | S3        | 458                | 201        | 0.839                   | 0.034  | 0.965             | 0.022  |
|       | S4        | 729                | 283        | 0.883                   | 0.032  | 0.969             | 0.021  |

**Table 1.** Performance of the AutoML-SM model in predicting soil moisture at different soil depths (10 cm, 20 cm, 30 cm, and 40 cm) in four different scenarios (S1, S2, S3, and S4) using metrics  $R^2$  and RMSE for the overall dataset and for data comprising only rainfall instances.



**Figure 12.** (a) Linear fit between the observed and predicted soil moisture values for soil depths 10, 20, 30, and 40 cm. The dashed black line represents the ideal 1:1 line, highlighting the perfect match between observed and predicted values. (b) Error histogram analysis showing the distribution of model errors for multiple soil depths. The vertical dashed black line indicates the zero-error line, with left and right regions exhibiting overestimates and underestimates, respectively.





wider spread compared to the 10 cm and 30 cm depths. It achieves a high  $R^2 = 0.97$ , suggesting strong correlation, RMSE of 2.1%, and a negative Bias of -0.021, suggesting slight underestimation at this depth.

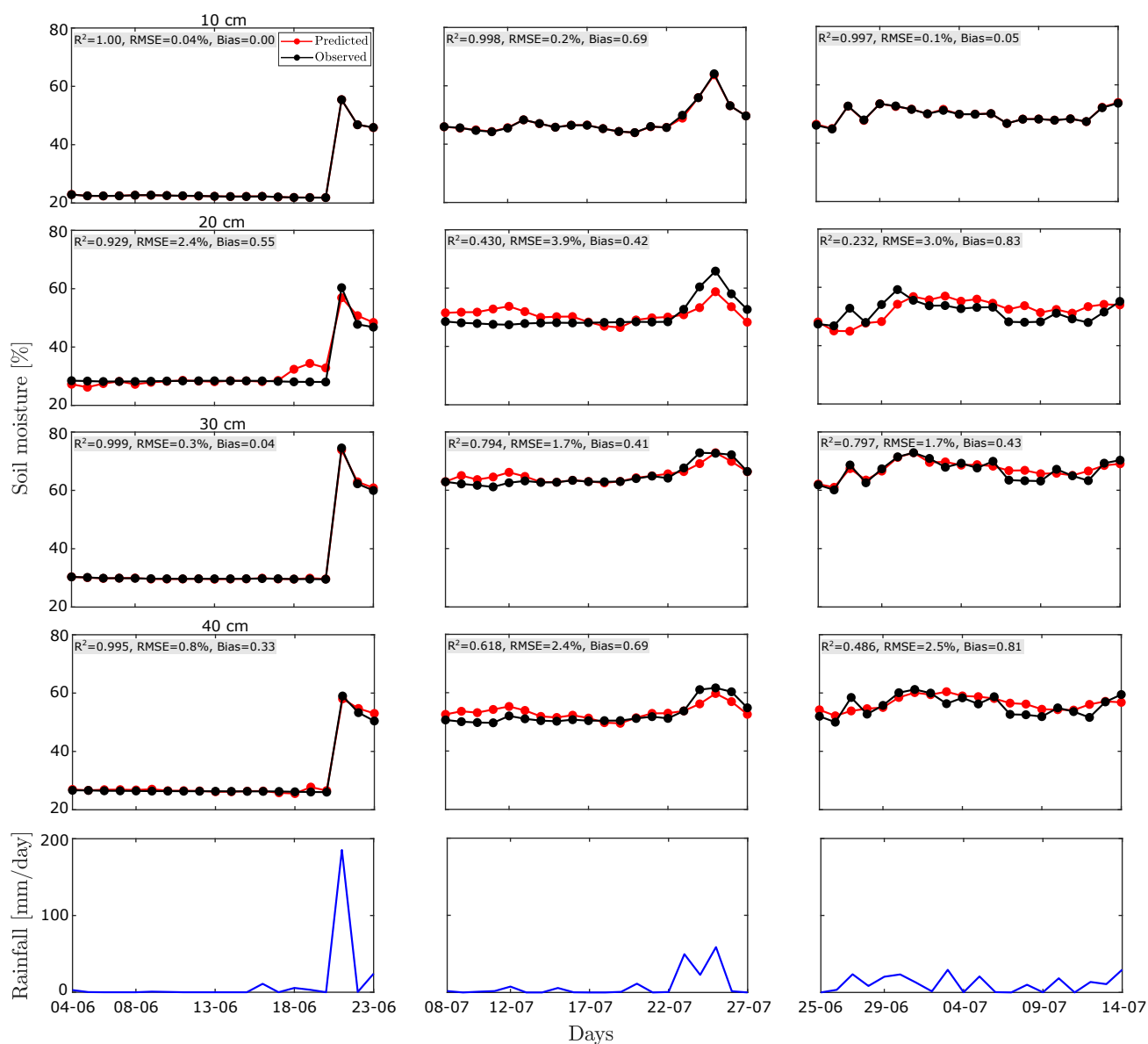
350 Additionally, we also performed an error histogram analysis illustrated through the histogram plot, which visualises the error distribution (Observed – Predicted) for soil moisture predictions at different depths fitted with Gaussian curves. The zero-error line (dashed black line) represents the ideal case where predictions perfectly match observations. 10 cm depth (blue curve) has the sharpest peak among all depths, suggesting higher instances of low errors. The error distribution is symmetric and centered around zero, indicating minimal bias. However, the Gaussian curve exhibits longer tails on both sides, indicating high variance  
355 and more outliers, which is evident from the scatter plot in which we observed more scattering in 10 cm for higher magnitude soil moisture as compared to the lower value. 20 cm depth (red curve) exhibits a larger spread-out distribution, with a slight skew towards the positive (underestimation) region, suggesting that the model tends to underpredict soil moisture at this depth. The Gaussian curve for the 30 cm depth (green) closely follows the trend of the 10 cm depth but is slightly wider. A minor negative skew suggests some overestimation with a slightly higher error variance. However, the peak remains prominent and  
360 centered near zero, indicating strong predictive accuracy. The 40 cm depth (black curve) exhibits a moderate peak, with an error distribution broader than those at 10 cm and 30 cm but narrower than at 20 cm. The Gaussian curve's tail extends slightly into the overestimation region, indicating occasional overestimation. However, the overall model performance remains strong.

## 4 Discussion

### 4.1 Assessing model performance: Event-based analysis

365 The proposed AutoML-SM framework exhibits high accuracy and robust predictive capabilities for the entire dataset and performed reliably when trained specifically on rainfall-influenced instances. Although the prediction accuracy decreases when tested on data subsets containing only non-zero rainfall values, this is primarily attributed to the limited number of rainfall instances included in the study. Nonetheless, we hypothesize that the model's predictive performance would improve with a higher density of rainfall observations. Since capturing and analysing rainfall-induced soil moisture variations is fundamental  
370 to understanding subsurface hydrodynamics, it is equally imperative to evaluate the model's reliability and predictive accuracy when applied to specific rainfall-driven events. To provide a clear visualisation of these dynamics, we plotted both observed and predicted soil moisture values at depths of 10, 20, 30, and 40 cm for rainfall events of varying intensity: high, moderate, and low. Each event spans a 20-day period, with each data point representing daily soil moisture values.

For the high-intensity rainfall event, a sharp increase in soil moisture is evident across all depths immediately following the  
375 rainfall peak. At 10 cm, the soil moisture rises steeply from nearly 20% to above 60%, reflecting the rapid infiltration of water into the surface layer. At 20 cm, a similar trend is observed, though the increase is slightly delayed compared to the surface layer. The model predictions align well with observations but slightly underestimate moisture levels near the peak. At 30 cm and 40 cm, the response is also well captured, though minor deviations between predicted and observed values are noticeable. Moisture level at 30 cm depth also increases by about 40% following the event, and the deeper layers show a more sustained  
380 increase in soil moisture, indicating water percolation over time.



**Figure 13.** Event-based evaluation of the AutoML-SM model's performance in predicting soil moisture at multiple depths. Observed and predicted soil moisture values are represented by black and red lines, respectively, for rainfall events of varying intensities: high, moderate, and low (left to right) where each event spans a 20-day period.





The moderate-intensity rainfall event shows that the soil moisture increase is more gradual compared to the high-intensity event. At 10 cm, the model follows the observed trend well. Soil moisture fluctuates slightly, with a noticeable rise occurring after the onset of rainfall, though less pronounced than in the high-intensity case. At 20 cm, the response is more evident, with soil moisture increasing steadily following the event. The model predictions align closely with observations, though there is a minor underestimation in some instances. At 30 cm and 40 cm, the soil moisture increase is further delayed, reflecting the slower infiltration of water into deeper layers. The model captures the overall trend but shows slight overestimation in small peaks and underestimation during rainfall duration.

For the low-intensity rainfall event, soil moisture variations are minimal compared to the other two cases. At 10 cm, there are small fluctuations in soil moisture but no sharp increases, reflecting the limited vertical movement of water under low rainfall conditions. Similar to other events, the predicted values align with the observed values in this event. At 20 cm, the response is similarly subdued, with only slight increases in soil moisture over time. The model performs well in capturing these small variations but exhibits occasional overpredictions. At 30 cm and 40 cm, the response is even less pronounced, with soil moisture remaining relatively stable throughout the event. The model predictions at these depths show good alignment with observations, though some overestimation is evident, likely due to the model's sensitivity to small changes in moisture levels.

## 4.2 Comparison with benchmark algorithms

We compared the performance of the AutoML-SM model with five benchmark machine learning algorithms across each soil depth based on metrics like  $R^2$ , RMSE and Bias. The AutoML-SM model consistently outperforms all other algorithms in predicting soil moisture, demonstrating superior accuracy at every depth (Table 2). Generalised regression neural network (GRNN), Generalised additive model (GAM), Gradient Boosted Decision Trees (BDT), Random Forest (RF) and Least-squares boosting (LSBoost) achieved  $R^2$  value between 0.73-0.84 for 10 cm, 0.73-0.80 for 20 cm, 0.85-0.92 for 30 cm and 0.77-0.89 for 40 cm whereas AutoML-SM recorded  $R^2$  of 0.98, 0.88, 0.98 and 0.97 for each soil depth progressing in the subsurface. In terms of RMSE, AutoML-SM recorded the lowest values across all depths (1.6 for 10 cm, 3.4 for 20 cm, 1.9 for 30 cm, and 2.1 for 40 cm). GRNN shows the lowest RMSE at 10 cm (5.38), 20 cm (5.64), and 40 cm (5.92), while GAM performs the worst at 30 cm (6.89). Random Forest emerged as the second-best model after AutoML-SM, with RMSE values ranging from 3.41 to 3.75 across depths, reflecting its relatively consistent performance. AutoML-SM model also exhibited minimal Bias across multiple depths, staying close to zero and ranging from -0.033 to 0.036. In contrast, GRNN and GAM showed relatively higher Bias from -0.058 to 0.111 at 10 and 30 cm depth. BDT and LSBoost also highlight large Bias values, especially at the topmost depth, while RF consistently performed better among all the benchmark algorithms to give lower Bias. These deviations indicate potential over or under predictions by the explainable models, specifically at shallower depths.

