Transpiration Insights: Estimating Transpiration Through Advanced Modeling

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Summery

- We conducted research to predict daily transpiration in crops by utilizing a combination of machine learning (ML) models and Big-Data from gravimetric load cells as well as ambient sensors. Our aim was to improve the accuracy of transpiration estimates.
- Data were collected from two semi-controlled greenhouses over seven years, measuring key physiological and meteorological variables at high frequency and accuracy. We trained Decision tree, Random Forest, XGBoost, and Neural Network models on this dataset to predict daily transpiration.
- The Random Forest and XGBoost models demonstrated high accuracy in predicting the whole plant transpiration, with R^2 values of 0.87 on the test set (cross-validation) and average of $R^2 = 0.79$ on holdout experiments. Ambient temperature was identified as the most influential environmental factors affecting transpiration.
- Our results emphasize the potential of ML for precise water management in agriculture, and simplify some of the complex and dynamic environmental forces that shape transpiration.

1. Introduction

Transpiration, the process of water evaporation from plants, has been a subject of scientific studies for centuries. It primarily occurs through leaves, facilitating a continuous transport of water and essential nutrients from roots. One remarkable aspect of transpiration is how plants regulate it in response to their surroundings through dynamic control mechanisms. This process is intricately linked to the behavior of stomata, small pores found on leaf surface. Stomata can adjust their aperture to manage the rate of transpiration (Lange et al., 1971). This adaptive response to the environment appears to have evolved as one of the protective mechanisms against excessive dehydration and physiological damage (Iqbal et al., 2020).

The dynamic ability of plants to regulate their transpiration rates plays a vital role in facilitating the exchange of carbon dioxide and water, thereby improving water use efficiency and optimizing growth. Various factors, both biologic, such as plant size (Geller & Smith, 1982) and environmental such as Solar Radiation (Pieruschka et al., 2010), temperature (Ben-Asher et al., 2008) , humidity (Rawson et al., 1977), soil water supply (Madhu & Hatfield, 2014) , carbon dioxide levels (Imai & Murata, 1976; Madhu & Hatfield, 2014), and wind speed (Dixon & Grace, 1984) , can impact the transpiration rates of different plants. The understanding of these influential factors holds paramount significance in the fields of agriculture and Eco physiological sciences.

Understanding and quantifying the factors which affects transpiration and plant-water relations has a key role in optimizing water management strategies in agricultural and greenhouse settings. Therefore, various modeling approaches have been employed to simulate and evaluate transpiration rates in plants. One common approach is the use of mechanistic models, which are based on physiological principles and the understanding of plant structure and function. For example, the semi-empirical Ball-Berry model integrates stomatal conductance and environmental variables to estimate transpiration rates (Ball et al., 1987). However, it's important to note that the Ball-Berry model simplifies the complex process, assuming a linear relationship between stomatal conductance and photosynthesis, which can significantly influence stomatal behavior and transpiration rates.

In contrast, process-based models like the Penman-Monteith equation take a more comprehensive approach. Process-based models represent a modeling approach that simulates natural processes by representing the underlying mechanisms. Penman-Monteith equation combine energy balance and aerodynamic principles to predict evapotranspiration (Monteith, 1965; Penman, 1948). The FAO56 Penman–Monteith is commonly used in the agriculture community to estimate transpiration (Landeras et al., 2008). However, previous studies have found daily FAO56 Penman–Monteith exhibited up to 22% discrepancy in accuracy compared to the lysimeters (Averbuch & Moshelion, 2024; López-Urrea

et al., 2006). These discrepancies underscore the ongoing need for improvement and refinement in modeling techniques to better understand and predict transpiration in different conditions and environments.

An alternative method involves developing models through machine learning algorithms, including artificial neural networks (ANN) and support vector regression (SVR). These have shown promising results in estimating transpiration based on environmental inputs and plant characteristics (Balasubramanian & Thirugnanam, 2023; de Meneses et al., 2020; Ferreira et al., 2019; Xing et al., 2022). However, these articles used estimated transpiration (such as FAO56 Penman–Monteith) or Synthetic data (Balasubramanian & Thirugnanam, 2023) in the models' training and not direct measurements of the plant interactions, therefore we believe that these models have refined and perhaps simplified equations predicting plant behaviour, they fall short in capturing the intricate complexities of actual plant responses.

Models predicting actual transpiration using lysimeters, which measure evapotranspiration (ET) or transpiration flux directly, can provide precise estimations and serve as benchmarks for calibrating other methods (Amani & Shafizadeh-Moghadam, 2023; Anapalli et al., 2016; Liu et al., 2017). Despite their benefits, most studies employing lysimeters tend to use a limited number of lysimeters and a small variety of crops due to the high costs of the system (Z. Chen et al., 2020).

In this study, we focused on daily measurements of transpiration for mediterranean summer and winter crops, tomato and cereals (Wheat and Barley), respectively. Over the past seven years, we have collected a big data set of continuous physiological traits from hundreds of plant specimens, along with corresponding environmental data. Leveraging this unique dataset, we employed machine learning models to predict the daily transpiration of well-irrigated plants. Our data is distinguished by its high scale frequency measurements (3-minute interval) and the use of actual quantified and annotated physiological measurements (e.g., whole plant transpiration g/day). These are obtained from an extensive array of load cells lysimeters soil and atmosphere adjesent conditions.

The objectives of this study are to leverage our dataset, which includes soil-plant-atmosphere continuum data, to (1) evaluate the effectiveness of conventional tree-based machine learning models, including Random Forest, a XGBoost model, and a neural network model, in predicting daily transpiration for tomato and cereal crops; and (2) determine the hierarchical significance of diverse ambient factors, thereby pinpointing the critical environmental factors that exert influence on transpiration.

2. Materials and methods

2.1 Research overview

In this study, we aimed to understand the determinants of daily transpiration in plants using a structured machine learning research workflow. Data collection took place within semi-commercial greenhouses using functional phenotyping platform composed of load-cells lysimeters. This platform provided essential information on several plant physiological traits (transpiration, plant weight, growth rate etc.) and ambient conditions. After essential data pre-processing steps, including outlier removal and transformation to daily values, we had 6237 observations (83% of the original data), split into training and testing sets. Machine learning models, including tree-based models and neural network, were trained to predict daily transpiration using the features: plant weight, temperature, humidity, Daily Light Integral (DLI), Vapor Pressure Deficit (VPD), greenhouse, plant type, and soil type. Model evaluation encompassed various metrics such as R^2 and Root Mean Square Error (RMSE). Model interpretation was accomplished through the analysis of feature importance using techniques like Permutation and Shapley Additive Explanations (SHAP; see 2.9). These methods hold major contribution in understanding the different features to the models' predictions and their impact on daily transpiration. This workflow allowed us to gain valuable insights into the determinants of daily transpiration in plants.

2.2 Experimental site

Data was collected from two semi-controled greenhouses located at the I-CORE centre for Functional Phenotyping of the Faculty of Agriculture, Food, and Environment in Rehovot, Israel (http://departments.agri.huji.ac.il/plantscience/icore.php). The 'main greenhouse' is a polycarbonate covered at coordinates 31°54'15.0"N, 34°48'03.6"E, is larger, covering 16 x 18 m^2 with a max height of 6 m. The secondary greenhouse' , also polycarbonate covered, located at 31°54'22.5"N, 34°48'10.6"E, spans 6 x 17 m^2 meters and reaches a height of 3 m. Both facilities feature natural daylight conditions and are equipped with a cooling pad along the northern wall to maintain temperatures below 35 degrees Celsius. To maintain a steady wind speed, the fans were continuously on, while the wetting of the pad was activated when the temperature reached 30°C. The experimental conditions varied, with natural Daily Light Integral (DLI) values ranging from 2 to 33 mol/(m^2·d) and mean daily temperatures fluctuating between 10 and 35°C (Table S1A).

