Efficient Hyperparameter Optimization for Reference Evapotranspiration Estimation with Limited Parameters: A Comparison of Optuna and Grid Search in the Doukkala Region, Morocco

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Abstract. Accurate estimation of reference evapotranspiration (ETo) is essential for irrigation scheduling and water resource management, particularly in semi-arid regions where meteorological data are often limited. In this study, we evaluate the performance of machine learning models—Support Vector Regression (SVR), Random Forest (RF), Extreme Gradient Boosting (XGB), and Artificial Neural Networks (ANN)—for daily ETo estimation in the Doukkala region of Morocco using only limited parameters (Julian day, maximum and minimum temperature, and relative humidity). Two hyperparameter optimization strategies, Grid Search and Optuna, were compared to assess their effectiveness and efficiency. Results show that all models achieved high predictive accuracy, with R^2 values ranging from 0.90 to 0.916 and RMSE between 0.53 and 0.56 mm/day. Optuna consistently matched or slightly outperformed Grid Search across all models while requiring fewer evaluations. For example, RF and SVR achieved R^2 of 0.9160 and 0.9118 respectively with Optuna, compared to 0.9156 and 0.9104 with Grid Search. Similarly, XGB improved from 0.9040 to 0.9137 with Optuna, while ANN performance remained stable around $R^2 \approx 0.913$. These findings highlight the effectiveness of Optuna as a more efficient and flexible alternative to Grid Search for hyperparameter tuning in ETo modeling.

1 Introduction

Reference evapotranspiration (ETo) represents the amount of water lost from a well-watered reference crop (usually grass or alfalfa) through the combined processes of soil evaporation and plant transpiration [1]. It is widely used as a standard indicator of the atmospheric

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demand for water, independent of crop type, soil, and management practices [2]. As such, ETo serves as a foundation for irrigation planning, crop water requirement estimation, and sustainable agricultural water management, particularly in semi-arid regions where water resources are under increasing pressure [3].

Direct measurements of evapotranspiration can be obtained using lysimeters or eddy covariance systems, which provide accurate estimates under controlled conditions [4]. However, these methods are expensive, technically demanding, and not feasible for large-scale or long-term monitoring in most agricultural areas [5]. To address this limitation, the Food and Agriculture Organization (FAO) recommends the Penman–Monteith equation as the standard indirect method for computing ETo, which combines meteorological variables such as air temperature, solar radiation, wind speed, and relative humidity into a physically based model [1]. While this approach is robust, its application is often constrained in developing regions where complete meteorological datasets are unavailable or contain significant gaps, reducing its practicality for routine irrigation management [6].

To overcome these limitations, researchers have increasingly investigated the use of machine learning (ML) models for ETo estimation using limited climatic inputs [7]. Studies have shown that temperature-based, radiation-based, and hybrid input combinations can provide satisfactory accuracy for ETo estimation when solar radiation or wind speed data are missing [8]. For instance, several works demonstrated that Support Vector Regression (SVR), Random Forest (RF), Extreme Gradient Boosting (XGB), and Artificial Neural Networks (ANN) can estimate ETo accurately using only temperature and relative humidity [9,10]. Such limited-parameter approaches are especially valuable in regions with sparse weather stations or unreliable radiation and wind measurements.

Despite these advances, hyperparameter tuning remains a critical challenge in applying ML models for ETo prediction. Grid Search is the most widely used method for hyperparameter optimization but becomes computationally expensive as the search space grows [11]. More recently, advanced optimization frameworks such as Optuna have been proposed, offering more efficient parameter search through techniques like Tree-structured Parzen Estimators (TPE) [12]. While some studies have compared different ML algorithms for ETo estimation under limited input conditions [13], few works have explicitly evaluated the impact of hyperparameter optimization strategies (Grid Search vs. Optuna) on model performance.