To ensure the validity of our analysis, we conducted the Kolmogorov–Smirnov normality test to evaluate the average model error for each algorithm. The findings evidently confirmed that all five algorithms at each depth conformed to a normal distribution. With this validation, we also performed the one-way ANOVA (Analysis of Variance) multiple comparison test, incorporating Tukey's Honestly Significant Difference (HSD) method as a rigorous post hoc analysis. By leveraging Tukey's

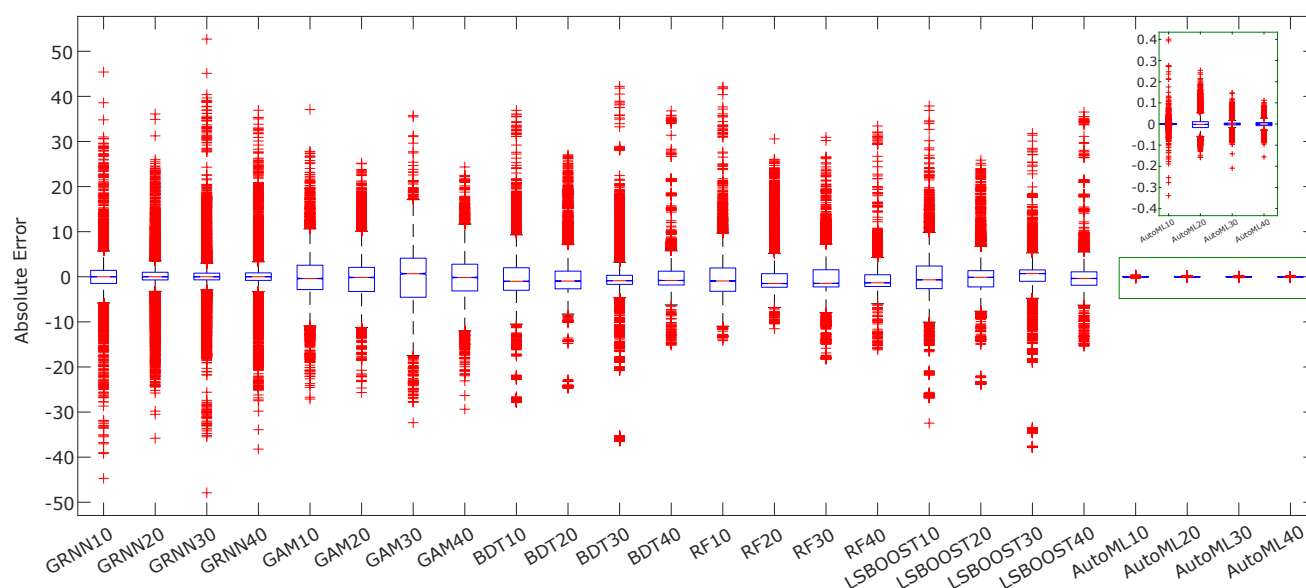


| Metrics        | Algorithms |       |        |       |         |        |       |       |        |        |       |        |
|----------------|------------|-------|--------|-------|---------|--------|-------|-------|--------|--------|-------|--------|
|                | GRNN       |       |        |       | GAM     |        |       |       | BDT    |        |       |        |
|                | 10 cm      | 20 cm | 30 cm  | 40 cm | 10 cm   | 20 cm  | 30 cm | 40 cm | 10 cm  | 20 cm  | 30 cm | 40 cm  |
| R <sup>2</sup> | 0.8        | 0.73  | 0.85   | 0.77  | 0.79    | 0.73   | 0.84  | 0.8   | 0.73   | 0.74   | 0.81  | 0.87   |
| RMSE           | 5.38       | 5.64  | 6.32   | 5.92  | 5.37    | 5.52   | 6.89  | 5.77  | 5.3    | 4.73   | 6.31  | 4.02   |
| Bias           | -0.058     | -0.07 | 0.077  | 0.008 | 0.111   | 0.043  | 0.086 | 0.037 | 0.072  | -0.024 | 0.069 | -0.051 |
| Metrics        | RF         |       |        |       | LSBoost |        |       |       | AutoML |        |       |        |
|                | 10 cm      | 20 cm | 30 cm  | 40 cm | 10 cm   | 20 cm  | 30 cm | 40 cm | 10 cm  | 20 cm  | 30 cm | 40 cm  |
|                | 10 cm      | 20 cm | 30 cm  | 40 cm | 10 cm   | 20 cm  | 30 cm | 40 cm | 10 cm  | 20 cm  | 30 cm | 40 cm  |
| R <sup>2</sup> | 0.84       | 0.8   | 0.92   | 0.89  | 0.78    | 0.79   | 0.85  | 0.89  | 0.98   | 0.88   | 0.98  | 0.97   |
| RMSE           | 3.59       | 3.74  | 3.75   | 3.41  | 5.34    | 4.68   | 6.02  | 3.83  | 1.6    | 3.4    | 1.9   | 2.1    |
| Bias           | -0.015     | 0.023 | -0.007 | 0.043 | -0.101  | -0.001 | -0.06 | 0.054 | 0.023  | -0.033 | 0.036 | -0.021 |

**Table 2.** Model performance of explainable benchmark machine learning algorithms and comparison with AutoML-SM model using R<sup>2</sup>, RMSE and Bias.

415 HSD, we systematically compared the mean model errors across different algorithms and derived adjusted p-values (Table A.1),  
ensuring a more precise and statistically robust assessment of algorithmic performance. The boxplot (Figure 14) illustrates the  
error distribution from the ANOVA analysis, facilitating the comparison of multiple models by identifying statistically signifi-  
cant differences in their absolute errors. The AutoML-SM model at all depths exhibits minimal errors and significantly fewer  
outliers relative to other benchmark algorithms, indicating superior prediction performance. Within the AutoML models, per-  
420 formance improves progressively with depth, with AutoML40 exhibiting the least error and outliers, followed by AutoML30  
outperforming AutoML20, while AutoML10 records the highest error among them. Conversely, other models like GRNN and  
BDT show numerous outliers, while GAM, RF, and LSBoost depict wider interquartile ranges, reflecting higher variability  
in prediction errors. Consequently, the AutoML-SM model demonstrates greater consistency and reliability in error reduction  
compared to traditional machine learning approaches.

425 To understand the efficiency and scalability of the model while working with large and complex datasets, it becomes critically  
important to consider the computation time of the algorithms. We evaluated all the machine learning models based on their  
computation time with a three-dimensional visualisation of all the key performance metrics in a bubble diagram (Figure 15)  
where size of the sphere represents the computation time of each model, averaged over 30 iterations. AutoML-SM exhibited  
the fastest computation time of 2.33 seconds at 10 cm depth and the longest time of 444.3 seconds at 30 cm, while requiring  
430 160.3 seconds and 125.7 seconds for 20 cm and 40 cm depths, respectively. These results highlight its efficiency in predicting  
surface soil moisture, although its performance became more computationally demanding at deeper subsurface levels. BDT and  
LSBoost consistently demonstrated lower computation times than AutoML-SM, averaging around 2.9 and 3.2 seconds across  
all depths, but at the cost of reduced accuracy. RF, however, maintained an effective balance between efficiency and accuracy,  
with moderate computation times ranging from 13.2 to 13.5 seconds across all depths, making it highly suitable for real-time  
435 predictions. GRNN processed data slightly faster than RF, at approximately 10.5 seconds, while GAM required more time,



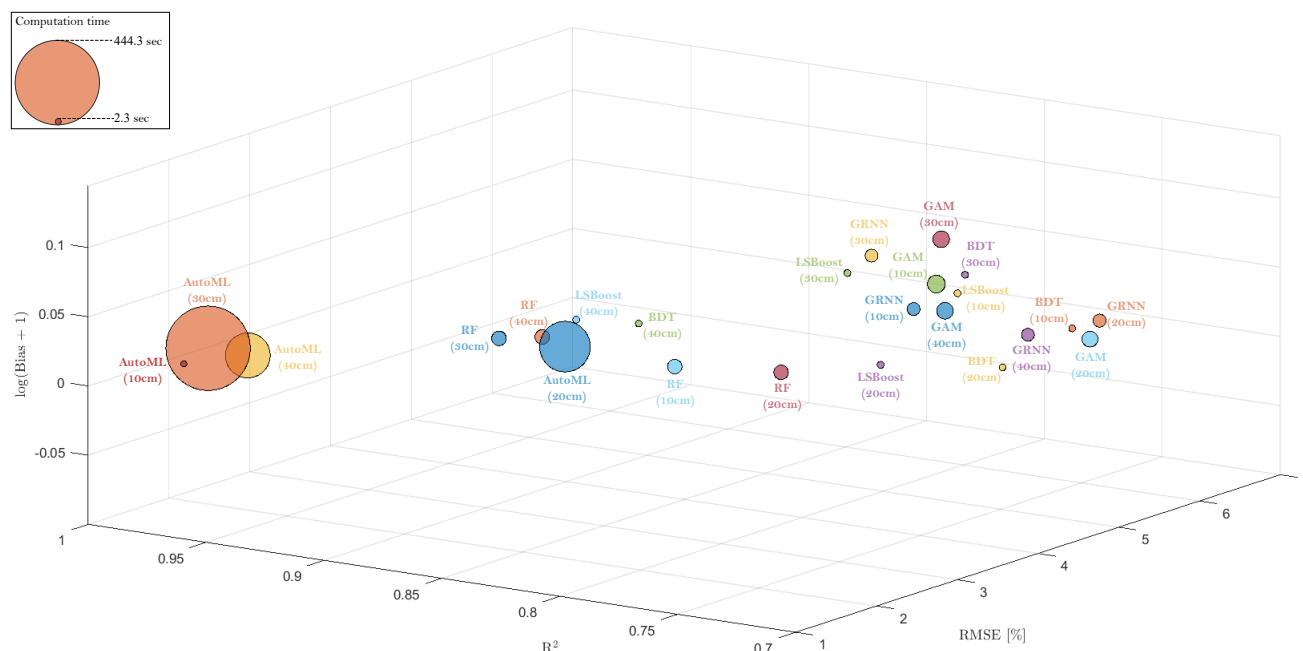
**Figure 14.** The boxplot illustrates the absolute model error analysed through ANOVA. The upper and lower edges of each box correspond to the 75th and 25th percentiles, respectively, while the line within the box marks the median of the sample. Outliers are indicated by red plus signs. The zoomed panel at top right show performance of AutoML at all depths relative to other algorithms.

ranging from 17.2 to 19.7 seconds. Despite their computational efficiency, GRNN and GAM are better suited for scenarios prioritizing processing speed over accuracy, given their lower predictive performance compared to RF.

