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Article

Predictive modeling of evapotranspiration using Long Short-Term Memory and explainable Artificial Intelligence

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Abstract: Evapotranspiration (ET) modeling plays a vital role in water resource management, agriculture, and climate adaptation. Accurate ET prediction is essential for effective irrigation planning and crop management. However, traditional methods often struggle to capture the complex relationships between environmental factors, resulting in less reliable forecasts. To address this, we implemented and optimized the Long Short-Term Memory (LSTM) network model to predict ET with improved accuracy of 98.8%, achieving a Mean Squared Error (MSE) of 0.12. Our approach incorporates SHapley Additive exPlanations (SHAP) to enhance model interpretability, offering insights into how key factors like solar radiation, wind speed, air temperature, and relative humidity impact ET predictions. The results showed that solar radiation had the highest impact on ET, followed by wind speed and air temperature. This improved understanding of key factors can help farmers and water managers make better decisions about irrigation, ensuring efficient water use and supporting sustainable agriculture. This provides a reliable and interpretable solution for ET prediction, aiding smarter irrigation strategies, improving resource efficiency, and supporting sustainable agricultural practices.

Keywords: evapotranspiration; SHAP; LSTM; deep learning; XGBoost; XAI; black-box

1. Introduction

Evapotranspiration (ET) is a vital process in the water cycle that represents the combined loss of water through evaporation from soil, water surfaces, and plant transpiration. It plays a significant role in maintaining the balance of moisture in the environment and directly influences weather patterns, climate conditions, and agricultural productivity. ET is a key factor in determining the amount of water required for crops to grow efficiently. In agriculture, accurate ET prediction is crucial for designing effective irrigation systems, ensuring crops receive sufficient amounts of water without overuse, and improving overall water resource management. The need for accurate ET prediction arises from its impact on several critical areas. First, in regions facing water scarcity, precise ET estimates help optimize irrigation scheduling, reducing water wastage while maintaining crop health. Second, understanding ET patterns can improve drought forecasting, enabling farmers to adopt proactive measures during dry periods. Additionally, ET modeling aids in managing groundwater resources by estimating the rate of water loss from the soil. In climate studies, ET data is essential for understanding energy balance, as it influences atmospheric relative humidity and air temperature.

Traditional ET estimation methods, such as the Penman-Monteith equation or empirical formulas, often rely on fixed assumptions that may not capture complex environmental interactions accurately. These methods can struggle with changing weather conditions, diverse soil types, and varying crop characteristics. As a result, they may produce less reliable predictions, especially in regions with dynamic climates. To overcome these limitations, machine learning models have gained attention for their ability to identify complex patterns in environmental data. However, these models are often considered "black box," making it difficult for users to understand how predictions are made. This lack of interpretability can hinder their adoption in real-world agricultural practices, where decision-makers need clear insights into the factors driving ET predictions.

Our research addresses this challenge by developing and optimizing predictive models using Long Short-Term Memory (LSTM) networks and eXtreme Gradient Boosting (XGBoost). To improve transparency, we employed SHapley Additive exPlanations (SHAP) values, which highlight the most influential features in ET prediction, such as solar radiation, wind speed, and air temperature. By combining accurate predictions with clear explanations, our approach provides actionable insights for improving irrigation strategies, supporting sustainable water management practices, and enhancing agricultural productivity.

2. Literature review

The field of evapotranspiration (ET) modeling has witnessed significant advancements due to the integration of machine learning and artificial intelligence [1]. Traditional methods of estimating ET, often reliant on empirical formulas, have been limited by their assumptions and localized applicability, as demonstrated by Fereres and García-Vila M. [2]. In contrast, machine learning approaches, including those utilizing dynamic neural networks, have demonstrated the ability to model complex relationships in soil moisture content, enhancing predictive irrigation scheduling, as shown by Ben Abdallah et al. [3]. This shift towards data-driven methods highlights the importance of leveraging sensor data and advanced algorithms to improve irrigation management and crop productivity, as noted by Goldstein et al. [4] and Goap et al. [5]. Explainable AI (XAI) has emerged as a critical area of research in this context, addressing the "black-box" nature of many machine learning models, as described by Arrieta et al. [6]. By providing insights into model decision-making processes, XAI facilitates a better understanding of the factors influencing ET predictions. Studies have shown that interpretability can enhance user trust and adoption of machine learning solutions in agricultural settings, as demonstrated by Chakraborty et al. [7] and Dikshit and Pradhan [8]. This has led to the development of frameworks that incorporate feature selection methods and ensemble learning approaches to optimize predictive accuracy while maintaining model transparency, supported by the use of the coefficient of determination (R^2) as presented by Di Bucchianico A. et al. [9]. Long Short-Term Memory (LSTM) networks have been widely recognized for their effectiveness in time series analysis, particularly in applications related to irrigation management, as demonstrated by Hochreiter and Schmidhuber [10]. These models excel at capturing temporal dependencies, making them well-suited for predicting ET based on historical meteorological data with ensemble methods like stacking and blending further enhancing estimation accuracy [11]. Recent studies have explored innovative approaches combining LSTM with explainable techniques to predict soil moisture and ET, aiming to enhance decision-making in smart agriculture, as shown by Koné et al. [12]. The integration of deep learning methods in environmental remote sensing has also shown promise in estimating daily reference evapotranspiration (ETo), as highlighted by Zhao et al. [13]. This reflects a broader trend towards utilizing hybrid models that combine various machine learning techniques to capture the complexity of environmental processes, as demonstrated by Acharki et al. [14]. Furthermore, research on learned features for monitoring plant water status emphasizes the potential of machine learning in addressing challenges related to irrigation and water resource management, as described by Zhuang et al. [15]. Recent advancements in evapotranspiration (ET) modeling highlight the integration of machine learning (ML) and artificial intelligence (AI), offering improved prediction accuracy for irrigation management and crop productivity [16]. The incorporation of Explainable AI (XAI) enhances model transparency, making it easier for users to understand decision-making processes and improving trust in ML models [17]. Long Short-Term Memory (LSTM) networks, particularly in hybrid models, have proven effective in capturing temporal dependencies for predicting ET based on historical meteorological data, showcasing their potential for smart agriculture applications [18]. Recent research on evapotranspiration (ET) modeling highlights the use of hybrid models combining machine learning and traditional methods. Vaz et al. [19] developed hybrid neural network models, improving ET prediction with limited weather parameters. Khairan et al. [20] reviewed parameter optimization-based hybrid models, enhancing reference ET accuracy. Additionally, Hu et al. [21] demonstrated the benefits of combining physical and data-driven models for better ET estimation.

