

Article

An Explainable XGBoost-Based Multi-Source Fusion Framework for Grape Leaf Fv/Fm Prediction

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Abstract

The chlorophyll fluorescence parameter Fv/Fm, representing the maximum photochemical efficiency of photosystem II, is an important indicator for evaluating plant photosynthetic performance and stress responses. However, rapid and non-destructive monitoring of Fv/Fm at the leaf scale remains challenging because conventional fluorescence measurements are time-consuming and require specialized equipment. Although spectral techniques provide an efficient alternative, existing spectral-based models mainly rely on single-source information and often lack sufficient integration of environmental conditions and physiological interpretability. Therefore, this study aimed to develop an explainable multi-source information fusion framework by integrating leaf spectral characteristics and environmental variables for accurate and interpretable estimation of grape leaf Fv/Fm. The grape cultivar ‘Queen Nina’ grown under protected cultivation was used as the experimental subject in this study. Visible–near-infrared reflectance spectra, measured Fv/Fm values, and environmental variables were synchronously collected under different water-stress conditions. Sensitive wavelengths were extracted by multiplicative scatter correction (MSC), competitive adaptive reweighted sampling (CARS), and the successive projections algorithm (SPA), and an XGBoost model incorporating both spectral and environmental features was established. The results demonstrated that: (1) the proposed multi-source fusion strategy effectively integrated spectral and environmental information for Fv/Fm prediction, with 12 sensitive wavelengths identified by MSC-CARS-SPA; (2) the XGBoost-EF model achieved R², RMSE, and MAE values of 0.906, 0.0432, and 0.0352, respectively, under vine-level five-fold cross-validation, outperforming the spectral-only XGBoost model; and (3) SHAP analysis provided an interpretable explanation of model predictions by quantifying the contributions of key spectral and environmental features, highlighting the importance of leaf temperature and red-edge wavelengths. It is concluded that the accuracy, robustness, and interpretability of non-destructive Fv/Fm monitoring in grape leaves can be substantially improved through multi-source information fusion.

Keywords: grape; Fv/Fm; multi-source information fusion; XGBoost; SHAP



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1. Introduction

The chlorophyll fluorescence parameter F_v/F_m , defined as the maximum photochemical efficiency of photosystem II (PSII), is a widely used indicator for evaluating the potential activity of the photosynthetic apparatus and the efficiency of light energy conversion in plants. It is highly sensitive to PSII reaction center damage and photoinhibition under adverse environmental conditions, and has therefore been extensively applied in the early diagnosis of abiotic stresses—such as drought, high temperature, and salinity—as well as in physiological status assessment and stress-tolerance evaluation of crops [1–7].

In recent years, precision viticulture has emerged as an important strategy for improving vineyard management by considering spatial and temporal variability within vineyards. Compared with conventional uniform management practices, precision viticulture aims to optimize irrigation, fertilization, and crop protection through the acquisition and analysis of multi-dimensional information related to vine growth, canopy structure, and physiological status. Various sensing technologies, including remote sensing platforms, imaging systems, and proximal sensors, have been applied to characterize vineyard variability from morphological and physiological perspectives. These approaches have provided valuable information for assessing canopy development, vegetation vigor, water status, and stress responses, thereby supporting site-specific management decisions [8,9]. However, challenges remain in accurately linking sensor-derived observations with plant physiological functions, particularly for parameters directly associated with photosynthetic performance. In addition, many existing sensing approaches mainly provide indirect indicators of plant status, while rapid and interpretable monitoring of physiological parameters at the leaf scale remains limited.

Spectral technology has become an important tool for estimating plant physiological traits owing to its rapid acquisition, non-destructive measurement, and relatively low cost [10–12]. The underlying principle is that the reflectance and absorption characteristics of plant leaves in the visible–near-infrared (VIS–NIR) region are closely related to variations in pigment content, water status, equivalent water thickness, and internal cellular structure [13–15]. Previous studies have successfully estimated several physiological traits, including chlorophyll content, nitrogen status, and light-use efficiency, using spectral reflectance data [16–19]. Spectral techniques have also demonstrated considerable potential for estimating chlorophyll fluorescence parameters. For F_v/F_m estimation, previous studies have explored different spectral-based strategies. Bartold and Kluczek [20] estimated and mapped F_v/F_m at a large spatial scale using Sentinel-2 satellite imagery combined with the XGBoost algorithm, demonstrating the feasibility of remote sensing approaches for monitoring photosynthetic performance. Liu et al. [21] investigated the relationship between vegetation indices and chlorophyll fluorescence parameters and found that indices such as the photochemical reflectance index could effectively estimate F_v/F_m using regression models. Zheng et al. [22] further explored hyperspectral vegetation indices for F_v/F_m estimation in *Suaeda salsa* and reported that D-690/D-1320 achieved promising prediction performance. These studies confirmed the correlation between spectral information and F_v/F_m ; however, vegetation indices usually contain only limited spectral information and may not fully exploit the complex spectral characteristics associated with physiological variation [23]. Recently, machine learning approaches based on full-spectrum information and feature wavelength selection have been increasingly applied to F_v/F_m prediction. Guo et al. [24] developed a one-dimensional convolutional neural network using hyperspectral data to assess drought tolerance in cotton genotypes. Li et al. [25] compared different preprocessing methods, feature selection algorithms, and machine learning models for predicting eggplant leaf F_v/F_m using visible–near-infrared spectra. Wang et al. [26] combined hyperspectral images with chlorophyll fluorescence images in pepper plants and proposed

an SG-SPA-BP strategy for efficient Fv/Fm image prediction. These studies demonstrate the potential of spectral and machine learning methods; however, most existing approaches primarily focus on extracting spectral information, while the environmental conditions driving photosynthetic variation are rarely incorporated into the prediction framework.

Although previous studies have laid an important foundation for the spectral estimation of Fv/Fm, several limitations remain. First, most existing models rely primarily on spectral information, which mainly reflects the integrated effects of leaf biochemical composition, structural characteristics, and physiological status. However, Fv/Fm represents the functional efficiency of PSII and is jointly regulated by internal physiological processes and external environmental conditions, including thermal status, radiation intensity, and water availability [27,28]. Environmental variables provide direct information about the stress-driving conditions, whereas spectral characteristics mainly describe the resulting changes in leaf optical properties. Therefore, spectral features alone may not fully represent the interactions among environmental drivers, leaf physiological responses, and photosynthetic efficiency. Integrating environmental variables with spectral information provides a complementary strategy for characterizing these relationships rather than simply increasing the number of input variables. Such multi-source information fusion may improve the representation of Fv/Fm variation under different environmental conditions. Second, most existing studies have focused mainly on prediction accuracy, while insufficient attention has been paid to model interpretability and the physiological mechanisms underlying Fv/Fm variation [29,30].

To address these issues, this study developed an explainable multi-source information fusion framework for predicting Fv/Fm in grape leaves under protected cultivation. Unlike conventional spectral-based models that mainly establish statistical relationships between reflectance characteristics and physiological parameters, this study aimed to integrate spectral responses with environmental information to better represent the interaction between external stress conditions and PSII photochemical performance. The main innovations of this study include: (1) the construction of a multi-source feature fusion strategy that combines leaf spectral characteristics and synchronous environmental variables to improve the representation of Fv/Fm variation under different stress conditions; (2) the development of an XGBoost-based prediction framework with feature optimization to capture nonlinear relationships between physiological responses and multi-dimensional information; and (3) the introduction of SHAP analysis to quantify the contributions of spectral and environmental features and provide interpretable insights into the factors affecting Fv/Fm prediction.