The purpose of this study is to evaluate the performance of SVR, RF, XGB, and ANN for daily ETo estimation in the Doukkala region of Morocco using limited meteorological parameters (Julian day, maximum and minimum temperature, and relative humidity). While previous research has demonstrated the potential of limited-input ETo modeling in other agro-climatic regions, it is essential to adapt and validate these approaches under local conditions. By systematically comparing Grid Search and Optuna as optimization strategies, this study aims to provide new insights into the efficiency and accuracy of ML-based ETo estimation frameworks tailored to data-scarce irrigation environments.

2 Materials and Methods

2.1 Study area

The study was conducted in Khemis Mettouh, located in the Doukkala region of northwestern Morocco (8.34° W, 32.67° N) at an altitude of 146.5 m above sea level (Fig. 1). The region is part of Morocco's semi-arid coastal plains, characterized by a Mediterranean climate with hot, dry summers and mild winters [14]. Agriculture is the dominant land use, with cereals,

sugar beet, and forage crops being the main cultivated species, heavily dependent on irrigation from both surface and groundwater resources [14].

Climatically, the Doukkala plain experiences high inter-annual variability in rainfall and frequent droughts, making efficient water management essential for sustaining agricultural productivity [15]. Reference evapotranspiration (ETo) is particularly relevant in this area, as irrigation demand represents a significant share of total water consumption.

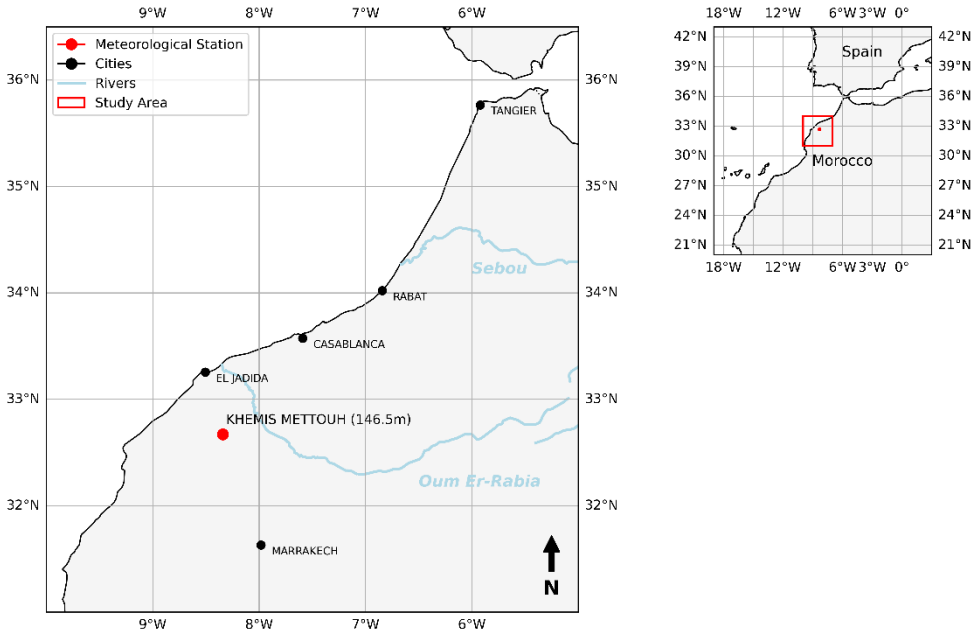

Fig. 1. The geographical location of the study site

2.2 Data

The dataset used in this study was obtained from the Regional Office of Agricultural Development of Doukkala (ORMVAD). It covers the period from September 1996 to September 2012, comprising a total of 5,844 daily records of meteorological observations at the Khemis Mettouh station. The collected variables include maximum air temperature (Tmax), minimum air temperature (Tmin), maximum relative humidity (RHmax), minimum relative humidity (RHmin), solar radiation (Rs), wind speed, and reference evapotranspiration (ETo).

A descriptive summary of the dataset is presented in Table 1, including the maximum, minimum, mean, and standard deviation (SD) for each variable.

For the modeling phase, only a subset of variables was used: Tmax, Tmin, RHmax, RHmin, and Julian day. This choice reflects a limited-parameter approach, motivated by the frequent unavailability or unreliability of solar radiation and wind speed measurements in many agricultural regions.