In summary, the literature [22–24] indicates a significant shift towards employing machine learning and explainable AI in evapotranspiration modeling. These approaches not only enhance predictive accuracy but also foster a deeper understanding of the underlying processes, thereby facilitating more informed decision-making in agricultural water management [25].

3. Methodology

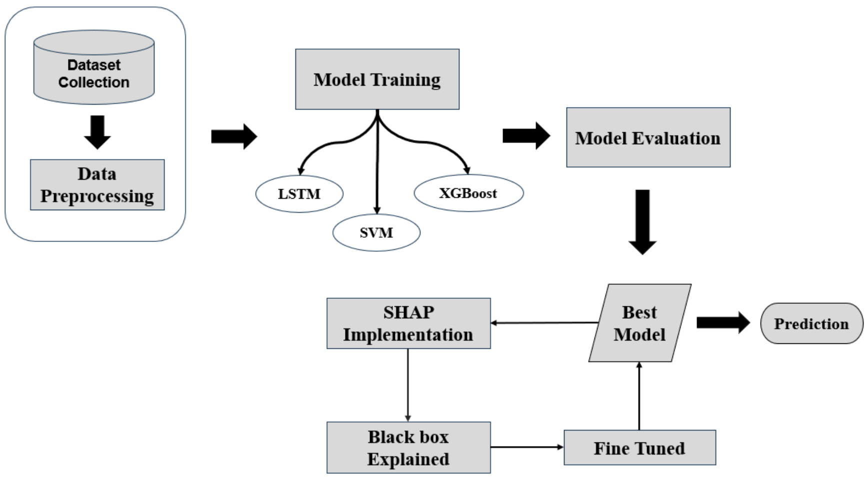

Figure 1. Overview of the architecture of the proposed system for potential evapotranspiration (PET) estimation using machine learning models with SHAP-based interpretability.

The architecture of the proposed system, as shown in **Figure 1**, has six sections: data collection and preprocessing, model selection and training, model evaluation, best model finding, explainable AI implementation, and prediction.

3.1. Data description

The dataset used in this study was obtained from the United States Geological Survey (USGS) website and consists of 10,850 records with 13 attributes spanning from 1994 to 2020. It includes continuous numeric values representing various environmental factors such as wind speed, solar radiation, air temperature, relative humidity, dew point temperature, and precipitation. The target variable, potential evapotranspiration (PET), measures water loss from soil and plants due to evaporation and transpiration. Key attributes include maximum wind gust, average wind speed, solar radiation, maximum and minimum air temperature, average air temperature, relative humidity (maximum, minimum, and sampled), average dew point temperature, and total precipitation.

The data was collected from a weather station (AWS) located at coordinates 39.8283° N, 98.5795° W, a central point in the United States. The wind sensors were positioned at a height of 10 m above the ground, while temperature and humidity sensors were placed at a height of 1.5 to 2 m to ensure accurate readings. The data was recorded at a daily frequency, with each record corresponding to one day's worth of measurements.

Data preprocessing

Data preprocessing is a crucial step in data analysis that involves cleaning and transforming raw data into a structured format suitable for analysis. It is necessary to improve data quality and ensure the dataset is ready for modeling [26]. In this study, dates appeared in various formats, which could lead to errors during analysis. To address this, all dates were converted into a consistent format to maintain accuracy. Additionally, missing values in the dataset were identified by checking for null or NaN entries. As all variables are continuous, such as wind speed, temperature, and humidity, missing data were filled using linear interpolation to preserve the continuity and accuracy of the time series. Other preprocessing steps, such as handling outliers, scaling numeric features, and encoding categorical data, were also performed to enhance data quality. These steps ensured the dataset was well-prepared for effective exploratory data analysis (EDA) and model development.

3.2. Exploratory data analysis

To understand the data better, various visualizations were employed. One key visualization is the line plot, as shown in **Figure 2**, which illustrates the average PET values across different years. This plot effectively shows long-term trends, highlighting any significant increases or decreases over time.