2.3 General experiment setup and Data collecting

The data was collected from June 2018 to March 2024. Using the functional phenotyping platform – PlantArray (PlantDitech, Israel) as described by Dalal et al., 2020; Halperin et al., 2017. Briefly, a load

cell lysimeter system was utilized, enabling continuous plant weight measurement and the derivation of both transpiration-induced water loss and daily plant mass accumulation. All data was automatically collected and uploaded to the cloud base SPAC analytics system (PlantDitech, Israel). The plants in the greenhouse were grown in pots (4L) filled with sand (Silica sand 20-30, Negev-Minerals, Israel) or soil (Bentel 11 garden mix, composed of (w/w) 55% peat, 20% tuff and 25% puffed coconut coir fiber (Tuff-Substrates, Israel). The experimental pots are set as described by (Dalal et al., 2020).

Meteorological data, consisting of three essential variables - temperature, light, and relative humidity (RH), were collected using weather station (Watchdog 2000 series ;Spectrum Technologies, Illinois, USA) connect to the PlantArray system. Within each greenhouse, The atmospheric sensors were positioned at the centre of the greenhouse, ~1 meter above the height of the pot surface.

Tomato, wheat and barley (cereals), were employed in this experiment. The tomato (*Solanum lycopersicum*) variety incorporated in the study was mainly M82 cultivar. The cereals included *T. turgidum subsp. durum 'Svevo'* and *T. aestivum cv. Gadish*, among others. Focusing on these commonly cultivated crops, ensuring multiple repetitions, and capturing the diversity of both winter and summer representations.

2.4 Data preprocessing

The data was initially collected at 3-minute intervals. For this research, it was further processed to generate daily values, covering the period from first light to last light (Table 1). This simplifies data interpretation, making it practical for applications such as irrigation decisions, much like other common methods, including the FAO56 Penman–Monteith model for irrigation management. Moreover, using daily values reduces the total data volume. Opting for daily intervals strikes a balance by capturing environmental variability while keeping data processing manageable.

Additionally, the type of potting media (sand or soil) and the specific plant species (tomato or cereal) were recorded. Light data in terms of Photosynthetically Active Radiation (PAR) was measured at 3-minute intervals. The Daily Light Integral (DLI) was calculated using the formula:

<u>Formula 1:</u>

$$DLI\left(\frac{mol}{m^2 * day}\right) = \frac{\sum PARlight\left(\frac{\mu mol}{m^2 s}\right)}{n} * 86400\left(\frac{sec}{day}\right) * \frac{1mol}{1000000\mu mol}$$

- *n* - number of samples in a full day (480 if sampled every 3 min).
- $\sum PARlight\left(\frac{\mu mol}{m^2 s}\right)$ is the sum of PAR light measurements throughout the day.

This calculation provided insights into the cumulative light exposure experienced by the plants over the course of a day. The Vapor Pressure Deficit (VPD) was calculated using the daily mean temperature and daily mean relative humidity (RH; Formula 2), to determine the daily water demand of the atmosphere. We originally intended to use VPD measurements every 3 minutes and calculate the daily mean. However, due to technical issues, we used the daily average temperature and relative humidity in the VPD formula. This resulted in minor differences in the outcomes (the correlation between the two calculation methods is greater than r = 0.9).

<u>Formula 2:</u>

$$VPD\ (kPa) = 0.6108 * e^{\frac{17.27 * T\ (°C)}{T\ (°C)+237.3}} - (0.6108 * e^{\frac{17.27 * T\ (°C)}{T\ (°C)+237.3}} * \frac{RH\ (\%)}{100})$$

- T - temperature in degrees Celsius (℃).
- RH- relative humidity in percentage (%).

Our dataset initially consisted of 7,547 observations (each observation consists of one plant on one day; Figure 1). After a comprehensive data cleaning process, we concluded with a total of 6,237 observations. This reduction was due to the removal of observations with missing values, extreme outliers, and those exhibiting irregular behaviours such as weight loss, water shortage, or illnesses. In our study, we meticulously ensured that the amount of water in the soil was above the transpiration limiting threshold (Halperin et. al., 2016). This was achieved by selecting data exclusively from control treatments and wild type (WT) plants, while deliberately excluding any data from plants that surpassed their pot's capacity, thereby ensuring non-pot effect of draught conditions. Therefore, we refined the data manually, removing entries where plants exhibited 'pot limitation', a scenario where a plant's transpiration plateaus due to reaching the pot's maximum available water capacity. While the total water-holding capacity is approximately 860 g in sand and 1700 g in potting media (Dalal et al., 2020), the actual available water for plants is lower: around 600 g/day in sand and 1200 g/day in soil, influenced by root structure and soil properties. The final variable and some preprocessing methods, such as daily aggregation of values and encoding, are detailed in Table 1.

2.5 Tuning, Training, and Testing Datasets

After preprocessing, the dataset comprised 6237 daily observations. Figure 1 illustrates a sample plant with 24 observations. The feature variables included Temperature, Relative Humidity (RH), vapor pressure deficit (VPD), Daily light Integral (DLI), plant type, and soil type, with the target variable being daily transpiration (Figure 1h, Table 1).

2.5.1 Validation Dataset (Holdout)

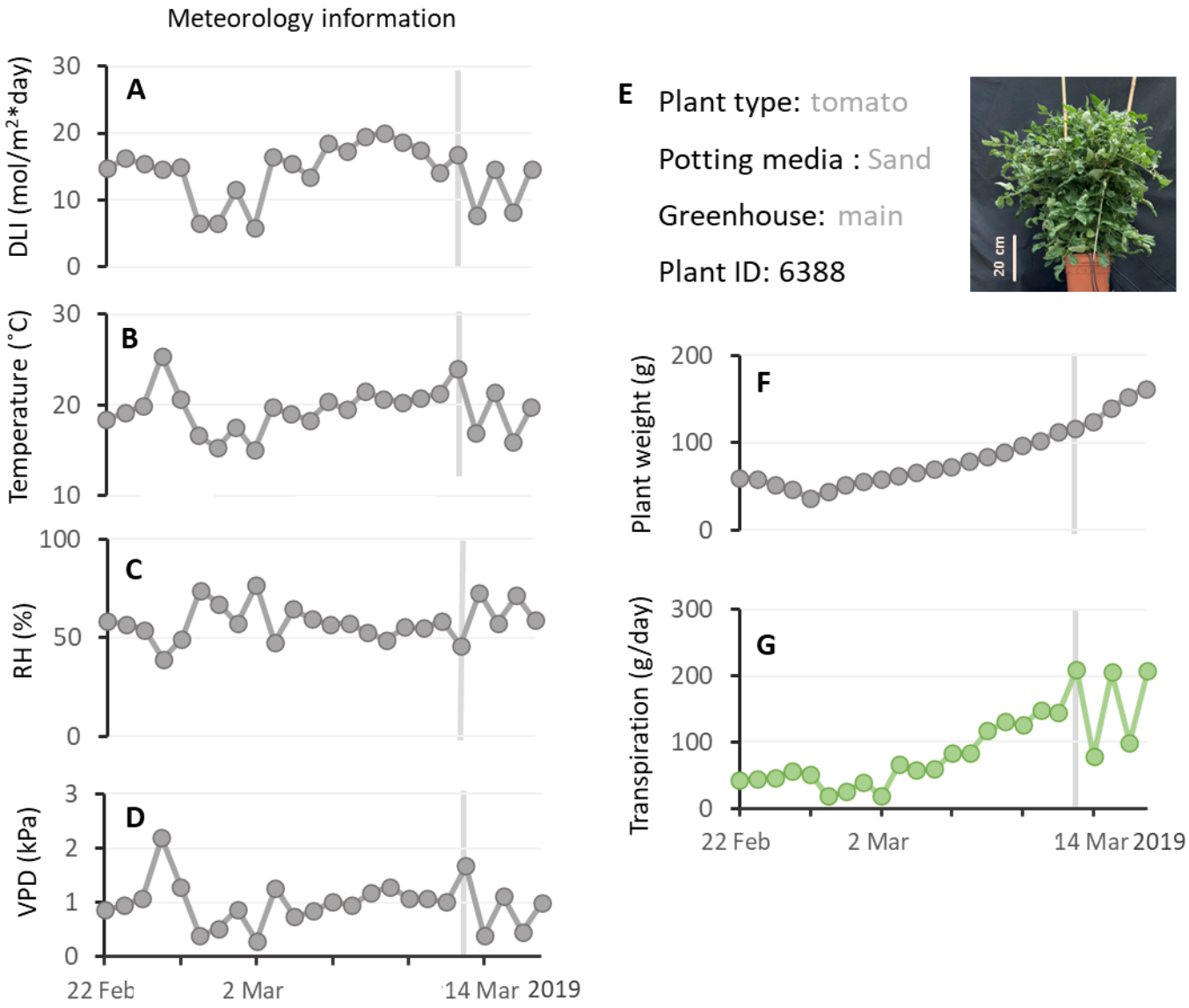
To assess the model's generalizability, a holdout dataset comprising 941 observations from 5 randomly selected experiments was established, a random seed function was set to ensure repeatability. This subset includes 213 observations related to tomato plants and 728 observations concerning cereal plants. The dataset distribution includes 883 observations in sand and 58 in soil (for more information see Table S1b and Figure S1b). This holdout dataset aims to reflect the model's performance and effectiveness on unseen data.