Specifically, the objectives of this study were to: (1) identify informative spectral features associated with grape leaf Fv/Fm using spectral preprocessing and wavelength selection methods; (2) establish and evaluate a multi-source information fusion model by integrating spectral and environmental variables, and compare its performance with spectral-only and conventional machine learning models; and (3) interpret the contribution of key spectral and environmental features to model predictions using SHAP analysis and improve the transparency of the proposed XGBoost framework. This study provides a potential approach for rapid, non-destructive, and interpretable monitoring of grape leaf photosynthetic performance under protected cultivation conditions and may support future precision management applications after further validation across diverse environmental conditions.

2. Materials and Methods

2.1. Experimental Site

The experiment was conducted from 1 June to 30 September 2025 at the protected grape cultivation base of the Guohe National Modern Agricultural Demonstration Zone, Lujiang County, Anhui Province, China. The experimental site is located at 31°27' N and 117°17' E and belongs to a subtropical monsoon humid climate zone, characterized by distinct seasons, abundant solar radiation, an annual mean temperature of approximately 16.5 °C, and an annual precipitation of approximately 1200 mm. The grapevines were grown in a multi-span plastic greenhouse system covered with polyolefin (PO) film, which provided a relatively stable protected cultivation environment for establishing different water-stress gradients.

2.2. Experimental Materials

The table grape cultivar 'Queen Nina', uniformly cultivated under protected conditions, was used as the experimental material. The grapevines were four years old and trained using a trellis system, with a row spacing of 4.0 m and a plant spacing of 1.0 m.

2.3. Experimental Design and Data Acquisition

To establish the response relationship between leaf photochemical efficiency and multi-source information, a water-stress gradient experiment was designed. Water availability is a key environmental factor affecting plant photosynthetic activity and PSII photochemical efficiency. Under water stress, stomatal closure can be induced, leaf transpiration can be reduced, chlorophyll content can be decreased, and leaf spectral characteristics and chlorophyll fluorescence parameters can be consequently altered. Therefore, three water treatments were established in this study: (1) full irrigation, in which soil water content was maintained at 75–80% of field capacity to simulate non-stress conditions; (2) mild drought stress, in which soil water content was maintained at 55–65% of field capacity; and (3) moderate drought stress, in which soil water content was maintained at 40–50% of field capacity. These treatments were designed for the systematic characterization of the photochemical responses of grape leaves under varying water conditions, yielding continuous response data of leaf photochemical efficiency across a gradient from non-stress to moderate stress. For each treatment, 10 grapevines with similar growth status were selected, and 15 healthy, mature, and pest-free functional leaves were randomly sampled from each vine, resulting in a total of 450 leaf samples. The selection of functional leaves was intended to reduce interference from non-physiological factors, such as leaf senescence, disease damage, and physical injury, while preserving physiological variations induced by different water-stress levels. Therefore, leaves subjected to different drought treatments, including those exhibiting reduced photosynthetic performance, were retained to establish the relationship between environmental stress and Fv/Fm variation.

2.3.1. Measurement of Leaf Spectral Reflectance

A VIS–NIR reflectance spectroscopy acquisition system was constructed, as shown in Figure 1. The system consisted of a spectrometer with a wavelength range of 200–1100 nm (Maya2000 Pro, Ocean Optics, Dunedin, FL, USA), a tungsten halogen light source (HL-2000, Ocean Optics, Dunedin, FL, USA), a reflection optical fiber, a reflection probe holder, a standard white reference panel, and a computer. Before measurement, the tungsten halogen lamp was preheated for 30 min to ensure stable light intensity. Dark-current correction was

then performed for the spectrometer, and white-reference calibration was carried out using the standard diffuse reflectance panel. The sample reflectance was calculated as follows:

$$R = \frac{I - I_b}{I_w - I_b} \quad (1)$$

where R is the spectral reflectance of the sample, I is the reflected spectral intensity of the sample, I_w is the reflected spectral intensity of the standard white reference panel, and I_b is the spectral intensity acquired by the spectrometer when the light source was turned off.

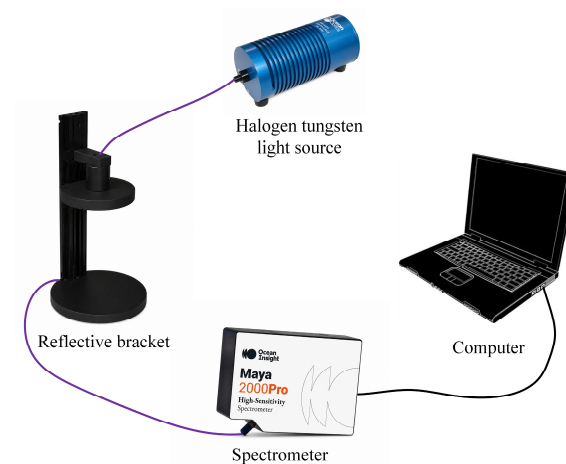


Figure 1. Visible–near-infrared reflectance spectroscopy data acquisition system. The purple line indicates the optical fiber connection, whereas the black line indicates the data cable connection.

OceanView software (version 2.0.18, Ocean Optics, Rochester, NY, USA) was used to set the spectral acquisition parameters. The spectral integration time was 200 ms, the number of scans averaged was 10, and the smoothing level was set to 5. Before measurement, the surface of each grape leaf was cleaned to avoid interference from dust and impurities. During measurement, the fiber-optic probe was vertically fixed above the target leaf using the probe holder, and the main vein was avoided. For each leaf, spectral reflectance was continuously collected from three points at the same physiological position. The average spectral reflectance of the three measurement points was used as the original spectral data of the leaf for subsequent analysis.

2.3.2. Measurement of Chlorophyll Fluorescence Parameters and Environmental Variables

A MultispeQ multifunctional plant phenotyping device (MultispeQ V2.0, PhotosynQ, East Lansing, MI, USA) was used to synchronously measure chlorophyll fluorescence parameters and key environmental variables. Data acquisition was performed using the PhotosynQ software (version 1.10.59.0). Before measurement, the leaf samples were dark-adapted for 20 min. The chlorophyll fluorescence parameter F_v/F_m was measured at the same leaf positions as the spectral measurements using the instrument probe, and the average value of three measurement points was taken as the F_v/F_m value of each leaf.

During each fluorescence measurement, the real-time environmental variables at the measurement point were simultaneously recorded by the built-in sensors of the device. These variables included photosynthetically active radiation (PAR, $\mu\text{mol m}^{-2}\cdot\text{s}^{-1}$), air temperature (T_a , $^{\circ}\text{C}$), leaf temperature (T_l , $^{\circ}\text{C}$), and relative humidity (RH, %).

2.4. Data Processing

2.4.1. Sample Set Division

To improve the signal-to-noise ratio of the spectral data, the unstable bands at both ends of the spectral range were removed, and 1339 bands within the range of 400–1000 nm were selected for analysis. To improve data quality before model development, a Monte Carlo cross-validation (MCCV)-based screening procedure was applied to identify samples showing unstable prediction behavior. Specifically, repeated random calibration-validation procedures were performed, and samples showing consistently high prediction errors across iterations were considered potential outliers and removed before final modeling [31,32]. This procedure aimed to reduce the influence of abnormal samples on model calibration rather than serving as a conventional statistical outlier detection method. Finally, 445 valid samples were retained. Considering the hierarchical structure of the experimental dataset, where multiple leaf samples were collected from the same grapevine, a vine-level five-fold cross-validation strategy was adopted. Specifically, grapevine identity was used as the grouping factor during dataset partitioning, ensuring that samples collected from the same vine were assigned exclusively to either the training or validation subset in each fold. This strategy prevented information leakage caused by the correlation among leaves from the same grapevine.