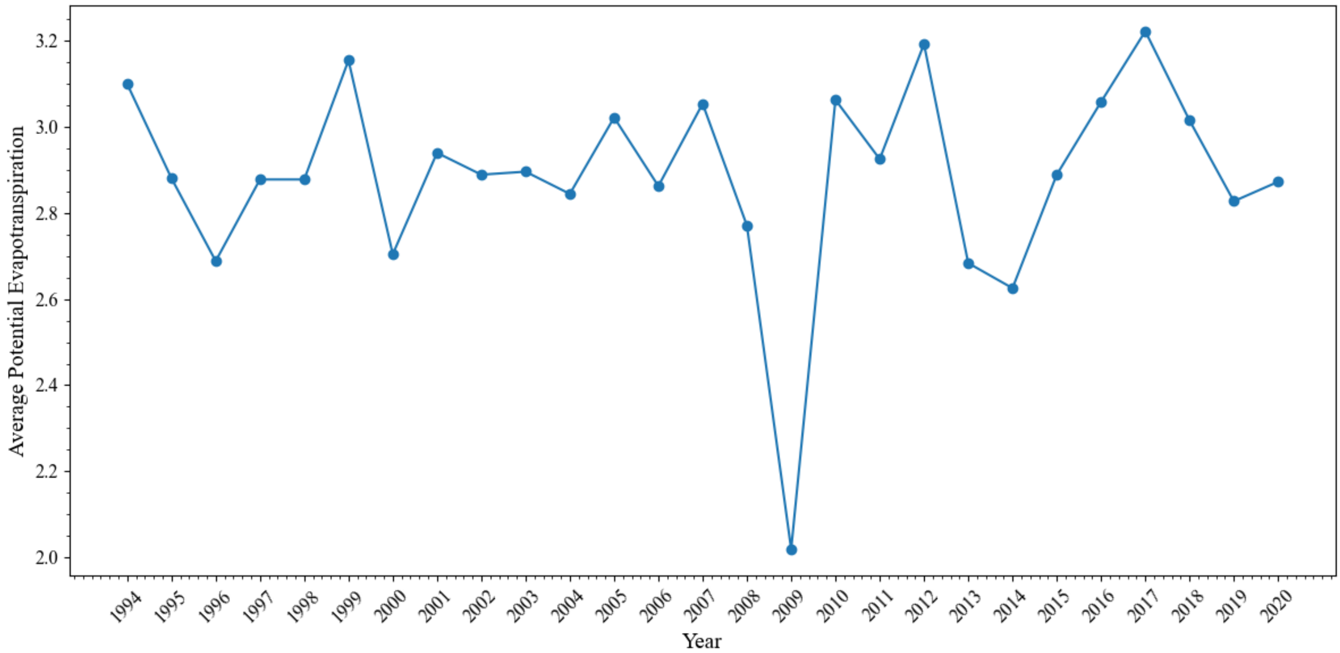

Figure 2. Line plot showing average PET over years.

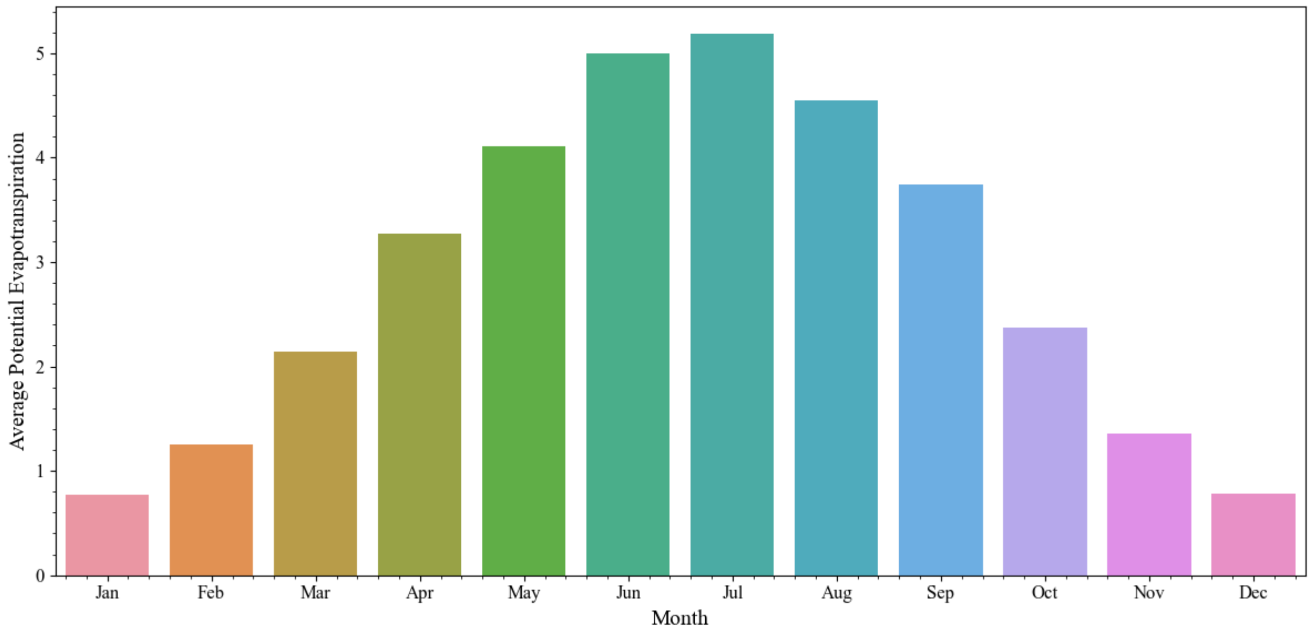

Figure 3. Bar plot of average potential evapotranspiration (PET) by month, highlighting seasonal variations in water loss.