### 4.3 Uncertainty analysis of the AutoML-SM

To evaluate the sensitivity of our proposed model and quantify how small uncertainties in key input features propagate into the model's output, we performed an uncertainty analysis by perturbing each input variable RH, WS, WD, SR, Rain, DP, and soil temperatures at 10 cm, 20 cm, 30 cm, and 40 cm (ST1, ST2, ST3, ST4)) by  $\pm 5\%$  and  $\pm 10\%$  (Figure 16). The subsequent percentage changes in the response variable were recorded and plotted to determine which parameters most strongly influence model behavior. This step is crucial for identifying the variables that require the most precise measurements and to determine potential weaknesses or instabilities in our predictive framework.

At 10 cm, moderate variations in RH (up to  $\approx 1.47\%$ ) and very slight changes due to WS, WD, SR, and EV (all roughly 0.35-0.36%) suggest that near-surface soil moisture is not extremely sensitive to small perturbations in these atmospheric variables. In contrast, DP shows an interesting asymmetry: a 10% decrease yields a 2.34% change in soil moisture, whereas smaller or positive perturbations lead to less pronounced shifts. This asymmetry suggests a threshold or non-linear relationship in the model, where sufficiently large negative deviations in atmospheric moisture can substantially influence soil moisture dynamics at 10 cm. Notably, soil temperature inputs (ST1, ST2, ST3, and ST4) produce some of the largest percentage changes (ranging from about 3.1% to 3.8%) indicates the dependency of the topsoil on the thermal dynamics. While rainfall exerts a major effect

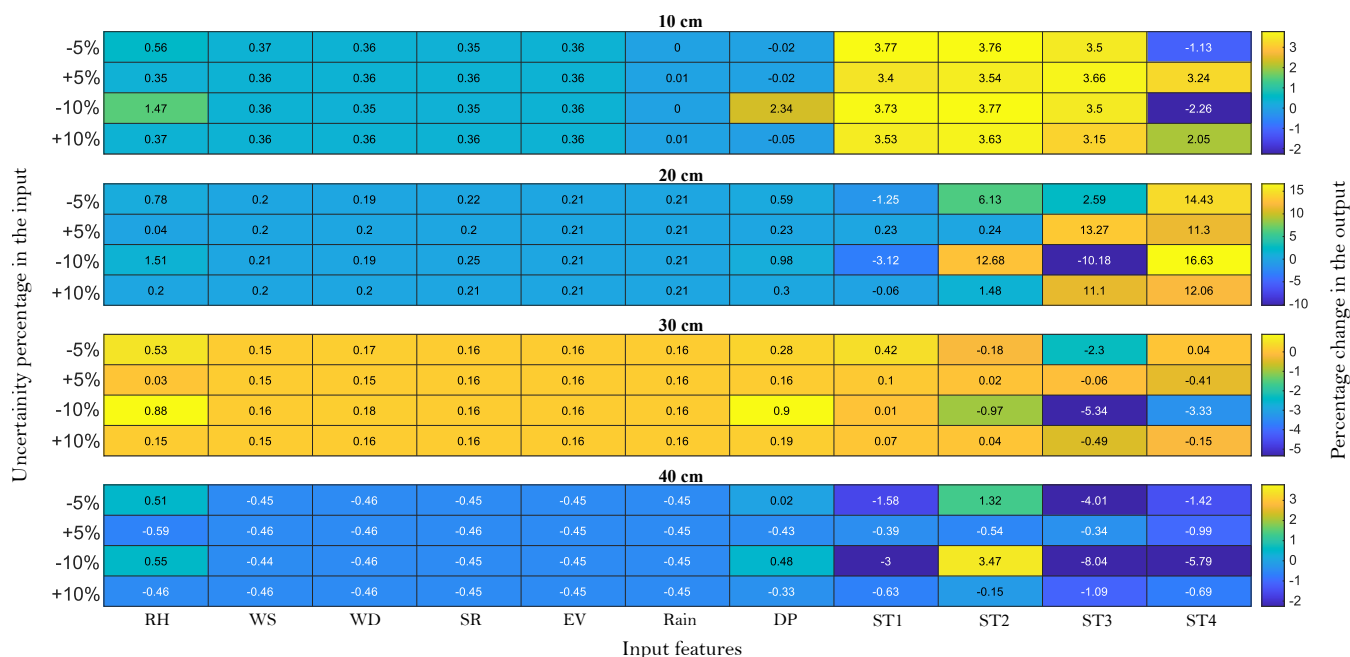


**Figure 15.** 3D bubble plot of RMSE,  $R^2$  and Bias (log-transformed) for the benchmark machine learning algorithms at all soil depths, with sphere size representing computation time.

on soil moisture at a broader scale, the results here (0.001-0.01%) indicate that in the short term or under specific conditions,  $\pm 5$ -10% rainfall errors have limited immediate impact at 10 cm. This could be tied to infiltration delays or antecedent moisture conditions.

455 Moving to 20 cm, the model's responses become more variable. ST4 exhibits exceptionally large positive swings (reaching over 14–16% in some perturbation scenarios), suggesting that deeper thermal conditions can significantly influence moisture at the 20 cm layer, possibly through upward heat flux or changes in hydraulic conductivity linked to temperature gradients. Changes in ST2 itself also range widely (e.g., from 0.24% to over 12%), reflecting strong self-sensitivity to the local temperature environment. DP occasionally shows higher magnitude changes (up to  $\approx 0.98\%$ ), especially under a 10% decrease, 460 reinforcing that reduced atmospheric moisture can enhance evaporation or vapour fluxes at this intermediate depth. Meanwhile, RH, WS, WD, SR, EV, and Rain display smaller or more moderate percentage changes (generally below 1% to 2%), indicating that, for this dataset, deeper infiltration or thermal dynamics overshadow the direct influence of small atmospheric perturbations.

At 30 cm, we observe a general decrease in overall percentage changes for many variables, reflecting a dampening effect 465 as moisture travels deeper into the profile. RH, WS, WD, SR, EV, and Rain mostly produce changes under  $\approx 0.5$ -0.9%. A notable exception is DP at -10%, which leads to a marked 0.90% surge in the model output, suggesting that sufficiently low atmospheric moisture can impact deeper soil layers, perhaps by modifying the vapour pressure gradient over a longer period.



**Figure 16.** Heatmap showing the average percentage change in output in response to the different levels of uncertainties in the input features across various soil depths.

Another key observation is the sensitivity to ST3: negative perturbations can yield changes as large as -5.34%, showing that a cooler-than-expected subsurface can significantly reduce local soil moisture content. This highlights the interconnected roles of temperature gradients, soil water retention, and possibly plant root uptake at mid-depths.

In the deepest monitored layer (40 cm), many variables appear with negative percentage changes under both  $\pm 5\%$  and  $\pm 10\%$  perturbations. WS, WD, SR, EV, and Rain consistently yield changes near -0.45% to -0.46%, likely reflecting a smaller direct impact at this depth. Interestingly, RH at  $\pm 10\%$  produces marginally positive (0.55%) or negative changes (-0.46%), signifying that moisture at 40 cm can still respond to humidity extremes but remains less affected by moderate perturbations. ST1, ST2, ST3, and ST4 also show a distinctly negative trend for certain scenarios, with large swings (e.g., -8.04% at ST3) when the soil temperatures are artificially lowered by 10%. This pattern implies that cooler subsurface temperatures can substantially affect moisture storage or movement at 40 cm, possibly due to reduced hydraulic conductivity or slowed percolation.

In summary, the uncertainty analysis reveals that soil temperature variables, in particular the deeper temperatures at 20-40 cm, can exert substantial influence on moisture predictions, sometimes exceeding 10-15% changes under  $\pm 10\%$  thermal perturbations. DP shows moderate but occasionally significant effects, particularly when decreased. Atmospheric drivers (RH, WS, WD, SR, EV, and Rain) generally induce more modest changes at all depths, although occasional outliers demonstrated potential non-linear interactions with local soil conditions. These findings emphasise the importance of accurate soil temperature measurements at multiple depths, as thermal gradients are a major driver of moisture distribution. Furthermore, ensuring that DP is well-estimated may be critical for conditions prone to low humidity episodes. Rainfall is important to the water



485 balance. However, at certain depths or during specific time periods, minor deviations ( $\pm 5$ -10%) may not cause significant moisture changes. This is likely due to infiltration delays or preexisting moisture conditions.