2.5.2 Training Dataset

Ninety percent (4766 observations) of the remaining data was randomly selected to tune the hyperparameters, as detailed in Section 2.7. This initial subset helped determining the optimal hyperparameters, allowing us to assess the effectiveness of the tuning process. After selecting the best hyperparameters, the models were then trained on the full dataset, excluding the holdout set. This approach ensures that the final model training incorporates the broadest data spectrum available while retaining an independent holdout set to evaluate the model (see 2.9).

Table 1: Dataset description and the main preprocessing methods.

category	variable	Units	Description
ID	Timestamp		Date
	Icore greenhouse		The greenhouse the data was collected from. Encoded as Main = 1 and secondary = 0.
	expId		Experiment number: each independent experiment contained 1-10 plants (repetitions) that the data was collected simultaneously from. A total of 48 independent experiments were used.
	plantId		The plant specific ID number, each plant was measured continuously for about 3-4 weeks. On average 23 daily observations per-plant. A total of 269 plants were used.
Meteorology	Temperture	˚C	The average temperature at daytime (from the first to last light).
	RH	%	The average Relative Humidity at daytime (from the first to last light).
	VPD	kPa	The average Vapor Pressure Deficit (VPD) at daytime was calculated using formula 2.
	DLI	mol/m^2*day	Daily Light Integral (DLI) was calculated using formula 1.
Others	Potting media		"Encoded soil" - dummy variables, 0 =silica sand, 1 = soil (4630 and 1607 observation respectively).
	Plant types		"Encoded plant" - dummy variable, 0 =tomato, 1 =cereal (4082 and 2155 observation respectively)
Plant weight	Plant Weight	gr	The net weight of the plant as calculated at 4AM, after soil field capacity (for details see Halperin et al 2017).
	Transpiration	gr	Daily water evaporating trough the plant (for details see Halperin et al 2017). This variable was used as output for the models.



H			X variables								Y variable
Date	expId	plantID	Icore greenhouse	Temp	RH	VPD	DLI	Encoded plant	Encoded soil	Plant Weight	Daily Transpiration
13/03/ 2019	103	6338	1	24.03	46.09	1.61	16.75	1	0	116.4561	210.19

Figure 1: Meteorological and physiological data derived from the I-core greenhouse PlantArray system. Daily average of (A) light integral, (B) temperature, (C) Relative humidity, and (D) vapor pressor deficit over a period of 22 days. (E) Plant identity information: plant type, potting media, ID number and plant picture at the end of the experiment. (F) Plant biomass - plant net weight (G) whole-plant daily transpiration, note the sensitivity of the transpiration to the methodological changes. (H) A single observation as it is documented it the data set. This observation is visually depicted in Figures A-F, on the 13th of March. X variables marked in gray and the y variable in green, representing the inputs and outputs used by computer models for learning and prediction.

2.6 Machine learning models for estimating daily transpiration.

2.6.1 Decision Tree:

Decision trees are a simple, yet powerful machine learning model used for classification and regression tasks. They recursively split the data into subsets based on the features to create a tree-like structure. At each node, the decision tree selects the feature and split point that minimizes impurity, aiming to create more homogenous subsets. The final predictions are made based on average value (for regression) of the samples in the leaf nodes. Decision trees are interpretable and can capture complex relationships in the data, but they may suffer from overfitting and lack generalization ability. The induction of decision trees is one of the oldest and most popular techniques for learning discriminatory models, which has been developed independently in the statistical (Breiman et al., 1984; Mingers, 1989) and machine learning (Quinlan, 1993) communities (Fürnkranz, 2011).

2.6.2 Random Forest:

Random Forest is an ensemble learning technique based on decision trees. It builds multiple decision trees, each trained on a random subset of the data and a random subset of the features. The final prediction is obtained by averaging (for regression) the predictions of individual trees. Random Forest overcomes the overfitting issue of decision trees and improves the model's performance and robustness. It can handle high-dimensional datasets and capture interactions between features, making it a popular choice for various applications.

The random forest or decision tree forest is an algorithm created in 1995 by Ho (Ho, 1995), then formally proposed by scientists in 2001 (Breiman, 2001; Cutler & Zhao, 2001).

2.6.1 XGBoost model

eXtreme Gradient Boosting (XGBoost) is a method, initially proposed by (T. Chen & Guestrin, 2016) , that generally generates high accuracy and fast processing time while being computationally less costly and less complex. The XGBoost model is a scalable machine learning system for tree boosting. The XGBoost model integrates several “weak” learners for developing a “strong” learner through additive learning. Parallel computation is automatically implemented during training to enhance computational efficiency (Fan et al., 2021).

2.6.3 Artificial neural networks:

Neural networks are a class of deep learning models inspired by the structure and function of the human brain (Haykin, 2009; Rosenblatt, 1958). They consist of interconnected nodes (neurons) organized into layers. Each node applies an activation function to the weighted sum of its inputs to

produce an output (Fukushima, 1969). As many ML models, Neural networks can learn complex and nonlinear relationships in the data through the process of forward and backward propagation during training (Leibniz, 1920).

2.7 Hyperparameters tuning:

Hyperparameter tuning is the process of discovering the optimal configuration for the hyperparameters of a machine learning model to achieve the best performance. Hyperparameters are external configuration settings established before the training process and are not learned from the data. Examples included learning rates, regularization strengths, and the number of trees in a random forest.

This process of hyperparameter tuning was carried out through cross-validation grid search on the training data. Grid search cross-validation is a method employed to systematically explore a vast array of combinations of hyperparameter values. By leveraging 5-fold cross-validation, the dataset was divided into 5 subsets, allowing for multiple rounds of training and validation. This approach aimed to find the optimal set of hyperparameter values and ensure the model's robustness by evaluating its performance across different subsets of the training data. The optimal hyperparameter values, and the options we tested are summarized in Table 2.

Table 2: Hyperparameters. Adjusting these parameters change the learning ability, so the model would not underfit neither overfit the dataset.