2.4.2. Spectral Data Preprocessing

To reduce spectral disturbances caused by measurement noise, baseline shifts, and scattering effects, three preprocessing methods were applied, including Savitzky–Golay (SG) smoothing, multiplicative scatter correction (MSC), and standard normal variate (SNV). Specifically, SG smoothing was used to reduce high-frequency random noise while preserving the main spectral characteristics. MSC was applied to correct multiplicative and additive scattering effects caused by differences in leaf surface structure, measurement geometry, and optical path conditions. SNV was employed to reduce spectral variation caused by scattering differences among samples by normalizing the spectral distribution of individual measurements. These preprocessing methods aimed to improve the signal-to-noise ratio and retain spectral information associated with Fv/Fm variation for subsequent feature selection and modeling.

2.4.3. Feature Wavelength Selection

To reduce the dimensionality of the hyperspectral data, eliminate noise and collinear variables, and identify feature wavelengths highly sensitive to grape leaf Fv/Fm, three feature selection algorithms and their combinations were used in this study: competitive adaptive reweighted sampling (CARS), the successive projections algorithm (SPA), uninformative variable elimination (UVE), CARS combined with SPA (CARS-SPA), and UVE combined with SPA (UVE-SPA).

Unlike vegetation indices that compress spectral information into ratios of several selected bands, this study retained the original reflectance values of informative wavelengths. This strategy was adopted because the objective of this study was leaf-scale Fv/Fm prediction using hyperspectral information rather than canopy-level vegetation monitoring. Retaining absolute reflectance values preserves detailed spectral responses associated with physiological variation, which can be further captured by nonlinear machine learning algorithms such as XGBoost.

2.4.4. Multicollinearity Analysis

To evaluate potential multicollinearity among the predictors included in the optimal multi-source model, Pearson correlation analysis and variance inflation factor (VIF) analysis were conducted for the selected spectral features and the four environmental variables

before model interpretation. Pearson correlation coefficients were calculated to assess pairwise relationships among predictors, while VIF values were calculated to evaluate multicollinearity considering the joint effects of the remaining variables. A VIF value below 5 was considered to indicate the absence of problematic multicollinearity.

2.5. Construction of Fv/Fm Prediction Models

2.5.1. XGBoost Regression Model

Extreme gradient boosting (XGBoost) is a decision-tree-based ensemble learning algorithm developed within the gradient boosting decision tree (GBDT) framework. Regularization terms, second-order Taylor expansion, and column block parallelization are introduced by XGBoost for improving training efficiency and generalization ability. Good performance is exhibited by XGBoost in handling high-dimensional and nonlinear data. Its core idea is the construction of an additive model using a forward stage-wise strategy: in each iteration, a new decision tree is generated for fitting the residuals between the predicted and observed values of the previous model, and the final prediction is obtained by summing the outputs of all trees [33].

$$\hat{y}_i = \sum_{k=1}^K f_k(x_i), f_k \in F \quad (2)$$

where $\hat{y}_i$ is the predicted value of the i -th sample, x_i is the input feature vector, K is the number of regression trees, and f_k represents the k -th decision tree. The objective function of XGBoost is defined as:

$$Obj = \sum_{i=1}^n l(y_i, \hat{y}_i) + \sum_{k=1}^K \Omega(f_k) \quad (3)$$

where l is the loss function, y_i is the measured value, and $\Omega(f_k)$ is the regularization term used to control model complexity and prevent overfitting. The regularization term can be expressed as:

$$\Omega(f) = \gamma J + \frac{1}{2} \lambda \sum_{j=1}^J w_j^2 \quad (4)$$

where J is the number of leaf nodes, w_j is the weight of the j -th leaf node, and γ and λ are regularization parameters.

During model construction, grid search combined with vine-level five-fold cross-validation was applied for hyperparameter optimization. The candidate ranges of key parameters, including the number of decision trees, maximum tree depth, learning rate, subsample ratio, feature sampling ratio, and regularization coefficients, were predefined according to the characteristics of the dataset and the recommended parameter ranges of XGBoost. Each parameter combination was evaluated based on the average validation RMSE obtained from the grouped cross-validation folds, and the combination achieving the lowest validation RMSE was selected as the optimal configuration. The optimal parameter combination was then used to train the XGBoost regression model for grape leaf Fv/Fm prediction.

2.5.2. Multi-Source Information Fusion Process

For the achievement of collaborative modeling with leaf reflectance spectra and real-time environmental variables, and for the improvement of the predictive performance and interpretability of the model under complex field conditions, a feature-level fusion strategy was adopted. Specifically, the extracted spectral features were concatenated with the real-time environmental variables and used as model inputs.

First, spectral feature extraction was performed. Preprocessing and feature selection algorithms were applied to reduce the dimensionality of the original spectral data and

remove redundant noise. Sensitive wavelengths related to Fv/Fm were then selected. Finally, m key wavelength reflectance values were extracted from each sample for the construction of a spectral feature vector.

Second, the environmental variables were normalized before feature concatenation. Because the four synchronously measured environmental variables, namely PAR, air temperature, leaf temperature, and relative humidity, had different dimensions and units, z-score normalization was applied to facilitate feature integration and comparison among heterogeneous variables. Although XGBoost is theoretically insensitive to monotonic transformations of input variables, normalization was retained as a consistent preprocessing step for organizing and integrating heterogeneous environmental variables within the feature-level fusion framework, rather than as a means of improving the predictive performance of XGBoost.

$$z_i = \frac{x_i - \mu}{\sigma} \quad (5)$$

where z_i is the standardized value, x_i is the original value of the i -th sample for a given feature, μ is the mean value of that feature, and σ is the standard deviation.

Third, feature concatenation and modeling were performed. The spectral feature vector and the environmental feature vector were directly concatenated at the feature level to form a joint feature vector. The spectral response of leaf photosynthetic physiology was integrated with the direct information of environmental stress by this joint vector, and was then used as the input for training the regression model (Figure 2).

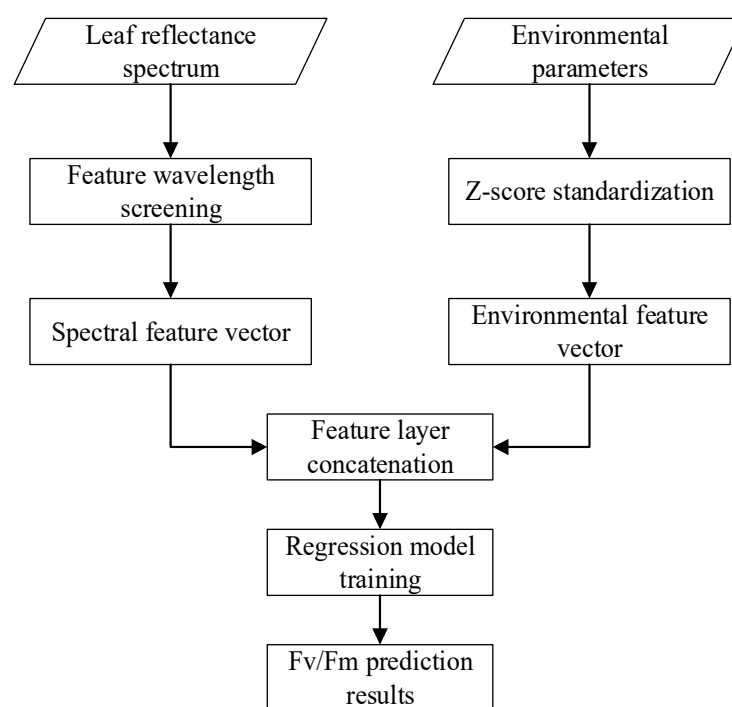


Figure 2. Process of environmental parameter fusion in the multi-source information model.