Another visualization, a bar plot that is shown in **Figure 3**, represents the average PET values for each month. This plot reveals seasonal patterns, such as higher PET rates in warmer months and lower rates during colder months. Together, these visualizations provide insights into both annual trends and seasonal variations.

3.3. Model training

Different machine learning models, including Support Vector Machine (SVM), XGBoost, and Long Short-Term Memory (LSTM), were used to predict potential evapotranspiration (PET).

Each model was chosen to explore its effectiveness in handling time series data. SVM and XGBoost were employed as baseline models due to their performance in regression tasks.

Hyperparameters like the regularization parameter in SVM and learning rate, maximum depth, and number of estimators in XGBoost were adjusted to achieve optimal results.

The LSTM model was chosen for its capacity to effectively capture temporal dependencies in time-series data. Since LSTM requires 3D input (samples, time steps, features), we transformed the dataset by creating lagged values for each feature to allow the model to learn from historical data. To optimize the lag values, we utilized 5-fold cross-validation for model evaluation, which involves splitting the dataset into five subsets and training the model on four subsets while validating it on the remaining one.

This process was repeated five times, ensuring that each fold serves as the validation set once. For lag optimization, we tested different lag values ranging from 1 to 7 days. The model's performance was evaluated using the Root Mean Squared Error (RMSE) on the validation set for each lag configuration.

The lag value that resulted in the lowest RMSE was selected as the optimal lag structure. After evaluating across all folds, the optimal lag of 3 days was chosen, as it consistently yielded the best performance across the folds, ensuring that the model captured relevant temporal patterns while avoiding overfitting.

This step allowed the model to recognize past patterns and improve prediction accuracy. The architecture was designed to handle sequential data and predict PET values effectively.

The LSTM architecture is designed to model temporal patterns in time-series data, making it suitable for predicting potential evapotranspiration (PET). As illustrated in **Figure 4**, it includes the following components:

- Input layer: Accepts 3D input (samples, time steps, features) formed by creating lagged sequences of environmental data.
- Forget gate: Filters out irrelevant information from the previous time step to prevent the accumulation of noise.
- Input gate: Determines which new information should be added to the cell state using sigmoid and tanh activations.
- Cell state: Serves as the memory component that carries essential information across time steps, updated by the forget and input gates.
- Output gate: Controls what information from the cell state is passed forward as the output and hidden state.
- Dropout layer: Reduces overfitting by randomly dropping neurons during training.
- Dense (output) layer: Outputs the final PET prediction based on the learned time-dependent patterns.

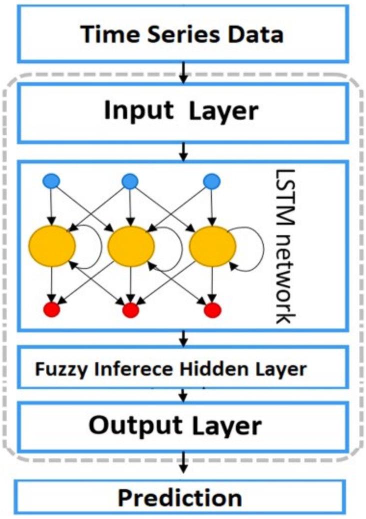

Figure 4. LSTM network diagram showing input, hidden layers with memory cells, and an output layer controlling information flow.

During training, one key challenge was reshaping the data into a suitable 3D format. Creating optimal lag values was crucial to ensure the model received enough historical context without overloading it with excessive data.

3.4. Model evaluation

Model evaluation is important to assess how well a model predicts outcomes. The model was evaluated using MSE (Equation (1)), RMSE (Equation (2)), and R^2. MSE shows the average squared difference between the actual and predicted values, helping to measure overall error.

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \tag{1}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \tag{2}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{3}$$

RMSE is the square root of MSE, making it easier to understand since it's in the same unit as the target. R^2 shows how well the model explains the data, with higher values meaning better performance. These metrics helped check how accurate and reliable the model is.

3.5. Explainable AI for model interpretation

Explainable AI (XAI) is a set of methods that make the decisions of machine learning models easier for humans to understand.

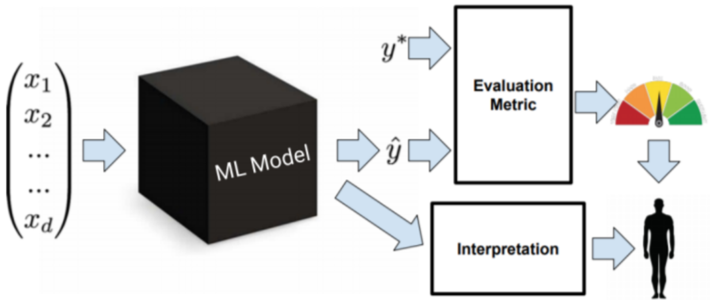

Figure 5. Illustration of a black box ML model where inputs lead to outputs without transparency in decision-making.