Table 1. Descriptive statistics of meteorological variables

Variable	Unit	Max	Min	Mean	SD
Tmax	°C	45.7	10	26.57	6.29
Tmin	°C	29	-3	13.76	5.61
RHmax	%	100	37	95.38	4.73
RHmin	%	98	6	49.33	15.53
Rs	MJ/m²	31.12	2.18	18.65	6.41
Wind Speed	m/s	7.1	0.2	1.99	0.88
ETo	mm/day	11.02	0.55	3.85	1.82

2.3 Machine Learning Models

Four machine learning algorithms were selected for daily ETo estimation:

2.3.1 Support Vector Regression (SVR)

A kernel-based regression method capable of modeling nonlinear relationships [16]. The tuned hyperparameters were the penalty parameter (C), the kernel type, and the kernel coefficient (γ).

2.3.2 Random Forest (RF)

An ensemble of decision trees trained on bootstrap samples with random feature selection [17]. The tuned hyperparameters were the number of trees (n_estimators) and the maximum depth of trees (max_depth).

2.3.3 Extreme Gradient Boosting (XGB)

A boosting algorithm that builds trees sequentially using gradient optimization [18]. The tuned hyperparameters were the number of trees (n_estimators), the maximum depth (max_depth), and the learning rate.

2.3.4 Artificial Neural Networks (ANN)

A class of computational models inspired by the structure and functioning of biological neural networks, designed to approximate complex nonlinear relationships between inputs and outputs [19]. In this study, ANN was implemented as a multilayer perceptron (MLP) with nonlinear activation functions. The tuned hyperparameters were the hidden layer size (hidden_layer_sizes), the activation function, and the regularization term (α).

2.4 Hyperparameter Optimization

Two hyperparameter optimization strategies were employed for all models in order to enable systematic comparison:

- **Grid Search:** A deterministic search technique that evaluates model performance across a predefined set of hyperparameter values. Although widely adopted, its

computational cost increases substantially as the dimensionality of the parameter space grows [11].

- **Optuna**: An optimization framework that uses adaptive sampling strategies, such as the Tree-structured Parzen Estimator (TPE), to explore the search space more efficiently. It includes mechanisms to prune less promising trials, which can reduce computational overhead compared to exhaustive methods [12].

Both strategies were applied under identical train/test data splits to ensure consistency in model evaluation.

2.5 Model Evaluation

Model performance was assessed on a test dataset using multiple statistical metrics:

- **Coefficient of Determination (R^2)**: Indicates the proportion of variance in observed ETo explained by the model.
- **Root Mean Square Error (RMSE)**: Measures the average magnitude of prediction error, with higher sensitivity to large deviations.
- **Mean Squared Error (MSE)**: Captures the squared differences between observed and predicted values.
- **Mean Absolute Error (MAE)**: Provides the average magnitude of prediction errors, less sensitive to outliers compared to RMSE.

3 Results and Discussion

3.1 Correlation Analysis

The correlation analysis (Fig. 2) provides insights into the linear relationships between meteorological variables and reference evapotranspiration (ETo). Maximum and minimum air temperatures (Tmax and Tmin) exhibited the strongest positive correlations with ETo, with coefficients of 0.85 and 0.73, respectively, while mean temperature (Tmean) also showed a similarly high correlation (0.84). These results confirm the dominant role of temperature in determining evaporative demand. Relative humidity variables, in contrast, were negatively correlated with ETo. Minimum relative humidity (RHmin) presented a strong negative correlation (−0.63), whereas maximum relative humidity (RHmax) showed a weaker but still significant negative correlation (−0.40). This suggests that dry air conditions, particularly during periods of low humidity, exert a stronger influence on evapotranspiration dynamics.