| Case    | Testing        |       |           |                |       |           |                |       |           |                |       |           |
|---------|----------------|-------|-----------|----------------|-------|-----------|----------------|-------|-----------|----------------|-------|-----------|
|         | 10 cm          |       |           | 20 cm          |       |           | 30 cm          |       |           | 40 cm          |       |           |
|         | R <sup>2</sup> | RMSE  | Bias      | R <sup>2</sup> | RMSE  | Bias      | R <sup>2</sup> | RMSE  | Bias      | R <sup>2</sup> | RMSE  | Bias      |
| rng(0)  | 0.972          | 0.019 | -8.02E-06 | 0.925          | 0.028 | 9.51E-05  | 0.979          | 0.023 | 1.97E-04  | 0.958          | 0.024 | -5.00E-05 |
| rng(1)  | 0.962          | 0.023 | 1.12E-04  | 0.938          | 0.026 | 1.67E-05  | 0.990          | 0.016 | -8.23E-05 | 0.968          | 0.022 | 2.84E-04  |
| rng(2)  | 0.958          | 0.024 | -3.00E-04 | 0.972          | 0.018 | 3.08E-04  | 0.995          | 0.012 | -2.45E-05 | 0.972          | 0.020 | 2.95E-04  |
| rng(3)  | 0.972          | 0.020 | 1.62E-05  | 0.973          | 0.018 | -6.10E-04 | 0.991          | 0.015 | -2.23E-04 | 0.991          | 0.011 | -3.22E-05 |
| rng(4)  | 0.923          | 0.032 | 1.79E-05  | 0.893          | 0.033 | 2.27E-04  | 0.980          | 0.022 | 1.87E-04  | 0.972          | 0.020 | -5.68E-05 |
| rng(5)  | 0.929          | 0.031 | -4.10E-04 | 0.923          | 0.029 | 6.56E-05  | 0.904          | 0.047 | 0.00117   | 0.972          | 0.020 | 2.84E-04  |
| rng(6)  | 0.976          | 0.018 | -2.90E-04 | 0.970          | 0.018 | -6.31E-04 | 0.995          | 0.011 | -7.51E-05 | 0.972          | 0.020 | -5.90E-04 |
| rng(7)  | 0.965          | 0.022 | -6.20E-04 | 0.919          | 0.030 | -3.89E-04 | 0.994          | 0.012 | 1.01E-05  | 0.957          | 0.024 | -6.19E-04 |
| rng(8)  | 0.949          | 0.026 | -2.30E-04 | 0.925          | 0.028 | -1.08E-03 | 0.972          | 0.027 | -4.21E-04 | 0.981          | 0.017 | -6.42E-04 |
| rng(9)  | 0.978          | 0.018 | -2.70E-05 | 0.932          | 0.027 | 5.58E-04  | 0.982          | 0.022 | 3.13E-04  | 0.993          | 0.011 | 1.82E-04  |
| rng(10) | 0.963          | 0.023 | -4.60E-04 | 0.971          | 0.018 | 5.34E-04  | 0.970          | 0.027 | 2.61E-04  | 0.989          | 0.013 | -2.05E-03 |
| rng(11) | 0.960          | 0.023 | -5.05E-05 | 0.938          | 0.026 | 4.56E-04  | 0.980          | 0.023 | 1.74E-04  | 0.977          | 0.018 | 4.21E-05  |
| rng(12) | 0.981          | 0.016 | -2.03E-04 | 0.849          | 0.038 | 5.88E-04  | 0.962          | 0.031 | 4.35E-04  | 0.994          | 0.010 | -3.90E-05 |
| rng(13) | 0.946          | 0.027 | -5.30E-04 | 0.913          | 0.030 | 1.49E-04  | 0.978          | 0.023 | -6.49E-05 | 0.994          | 0.009 | -2.31E-04 |
| rng(14) | 0.976          | 0.018 | -2.85E-04 | 0.965          | 0.020 | -5.08E-04 | 0.974          | 0.025 | -7.63E-04 | 0.913          | 0.033 | -2.05E-03 |
| rng(15) | 0.948          | 0.027 | -4.58E-04 | 0.898          | 0.033 | 3.35E-04  | 0.973          | 0.026 | 3.54E-04  | 0.989          | 0.012 | -1.48E-05 |
| rng(16) | 0.967          | 0.021 | 2.26E-04  | 0.972          | 0.018 | 2.00E-04  | 0.960          | 0.031 | 6.73E-04  | 0.994          | 0.009 | 4.44E-05  |
| rng(17) | 0.890          | 0.037 | -9.64E-05 | 0.972          | 0.017 | 1.36E-04  | 0.993          | 0.013 | 2.25E-04  | 0.994          | 0.009 | 9.58E-05  |
| rng(18) | 0.940          | 0.028 | -6.14E-04 | 0.938          | 0.026 | -1.70E-04 | 0.992          | 0.014 | -1.51E-04 | 0.981          | 0.017 | -1.70E-04 |
| rng(19) | 0.951          | 0.026 | -2.86E-04 | 0.919          | 0.030 | 6.44E-04  | 0.985          | 0.019 | -1.93E-04 | 0.980          | 0.017 | -2.82E-04 |
| rng(20) | 0.929          | 0.031 | -1.79E-04 | 0.974          | 0.017 | 1.84E-04  | 0.995          | 0.011 | -2.90E-04 | 0.979          | 0.017 | -1.04E-04 |
| rng(21) | 0.974          | 0.019 | 3.35E-05  | 0.972          | 0.018 | -1.93E-04 | 0.894          | 0.049 | 1.67E-04  | 0.978          | 0.018 | -3.37E-05 |
| rng(22) | 0.864          | 0.041 | 1.30E-04  | 0.972          | 0.018 | -2.65E-04 | 0.994          | 0.012 | -1.74E-04 | 0.993          | 0.010 | -1.15E-04 |
| rng(23) | 0.976          | 0.018 | -2.85E-04 | 0.918          | 0.030 | -6.28E-04 | 0.979          | 0.023 | -2.97E-04 | 0.967          | 0.022 | -2.60E-04 |
| rng(24) | 0.973          | 0.019 | 1.55E-05  | 0.976          | 0.016 | 1.82E-04  | 0.992          | 0.014 | 1.11E-05  | 0.993          | 0.010 | 2.90E-06  |
| rng(25) | 0.976          | 0.018 | -2.85E-04 | 0.974          | 0.017 | 3.51E-05  | 0.972          | 0.026 | 2.45E-04  | 0.992          | 0.011 | -1.12E-04 |
| rng(26) | 0.978          | 0.017 | -2.78E-04 | 0.977          | 0.016 | -6.26E-05 | 0.974          | 0.026 | 1.72E-04  | 0.984          | 0.016 | 1.77E-04  |
| rng(27) | 0.968          | 0.021 | -2.56E-04 | 0.915          | 0.030 | 1.45E-04  | 0.973          | 0.026 | 3.73E-04  | 0.960          | 0.024 | 1.85E-04  |
| rng(28) | 0.942          | 0.028 | -9.81E-04 | 0.944          | 0.025 | -6.33E-05 | 0.995          | 0.011 | 3.52E-05  | 0.992          | 0.011 | -6.81E-05 |
| rng(29) | 0.975          | 0.018 | -5.26E-05 | 0.918          | 0.029 | 1.42E-04  | 0.978          | 0.023 | 2.48E-04  | 0.969          | 0.021 | 2.97E-04  |