Many advanced models, like deep learning networks and ensemble methods, act as "black-box," as shown in **Figure 5**, meaning they provide accurate predictions but without clear explanations for how those predictions are made. This lack of transparency can be risky, especially in important areas like healthcare, finance, or criminal justice, where decisions can significantly impact people's lives.

Figure 6 highlights the growing need for interpretability in ML systems. It presents a typical workflow from training data and learning algorithms to predictions and illustrates how users may question outputs when the decision-making process is not transparent. In high-stakes scenarios, users often ask, "Why did the model make this prediction?", "Can I trust this output?", or "Which features contributed the most?" Such uncertainty can undermine trust and lead to rejection of AI solutions. Therefore, incorporating interpretable methods like SHAP not only helps improve model accuracy and transparency but also ensures that AI systems are trustworthy, ethical, and aligned with human values.

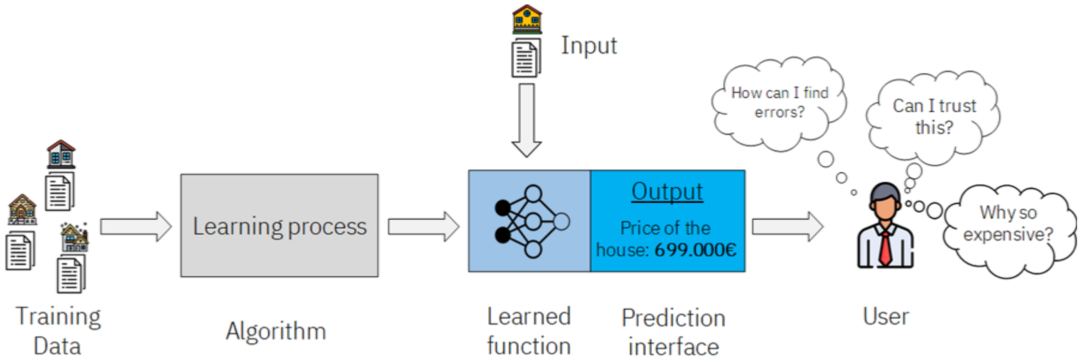

Figure 6. The need for model interpretability, as users question ML predictions due to a lack of transparency.

XAI methods, such as SHAP (SHapley Additive exPlanations), are designed to explain the contribution of each input feature to the model's output. SHAP values calculate how much each feature influences a prediction by averaging its impact across all possible feature combinations. Using SHAP values helps to identify which features have the most impact, allowing us to refine models and improve accuracy. By improving understandability, XAI and SHAP values ensure that AI models are not just powerful but also safe, ethical, and aligned with human values.

3.6. SHAP implementation

After training the model, SHAP values were used to explain how different features influenced the predictions. Several SHAP plots were created to better understand these effects. The summary plot showed which features were most important and how they affected the target value. The dependence plot helped reveal how one feature's effect changes based on another feature.

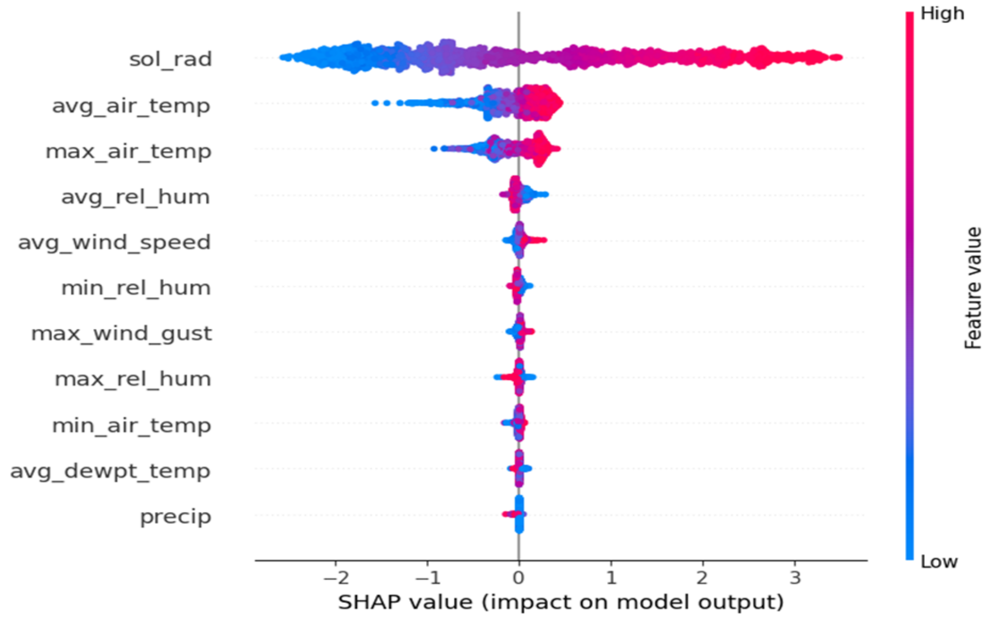

Figure 7. SHAP Beeswarm Plot illustrating how individual features contribute to the model's prediction.