2.5.3. Model Interpretability Analysis

To address the limitation of conventional XGBoost models as black-box predictors and reveal the contribution mechanisms of multi-source features to Fv/Fm prediction in grape leaves, SHapley Additive exPlanations (SHAP), which is based on cooperative game theory, were used to interpret the optimal model. A specific Shapley value is assigned to each feature by SHAP, by which the contribution of that feature to a particular prediction relative to the average prediction is represented. The SHAP results were used to quantify

the contribution of each spectral and environmental feature to the model prediction and to improve the transparency of the proposed multi-source information fusion framework.

$$\phi_i = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|!(|N|-|S|-1)!}{|N|!} [f_x(S \cup \{i\}) - f_x(S)] \quad (6)$$

$f_x(S)$ where N is the set of all features, S is a subset of features excluding feature i , and is the model prediction based on the feature subset S . By combining global and local SHAP analyses, confirmation was sought in this study not only that the model prediction depended on spectral features and environmental variables with clear physiological significance, but also for intuitive and quantitative attribution explanations to be provided at the individual-sample level.

2.6. Experimental Environment and Model Evaluation Metrics

All experiments were conducted on a 64-bit Windows 11 operating system, and all programs were developed and executed in Python 3.10. The hardware configuration included an Intel Core i7-12700H central processing unit (CPU), an NVIDIA GeForce RTX 5060 graphics processing unit (GPU), and 32 GB of RAM.

For the comprehensive and objective evaluation and comparison of the prediction performance, goodness of fit, and generalization ability of different models, three metrics were employed, namely: coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE). These metrics were calculated as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (7)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (8)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (9)$$

where y_i is the measured Fv/Fm value of the i -th sample, $\hat{y}_i$ is the predicted value, $\bar{y}$ is the mean of the measured values, and n is the number of samples. A higher R^2 and lower RMSE and MAE indicate better prediction performance.

3. Results and Discussion

3.1. Spectral Characteristics of Grape Leaves

After removing the unstable bands at both ends of the spectral range, the original reflectance spectra of grape leaves are shown in Figure 3. The typical reflectance characteristics of green plants were exhibited by all spectral curves. A distinct reflectance peak was observed near 550 nm, corresponding to the green peak, while a reflectance trough was observed near 680 nm due to strong chlorophyll absorption. In the range of 700–750 nm, reflectance was sharply increased, forming the red-edge region, which is highly sensitive to changes in photosynthetic physiological status. In the near-infrared (NIR) region of 760–1000 nm, reflectance was maintained at a relatively high level with slight fluctuations. Differences in spectral reflectance were observed among samples, particularly in the visible region of 550–680 nm and in the red-edge region. Differences in pigment content, water status, and cellular structure of grape leaves under different water-stress treatments are likely reflected by these variations, whereby a spectral information basis for estimating Fv/Fm was provided.

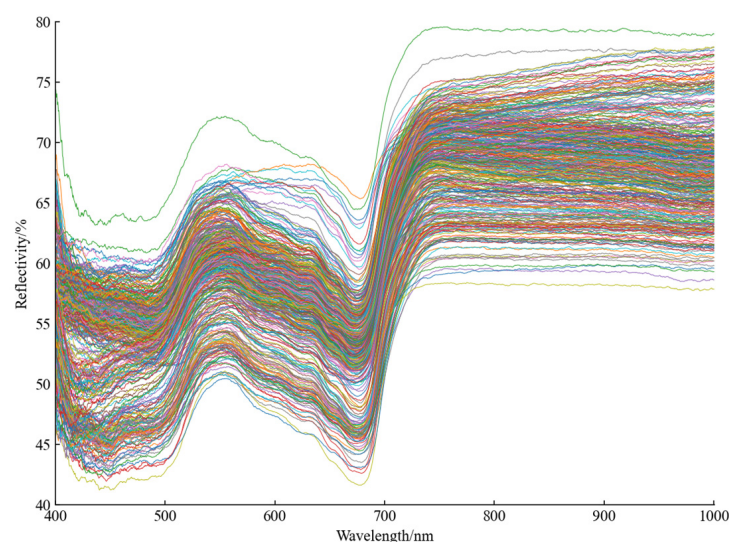


Figure 3. Spectral curves of grape leaves. Different colored lines represent individual reflectance spectra.

3.2. Comparison of Prediction Performance Among Different Models

To reduce the dimensionality of the spectral data, eliminate redundant information, and select wavelength variables sensitive to Fv/Fm, the original spectra were preprocessed using Savitzky–Golay (SG) smoothing, multiplicative scatter correction (MSC), and standard normal variate (SNV) transformation. Subsequently, five feature wavelength selection methods—namely, SPA, CARS, UVE, CARS-SPA, and UVE-SPA—were applied to the preprocessed spectra. The distribution of feature wavelengths selected by each method across the full-wavelength spectral curves is shown in Figure 4.

Using the feature wavelength matrices obtained from different combinations of pre-processing and feature selection methods as input variables, partial least squares regression (PLSR) models were established for predicting grape leaf Fv/Fm. To account for the hierarchical structure of the dataset, vine-level five-fold cross-validation was consistently applied to all preprocessing and feature-selection combinations. Grapevine identity was used as the grouping factor, ensuring that all leaf samples collected from the same vine were assigned to the same fold and were not simultaneously included in the calibration and validation subsets. Model performance was evaluated using the coefficient of determination (R^2) and root mean square error (RMSE) obtained from the grouped validation folds.

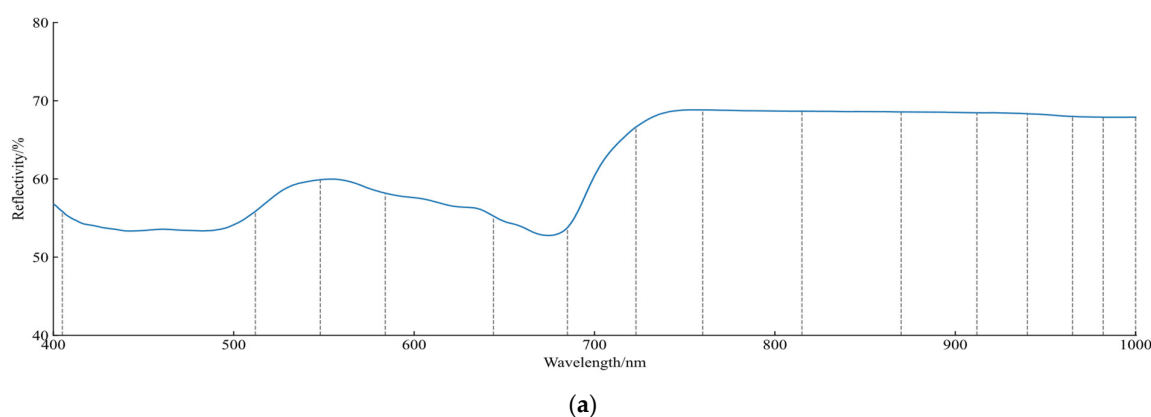


Figure 4. Cont.