Solar radiation (Rs) was also strongly correlated with ETo (0.84), indicating its significant influence as a driver of evapotranspiration. However, Rs was not included among the selected predictors in this study, as solar radiation data are often unavailable or incomplete in many developing regions or countries, limiting their operational use for data-driven irrigation management. Wind speed exhibited a weaker positive correlation (0.32), and rainfall showed a slight negative relationship (−0.23), indicating that these variables were less influential in this dataset compared to temperature and humidity.

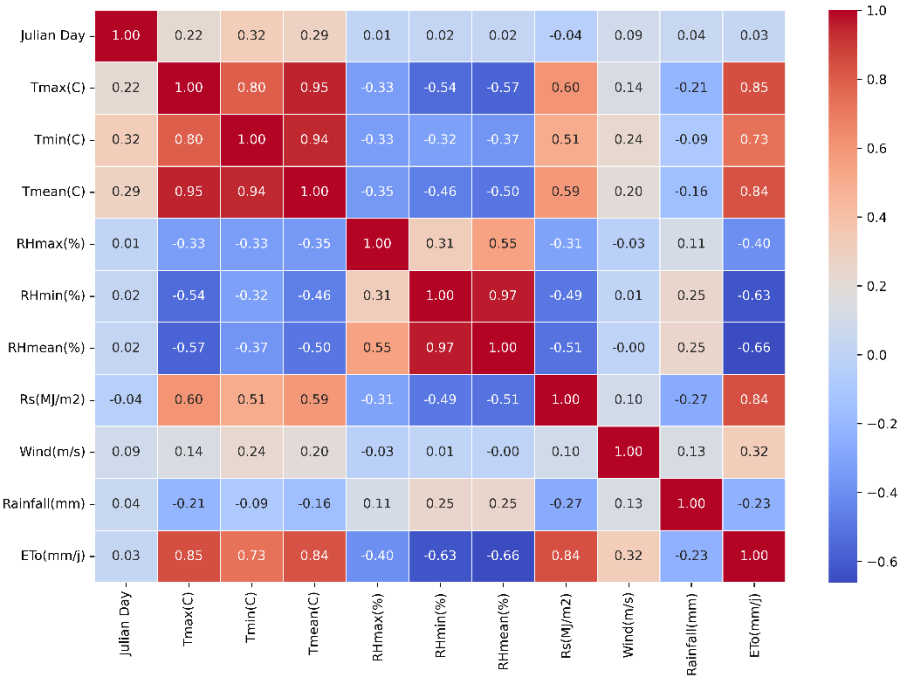

Fig. 2. Correlation heatmap of meteorological variables and ETo

3.2 Predictive Accuracy of Machine Learning Models

The predictive performance of the models is summarized in Table 2. All models achieved high accuracy, with R^2 ranging from 0.90 to 0.916 and RMSE values between 0.53 and 0.57 mm/day. Random Forest (Optuna) achieved the highest overall accuracy ($R^2 = 0.916$, RMSE = 0.529 mm/day), closely followed by ANN and XGB with $R^2 \approx 0.913$. SVR also performed robustly, with $R^2 \approx 0.912$.

Table 2. Performance metrics of ML models under Grid Search and Optuna optimization.

Model	Optimizer	R2	RMSE	MSE	MAE
SVR	Grid Search	0.910408	0.546166	0.298297	0.39264
SVR	Optuna	0.911838	0.54179	0.293536	0.390891
RF	Grid Search	0.915575	0.530185	0.281096	0.387256
RF	Optuna	0.916017	0.528794	0.279623	0.386788
XGB	Grid Search	0.904013	0.565324	0.319592	0.405214
XGB	Optuna	0.913731	0.535943	0.287235	0.38951
ANN	Grid Search	0.912035	0.541185	0.292881	0.397526
ANN	Optuna	0.913396	0.536981	0.288349	0.392381

3.3 Hyperparameter Optimization Performance

The convergence plots (Fig. 3) illustrate the evolution of the R^2 score across Optuna trials for each model. In general, Optuna achieved comparable or superior performance to Grid Search while requiring fewer evaluations. For SVR and RF, the best Optuna trials slightly outperformed Grid Search, with R^2 values of 0.912 and 0.916, respectively. XGB also benefited from Optuna tuning, improving from 0.904 to 0.914. ANN showed stable performance under both optimization strategies, with marginal gains from Optuna. The dashed red lines in Fig. 3 represent the best Grid Search performance, which was matched or exceeded by Optuna in most cases.