The Beeswarm plot as shown in **Figure 7** explained individual predictions by showing how each feature increased or decreased the final result. The waterfall plot broke down the prediction step by step, showing each feature's contribution. These visualizations made it easier to understand the model's behavior and identify key factors influencing its predictions.

3.7. Prediction of potential evapotranspiration

After improving the model using SHAP values to understand which factors impact potential evapotranspiration the most, we moved on to predicting future values. Using this improved model, we predicted the potential evapotranspiration (PET) rates for the next five years.

4. Result and discussion

Our study focused on predicting potential evapotranspiration (PET) using an LSTM model, which demonstrated superior performance compared to XGBoost and SVM. Given the time-series nature of PET data, deep learning models like LSTM are well-suited for capturing temporal dependencies and complex patterns. The comparison of model accuracy and Mean Squared Error (MSE) is presented in **Table 1**.

Table 1. Comparison of accuracy and MSE of different models.

	MSE	RMSE	MAE	R^2	Accuracy
LSTM	0.12	0.35	0.08	0.98	98.8
XGBoost	0.28	0.53	0.15	0.94	96
SVM	0.45	0.67	0.20	0.89	92

The results indicate that the LSTM model achieved the lowest Mean Squared Error (MSE) of 0.12, demonstrating its ability to learn intricate relationships in the data.

In contrast, XGBoost and SVM recorded higher errors of 0.28 and 0.45, respectively, highlighting their limitations in handling sequential dependencies. The superior accuracy of 98.8% achieved by LSTM underscores its effectiveness in forecasting PET values with minimal deviation. The 98.8% accuracy metric was derived using a train-test split methodology. The dataset was divided into two parts: a training set and a test set. The training set, comprising 70% of the data, was used to train the LSTM model, while the remaining 30% was reserved for testing. The train loss plot of **Figure 8** showed a smooth decline in error, confirming the model's stable learning process. This separation ensured that the model was trained on one subset of the data and evaluated on a completely different subset, which helps in assessing the model's generalization ability.

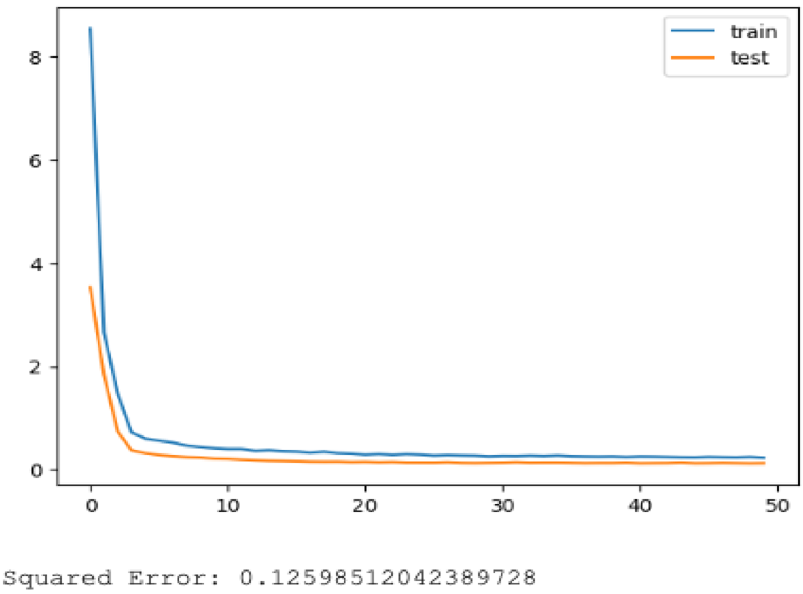

Figure 8. Learning curve for the LSTM model illustrating the training and testing loss over epochs.

Once the model was trained, its performance was evaluated by comparing the predicted PET values against the actual observed values from the test set. The accuracy was calculated as the percentage of correct predictions made by the model on the test data, providing an estimate of how well the model could forecast unseen data. This method offers a reliable measure of the model's ability to generalize to new, unseen data, ensuring that the high accuracy observed reflects the model's true predictive capability.

This enhanced performance can be attributed to LSTM's gated memory units, which allow it to retain relevant past information while filtering out noise. Unlike XGBoost, which relies on gradient boosting techniques, and SVM, which constructs decision boundaries in high-dimensional space, LSTM dynamically adjusts its parameters through sequential learning. This adaptability makes it more suitable for capturing long-term dependencies in climate-related datasets.

To understand which features influenced PET the most, a pie chart, as shown in **Figure 9**, revealed that solar radiation, average air temperature, and wind speed had the strongest impact.