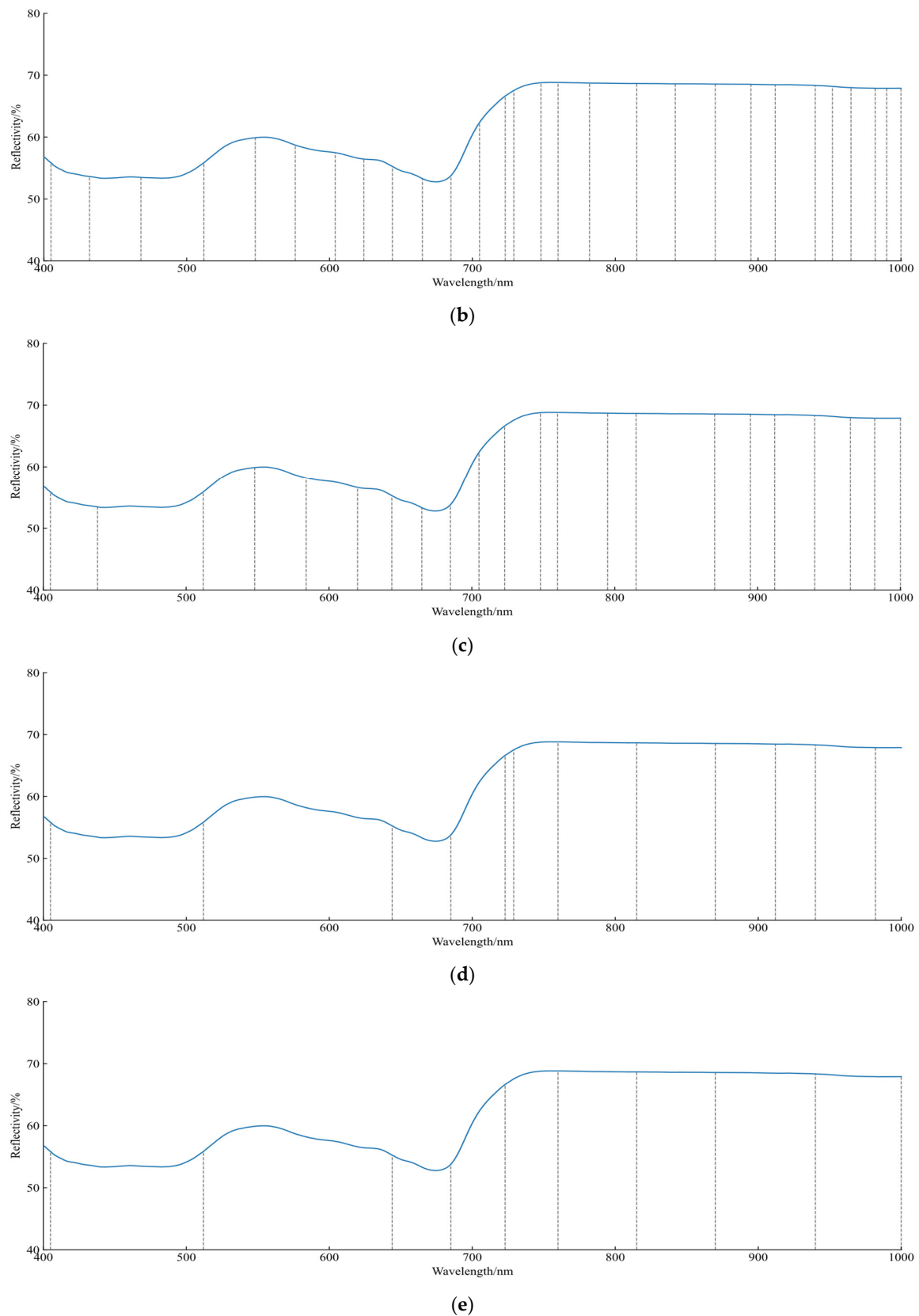


Figure 4. Distribution of feature wavelengths selected by different algorithms across the full-wavelength spectral curves. Dashed vertical lines indicate the wavelengths selected as spectral features by the corresponding feature-selection algorithms. (a) Feature wavelengths selected by SPA; (b) feature wavelengths selected by CARS; (c) feature wavelengths selected by UVE; (d) feature wavelengths selected by CARS-SPA; (e) feature wavelengths selected by UVE-SPA.

As shown in Table 1, model accuracy was improved by MSC and SNV preprocessing compared with both the original spectra and SG preprocessing, indicating that scattering effects in the spectral data were effectively reduced by these methods. Among the feature selection methods, SPA selected the fewest variables; however, this substantial reduction in dimensionality resulted in a decrease in prediction performance. For example, under MSC preprocessing, SPA reduced the number of variables from 1339 to 13, corresponding to a 99.0% reduction in spectral variables. Meanwhile, the validation R^2 decreased from 0.826 to 0.747, and the RMSE increased from 0.0585 to 0.0701. These results indicate that although SPA effectively reduced spectral dimensionality, excessive variable compression may lead to the loss of informative spectral features associated with Fv/Fm variation. Wavelengths related to Fv/Fm were selected by CARS and UVE, but the number of retained variables was kept relatively large. In contrast, the number of variables was substantially reduced by the CARS-SPA combination while relatively high prediction accuracy was maintained. Among all combinations, the best overall performance was achieved by the PLSR model based on MSC preprocessing and CARS-SPA feature selection, with a validation R^2 of 0.823 and a validation RMSE of 0.0590 obtained from vine-level five-fold cross-validation. Only 12 feature wavelengths were selected by this method—namely 402, 405, 450, 512, 580, 644, 685, 708, 723, 729, 820, and 940 nm—accounting for only 0.9% of the full spectral bands. Therefore, MSC-CARS-SPA was adopted as the feature extraction strategy for subsequent modeling.

Table 1. Prediction performance of PLSR models under different combinations of preprocessing and feature selection methods.

Preprocessing	Screening Method	Number of Variables	Calibration		Validation	
			R^2	RMSE	R^2	RMSE
RAW	Full spectrum	1339	0.832	0.0573	0.803	0.0621
	SPA	15	0.746	0.0702	0.721	0.0738
	CARS	28	0.801	0.0621	0.777	0.0659
	UVE	22	0.785	0.0645	0.758	0.0687
	CARS-SPA	12	0.809	0.0608	0.788	0.0643
	UVE-SPA	10	0.791	0.0635	0.767	0.0674
SG	Full spectrum	1339	0.828	0.0578	0.798	0.0627
	SPA	14	0.737	0.0714	0.712	0.0752
	CARS	31	0.789	0.0638	0.765	0.0677
	UVE	24	0.774	0.0662	0.747	0.0701
	CARS-SPA	13	0.796	0.0627	0.773	0.0666
	UVE-SPA	11	0.781	0.0651	0.756	0.0689
MSC	Full spectrum	1339	0.853	0.0534	0.826	0.0585
	SPA	13	0.770	0.0666	0.747	0.0701
	CARS	27	0.822	0.0586	0.802	0.0621
	UVE	20	0.809	0.0608	0.787	0.0644
	CARS-SPA	12	0.839	0.0558	0.823	0.0590
	UVE-SPA	10	0.814	0.0599	0.793	0.0635
SNV	Full spectrum	1339	0.847	0.0545	0.819	0.0597
	SPA	14	0.764	0.0675	0.739	0.0713
	CARS	26	0.817	0.0594	0.795	0.0632
	UVE	21	0.802	0.0619	0.779	0.0656
	CARS-SPA	12	0.831	0.0572	0.812	0.0606
	UVE-SPA	11	0.808	0.0609	0.785	0.0647

Based on the MSC-CARS-SPA combination, five prediction models were further established: partial least squares regression (PLSR), back propagation neural network (BP), extreme learning machine (ELM), support vector regression (SVR), and extreme gradient boosting (XGBoost). The same vine-level fold assignments were used for all models to en-

sure a fair comparison. Grapevine identity was retained as the grouping factor throughout hyperparameter optimization and model evaluation. Key hyperparameters of each machine learning model were optimized using grid search combined with vine-level five-fold cross-validation, with the minimum validation RMSE serving as the criterion for parameter selection (Table 2).