|                  |                                                                                |       |           |                                                                                |       |           |                |       |           |                |        |           |
|------------------|--------------------------------------------------------------------------------|-------|-----------|--------------------------------------------------------------------------------|-------|-----------|----------------|-------|-----------|----------------|--------|-----------|
| $\mu \pm \sigma$ | 0.955 $\pm$ 0.023 $\pm$ -2.21E-04 $\pm$ 0.941 $\pm$ 0.024 $\pm$ 1.34E-05 $\pm$ |       |           | 0.976 $\pm$ 0.022 $\pm$ 8.31E-05 $\pm$ 0.978 $\pm$ 0.016 $\pm$ -1.15E-04 $\pm$ |       |           |                |       |           |                |        |           |
|                  | 0.027                                                                          | 0.006 | 2.62E-04  | 0.032                                                                          | 0.006 | 4.11E-04  | 0.023          | 0.009 | 3.55E-04  | 0.017          | 0.005  | 4.43E-04  |
| Case             | Training                                                                       |       |           |                                                                                |       |           |                |       |           |                |        |           |
|                  | 10 cm                                                                          |       |           | 20 cm                                                                          |       |           | 30 cm          |       |           | 40 cm          |        |           |
|                  | R <sup>2</sup>                                                                 | RMSE  | Bias      | R <sup>2</sup>                                                                 | RMSE  | Bias      | R <sup>2</sup> | RMSE  | Bias      | R <sup>2</sup> | RMSE   | Bias      |
| rng(0)           | 0.980                                                                          | 0.017 | 2.30E-05  | 0.934                                                                          | 0.026 | 1.66E-06  | 0.981          | 0.021 | -3.42E-05 | 0.960          | 0.024  | -7.53E-05 |
| rng(1)           | 0.902                                                                          | 0.035 | -1.16E-04 | 0.923                                                                          | 0.029 | 4.48E-05  | 0.974          | 0.974 | -2.63E-05 | 0.967          | 0.022  | 1.38E-05  |
| rng(2)           | 0.932                                                                          | 0.030 | -1.05E-04 | 0.925                                                                          | 0.028 | 7.89E-05  | 0.979          | 0.023 | -2.07E-06 | 0.974          | 0.019  | 6.98E-05  |
| rng(3)           | 0.980                                                                          | 0.017 | -1.37E-11 | 0.931                                                                          | 0.027 | -6.78E-06 | 0.962          | 0.031 | 1.06E-04  | 0.967          | 0.022  | 2.77E-05  |
| rng(4)           | 0.950                                                                          | 0.026 | -3.26E-04 | 0.905                                                                          | 0.032 | -2.06E-04 | 0.979          | 0.023 | -2.62E-05 | 0.972          | 0.020  | -7.67E-05 |
| rng(5)           | 0.936                                                                          | 0.029 | -2.67E-04 | 0.912                                                                          | 0.030 | -1.11E-05 | 0.979          | 0.023 | -7.84E-05 | 0.973          | 0.020  | 5.27E-05  |
| rng(6)           | 0.981                                                                          | 0.016 | -1.19E-04 | 0.931                                                                          | 0.027 | -8.51E-05 | 0.980          | 0.023 | -5.02E-05 | 0.974          | 0.019  | -4.12E-05 |
| rng(7)           | 0.985                                                                          | 0.014 | -6.76E-15 | 0.943                                                                          | 0.025 | -1.32E-06 | 0.952          | 0.034 | 1.12E-04  | 0.956          | 0.025  | -2.64E-05 |
| rng(8)           | 0.958                                                                          | 0.024 | -1.23E-04 | 0.944                                                                          | 0.025 | 1.84E-04  | 0.979          | 0.023 | -4.79E-05 | 0.983          | 0.016  | 9.69E-06  |
| rng(9)           | 0.944                                                                          | 0.027 | -4.16E-05 | 0.952                                                                          | 0.023 | -6.24E-05 | 0.999          | 0.005 | 4.05E-16  | 0.999          | 0.003  | 1.87E-16  |
| rng(10)          | 0.985                                                                          | 0.014 | -7.02E-15 | 0.963                                                                          | 0.020 | -5.84E-05 | 0.997          | 0.009 | 4.45E-16  | 0.983          | 0.016  | 7.11E-05  |
| rng(11)          | 0.974                                                                          | 0.019 | 4.10E-05  | 0.980                                                                          | 0.015 | -1.32E-14 | 0.984          | 0.020 | -7.98E-05 | 0.979          | 0.017  | 2.99E-05  |
| rng(12)          | 0.996                                                                          | 0.008 | -1.02E-16 | 0.919                                                                          | 0.030 | -8.36E-06 | 0.993          | 0.013 | -2.22E-12 | 0.978          | 0.0176 | 4.16E-05  |
| rng(13)          | 0.945                                                                          | 0.027 | 2.19E-04  | 0.914                                                                          | 0.030 | -5.66E-05 | 0.975          | 0.025 | 4.73E-05  | 0.974          | 0.019  | -8.34E-05 |
| rng(14)          | 0.944                                                                          | 0.027 | 5.53E-05  | 0.904                                                                          | 0.032 | 7.64E-05  | 0.973          | 0.026 | -7.80E-05 | 0.918          | 0.032  | -3.19E-04 |
| rng(15)          | 0.950                                                                          | 0.026 | -1.32E-05 | 0.920                                                                          | 0.029 | 1.81E-04  | 0.993          | 0.013 | -3.39E-12 | 0.984          | 0.015  | -3.89E-05 |
| rng(16)          | 0.982                                                                          | 0.016 | -9.87E-13 | 0.965                                                                          | 0.020 | -1.34E-04 | 0.961          | 0.031 | 3.19E-05  | 0.999          | 0.004  | 1.63E-16  |
| rng(17)          | 0.995                                                                          | 0.008 | -9.96E-17 | 0.978                                                                          | 0.016 | -1.00E-12 | 0.994          | 0.012 | -1.60E-13 | 0.999          | 0.004  | 1.42E-16  |
| rng(18)          | 0.980                                                                          | 0.017 | -7.28E-12 | 0.977                                                                          | 0.016 | -3.54E-12 | 0.993          | 0.013 | -8.74E-12 | 0.986          | 0.014  | 1.55E-05  |
| rng(19)          | 0.979                                                                          | 0.017 | -3.19E-11 | 0.966                                                                          | 0.020 | -4.94E-05 | 0.991          | 0.015 | -4.79E-06 | 0.984          | 0.015  | 5.41E-05  |
| rng(20)          | 0.982                                                                          | 0.016 | -3.39E-14 | 0.982                                                                          | 0.014 | -5.14E-16 | 0.998          | 0.007 | 5.01E-16  | 0.981          | 0.017  | -2.15E-04 |
| rng(21)          | 0.981                                                                          | 0.016 | -1.85E-12 | 0.925                                                                          | 0.028 | 1.18E-04  | 0.899          | 0.048 | -1.78E-04 | 0.982          | 0.016  | -7.19E-05 |
| rng(22)          | 0.948                                                                          | 0.026 | 7.66E-05  | 0.981                                                                          | 0.014 | -7.87E-15 | 0.999          | 0.004 | 4.30E-16  | 0.992          | 0.010  | -6.83E-13 |
| rng(23)          | 0.923                                                                          | 0.031 | 1.60E-05  | 0.997                                                                          | 0.005 | 1.72E-16  | 0.980          | 0.022 | -2.50E-04 | 0.966          | 0.022  | 6.73E-06  |
| rng(24)          | 0.919                                                                          | 0.032 | 1.71E-04  | 0.981                                                                          | 0.015 | -7.70E-15 | 0.994          | 0.012 | -1.96E-13 | 0.998          | 0.005  | 3.01E-16  |
| rng(25)          | 0.955                                                                          | 0.025 | -2.38E-05 | 0.960                                                                          | 0.021 | 9.27E-05  | 0.974          | 0.025 | -2.28E-04 | 0.998          | 0.006  | 2.38E-16  |
| rng(26)          | 0.979                                                                          | 0.017 | -2.87E-11 | 0.972                                                                          | 0.018 | -1.72E-11 | 0.974          | 0.025 | -1.69E-04 | 0.987          | 0.014  | 4.44E-05  |
| rng(27)          | 0.969                                                                          | 0.020 | -1.56E-04 | 0.923                                                                          | 0.029 | 3.09E-05  | 0.967          | 0.029 | 1.94E-05  | 0.959          | 0.024  | -6.37E-06 |
| rng(28)          | 0.916                                                                          | 0.033 | 1.15E-04  | 0.910                                                                          | 0.031 | 1.54E-05  | 0.999          | 0.004 | 5.22E-16  | 0.998          | 0.005  | 2.85E-16  |
| rng(29)          | 0.983                                                                          | 0.015 | -7.66E-15 | 0.940                                                                          | 0.025 | -1.66E-04 | 0.979          | 0.023 | -1.06E-04 | 0.970          | 0.021  | 8.18E-05  |



|                  |                                                                                                                 |
|------------------|-----------------------------------------------------------------------------------------------------------------|
| $\mu \pm \sigma$ | 0.961 ± 0.021 ± -1.91E-05 ± 0.945 ± 0.023 ± -7.23E-07 ± 0.979 ± 0.051 ± -3.47E-05 ± 0.978 ± 0.016 ± -1.45E-05 ± |
|                  | 0.025   0.007   1.10E-04   0.027   0.006   8.56E-05   0.019   0.174   8.37E-05   0.016   0.007   8.25E-05       |

Table 3: Performance metrics ( $R^2$ , RMSE, and Bias) for training and testing data across different depths (10 cm, 20 cm, 30 cm, and 40 cm) obtained from temporal distribution analysis using 30 different random seeds.

#### 4.4 Temporal distribution analysis

Temporal distribution analysis is essential to assess the robustness and generalisability of the model across different training and testing splits. By varying the random seed (rng(0) to rng(29)) and analysing performance across multiple iterations, we ensure that the model's success is not due to chance but rather its ability to consistently capture underlying patterns in the data, leading to reliable predictions across varying conditions and different depths (10 cm, 20 cm, 30 cm, and 40 cm). We tabulated the training and testing accuracy ( $R^2$ , RMSE, and Bias) for all the thirty cases corresponding to different random seeds (Table 3).

The results indicate that the model achieves high accuracy across all depths, with mean  $R^2$  values ranging from 0.941 to 0.978 in testing and 0.945 to 0.979 in training, confirming strong predictive performance. However, there is a noticeable trend where deeper depths (30 cm and 40 cm) outperform shallower depths (10 cm and 20 cm). The 40 cm depth exhibits the highest testing accuracy ( $R^2 = 0.978 \pm 0.017$ ) with the lowest RMSE ( $0.016 \pm 0.005$ ), followed closely by the 30 cm depth ( $R^2 = 0.976 \pm 0.023$ , RMSE =  $0.022 \pm 0.009$ ). In contrast, the shallower depths show slightly higher variability, with 10 cm having a wider range of  $R^2$  ( $0.955 \pm 0.027$ ) and RMSE ( $0.023 \pm 0.006$ ), while 20 cm also demonstrates slightly higher uncertainty ( $R^2 = 0.941 \pm 0.032$ , RMSE =  $0.024 \pm 0.006$ ). This suggests that shallow soil moisture is more susceptible to external influences such as precipitation, evaporation, and surface temperature fluctuations, leading to greater variability in predictions.

A comparison between training and testing metrics further supports the robustness of the model. The training RMSE values closely align with testing RMSE values across all depths, indicating that the model generalises well without overfitting. The bias remains close to zero for all depths, confirming that the model does not systematically over- or under-predict soil moisture values. However, a slightly higher variability in bias is observed at 20 cm and 40 cm depths, suggesting that while the model remains stable, it might be sensitive to certain data distributions at these depths.

The higher predictability at deeper depths aligns with the physical understanding of soil moisture behaviour, as moisture at greater depths is less influenced by short-term weather fluctuations and tends to have more stable temporal patterns. It suggests that the model is particularly well-suited for predicting subsurface moisture. In contrast, shallow soil layers are more dynamic and influenced by immediate environmental conditions, leading to higher variability in model performance. In conclusion, the results confirm that the model is robust and reliable in predicting soil moisture at different depths.



| Input feature sets         | Depth (cm) | Testing |          |          | Training |          |          |
|----------------------------|------------|---------|----------|----------|----------|----------|----------|
|                            |            | R       | RMSE [%] | Bias [%] | R        | RMSE [%] | Bias [%] |
| RH, ST2                    | 10         | 0.943   | 3.8      | 0.034    | 0.956    | 3.3      | 2.0E-11  |
|                            | 20         | 0.943   | 3.4      | 0.063    | 0.954    | 3.0      | 9.1E-15  |
|                            | 30         | 0.971   | 3.7      | 0.014    | 0.976    | 3.4      | 9.0E-13  |
|                            | 40         | 0.969   | 3.0      | 0.031    | 0.965    | 3.1      | 9.0E-15  |
| RH, ST2, DP                | 10         | 0.975   | 2.5      | 0.040    | 0.978    | 2.4      | 1.5E-14  |
|                            | 20         | 0.967   | 2.6      | 0.055    | 0.988    | 1.7      | -4.7E-15 |
|                            | 30         | 0.986   | 2.6      | 0.021    | 0.990    | 2.2      | -3.2E-14 |
|                            | 40         | 0.982   | 2.2      | -2.3E-03 | 0.994    | 1.3      | -5.0E-02 |
| RH, ST2, DP, ST4           | 10         | 0.989   | 1.7      | -0.0076  | 0.997    | 0.9      | 5.5E-15  |
|                            | 20         | 0.982   | 2.0      | -0.0053  | 0.995    | 1.0      | -2.6E-14 |
|                            | 30         | 0.995   | 1.5      | 0.039    | 1.000    | 0.3      | -3.1E-14 |
|                            | 40         | 0.996   | 1.0      | -3.1E-03 | 0.999    | 0.6      | -1.9E-14 |
| RH, ST2, DP, ST4, ST3      | 10         | 0.989   | 1.7      | 3.2E-04  | 0.996    | 1.0      | 5.9E-15  |
|                            | 20         | 0.989   | 1.6      | 0.023    | 1.000    | 0.2      | -2.5E-14 |
|                            | 30         | 0.996   | 1.4      | 0.021    | 0.999    | 0.8      | -4.0E-14 |
|                            | 40         | 0.997   | 1.0      | -1.1E-03 | 1.000    | 0.2      | -1.6E-14 |
| RH, ST2, DP, ST4, ST3, ST1 | 10         | 0.989   | 1.7      | 0.007    | 0.998    | 0.8      | 1.0E-14  |
|                            | 20         | 0.988   | 1.6      | 0.023    | 1.000    | 0.2      | -2.4E-14 |
|                            | 30         | 0.997   | 1.3      | 0.045    | 1.000    | 0.2      | -4.4E-14 |
|                            | 40         | 0.997   | 0.9      | 2.3E-04  | 0.999    | 0.5      | -2.3E-14 |
| All 11 features            | 10         | 0.990   | 1.6      | 0.023    | 0.831    | 5.8      | 1.1E-02  |
|                            | 20         | 0.938   | 3.4      | -0.033   | 0.954    | 3.1      | 6.7E-10  |
|                            | 30         | 0.990   | 1.9      | 0.036    | 0.992    | 1.9      | 1.8E-02  |
|                            | 40         | 0.985   | 2.1      | -0.021   | 0.971    | 2.8      | 3.4E-04  |