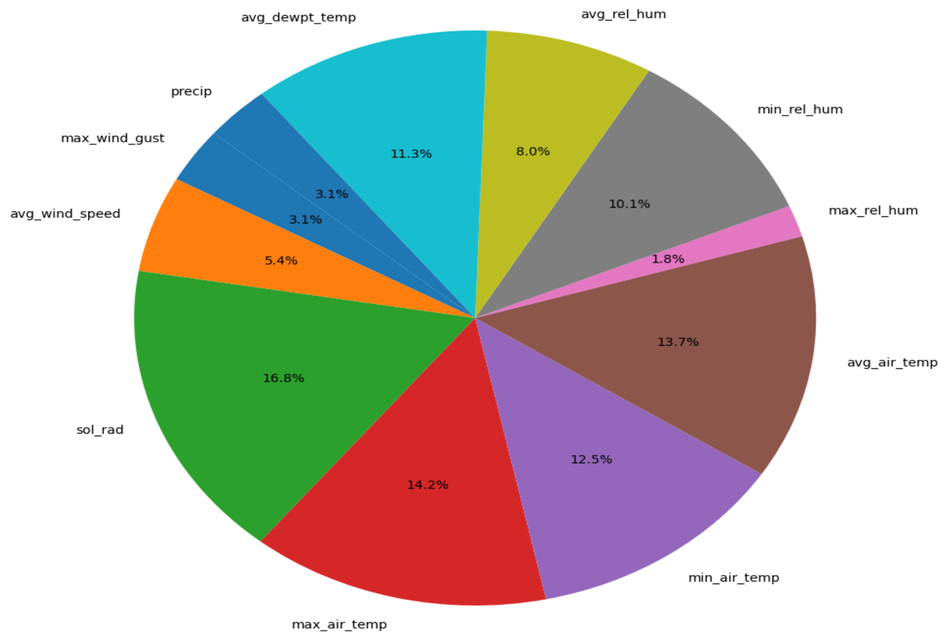

Figure 9. Feature contribution to potential evapotranspiration.

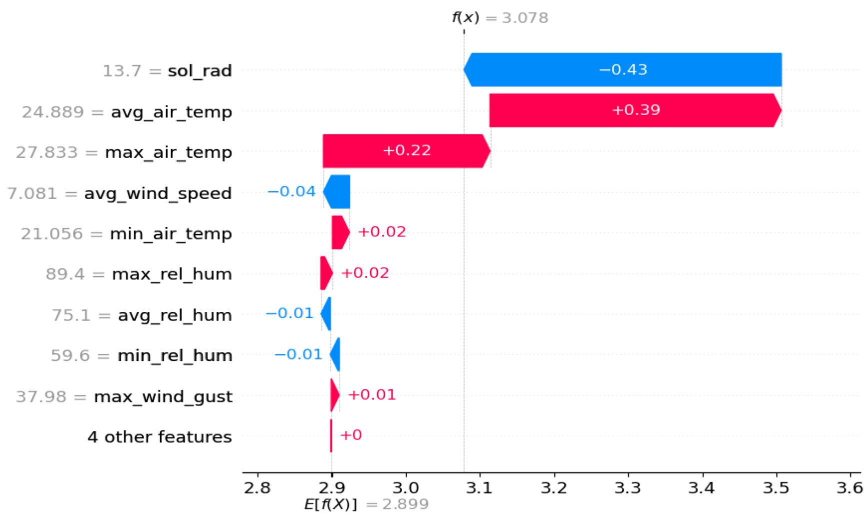

Figure 10. SHAP waterfall plot explaining a single prediction for PET.

Additionally, SHAP plots provided deeper insights into these feature contributions. The waterfall plot, as shown in **Figure 10**, highlighted the most influential features, while the dependence plot showed how they interacted with each other.

The SHAP summery plot, as shown in **Figure 11**, shows the overall feature importance, showing which factors had the most influence on the predicted PET values. These plots helped identify key contributors by highlighting how different features impacted the model's predictions.

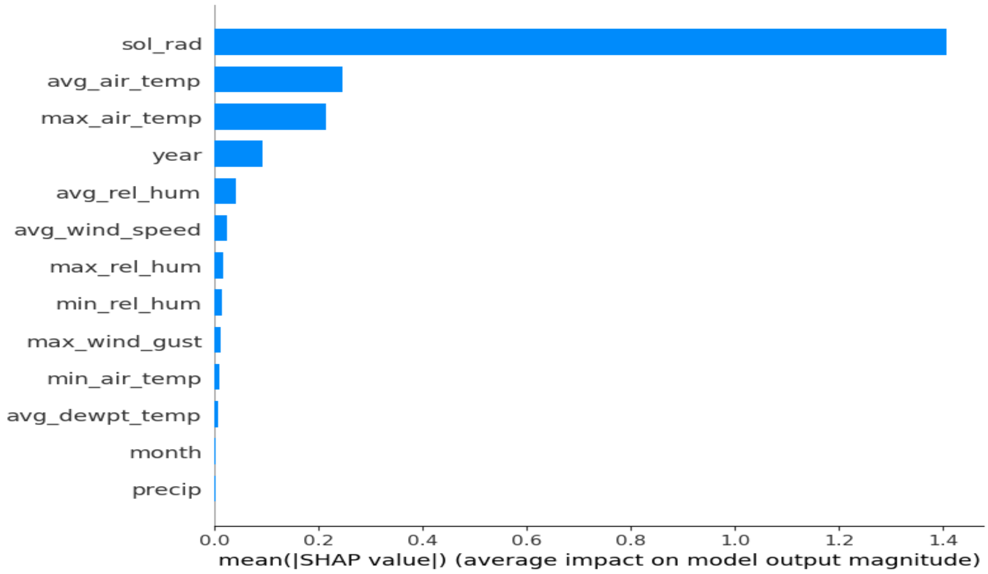

Figure 11. SHAP summary plot for feature importance in PET prediction.