Implementing GridSearch cross-validation on the training data set. Systematically all the possible combinations of the Hyperparameter options were evaluated and the optimal setting was retained. We used the 5-fold cross validation splitting strategy to test the optimal parameters on 5 different subsets of the training dataset.

model	Hyperparameter	Explanation	Options	Optimal value	Combinations
Decision Tree	min_samples_split	The minimum number of samples required to split an internal node.	[2,3,4]	2	60 candidates * 5 folds = 300 fits
	min_samples_leaf	The minimum number of samples required to be at a leaf node of the trees.	[1,2,3,4]	4	
	max_depth	The maximum depth of a decision tree.	[5,7,10,12,15]	10	
Random Forest	n_estimators	The number of decision trees (estimators) or boosting rounds in the random forest ensemble.	[50,60,70,80]	70	192 candidates * 5 folds = 960 fits
	min_samples_split	Explained above	[2,3,4,5]	2	
	min_samples_leaf	Explained above	[1, 2]	1	
	max_depth	Explained above	[12,15,17]	12	
	bootstrap	This hyperparameter determines whether bootstrap samples (sampling with replacement) are used when building trees in the random forest.	[True, False]	True	
XGBoost	n_estimators	Explained above	[60, 80, 100]	100	972 candidates*5 folds = 30,000 fits
	min_child_weight	Minimum sum of sample weight (hessian) of the smallest leaf node. Larger values, preventing splits that have a smaller hessian value.	[1, 2, 4, 5]	4	
	max_depth	Explained above	[3, 5, 7]	7	
	gamma	Minimum loss reduction required to make a further partition on a leaf node of the tree (helps in pruning the tree).	[0, 0.1, 0.2]	0.2	

	reg_lambda	L2 regularization term on weights. It adds a penalty to the loss function based on the size of the weights.	[0, 1, 2]	0	
	learning_rate	scales the contribution of each tree in the ensemble. A smaller learning rate makes the algorithm more robust by reducing the step size.	[0.2, 0.1, 0.01]	0.1	
Neural Network	num_units – layer 1	controls the number of units (neurons) in each hidden layer of the neural network. It represents the width of the network.	[32, 64, 96, 128, 160, 192, 224, 256, 288]	32	1296 candidates * 40 epoch = 51,840 fits
	num_units – layer 2	Explained above	[32, 64, 96, 128, 160, 192, 224, 256 ,288]	224	
	optimizer	determines the optimization algorithm used to update the model's weights during training. The code considers two options: 'adam' (Adaptive Moment Estimation) and 'rmsprop' (Root Mean Square Propagation)	['adam', 'rmsprop']	rmsprop	
	Activation - Layer1	The activation function applied to the output of each neuron in the hidden layers. Common choices are 'relu' (Rectified Linear Unit) and 'tanh' (Hyperbolic Tangent). Activation functions introduce non-linearity to the network, enabling it to learn complex patterns.	['relu', 'tanh']	tanh	
	Activation- Layer 2	Explained above	['relu', 'tanh']	tanh	
	learning_rate	The learning rate controls the step size at which the optimizer updates the model's weights in each iteration during training. It is a crucial hyperparameter as it affects the speed and stability of training.	[0.001, 0.01]	0.01	
	batch_size	The batch size specifies the number of samples used in each update of the model during training.	[10]	10	

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2.8 Modelling process

We implemented our models using a robust set of Python libraries tailored for statistical computing, data manipulation, and machine learning. Specifically, we used: Scipy (Virtanen et al., 2020), for conducting statistical tests, Numpy (Harris et al., 2020), for high-performance numerical operations, Pandas (Mckinney, 2010; The pandas development team, 2020), for data handling and manipulation, Sklearn (Pedregosa et al., 2011) for machine learning algorithms and model evaluation tools, Keras (Chollet, 2015) and TensorFlow (Abadi et al., 2016) for building and training neural network models.

2.9 Cross-Validation and Performance Evaluation

Cross-validation was conducted on the dataset to validate model stability and reliability. We used 10-fold cross-validation, allowing each subset of data to be used as both training and testing sets iteratively, ensuring comprehensive performance assessment. This method not only helps in assessing the performance across different slices of data but also in comparing the effectiveness of different models under varying conditions (Table 3).

The final model evaluation was performed on the holdout set, using metrics such as Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and the R^2 statistic to compare the predictions and actual measurements (Table 4). These metrics provided a detailed measure of model accuracy, prediction error, and the proportion of variance explained by the model.

2.10 feature importance

To interpret the predictions and understand the importance and contribution of each feature to building the models several feature important tests were presented:

2.10.1 Impurity-based feature importance

Impurity-based feature importance is a technique commonly employed in decision tree-based machine learning models, to assess the significance of individual features in making predictions. The method calculates the contribution of each feature by measuring how much it reduces the impurity (e.g., Gini impurity or entropy) in the model's decision nodes. This approach is simple, computational efficient, and interpretable, as it provides a clear ranking of features based on their impact. However, Impurity-based feature importance tends to favor variables with more categories or levels, which can lead to biases.

2.10.2 Permutation feature importance

Permutation feature importance is a technique used to evaluate the significance of individual features in a machine learning model. The process involves systematically shuffling the values of a single feature

in the dataset and observing the impact on the model's performance. By comparing the model's performance before and after the permutation, a decrease in performance indicates that the feature is crucial, as its alteration disrupts the model's predictive accuracy. This approach does not require retraining the model and can be applied to various algorithms (not just tree-based models). However, it may not capture feature interactions and is most effective when dealing with uncorrelated features. In our study, the “sklearn.inspection.permutation_importance” was used.

2.10.3 SHapley Additive exPlanations (SHAP)

SHapley Additive exPlanations (SHAP) by Lundberg et al., 2017 is a method to explain individual predictions. SHAP is based on the game theoretically optimal Shapley values (Molnar, 2022). Shapley values provide a mathematically fair and unique method to attribute the payoff of a cooperative game to the players of the game (Merrick & Taly, 2020; Shapley, 1953). SHAP values help us understand the role of each feature in a prediction by calculating how much each feature has pushed the prediction higher or lower, compared to prediction without that feature. For instance, applying SHAP to our model (Figure S2 and see Figure 4) revealed that temperature significantly influences predicted daily transpiration. Lower temperatures (depicted in blue) correlate with negative SHAP values, pushing predictions downward, while higher temperatures (depicted in red) associate with positive SHAP values, pushing predictions upward. Therefore, in this context, the model suggests that transpiration tends to be lower at lower temperatures. The SHAP library in python was used (Lundberg et al., 2017). For more info see https://shap.readthedocs.io/en/latest/example_notebooks/api_examples/plots/beeswarm.html#

2.11 Statistical Analysis:

Several statistical methods were employed in this study. To assess the correlation between features, we used the correlation coefficient (r), which measures the strength and direction of the linear relationship between two variables. For evaluating model performance, we used R^2 (coefficient of determination), which represents the proportion of variance in the dependent variable that is predictable from the independent variables. T-tests were used to compare the means of two groups and to assess whether there were significant differences between them. P-values (Pv) associated with the t-tests were used to determine statistical significance, with a threshold of $Pv < 0.05$ considered significant.

For categorical variables, we used a chi-square test to evaluate associations between categories. The chi-square value indicates the magnitude of the discrepancy between observed and expected values, while the p-value reveals whether this discrepancy is statistically significant. To compare multiple groups and determine whether their means differed significantly, we applied ANOVA (Analysis of Variance), calculating the F-statistic and corresponding Pv to evaluate overall model significance. Additionally, when group variances were unequal, we used Welch's test as a robust alternative to ANOVA, reporting the F-ratio and Pv to verify the statistical significance of the differences.