**Table 4.** Input ablation results for various feature sets across all depths.

#### 4.5 Ablation analysis

A critical aspect of refining predictive models is determining which input variables most significantly influence model accuracy, a process commonly known as input ablation. By systematically removing or adding features, we can identify the smallest subset of inputs that yields near-optimal or optimal model performance. This approach not only helps streamline data collection efforts but also reveals interactions among variables and potential redundancies within the feature space. In the context of soil moisture modelling, understanding exactly which environmental factors (e.g., soil temperatures, atmospheric conditions, moisture indices) drive the model's predictive capability is essential for both practical deployment and scientific interpretation.

Table 4 presents the results of the input ablation by considering six scenarios ranging from just two input variables (RH and ST2) to the full set of 11 features. Interestingly, certain reduced-feature subsets yield results that are comparable to or even



surpass those of the complete feature set. For instance, adding DP and deeper soil temperatures (ST3 and ST4) in progressive steps consistently improves testing R values and lowers RMSE across depths, often achieving exceptionally high R-value ( $\geq 0.98$ ) in the topsoil layers (10-30 cm). Such consistent gains in performance from the inclusion of specific soil temperature features confirm the important role of subsurface thermal conditions in driving near-surface moisture dynamics, which is also evident from the uncertainty analysis results observed in Section 4.3.

Despite these encouraging results for smaller subsets, there are valid reasons for maintaining a comprehensive set of input features in certain modelling scenarios. First, complete feature models can be more robust when conditions deviate from the historical range of data, such as atypical weather extremes, changes in land cover, or altered rainfall patterns. Second, including the full range of meteorological and soil variables can capture complete interactions that might not be evident during typical conditions or within a limited dataset. Although some of these features do not exhibit high importance under current conditions, particularly rainfall, which shows lower importance due to a relatively small number of rain events in the dataset, they remain physically meaningful variables. Consequently, rainfall does not emerge as a key driver within this particular modelling window, and thus, it is not included in the ablation subsets. However, this finding should not be interpreted to mean rainfall is universally unimportant. In a climate or season with more frequent or heavier precipitation, rainfall would likely rise in importance and substantially influence model output. Hence, retaining rainfall as part of the full feature set can be crucial for broader applicability, especially if the modelling framework is to remain robust under varying climatic conditions.

## 5 Conclusion

This study integrates an event-based approach to explore the subsurface soil moisture dynamics. Single peak and multiple peak events overall suggest that the soil has a moderate infiltration rate where high-intensity rainfall leads to sharp and immediate peaks, suggesting quick infiltration and possible saturation at deeper layers. In contrast, medium- and low-intensity rainfall events result in gradual moisture accumulation, with deeper layers showing limited response, indicating restricted percolation likely due to soil texture and composition. Global feature sensitivity analysis shows humidity and dew point strongly enhance soil moisture, while wind speed and direction have minimal impact. Solar radiance and evaporation cause drying, while rainfall increases soil moisture, with stronger effects at the shallower depths. Soil temperature generally show a negative correlation, though slight recoveries appear at higher thresholds.

Further evaluation of the model's performance in reconstructing soil moisture across various depths and rainfall events demonstrates that the AutoML-SM approach consistently captures soil moisture dynamics and outperforms conventional benchmark algorithms, as supported by our statistical analysis. The model also provides accurate estimates for high-intensity rainfall events at all depths, but its performance declines at deeper layers for medium and low-intensity events. Inducing small perturbations in the input variables clearly affirmed that soil temperature is the key driver whereas rainfall deviations have limited impact likely due to infiltration delays or existing moisture conditions. The temporal distribution analysis further highlights the model's robustness and stability across different soil depths, with notably higher accuracy at deeper layers. Overall,



our study shows the potential of AutoML-SM in advancing soil moisture modelling, providing a reliable and scalable approach  
555 for hydrological and agricultural applications.

Despite the strong performance of the AutoML-SM model, there are some limitations. The model relies heavily on the  
availability of input data, meaning that missing data can affect its predictions. Additionally, while the model performed well  
across different depths, further investigation is needed to understand its performance in extreme weather conditions, such as  
droughts or prolonged heavy rainfall. For future work, we plan to test the model in different geographical regions to assess its  
560 adaptability and reliability under varying climate conditions. Lastly, integrating physics-based constraints with AutoML-SM  
could improve the interpretability and generalisation of the model, making it even more effective for real-world applications.

#### Appendix A Table for the statistical comparison.

| Group A | Group B   | Lower Limit | Upper Limit | A-B  | p-value | Group A | Group B   | Lower Limit | Upper Limit | A-B  | p-value |
|---------|-----------|-------------|-------------|------|---------|---------|-----------|-------------|-------------|------|---------|
| GRNN10  | GRNN20    | -0.28       | 0.01        | 0.31 | 1       | GAM30   | AutoML30  | -0.38       | -0.09       | 0.21 | 1       |
| GRNN10  | GRNN30    | -0.43       | -0.13       | 0.16 | 0.99    | GAM30   | AutoML40  | -0.38       | -0.09       | 0.21 | 1       |
| GRNN10  | GRNN40    | -0.36       | -0.07       | 0.23 | 1       | GAM40   | BDT10     | -0.26       | 0.03        | 0.33 | 1       |
| GRNN10  | GAM10     | -0.24       | 0.05        | 0.35 | 1       | GAM40   | BDT20     | -0.36       | -0.06       | 0.23 | 1       |
| GRNN10  | GAM20     | -0.31       | -0.01       | 0.28 | 1       | GAM40   | BDT30     | -0.26       | 0.03        | 0.33 | 1       |
| GRNN10  | GAM30     | -0.27       | 0.03        | 0.32 | 1       | GAM40   | BDT40     | -0.38       | -0.09       | 0.21 | 1       |
| GRNN10  | GAM40     | -0.32       | -0.02       | 0.27 | 1       | GAM40   | RF10      | -0.32       | -0.02       | 0.27 | 1       |
| GRNN10  | BDT10     | -0.28       | 0.01        | 0.31 | 1       | GAM40   | RF20      | -0.35       | -0.06       | 0.23 | 1       |
| GRNN10  | BDT20     | -0.38       | -0.08       | 0.21 | 1       | GAM40   | RF30      | -0.33       | -0.03       | 0.26 | 1       |
| GRNN10  | BDT30     | -0.28       | 0.01        | 0.31 | 1       | GAM40   | RF40      | -0.37       | -0.08       | 0.21 | 1       |
| GRNN10  | BDT40     | -0.40       | -0.11       | 0.19 | 1       | GAM40   | LSBoost10 | -0.23       | 0.06        | 0.36 | 1       |
| GRNN10  | RF10      | -0.34       | -0.04       | 0.25 | 1       | GAM40   | LSBoost20 | -0.33       | -0.04       | 0.26 | 1       |
| GRNN10  | RF20      | -0.38       | -0.08       | 0.21 | 1       | GAM40   | LSBoost30 | -0.27       | 0.02        | 0.32 | 1       |
| GRNN10  | RF30      | -0.35       | -0.05       | 0.24 | 1       | GAM40   | LSBoost40 | -0.39       | -0.09       | 0.20 | 1       |
| GRNN10  | RF40      | -0.39       | -0.10       | 0.19 | 1       | GAM40   | AutoML10  | -0.33       | -0.04       | 0.26 | 1       |
| GRNN10  | LSBoost10 | -0.25       | 0.04        | 0.34 | 1       | GAM40   | AutoML20  | -0.33       | -0.04       | 0.26 | 1       |
| GRNN10  | LSBoost20 | -0.35       | -0.06       | 0.24 | 1       | GAM40   | AutoML30  | -0.33       | -0.04       | 0.26 | 1       |
| GRNN10  | LSBoost30 | -0.29       | 0.00        | 0.30 | 1       | GAM40   | AutoML40  | -0.33       | -0.04       | 0.26 | 1       |
| GRNN10  | LSBoost40 | -0.41       | -0.11       | 0.18 | 1       | BDT10   | BDT20     | -0.39       | -0.10       | 0.20 | 1       |
| GRNN10  | AutoML10  | -0.35       | -0.06       | 0.24 | 1       | BDT10   | BDT30     | -0.30       | 0.00        | 0.29 | 1       |