Table 2. Hyperparameter search ranges and optimal parameter settings of different machine learning models.

Model	Main Hyperparameters	Search Range	Optimal Parameters
PLSR	Number of components	1–12	8
	Number of hidden layer nodes	5, 10, 15, 20, 25, 30	20
BP	Learning rate	0.001, 0.005, 0.01, 0.05	0.01
	Maximum number of iterations	500, 1000, 1500, 2000	1000
ELM	Number of hidden layer nodes	20, 40, 60, 80, 100	80
	Activation function	Sigmoid, tanh, relu	sigmoid
SVR	Kernel function	Linear, rbf, poly	rbf
	Penalty coefficient	0.1, 1, 10, 50, 100	10
	Kernel function parameter	0.001, 0.01, 0.1, 1	0.01
	Insensitivity loss coefficient	0.001, 0.01, 0.05, 0.1	0.05
XGBoost	Number of decision trees	50, 100, 150, 200, 300	200
	Maximum tree depth	2, 3, 4, 5, 6	3
	Learning rate	0.01, 0.03, 0.05, 0.1	0.05
	Subsample ratio	0.6, 0.8, 1.0	0.8
	Feature sampling ratio	0.6, 0.8, 1.0	0.8
	L1 regularization coefficient	0, 0.01, 0.1, 1	0.1
	L2 regularization coefficient	0.1, 1, 5, 10	1

As shown in Table 3, compared with traditional regression models (PLSR) and other machine learning approaches (BP, ELM, and SVR), XGBoost achieved superior prediction performance for grape leaf Fv/Fm estimation. This improvement may be attributed to the capability of XGBoost to capture nonlinear relationships between spectral characteristics and physiological responses through ensemble decision trees. In contrast, linear models such as PLSR may have limited ability to describe complex interactions among spectral variables, while neural network and kernel-based models may be more sensitive to parameter optimization and sample size. The improved performance of the proposed model indicates that nonlinear machine learning approaches are more suitable for modeling the complex relationships associated with Fv/Fm variation. Therefore, XGBoost was adopted as the base model for subsequent multi-source information fusion.

Table 3. Prediction performance of different machine learning models for Fv/Fm.

Model	Calibration			Validation		
	R ²	RMSE	MAE	R ²	RMSE	MAE
PLSR	0.839	0.0558	0.0457	0.823	0.0590	0.0494
BP	0.872	0.0497	0.0407	0.841	0.0558	0.0457
ELM	0.858	0.0523	0.0429	0.832	0.0575	0.0471
SVR	0.879	0.0473	0.0395	0.856	0.0531	0.0435
XGBoost	0.891	0.0459	0.0375	0.868	0.0510	0.0418

3.3. Performance Analysis of the Multi-Source Information Fusion XGBoost Model

To further improve the adaptability of the model to complex field environments, real-time environmental variables were incorporated into the modeling process, and a multi-source information fusion XGBoost model integrating spectral features and environmental parameters—referred to as XGBoost-EF—was constructed. The four synchronously

measured environmental variables—namely, PAR, air temperature, leaf temperature, and relative humidity—were first standardized using Z-score normalization to eliminate dimensional effects. The standardized environmental variables were then concatenated with the feature wavelength reflectance values selected by MSC-CARS-SPA, generating a 16-dimensional joint feature vector.

The hyperparameters of the model were kept consistent with the optimal parameter combination determined previously: 200 decision trees, a maximum tree depth of 3, a learning rate of 0.05, a subsample ratio of 0.8, a feature sampling ratio of 0.8, an L1 regularization coefficient of 0.1, and an L2 regularization coefficient of 1.0. The same vine-level five-fold cross-validation strategy was adopted. The model was evaluated using vine-level five-fold cross-validation, and the reported performance metrics represent the aggregated prediction results from all validation folds. The fitting results of the XGBoost-EF model are shown in Figure 5.

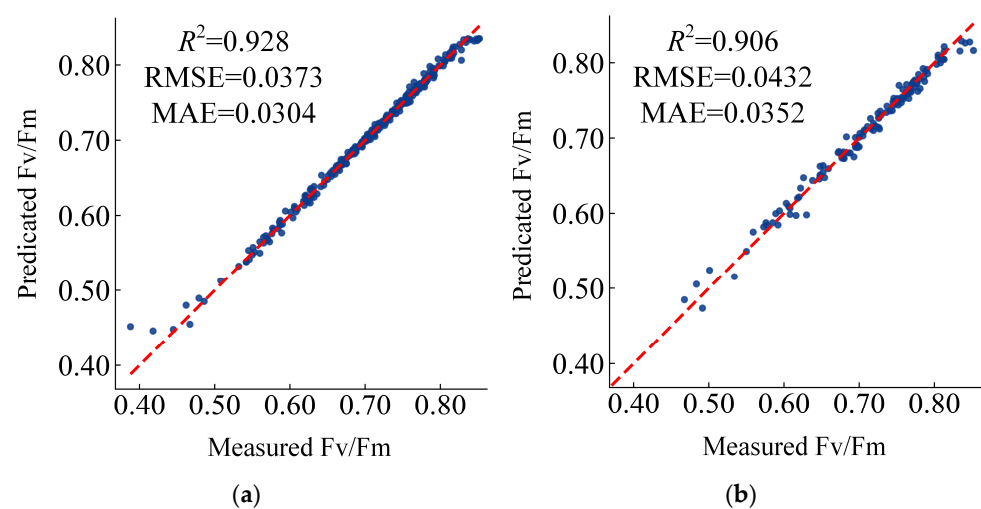


Figure 5. Fitting results of the XGBoost-EF prediction model. (a) Comparison between measured and predicted values in the calibration folds; (b) Comparison between measured and predicted values in the validation folds.

As shown in Figure 5, the prediction performance of the XGBoost-EF model was significantly improved after incorporating environmental variables. Compared with the spectral-only XGBoost model, the cross-validation R^2 of XGBoost-EF increased from 0.868 to 0.906, representing a relative improvement of 4.4%; the RMSE was decreased from 0.0510 to 0.0432, a reduction of 15.3%; and the MAE was decreased from 0.0418 to 0.0352, a reduction of 15.8%. It is indicated by these results that the proposed multi-source XGBoost-EF model provided accurate estimation of grape leaf Fv/Fm and the ability to estimate leaf Fv/Fm was significantly enhanced by the multi-source information fusion strategy.

To further evaluate the robustness of the multi-source information fusion model to slight spectral disturbances and noise, two data augmentation methods—namely, shift augmentation and Gaussian noise augmentation—were used to simulate spectral variations caused by instrument drift, environmental fluctuations, or operational errors during field measurement. For shift augmentation, each original spectrum was randomly shifted along the wavelength axis by 1–6 nm in either the left or right direction. For Gaussian noise augmentation, random noise following a normal distribution was added to the spectral variables, where the standard deviation of the added noise was randomly set to 1–5% of the original standard deviation at each wavelength. The augmented samples generated by each method were mixed with the original calibration folds at a ratio of 1:1 to construct the shift-augmented and noise-augmented datasets (Figure 6).