3. Results

From June 2018 to March 2024, multiple experiments were conducted in our greenhouses using the PlantArray systems. These experiments yielded continuous data on both plant physiology and environmental conditions. We collected, cleaned, labeled, and averaged the data to obtain daily values, as described in the methods section (Table 1). For this research we have used only well irrigated cleaned data, the resulting dataset composes 6237 observations, with each observation representing a single plant, and its ambient conditions in a day of measurement.

This article investigates the environmental responses of tomato and cereal crops, cultivated during summer and winter seasons respectively. Our findings reveal significant differences in environmental conditions between the two. Tomato plants were exposed to significantly higher summer temperatures (grand mean 25.1°C for tomatoes and 18.6°C for cereals, $p < 0.001$; Fig. 2a1) and relative humidity (grand mean 56.2% for tomatoes and 52.47% for cereals, $p < 0.001$; Fig. 2a2) compared to the winter conditions experienced by the cereals. Consequently, tomatoes plants were exposed to higher daily average vapor pressure deficit (VPD) than cereals (grand mean 1.43 kPa and 1.08 Kpa respectively; Pv<0.001 ; Fig. 2a3). The Daily Light Integral (DLI) for tomatoes was also greater (Pv<0.001), with an average of 18.18 mol/m²/day and a peak of 33.99 mol/m²/day, whereas cereals recorded a lower average DLI of 11.37 mol/m²/day and a maximum of 28.96 mol/m²/day (Fig 2. A4).

Despite cereals having a higher average plant weight (151.11 g) compared to tomatoes (110.15 g), their transpiration rates were significantly lower than those of tomatoes (average 160.38 g/day and 312.59 g/day respectively; Pv <0.001; Fig. 2a5, a6). This comparative analysis underscores the distinct environmental adaptabilities and physiological responses of these crops under varying seasonal conditions.

The data, presents a relatively high correlation between DLI and temperature ($r = 0.75$) and a minor correlation between transpiration and plant weight ($r = 0.6$; Fig. 2b). VPD is relatively corelated to temperature ($r = 0.74$), RH ($r = - 0.67$) and DLI ($r = 0.61$) but not to transpiration ($r = 0.24$; Fig. 2b).

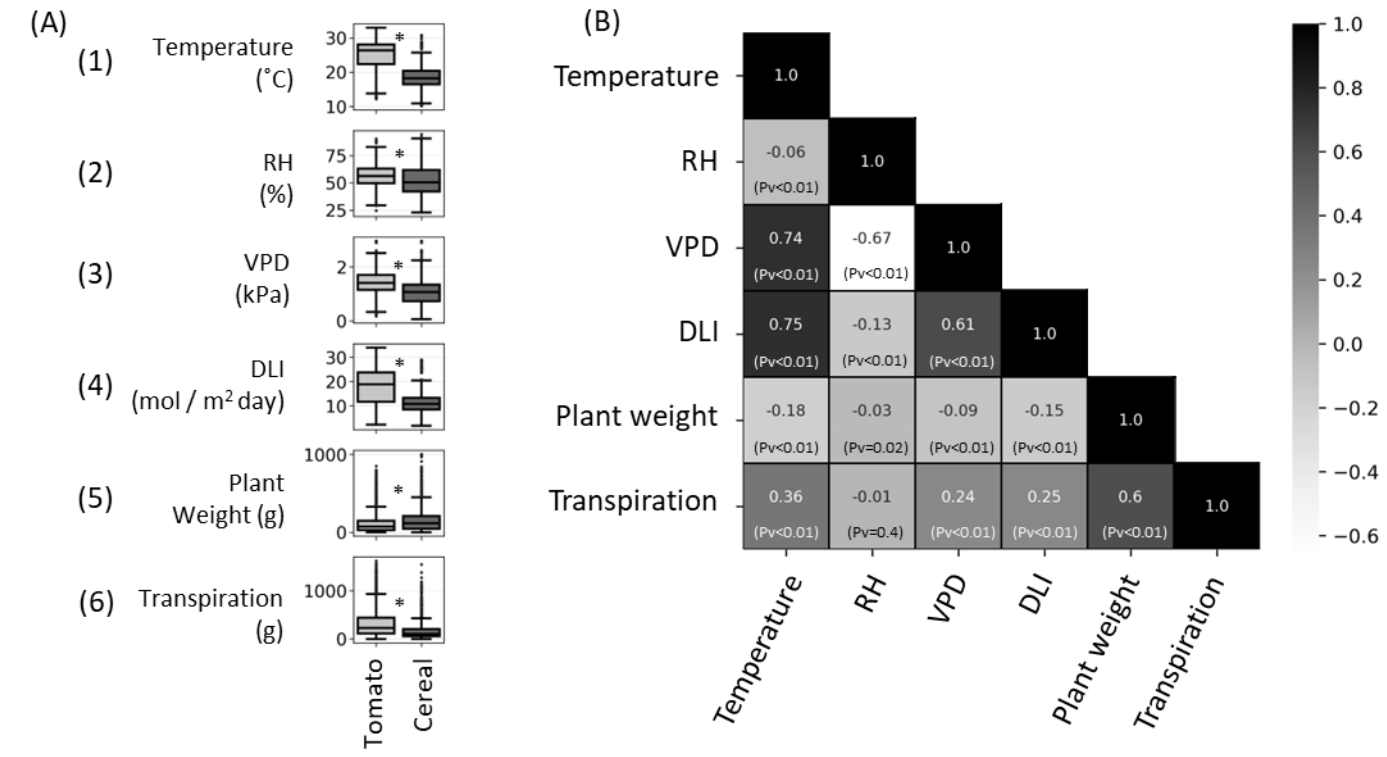

Figure 2: Data visualization. The data was collected between June 2018 and February 2022, by the lysimeter system, and preprocess to daily values. (A) Data variety between tomato and cereals crops (3057 / 1601 observations respectively). Box and Whisker of daily (A1) temperature, (A2) RH, (A3) VPD, (A4) DLI, (A5) plant weight and (A6) plant transpiration. Asterisks indicate statistical difference, t test; Pv<=0.001. (B) Pearson correlation coefficient chart of continuous features: Temperature, RH, VPD, DLI, plant weight and transpiration (for expansion see Figure S1). P-values (Pv) are presented in bracket.

3.1 Model precision and accuracy

Machine learning models were trained using the features: plant weight, temperature, RH, VPD, DLI, plant type, and soil type to predict daily transpiration (Table 1.). Hyperparameters for all models were finely tuned using a Cross-Validation Grid Search on the training dataset.

Our final models underwent rigorous evaluation through a 10-fold cross-validation process. This involved partitioning the dataset into 10 subsets, with 90% allocated for training and the remaining 10% for testing, repeated across 10 iterations. Such meticulous methodology facilitated comprehensive assessment under diverse training scenarios. To ensure robust performance evaluation, we conducted statistical analyses, including Root Mean Square Error (RMSE) and R^2 calculations across the 10 folds. Notably, while the Decision Tree model displayed respectable performance, the models Random Forest, XGBoost, and Neural Network showcased significant accuracy ($Pv < 0.05$, Table 3). Random Forest with the mean R^2 of 0.878 and an RMSE of 88.01. Similarly, XGBoost and Neural Network models yielded competitive mean R^2 values of 0.873 and 0.876, respectively, with RMSE values of 86.41 and 86.58. Neural Network, however, distinguished itself as the slowest model, completing the 10-fold cross-validation in 9.7 min ($Pv < 0.05$, Table 3).

Table 3: Comparison of evaluation scores among the four methods models.
The average of 10-fold Cross validations are presented.