|                  |       |       |      |      |       |           |       |       |      |   |
|------------------|-------|-------|------|------|-------|-----------|-------|-------|------|---|
| GRNN10 AutoML20  | -0.35 | -0.06 | 0.24 | 1    | BDT10 | BDT40     | -0.42 | -0.12 | 0.17 | 1 |
| GRNN10 AutoML30  | -0.35 | -0.06 | 0.24 | 1    | BDT10 | RF10      | -0.35 | -0.06 | 0.24 | 1 |
| GRNN10 AutoML40  | -0.35 | -0.06 | 0.24 | 1    | BDT10 | RF20      | -0.39 | -0.09 | 0.20 | 1 |
| GRNN20 GRNN30    | -0.44 | -0.15 | 0.15 | 0.98 | BDT10 | RF30      | -0.36 | -0.07 | 0.23 | 1 |
| GRNN20 GRNN40    | -0.37 | -0.08 | 0.22 | 1    | BDT10 | RF40      | -0.41 | -0.11 | 0.18 | 1 |
| GRNN20 GAM10     | -0.25 | 0.04  | 0.34 | 1    | BDT10 | LSBoost10 | -0.27 | 0.03  | 0.32 | 1 |
| GRNN20 GAM20     | -0.32 | -0.03 | 0.27 | 1    | BDT10 | LSBoost20 | -0.37 | -0.07 | 0.22 | 1 |
| GRNN20 GAM30     | -0.28 | 0.02  | 0.31 | 1    | BDT10 | LSBoost30 | -0.31 | -0.01 | 0.28 | 1 |
| GRNN20 GAM40     | -0.33 | -0.03 | 0.26 | 1    | BDT10 | LSBoost40 | -0.42 | -0.13 | 0.17 | 1 |
| GRNN20 BDT10     | -0.29 | 0.00  | 0.30 | 1    | BDT10 | AutoML10  | -0.37 | -0.07 | 0.22 | 1 |
| GRNN20 BDT20     | -0.39 | -0.09 | 0.20 | 1    | BDT10 | AutoML20  | -0.37 | -0.07 | 0.22 | 1 |
| GRNN20 BDT30     | -0.30 | 0.00  | 0.29 | 1    | BDT10 | AutoML30  | -0.37 | -0.07 | 0.22 | 1 |
| GRNN20 BDT40     | -0.42 | -0.12 | 0.17 | 1    | BDT10 | AutoML40  | -0.37 | -0.07 | 0.22 | 1 |
| GRNN20 RF10      | -0.35 | -0.05 | 0.24 | 1    | BDT10 | BDT30     | -0.20 | 0.09  | 0.39 | 1 |
| GRNN20 RF20      | -0.39 | -0.09 | 0.20 | 1    | BDT20 | BDT40     | -0.32 | -0.03 | 0.27 | 1 |
| GRNN20 RF30      | -0.36 | -0.06 | 0.23 | 1    | BDT20 | RF10      | -0.26 | 0.04  | 0.33 | 1 |
| GRNN20 RF40      | -0.41 | -0.11 | 0.18 | 1    | BDT20 | RF20      | -0.29 | 0.00  | 0.30 | 1 |
| GRNN20 LSBoost10 | -0.26 | 0.03  | 0.33 | 1    | BDT20 | RF30      | -0.26 | 0.03  | 0.33 | 1 |
| GRNN20 LSBoost20 | -0.36 | -0.07 | 0.23 | 1    | BDT20 | RF40      | -0.31 | -0.02 | 0.28 | 1 |
| GRNN20 LSBoost30 | -0.30 | -0.01 | 0.28 | 1    | BDT20 | LSBoost10 | -0.17 | 0.13  | 0.42 | 1 |
| GRNN20 LSBoost40 | -0.42 | -0.12 | 0.17 | 1    | BDT20 | LSBoost20 | -0.27 | 0.02  | 0.32 | 1 |
| GRNN20 AutoML10  | -0.36 | -0.07 | 0.22 | 1    | BDT20 | LSBoost30 | -0.21 | 0.08  | 0.38 | 1 |
| GRNN20 AutoML20  | -0.36 | -0.07 | 0.23 | 1    | BDT20 | LSBoost40 | -0.32 | -0.03 | 0.27 | 1 |
| GRNN20 AutoML30  | -0.36 | -0.07 | 0.22 | 1    | BDT20 | AutoML10  | -0.27 | 0.02  | 0.32 | 1 |
| GRNN20 AutoML40  | -0.36 | -0.07 | 0.22 | 1    | BDT20 | AutoML20  | -0.27 | 0.02  | 0.32 | 1 |
| GRNN30 GRNN40    | -0.23 | 0.07  | 0.36 | 1    | BDT20 | AutoML30  | -0.27 | 0.02  | 0.32 | 1 |
| GRNN30 GAM10     | -0.11 | 0.19  | 0.48 | 0.81 | BDT20 | AutoML40  | -0.27 | 0.02  | 0.32 | 1 |
| GRNN30 GAM20     | -0.17 | 0.12  | 0.41 | 1    | BDT30 | BDT40     | -0.41 | -0.12 | 0.17 | 1 |
| GRNN30 GAM30     | -0.13 | 0.16  | 0.46 | 0.95 | BDT30 | RF10      | -0.35 | -0.05 | 0.24 | 1 |
| GRNN30 GAM40     | -0.18 | 0.11  | 0.41 | 1    | BDT30 | RF20      | -0.39 | -0.09 | 0.20 | 1 |
| GRNN30 BDT10     | -0.15 | 0.15  | 0.44 | 0.98 | BDT30 | RF30      | -0.36 | -0.06 | 0.23 | 1 |
| GRNN30 BDT20     | -0.24 | 0.05  | 0.35 | 1    | BDT30 | RF40      | -0.41 | -0.11 | 0.18 | 1 |



|        |           |       |       |      |      |       |           |       |       |      |      |
|--------|-----------|-------|-------|------|------|-------|-----------|-------|-------|------|------|
| GRNN30 | BDT30     | -0.15 | 0.15  | 0.44 | 0.98 | BDT30 | LSBoost10 | -0.26 | 0.03  | 0.33 | 1    |
| GRNN30 | BDT40     | -0.27 | 0.03  | 0.32 | 1    | BDT30 | LSBoost20 | -0.36 | -0.07 | 0.23 | 1    |
| GRNN30 | RF10      | -0.20 | 0.09  | 0.39 | 1    | BDT30 | LSBoost30 | -0.30 | -0.01 | 0.29 | 1    |
| GRNN30 | RF20      | -0.24 | 0.05  | 0.35 | 1    | BDT30 | LSBoost40 | -0.42 | -0.12 | 0.17 | 1    |
| GRNN30 | RF30      | -0.21 | 0.08  | 0.38 | 1    | BDT30 | AutoML10  | -0.36 | -0.07 | 0.23 | 1    |
| GRNN30 | RF40      | -0.26 | 0.03  | 0.33 | 1    | BDT30 | AutoML20  | -0.36 | -0.07 | 0.23 | 1    |
| GRNN30 | LSBoost10 | -0.12 | 0.18  | 0.47 | 0.87 | BDT30 | AutoML30  | -0.36 | -0.07 | 0.23 | 1    |
| GRNN30 | LSBoost20 | -0.22 | 0.08  | 0.37 | 1    | BDT30 | AutoML40  | -0.36 | -0.07 | 0.23 | 1    |
| GRNN30 | LSBoost30 | -0.16 | 0.14  | 0.43 | 0.99 | BDT40 | RF10      | -0.23 | 0.07  | 0.36 | 1    |
| GRNN30 | LSBoost40 | -0.27 | 0.02  | 0.32 | 1    | BDT40 | RF20      | -0.27 | 0.03  | 0.32 | 1    |
| GRNN30 | AutoML10  | -0.22 | 0.08  | 0.37 | 1    | BDT40 | RF30      | -0.24 | 0.06  | 0.35 | 1    |
| GRNN30 | AutoML20  | -0.22 | 0.08  | 0.37 | 1    | BDT40 | RF40      | -0.29 | 0.01  | 0.30 | 1    |
| GRNN30 | AutoML30  | -0.22 | 0.08  | 0.37 | 1    | BDT40 | LSBoost10 | -0.14 | 0.15  | 0.45 | 0.97 |
| GRNN30 | AutoML40  | -0.22 | 0.08  | 0.37 | 1    | BDT40 | LSBoost20 | -0.24 | 0.05  | 0.35 | 1    |
| GRNN40 | GAM10     | -0.18 | 0.12  | 0.41 | 1    | BDT40 | LSBoost30 | -0.18 | 0.11  | 0.41 | 1    |
| GRNN40 | GAM20     | -0.24 | 0.05  | 0.35 | 1    | BDT40 | LSBoost40 | -0.30 | 0.00  | 0.29 | 1    |
| GRNN40 | GAM30     | -0.20 | 0.09  | 0.39 | 1    | BDT40 | AutoML10  | -0.24 | 0.05  | 0.35 | 1    |
| GRNN40 | GAM40     | -0.25 | 0.05  | 0.34 | 1    | BDT40 | AutoML20  | -0.24 | 0.05  | 0.35 | 1    |
| GRNN40 | BDT10     | -0.21 | 0.08  | 0.38 | 1    | BDT40 | AutoML30  | -0.24 | 0.05  | 0.35 | 1    |
| GRNN40 | BDT20     | -0.31 | -0.02 | 0.28 | 1    | BDT40 | AutoML40  | -0.24 | 0.05  | 0.35 | 1    |
| GRNN40 | BDT30     | -0.22 | 0.08  | 0.37 | 1    | RF10  | RF20      | -0.33 | -0.04 | 0.26 | 1    |
| GRNN40 | BDT40     | -0.34 | -0.04 | 0.25 | 1    | RF10  | RF30      | -0.30 | -0.01 | 0.29 | 1    |
| GRNN40 | RF10      | -0.27 | 0.02  | 0.32 | 1    | RF10  | RF40      | -0.35 | -0.06 | 0.24 | 1    |
| GRNN40 | RF20      | -0.31 | -0.01 | 0.28 | 1    | RF10  | LSBoost10 | -0.21 | 0.09  | 0.38 | 1    |
| GRNN40 | RF30      | -0.28 | 0.01  | 0.31 | 1    | RF10  | LSBoost20 | -0.31 | -0.01 | 0.28 | 1    |
| GRNN40 | RF40      | -0.33 | -0.03 | 0.26 | 1    | RF10  | LSBoost30 | -0.25 | 0.05  | 0.34 | 1    |
| GRNN40 | LSBoost10 | -0.18 | 0.11  | 0.40 | 1    | RF10  | LSBoost40 | -0.36 | -0.07 | 0.23 | 1    |
| GRNN40 | LSBoost20 | -0.29 | 0.01  | 0.30 | 1    | RF10  | AutoML10  | -0.31 | -0.02 | 0.28 | 1    |
| GRNN40 | LSBoost30 | -0.23 | 0.07  | 0.36 | 1    | RF10  | AutoML20  | -0.31 | -0.01 | 0.28 | 1    |
| GRNN40 | LSBoost40 | -0.34 | -0.05 | 0.25 | 1    | RF10  | AutoML30  | -0.31 | -0.02 | 0.28 | 1    |
| GRNN40 | AutoML10  | -0.29 | 0.01  | 0.30 | 1    | RF10  | AutoML40  | -0.31 | -0.01 | 0.28 | 1    |
| GRNN40 | AutoML20  | -0.29 | 0.01  | 0.30 | 1    | RF20  | RF30      | -0.27 | 0.03  | 0.32 | 1    |