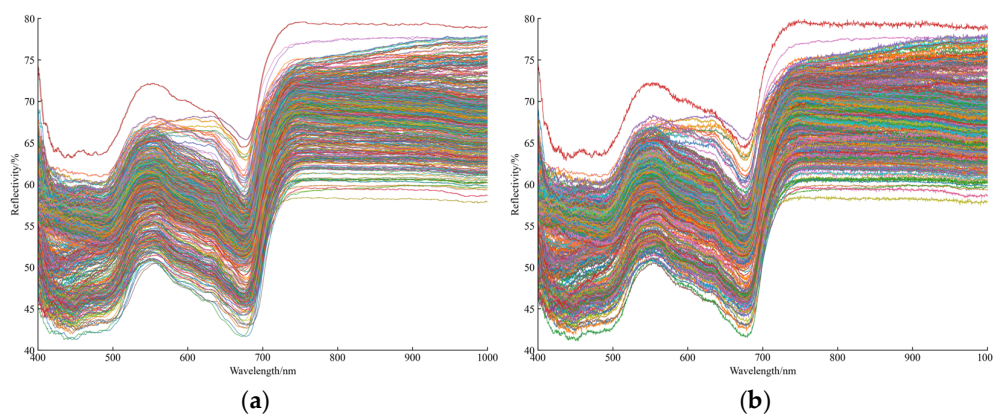


Figure 6. Spectral curves after data augmentation. Different colored lines represent individual augmented reflectance spectra. (a) Shift augmentation; (b) Gaussian noise augmentation.

As shown in Table 4, a decrease in the prediction accuracy of both models was observed, as expected, when the training spectral data were affected by shift or noise disturbances. However, the performance degradation of the XGBoost-EF model was consistently smaller than that of the spectral-only XGBoost model. Under the shift-augmented dataset, the validation R^2 obtained from vine-level five-fold cross-validation of XGBoost-EF was 0.889, decreasing by only 1.9% compared with its performance on the original calibration folds, whereas the R^2 of the XGBoost model was decreased from 0.868 to 0.841, corresponding to a reduction of 3.1%. For RMSE, an increase from 0.0432 to 0.0468 was observed in XGBoost-EF, while an increase from 0.0510 to 0.0557 was observed in XGBoost. A similar trend was observed under Gaussian noise augmentation: the decrease in the R^2 of XGBoost-EF was 2.5%, whereas that of XGBoost was 3.9%; the RMSE of XGBoost-EF was increased from 0.0432 to 0.0491, while that of XGBoost was increased from 0.0510 to 0.0569. It is suggested by these results that greater stability was maintained by XGBoost-EF than by the spectral-only XGBoost model under both disturbance conditions, indicating that model generalization and reliability in complex field environments were improved by multi-source information fusion.

Table 4. Comparison of validation performance obtained from vine-level five-fold cross-validation between XGBoost and XGBoost-EF under data augmentation conditions.

Data Augmentation Methods	Model	R^2	RMSE	MAE
No augmentation	XGBoost	0.868	0.0510	0.0418
	XGBoost-EF	0.906	0.0432	0.0352
Shift augmentation	XGBoost	0.841	0.0557	0.0456
	XGBoost-EF	0.889	0.0468	0.0383
Gaussian noise augmentation	XGBoost	0.834	0.0569	0.0465
	XGBoost-EF	0.883	0.0491	0.0394

3.4. Multicollinearity Assessment of Spectral and Environmental Variables

To evaluate whether correlations among the selected spectral and environmental variables could affect model construction and subsequent SHAP interpretation, Pearson correlation analysis and variance inflation factor (VIF) analysis were performed for the predictors included in the optimal XGBoost-EF model. The analyzed variables consisted of the 12 spectral wavelengths selected by the MSC-CARS-SPA method and four environmental variables, namely photosynthetically active radiation (PAR), air temperature (T_a), leaf temperature (T_l), and relative humidity (RH).

As shown in Figure 7, relatively strong correlations were observed among several selected spectral wavelengths. The highest pairwise correlation occurred between 723 nm

and 729 nm ($r = 0.91$), followed by 402 nm and 405 nm ($r = 0.90$), and 708 nm and 723 nm ($r = 0.89$). These relatively high correlations were expected because adjacent or physiologically related spectral regions may contain partially overlapping optical information. Although the reflectance values at 723 nm and 729 nm showed a high correlation due to their close spectral positions, both wavelengths were retained because they were independently selected by the feature-selection procedure and may represent slightly different spectral responses within the red-edge transition region. For nonlinear models such as XGBoost, correlated variables do not necessarily provide redundant information if they contribute complementary patterns for prediction. In addition, as shown in Table 5, the VIF analysis showed that the multicollinearity introduced by these variables remained within an acceptable range ($VIF < 5$), suggesting that retaining both wavelengths did not substantially compromise model stability. Among the environmental variables, air temperature and leaf temperature exhibited a strong positive correlation ($r = 0.86$), whereas relative humidity was moderately negatively correlated with leaf temperature ($r = -0.52$) and air temperature ($r = -0.46$). In contrast, correlations between the selected spectral variables and environmental variables were generally weak. The maximum absolute cross-source correlation coefficient was 0.32, observed between the reflectance at 940 nm and leaf temperature. These results indicate that, although correlations existed within the spectral and environmental feature groups, the degree of direct redundancy between the two information sources was limited.

Table 5. Variance inflation factor (VIF) values for the 16 input features in the XGBoost-EF model.

Feature	VIF	Feature	VIF
723 nm	3.87	729 nm	2.94
685 nm	3.52	405 nm	2.31
940 nm	3.18	Tl	1.89
820 nm	3.05	644 nm	1.76
512 nm	2.98	PAR	1.52
580 nm	2.96	Ta	1.41
450 nm	2.45	RH	1.36
708 nm	2.38	402 nm	1.24

The VIF values of all predictors ranged from 1.24 to 3.87, and none exceeded the threshold of 5 (Table 5). The highest VIF was observed for the reflectance at 723 nm ($VIF = 3.87$), followed by 685 nm ($VIF = 3.52$) and 940 nm ($VIF = 3.18$). Among the environmental variables, leaf temperature showed the highest VIF value of 1.89. These results indicate that no problematic multicollinearity was present in the combined predictor set when the joint effects of the remaining variables were considered.

Overall, the correlation analysis and VIF diagnostics collectively indicate that, although moderate correlations exist among certain spectral predictors—which is an inherent characteristic of hyperspectral reflectance data—none of the predictors exhibited VIF values exceeding the commonly accepted threshold of 5. This suggests that multicollinearity is unlikely to severely compromise the stability of the SHAP-based feature importance interpretation. Therefore, the subsequent SHAP analysis can be considered a reliable basis for identifying the dominant spectral and environmental drivers of Fv/Fm variation in grape leaves.

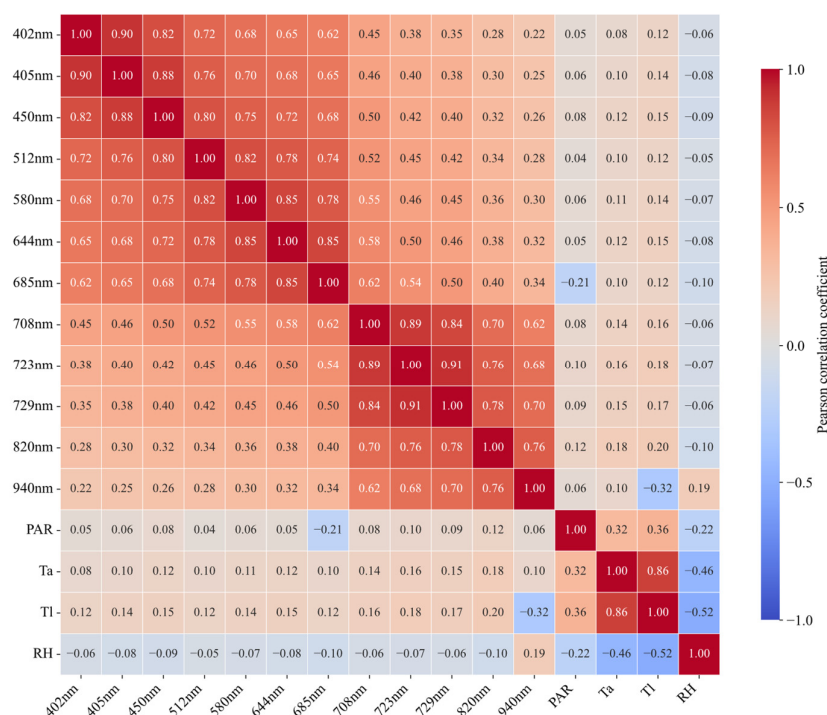


Figure 7. Pearson correlation matrix among the 12 selected spectral wavelengths and four environmental variables included in the XGBoost-EF model.