Model	RMSE	R^2	Run time (sec)
Decision tree	103.65 [a]	0.832 [a]	0.01 [a]
Random forest	88.01 [b]	0.878 [b]	1.08 [a]
XGBoost	86.41 [b]	0.873 [b]	0.25 [a]
Neural Network	86.58 [b]	0.876 [b]	58.59

An ANOVA test was conducted to statistically evaluate performance differences among the 10-fold models scores, followed by Tukey's Honest Significant Difference (HSD), differences are indicated by letters.

3.2 Testing the models using hold out experiments.

Randomly selected experiments were separated from the rest of the data to serve as a validation dataset for testing the models' performance on unseen data. The hold out data structure was different from the data used to tune and train the models; with a lower temperature (T test = 21, $p \leq 0.001$), different ratio of Tomato: Cereal (Chi-square = 1225, $Pv < 0.001$), and a lower correlation between plant weight and transpiration (Table S1, Figure S1). Moreover, the distribution of transpiration values in the holdout data significantly differed from those in the training dataset ($Pv <0.001$). Notably, the upper quartiles of transpiration in the training and holdout datasets were 379g and 224g respectively (Fig. S3 and 3a). When the trained models were applied to this new dataset, the Random Forest model

demonstrated high accuracy in predicting transpiration, with a correlation coefficient (r) value of 0.88 (Figure 3b). The residual plot (Figure 3c) shows that the model's residuals are mostly centred around zero, indicating good predictive performance. Note that the distribution is wider where the transpiration is over 400 gr. The XGBoost exhibited the highest R^2 (0.8) and the lowest RMSE (92.89 g) among all models (Table 4, N.S.). The Random Forest Regressor model also performed well (R^2= 0.78, RMSE = 96.61 g). Conversely, the Neural Network exhibited higher errors (N. S.), with an RMSE of 114.42 g and an MAE of 82.21 g. On the holdout data, Tukey HSD test revealed no significant differences between models (Fig. S4. ANOVA: F= 0.7, Pv = 0.54).

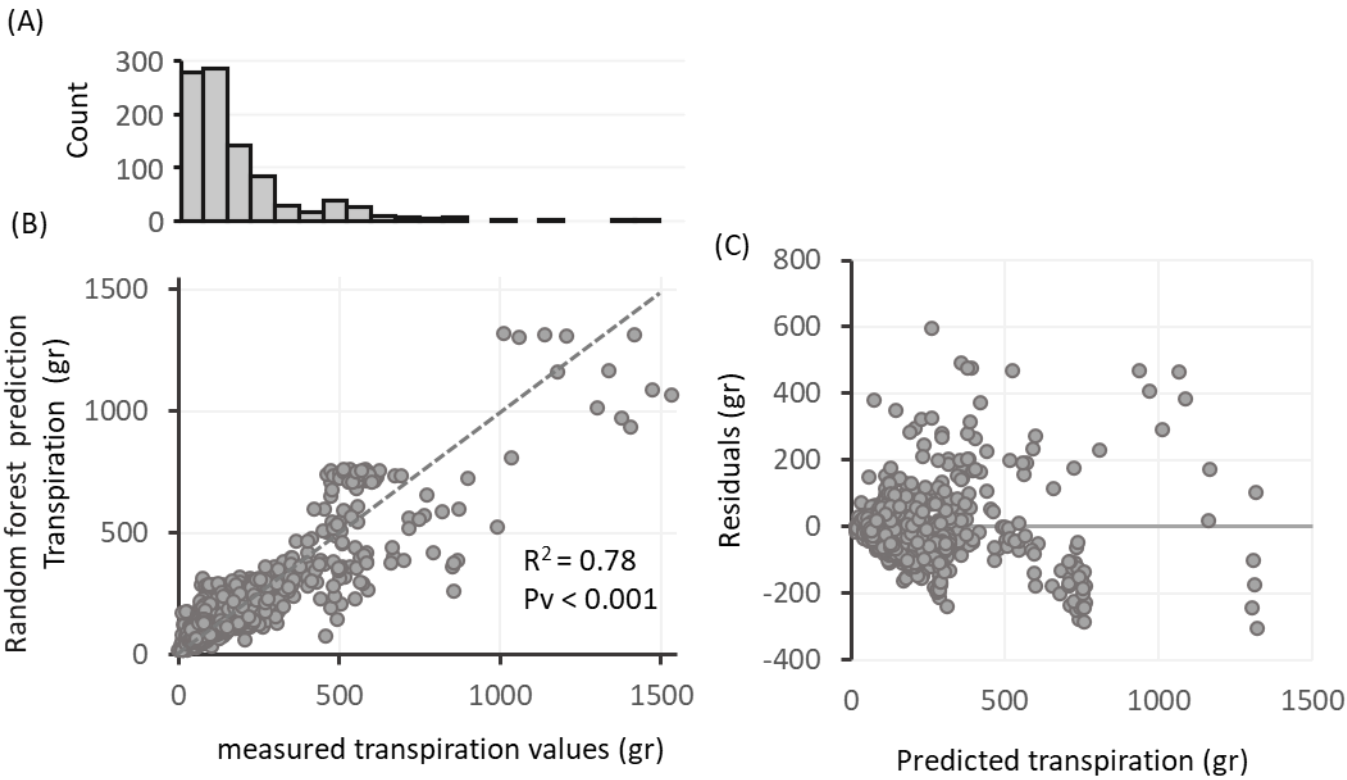

Figure 3: Random forest model evaluation on five holdout experiments (A) Histogram distribution of daily transpiration measured in the holdout data. (B) Goodness of fit for the Random Forest model predictions, comparing predicted against observed values. The dashed gray line represents an exact fit (Y=X), indicating where the model's predictions perfectly match the observations. The R^2 and the associated p-value (Pv) are stated on the graph to indicate the strength and significance of the relationship. (C) Residuals (observed minus predicted values) plotted against predicted values to assess any systematic deviations from the model. Higher values, which are less frequent as shown in (A), exhibit increased scatter and reduced correlation, as illustrated in (B) and (C).

Table 4: model evaluation statistics on the holdout experiments data.

Model	R^2	RMSE (g)	MAE	Relative error[1] (%)	Residual[2] (g)	Residual[2] (%)	Tukey HSD[3]
Decision Tree	0.67	119.29	76.13	57.83	76.13	57.83	a
Random Forest	0.78	96.61	64.70	56.25	64.70	56.25	a
XGBoost	0.80	92.89	61.34	51.83	61.34	51.83	a
Neural Network	0.69	114.42	82.21	69.52	82.21	69.52	a

[1] Relative error, also known as the Relative RMSE, is a measure that quantifies the accuracy of predictions relative to the scale of the actual values. is calculated as the RMSE divided by the mean of the actual values

[2] The mean absolute residual was calculated.

[3] Tukey test on the residuals between the predicted and actual values. Different letters indicate significant difference in Tukey HSD test Pv<0.05.

3.3 Feature importance

Feature importance was assessed through various techniques. For tree-based models, impurity metrics were employed, permutation and SHAP values were used. Interestingly, plant weight and temperature were identified as crucial predictors for transpiration (Figure 4a) and the SHAP feature importance test (Figure 4b) on the Random Forest model predicting transpiration. The horizontal spread of dots for each feature indicates the range of SHAP values, with a wider spread denoting greater impact variability on model output. Color signifies feature value magnitude, with red indicating high and blue indicating low values. Plant weight, temperature, and potting media are the most influential features in predicting transpiration, as evidenced by the wider spread of SHAP values, indicating a stronger effect on model predictions. In contrast, DLI shows a narrow spread with randomly distributed colors, suggesting a small and uniform influence on model output. Divergent color patterns in potting media reveal varying impacts on predictions, with soil (encoded as 1) increasing transpiration and sand (encoded as 0) decreasing it. Furthermore, the main, large greenhouse (encoded as 1) and cereal plant type (encoded as 1) are associated with reduced transpiration, while the secondary, smaller greenhouse (encoded as 0) and tomato (encoded as 0) contribute to increased transpiration.