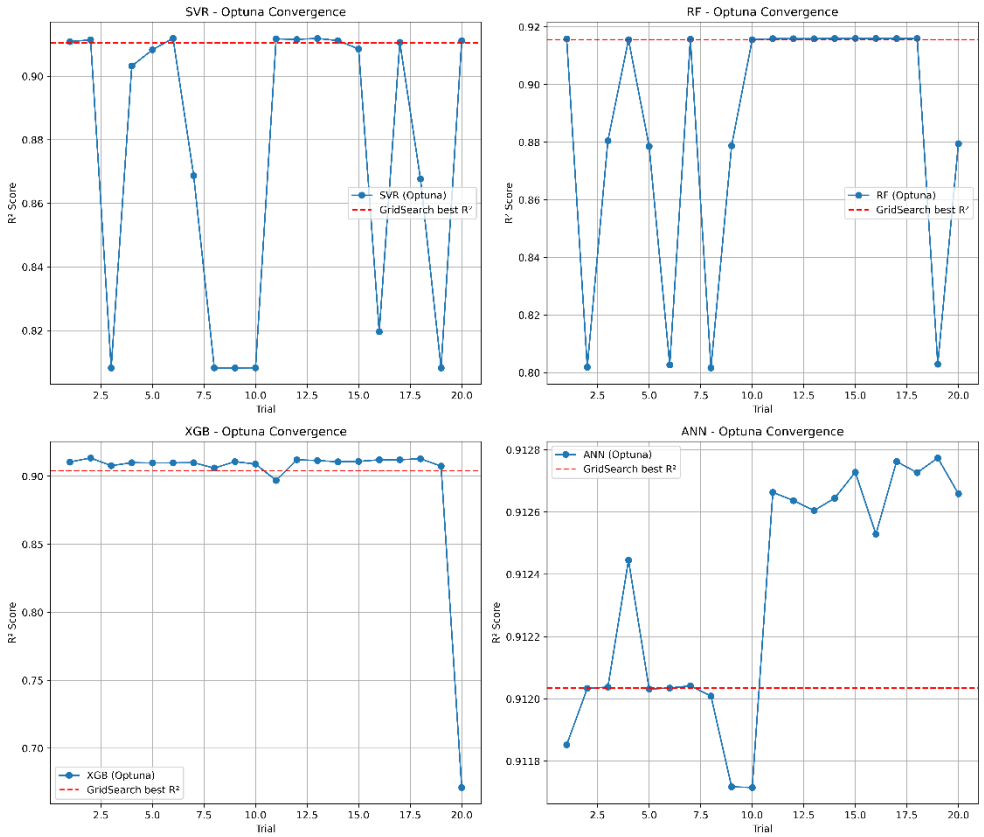

Fig. 3. Optuna convergence curves compared with Grid Search

3.4 Predicted vs. Actual ETo

Scatterplots of predicted versus observed daily ETo values (Fig. 4) further illustrate model performance. All models demonstrated strong alignment along the 1:1 reference line, with relatively small dispersion around the diagonal. This confirms the capacity of the selected ML approaches to reproduce observed ETo values even when trained on a limited set of input parameters (Julian day, Tmax, Tmin, RHmax, RHmin).

Overall, the results indicate that tree-based methods (RF and XGB) and ANN slightly outperform SVR in terms of predictive accuracy, although differences remain modest.

Importantly, Optuna provided consistent improvements over Grid Search across all models, validating its effectiveness as a hyperparameter optimization strategy.