|        |           |       |       |      |      |           |           |       |       |      |      |
|--------|-----------|-------|-------|------|------|-----------|-----------|-------|-------|------|------|
| GRNN40 | AutoML30  | -0.29 | 0.01  | 0.30 | 1    | RF20      | RF40      | -0.31 | -0.02 | 0.27 | 1    |
| GRNN40 | AutoML40  | -0.29 | 0.01  | 0.30 | 1    | RF20      | LSBoost10 | -0.17 | 0.12  | 0.42 | 1    |
| GAM10  | GAM20     | -0.36 | -0.07 | 0.23 | 1    | RF20      | LSBoost20 | -0.27 | 0.02  | 0.32 | 1    |
| GAM10  | GAM30     | -0.32 | -0.02 | 0.27 | 1    | RF20      | LSBoost30 | -0.21 | 0.08  | 0.38 | 1    |
| GAM10  | GAM40     | -0.37 | -0.07 | 0.22 | 1    | RF20      | LSBoost40 | -0.33 | -0.03 | 0.26 | 1    |
| GAM10  | BDT10     | -0.33 | -0.04 | 0.26 | 1    | RF20      | AutoML10  | -0.27 | 0.02  | 0.32 | 1    |
| GAM10  | BDT20     | -0.43 | -0.13 | 0.16 | 0.99 | RF20      | AutoML20  | -0.27 | 0.02  | 0.32 | 1    |
| GAM10  | BDT30     | -0.34 | -0.04 | 0.25 | 1    | RF20      | AutoML30  | -0.27 | 0.02  | 0.32 | 1    |
| GAM10  | BDT40     | -0.46 | -0.16 | 0.13 | 0.95 | RF20      | AutoML40  | -0.27 | 0.02  | 0.32 | 1    |
| GAM10  | RF10      | -0.39 | -0.10 | 0.20 | 1    | RF30      | RF40      | -0.34 | -0.05 | 0.25 | 1    |
| GAM10  | RF20      | -0.43 | -0.13 | 0.16 | 0.99 | RF30      | LSBoost10 | -0.20 | 0.09  | 0.39 | 1    |
| GAM10  | RF30      | -0.40 | -0.10 | 0.19 | 1    | RF30      | LSBoost20 | -0.30 | -0.01 | 0.29 | 1    |
| GAM10  | RF40      | -0.45 | -0.15 | 0.14 | 0.97 | RF30      | LSBoost30 | -0.24 | 0.05  | 0.35 | 1    |
| GAM10  | LSBoost10 | -0.30 | -0.01 | 0.29 | 1    | RF30      | LSBoost40 | -0.35 | -0.06 | 0.23 | 1    |
| GAM10  | LSBoost20 | -0.40 | -0.11 | 0.18 | 1    | RF30      | AutoML10  | -0.30 | -0.01 | 0.29 | 1    |
| GAM10  | LSBoost30 | -0.35 | -0.05 | 0.24 | 1    | RF30      | AutoML20  | -0.30 | -0.01 | 0.29 | 1    |
| GAM10  | LSBoost40 | -0.46 | -0.16 | 0.13 | 0.94 | RF30      | AutoML30  | -0.30 | -0.01 | 0.29 | 1    |
| GAM10  | AutoML10  | -0.41 | -0.11 | 0.18 | 1    | RF30      | AutoML40  | -0.30 | -0.01 | 0.29 | 1    |
| GAM10  | AutoML20  | -0.41 | -0.11 | 0.18 | 1    | RF40      | LSBoost10 | -0.15 | 0.14  | 0.44 | 0.99 |
| GAM10  | AutoML30  | -0.41 | -0.11 | 0.18 | 1    | RF40      | LSBoost20 | -0.25 | 0.04  | 0.34 | 1    |
| GAM10  | AutoML40  | -0.41 | -0.11 | 0.18 | 1    | RF40      | LSBoost30 | -0.19 | 0.10  | 0.40 | 1    |
| GAM20  | GAM30     | -0.25 | 0.04  | 0.34 | 1    | RF40      | LSBoost40 | -0.31 | -0.01 | 0.28 | 1    |
| GAM20  | GAM40     | -0.30 | -0.01 | 0.29 | 1    | RF40      | AutoML10  | -0.25 | 0.04  | 0.34 | 1    |
| GAM20  | BDT10     | -0.27 | 0.03  | 0.32 | 1    | RF40      | AutoML20  | -0.25 | 0.04  | 0.34 | 1    |
| GAM20  | BDT20     | -0.36 | -0.07 | 0.23 | 1    | RF40      | AutoML30  | -0.25 | 0.04  | 0.34 | 1    |
| GAM20  | BDT30     | -0.27 | 0.03  | 0.32 | 1    | RF40      | AutoML40  | -0.25 | 0.04  | 0.34 | 1    |
| GAM20  | BDT40     | -0.39 | -0.09 | 0.20 | 1    | LSBoost10 | LSBoost20 | -0.40 | -0.10 | 0.19 | 1    |
| GAM20  | RF10      | -0.32 | -0.03 | 0.27 | 1    | LSBoost10 | LSBoost30 | -0.34 | -0.04 | 0.25 | 1    |
| GAM20  | RF20      | -0.36 | -0.07 | 0.23 | 1    | LSBoost10 | LSBoost40 | -0.45 | -0.16 | 0.14 | 0.97 |
| GAM20  | RF30      | -0.33 | -0.04 | 0.26 | 1    | LSBoost10 | AutoML10  | -0.40 | -0.10 | 0.19 | 1    |
| GAM20  | RF40      | -0.38 | -0.09 | 0.21 | 1    | LSBoost10 | AutoML20  | -0.40 | -0.10 | 0.19 | 1    |
| GAM20  | LSBoost10 | -0.24 | 0.06  | 0.35 | 1    | LSBoost10 | AutoML30  | -0.40 | -0.10 | 0.19 | 1    |



|       |           |       |       |      |      |           |           |       |       |      |   |
|-------|-----------|-------|-------|------|------|-----------|-----------|-------|-------|------|---|
| GAM20 | LSBoost20 | -0.34 | -0.04 | 0.25 | 1    | LSBoost10 | AutoML40  | -0.40 | -0.10 | 0.19 | 1 |
| GAM20 | LSBoost30 | -0.28 | 0.02  | 0.31 | 1    | LSBoost20 | LSBoost30 | -0.24 | 0.06  | 0.35 | 1 |
| GAM20 | LSBoost40 | -0.39 | -0.10 | 0.20 | 1    | LSBoost20 | LSBoost40 | -0.35 | -0.05 | 0.24 | 1 |
| GAM20 | AutoML10  | -0.34 | -0.04 | 0.25 | 1    | LSBoost20 | AutoML10  | -0.30 | 0.00  | 0.29 | 1 |
| GAM20 | AutoML20  | -0.34 | -0.04 | 0.25 | 1    | LSBoost20 | AutoML20  | -0.30 | 0.00  | 0.29 | 1 |
| GAM20 | AutoML30  | -0.34 | -0.04 | 0.25 | 1    | LSBoost20 | AutoML30  | -0.30 | 0.00  | 0.29 | 1 |
| GAM20 | AutoML40  | -0.34 | -0.04 | 0.25 | 1    | LSBoost20 | AutoML40  | -0.30 | 0.00  | 0.29 | 1 |
| GAM30 | GAM40     | -0.34 | -0.05 | 0.25 | 1    | LSBoost30 | LSBoost40 | -0.41 | -0.11 | 0.18 | 1 |
| GAM30 | BDT10     | -0.31 | -0.01 | 0.28 | 1    | LSBoost30 | AutoML10  | -0.35 | -0.06 | 0.23 | 1 |
| GAM30 | BDT20     | -0.40 | -0.11 | 0.18 | 1    | LSBoost30 | AutoML20  | -0.35 | -0.06 | 0.23 | 1 |
| GAM30 | BDT30     | -0.31 | -0.02 | 0.28 | 1    | LSBoost30 | AutoML30  | -0.36 | -0.06 | 0.23 | 1 |
| GAM30 | BDT40     | -0.43 | -0.14 | 0.16 | 0.99 | LSBoost30 | AutoML40  | -0.35 | -0.06 | 0.23 | 1 |
| GAM30 | RF10      | -0.37 | -0.07 | 0.22 | 1    | LSBoost40 | AutoML10  | -0.24 | 0.05  | 0.35 | 1 |
| GAM30 | RF20      | -0.40 | -0.11 | 0.19 | 1    | LSBoost40 | AutoML20  | -0.24 | 0.05  | 0.35 | 1 |
| GAM30 | RF30      | -0.37 | -0.08 | 0.22 | 1    | LSBoost40 | AutoML30  | -0.24 | 0.05  | 0.35 | 1 |
| GAM30 | RF40      | -0.42 | -0.13 | 0.17 | 1    | LSBoost40 | AutoML40  | -0.24 | 0.05  | 0.35 | 1 |
| GAM30 | LSBoost10 | -0.28 | 0.02  | 0.31 | 1    | AutoML10  | AutoML20  | -0.29 | 0.00  | 0.30 | 1 |
| GAM30 | LSBoost20 | -0.38 | -0.08 | 0.21 | 1    | AutoML10  | AutoML30  | -0.29 | 0.00  | 0.29 | 1 |
| GAM30 | LSBoost30 | -0.32 | -0.03 | 0.27 | 1    | AutoML10  | AutoML40  | -0.29 | 0.00  | 0.30 | 1 |
| GAM30 | LSBoost40 | -0.43 | -0.14 | 0.16 | 0.99 | AutoML20  | AutoML30  | -0.30 | 0.00  | 0.29 | 1 |
| GAM30 | AutoML10  | -0.38 | -0.09 | 0.21 | 1    | AutoML20  | AutoML40  | -0.29 | 0.00  | 0.29 | 1 |
| GAM30 | AutoML20  | -0.38 | -0.09 | 0.21 | 1    | AutoML30  | AutoML40  | -0.29 | 0.00  | 0.30 | 1 |

Table .1: Benchmark algorithm intercomparison results through post-hoc test.

*Code availability.* The code developed in this study will be made publicly available (<https://abhilashsingh.net/codes.html>) after acceptance of this manuscript.

565 *Data availability.* The data will be made available with the code.



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