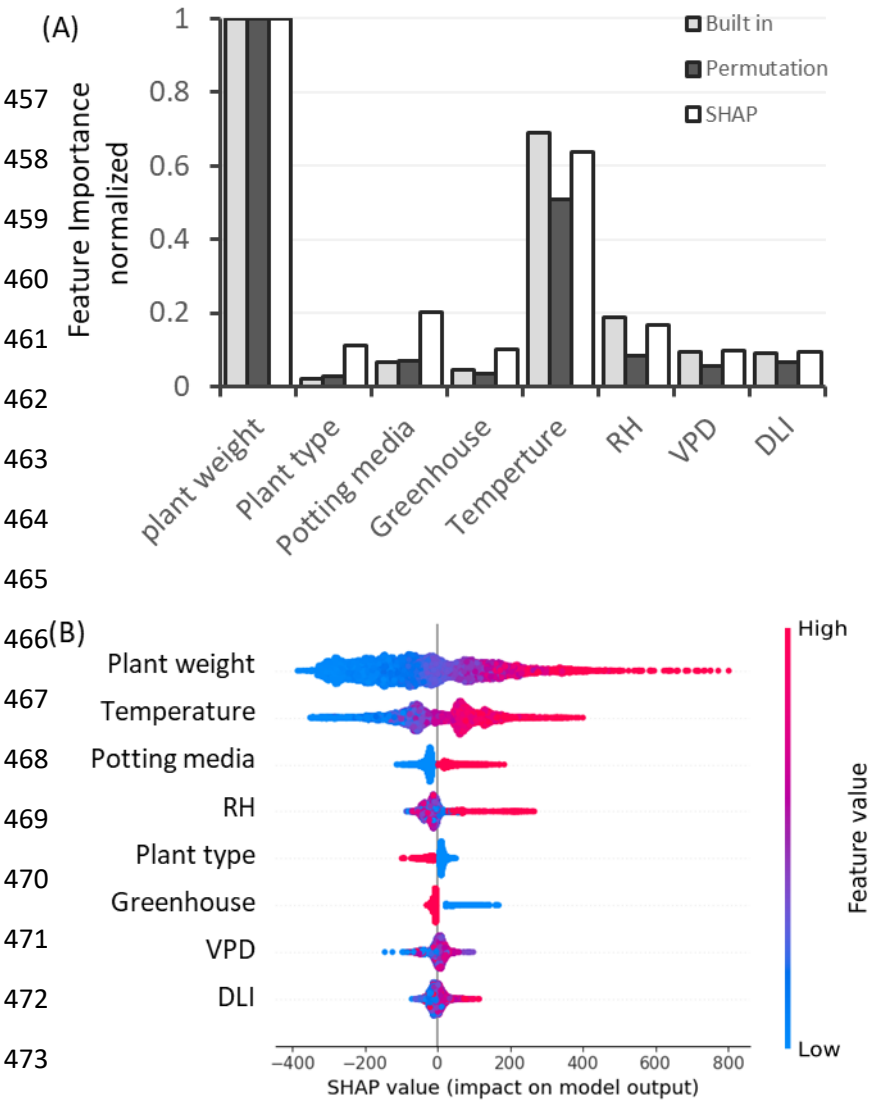

Figure 4: Feature importance contribution to the model prediction accuracy. Plant weight and temperature have a high importance overall. Testing feature significance in **Random Forest** model; (A) Feature importance using built in impurity test (gray), permutation (black) and SHAP values (white). Y axes are the feature importance scores normalized by a Min-Max scaling method, High score is given to the more influential features. (B) SHAP presentation of Feature importance. Every observation has one dot in each row. The position of the dot on the x-axis is the impact of that feature on the model's prediction for the observation, and the color of the dot represents the value of that feature for the observation. A larger spread of dots suggests that the feature has a more significant impact on the model's predictions.

3.4 Holdout data splitting methods.

In this section, we assess the robustness of our data analysis using three distinct partitioning strategies: temporal splits, greenhouse-based splits, and random experiment-based splits. These methods help us evaluate how reliable is our data and how well our models perform across different timeframes, environmental conditions, and experimental setups.

For data partitioning, the temporal split involved segregating data by leaving out a different year for each iteration, using the remaining years for training and testing. This approach allowed us to assess the model's ability to adapt to temporal variations. The greenhouse-based split used data from one greenhouse for training and testing, while data from another was held out, enabling evaluation of model generalizability across different greenhouse environments. In the random experiment-based split, experiments were randomly selected as holdouts, with the remaining used for training and testing, aiming to gauge the model's robustness across diverse experimental setups. R^2 scores analysis indicated no significant performance differences among the splitting methods: temporal split scored approximately 0.63, random experiment-based split achieved a mean of 0.64 (median 0.69), and

greenhouse-based split averaged 0.6 (Figure 5; Welch's test: F = 0.69, Pv = 0.52). Notably, variations in the random seed introduced considerable variability in the randomly selected holdout sets, while changes across different years also added diversity.

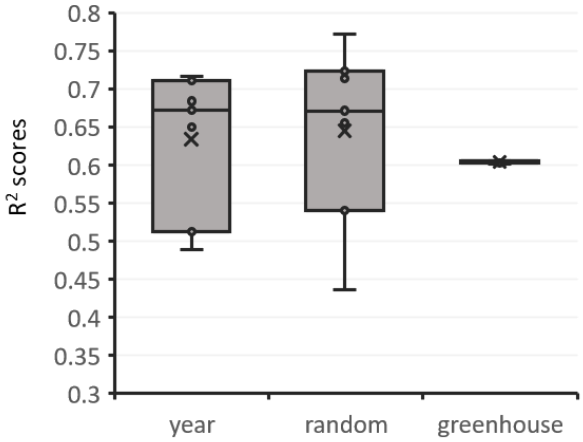

Figure 5: Comparing Data Splitting Methods for Holdout Data Set. The distribution of R2 scores for a tuned random forest model, evaluated using three distinct data splitting methods. The "Year" method separates the data chronologically, training on observations from six years while holdout data was from one excluded year, repeatedly applied across all available years. The "Random" method involves randomly selecting entire experiments as the holdout dataset. Different random seeds lead to varied holdout experiments, resulting in a broad range of scores. The "Greenhouse" method uses data from the main greenhouse for training and data from a secondary, different-sized greenhouse for testing.

4. Discussion

In this study, we explored the dynamic of daily transpiration in well-irrigated plants using advance machine learning models. Our unique dataset, collected over seven years, included high-resolution physiological traits and meteorological measurements from two greenhouses. Our findings indicate that our ML models, particularly Random Forest and XGBoost, showed respectable performance in predicting daily transportation. Additionally, both SHAP and feature importance scores revealed that plant weight and daily mean temperature are the most influential factors in these predictions. This discussion addresses these findings and their potential applications in agriculture.

4.1. Seasonal Environmental Effects on Plant Weight and Transpiration

Figure 2 highlights the distinct environmental parameters experienced by summer tomato and winter cereal, as well as the significantly higher daily transpiration of the tomatoes. Interestingly, the plant weight (Figure 2a5) of cereals was significantly higher than that of tomatoes, with averages of 151.11 g and 110.5 g, respectively. This result was unexpected, given the common correlation between larger annual plant size—which is closely related to transpiring leaf area (Halperin et al., 2017)—and higher transpiration rates (Figure 2b; Transpiration-Plant Weight; r=0.6). However, this discrepancy highlights how seasonal environmental variations can influence transpiration.