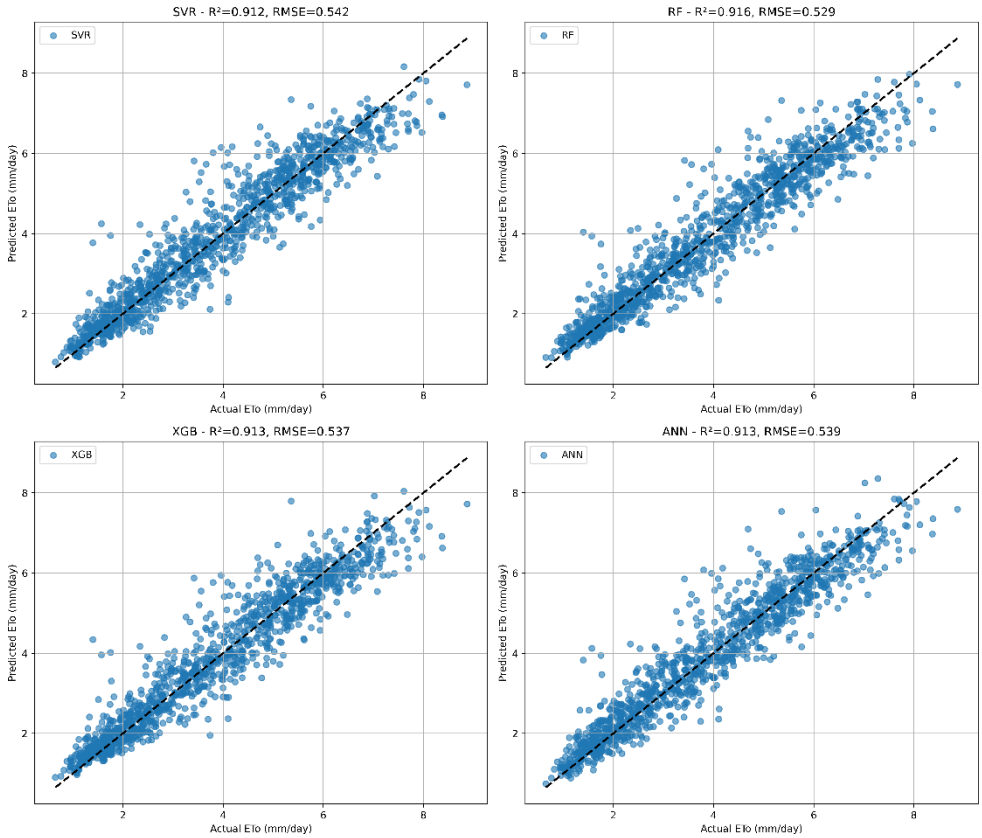

Fig. 4. Scatterplots of predicted versus observed daily ETo

4 Conclusion

This study assessed the performance of four machine learning models—Support Vector Regression (SVR), Random Forest (RF), Extreme Gradient Boosting (XGB), and Artificial Neural Networks (ANN)—for estimating daily reference evapotranspiration (ETo) in the Doukkala region of Morocco using limited meteorological inputs (Julian day, maximum and minimum temperature, and relative humidity). Two hyperparameter optimization strategies, Grid Search and Optuna, were compared to evaluate their efficiency and effectiveness.

The results demonstrated that all models achieved high predictive accuracy, with R^2 values consistently above 0.90 and RMSE ranging between 0.53 and 0.56 mm/day. Among the tested algorithms, RF and XGB slightly outperformed others, while ANN showed stable performance across optimizers. Optuna consistently matched or improved upon Grid Search results while requiring fewer evaluations, highlighting its value as a flexible and efficient optimization framework.

These findings confirm that reliable ETo estimation is possible even with limited meteorological inputs, which is particularly relevant in semi-arid regions where complete

datasets are often unavailable. The integration of machine learning models with efficient hyperparameter optimization thus provides a robust alternative to conventional approaches and supports more effective irrigation planning and water resource management.

Future research should extend this framework by integrating additional agro-climatic zones, testing transferability across regions, and exploring hybrid or ensemble approaches to further improve accuracy and generalization capacity.

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