The force plot and waterfall plot explained individual predictions, helping to visualize how each feature increased or decreased the predicted PET value. When predicting PET for the next five years, the values ranged between 0.41656 and 0.41910, indicating a stable trend. This stable prediction can support better planning in agriculture and water resource management, ensuring efficient use of resources based on future climate patterns.

Using the trained LSTM model, we forecasted the potential evapotranspiration rates for the next five years. The predicted value range can increase between 0.41656 and 0.41910, as shown in **Figure 12**, suggesting a stable trend in PET within this range. These findings can help in better water resource planning and agricultural management by providing insights into future evapotranspiration patterns. By combining deep learning-based forecasting with explainability techniques like SHAP, this study enhances the interpretability of PET predictions, allowing researchers and decision-makers to focus on the most influential environmental factors.

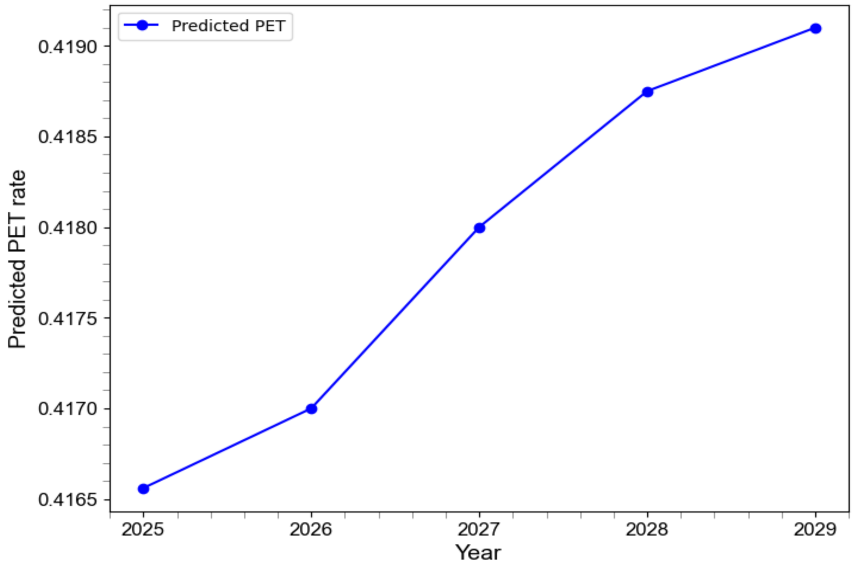

Figure 12. SHAP summary plot for feature importance in PET prediction.

5. Limitations and future work

5.1. Limitations

Although this study provides useful insights, there are some limitations to consider. The model mainly relies on weather data, but factors like plant types and land conditions, which also impact evapotranspiration, were not included. The model's accuracy depends on reliable weather records, so missing or inconsistent data may reduce its effectiveness. Since the model was trained on data from specific locations, it may need adjustments to perform well in different regions as presented by Sun G et al. [27]. Regional differences in climate, soil type, and vegetation can introduce bias if the model is not retrained accordingly. Additionally, missing information on plant types and soil characteristics of evapotranspiration can lead to incomplete or biased predictions. The model's performance may also vary during extreme weather events, as sudden changes are harder to predict accurately. Furthermore, the limited availability of high-resolution environmental data can reduce the model's overall precision. Furthermore, the model's reliance on past trends may overlook unexpected environmental shifts or new agricultural practices. The accuracy might also decrease if input data sources change or are updated inconsistently [28].

5.2. Future work

To improve our model and make it more useful in the future, several steps can be taken:

- Training models with more factors: Including additional environmental data like soil moisture and plant types can improve prediction accuracy.
- Hyperparameter tuning: Adjusting the model settings and trying advanced methods like ensemble models can make the model more reliable.
- Long-term predictions: Building models that consider seasonal changes and climate trends can help predict evapotranspiration over longer periods.
- Real-time use case: Adding the model to real-time systems for irrigation

management can help farmers get quick and accurate advice based on current weather and soil conditions.

- Mobile app deployment: Creating cloud-based or mobile-friendly tools can make the model easier for farmers and agricultural experts to use, even in remote areas.
- Testing in different regions: Running tests in different climates and soil conditions will help ensure the model works well in various locations.

6. Conclusion

This study concluded that deep learning models, particularly LSTM, can effectively predict potential evapotranspiration. The outcomes suggested that LSTM performed better than other models, indicating that it is a good fit for time series data. By analyzing feature importance using SHAP, we identified that the key factor influencing the model's predictions is solar radiation, which allowed us to refine the model and improve its accuracy. This approach not only enhanced prediction performance but also provided valuable insights into the environmental factors driving evapotranspiration. These findings highlight the importance of combining predictive models with clear explanations to ensure accurate and understandable outcomes, which may assist in improved decision-making in environmental studies.

Author contributions: Conceptualization, SS and AK; methodology, SS; software, AK; validation, SS and AK; formal analysis, SS; resources, AK; data curation, AK; writing—original draft preparation, SS and AK; writing—review and editing, SS and AK; visualization, SS; supervision, AK; project administration, SS and AK. All authors have read and agreed to the published version of the manuscript.

Conflict of interest: The authors declare no conflict of interest.

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