4.2. Model performance and Accuracy

The effectiveness of ML models in predicting daily transpiration was tested. Hyperparameters tuning (table 2) was critical for optimizing our models performance. Although the difference between tuned and untuned models was minor, it was significant with a mean difference in RMSE of 1.4 g and a pv = 0.0043 (Figure S5). The tuned models were trained and evaluated using 10-fold cross-validation. Random Forest and XGBoost performed similarly, with XGBoost being 4.5 times faster (Table 3). The XGBoost model achieved an RMSE of 86.41 g with and R^2=0.873. Neural Networks had comparable accuracy but much longer runtimes.

Testing our model on a holdout dataset, to further validate our model accuracy and generalizability. The XGBoost model demonstrates the strongest performance in predicting the daily transpiration (R^2 = 0.8, RMSE = 92.8 g). Although there is no significant difference in the residuals, the XGBoost shows the lowest residuals values followed by the Random Forest (51.83 % and 56.25 % respectively). These results, along with the detailed analysis of model performance, are included in Section S2.1 .

Our results align with other ML models that have predicted actual transpiration. For instance, Pagano et al. (2023) reported that their model had R^2 = 0.84, using Eddy Covariance flux tower. Similarly, Fan et al. (2021) achieved R^2 values from 0.816 to 0.95, using sap flow data from maize. Pagano et al. (2023) present a table summarizing several studies that predicted actual transpiration, with an average maximum R^2 of 0.87 for these predictions. We propose that the accuracy of our models (R^2 = 0.8-0.87) can be attributed to the precision of our transpiration measurements, the size of our dataset, and the specific features used during model training (Table. 1). Overall, these findings validate the possibility of using ML models to predict daily transpiration.

4.3 Key factors Influencing transpiration.

Artificial Intelligence models are often considered “black boxes” due to their complexity, consideration of multiple parameters, and the intricate statistical calculations involved in their algorithms (Azodi et al., 2020). Feature importance analysis enables us to understand the strength of each feature in the model’s predictions and in the transpiration processes.

Our Feature importance analysis indicates that **plant weight** plays the most significant role in predicting daily transpiration (Figure 4). We find this result very rational as the correlation between plant biomass and transpiration is well known (Lambers et al., 2008; Taiz & Zeiger, 2003). As larger plants have more leaves (and thus more stomata) leading to more water loss. Similarly, other studies have found that canopy size in olives (Sperling et al., 2023) and plant height in maize (Z. Chen et al., 2020) are crucial factors. Additionally, leaf area index has been effectively used in other studies to

predict sap flow, highlighting the broader applicability of leaf and plant size in transpiration models (Balasubramanian & Thirugnanam, 2023).

While plant age might replace plant weight for ease, as higher transpiration rates are often observed during late vegetative stages (Grulke & Retzlaff, 2001; Juárez-López et al., 2008). However, in our data, the correlation between plant age and transpiration is weak (days-transpiration; r=0.4, Figure S1). This due to inconsistencies in documenting plant age in our database, including it as a feature may introduce bias.

Temperature was the second most important factor in our feature importance hierarchy, making it our most critical environmental predictor of daily transpiration (Figure 4). This aligns with its previously observed effects on physiological processes, as high temperatures drive transpiration by increasing water vapor pressure (Peres et al., 2023; Liu et al., 2020). Additionally, it directly affects the physiological responses of plants, such as stomatal conductance (Haijun et al., 2015). Some researchers even found temperature to be the most critical factor influencing evapotranspiration (ET0), especially in spring and summer season when it contributes to as much as 46% of the variance of ET0 (Peres et al., 2023, Liu 2020, Zhang et al., 2020). Furthermore, temperature can be continuously monitored with high accuracy using small, portable sensors. This ease of measurement makes temperature an accessible and reliable variable for predictive models of plant water use, which are essential for efficient irrigation management and agricultural planning.

We were surprised to find **plant type** the least important feature for predicting transpiration (Figure 4a). Genotype by Environment (GxE) interactions suggest that different crops like tomatoes and cereals, with potential variations in stomatal density, would influence transpiration rates (Des Marais et al., 2013; Fournier-Level et al., 2011). A possible explanation is that the model may indemnity plant type indirectly through weight (Figure 2a5, Figure4a). However, if the model's assessment holds, it could signal a groundbreaking insight into the plant transpiration prediction.

Exploration of Potting media, VPD, and greenhouse feature importance are presented in the supplementary section S2.2.

The low importance score of the **Daily Light Integral (DLI)** was unexpected, as it contradicts the common understanding of the high significance of solar radiation (Tanny, 2013). It is possible that in indirect models based on eddy covariance (Pagano et al., 2023) and FAO56 estimation (Başağaoğlu et al., 2021), radiation plays a more crucial role, whereas in models using direct measurements such as sap and lysimeters (current article), its importance may be less pronounced. Another consideration is that daily averaging might diminish the perceived importance of light, while more granular data

collected at hourly or minute intervals may reveal its greater significance (as in these works: Li et al., 2020).

Future studies should explore the use of more granular data, such as hourly or minute-level measurements, instead of daily averages, to better capture the influence of all meteorological parameters on transpiration. Daily averaging can obscure the dynamic effects of factors like solar radiation, temperature, and humidity, potentially underestimating their true importance. By analyzing shorter time intervals, researchers may uncover stronger correlations between these variables and transpiration, providing a clearer understanding of their interactions.

4.4 Splitting methods.

Splitting the data into train and validation sets can significantly impact model performance and generalizability (Shi et al., 2022). We explored three distinct data sampling methods: year (temporal), random, and greenhouse (spatial). Although the models' accuracy results didn't show a significant difference between them, each method offered unique insights into the models' ability to accurately predict transpiration (Figure 5). The year split had a median accuracy (R^2) of 0.58, impacted by greenhouse differences, equipment aging, and yearly meteorological variation. Random sampling yielded a higher median accuracy of 0.69, benefiting from broader variation. Greenhouse-based splitting achieved 0.63, as the model effectively predicted transpiration in the secondary greenhouse using data from the main one, suggesting good generalizability across similar coupled setups.

4.5. Application and limitations

Our study has implications for irrigation management, water conservation, and greenhouse control. Integrating ML and artificial intelligence models into precision agriculture systems can provide real-time irrigation recommendations based on actual transpiration measured by lysimeters (load cells), which might be positioned in the greenhouse as supplementary sensors.

In conclusion, our study demonstrates the high potential of ML models to optimizing irrigation and enhancing crop management. Future research should aim to improve data quality with advanced sensor technology to capture the full spatial and temporal changes of environmental variables Moreover, future research should investigate whether these models can detect suboptimal plant behaviour and provide early warnings for plant stress.

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Competing interests

None declared.

Author contributions

SF and MM designed the study. SF collected the data and performed the data analyses. TN conducted the initial coding and data cleaning. SF and NA adjusted the workflow and tested the statistical models. SF wrote the first draft of the manuscript. MM (Corresponding Author) oversaw manuscript revisions, project management, and secured funding. SF, NA and MM contributed substantially to revisions.

Data availability

Data available on request due to privacy/ethical restrictions

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Supporting Information

Supplementary Table 1: Description of the training and holdout datasets used for model training and evaluation.

Supplementary Figure 1: Correlation charts of the training and holdout datasets, showing the Pearson correlation coefficients.

Supplementary Figure 2: SHAP analysis showing the feature importance for predicting plant transpiration.

Supplementary Figure 3: Box and whisker plots illustrating the distribution of transpiration in the training and holdout datasets.

Supplementary Figure 4: Predictions from different models compared to actual transpiration and corresponding environmental data across four holdout experiments.

Supplementary Figure 5: Comparison of model performance before and after hyperparameter tuning using Random Forest, demonstrating improvements in RMSE.

Supplementary section 2.1: Model performance and Accuracy.

Supplementary section 2.2: Factors Influencing transpiration