3.5. SHAP-Based Interpretation of Model

3.5.1. Global Feature Importance Analysis

Based on the samples from all validation folds, the SHAP values of all input features were calculated, and the mean absolute SHAP value was used to derive the global feature importance ranking, as shown in Figure 8. The horizontal axis represents the mean absolute SHAP value, and the top 10 input features contributing most to the model prediction are listed on the vertical axis.

As shown in Figure 8, the top 10 features contributing to the model prediction were composed of seven spectral wavelengths—namely, 723, 685, 940, 512, 729, 405, and 644 nm—and three environmental variables—namely, leaf temperature, PAR, and air temperature. Among these features, the highest importance was held by the 723 nm wavelength located in the red-edge region, with a mean SHAP value of 0.021, indicating that the most critical spectral feature for predicting Fv/Fm was represented by the reflectance at this wavelength.

Consistency was observed between these results and the established spectral characteristics of vegetation. The red-edge region (approximately 680–750 nm) represents the transition between strong chlorophyll absorption in the red region and high reflectance in the near-infrared region. Therefore, variations in reflectance within this region are generally considered sensitive to changes in leaf physiological status. In addition, near-infrared reflectance is affected by leaf internal structure, water status, and light scattering properties. These spectral responses may contribute to the ability of the model to capture Fv/Fm variation under different water-stress conditions [34–36]. However, direct measurements of chlorophyll concentration, leaf anatomical characteristics, or leaf water status were not performed in this study; therefore, the physiological mechanisms underlying the contribution of these wavelengths require further validation. The second and third most important features were 685 nm, located in the chlorophyll absorption region, and 940 nm, located in the near-infrared water absorption region, with mean SHAP values of 0.018 and 0.016, respectively. These wavelengths may reflect spectral variations associated with pigment-related absorption and leaf water conditions, although their specific physio-

logical contributions to Fv/Fm variation cannot be directly confirmed without additional biochemical measurements.

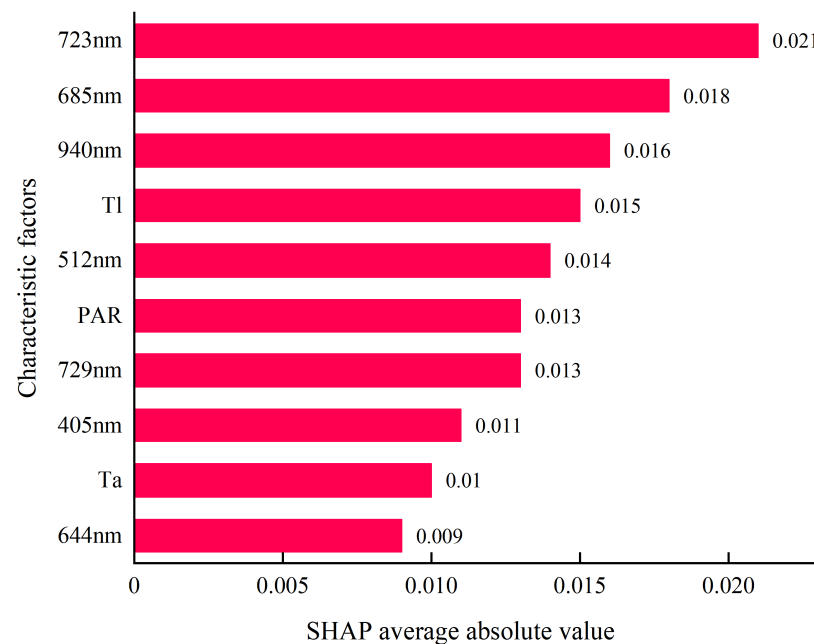


Figure 8. Global SHAP feature importance ranking plot.

Among the environmental variables, the fourth and sixth ranks were held by leaf temperature and PAR, respectively, and their importance was notably higher than that of air temperature and relative humidity. The first rank among the environmental factors was held by leaf temperature, as a direct indicator of leaf thermal stress. A high degree of consistency is exhibited between this result and the physiological mechanism by which PSII photochemical efficiency is reduced by high temperature [37]. It is indicated by these findings that spectral information was not only captured by the model but also that the direct effects of light and temperature on photosynthesis were effectively incorporated, whereby the advantage of multi-source information fusion was highlighted.

3.5.2. Local Explanation and Attribution Analysis

To intuitively illustrate the prediction reasoning process for an individual sample, a representative sample from the validation folds was selected for local explanation. This sample was obtained from the mild drought stress treatment. Its measured Fv/Fm value was 0.58, indicating relatively low photosynthetic efficiency, while the predicted value was 0.60, yielding a small prediction error. The SHAP waterfall plot for this sample is shown in Figure 9, in which how the model output was shifted by individual features from the baseline value (the mean prediction of all samples, approximately 0.75) to the final predicted value of 0.60 is illustrated.

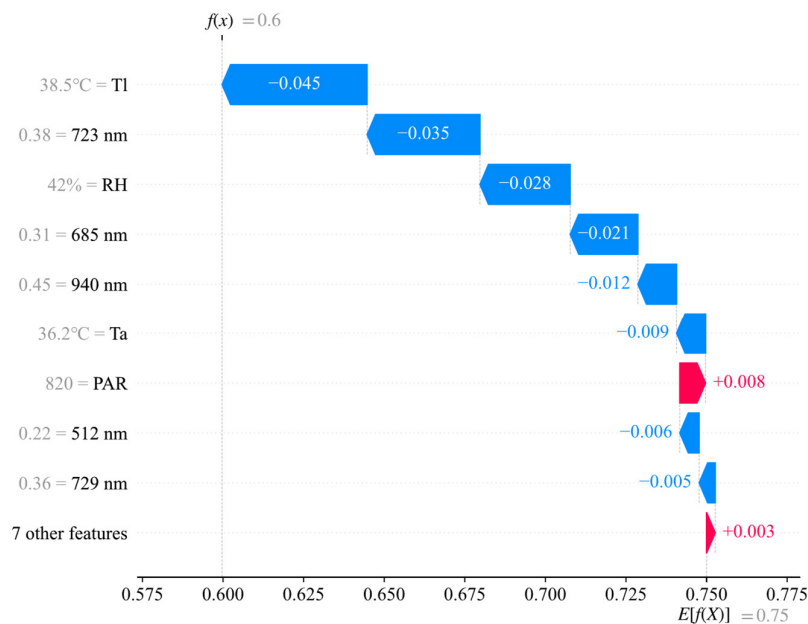


Figure 9. SHAP waterfall plot for a representative sample. Blue and pink bars indicate negative and positive contributions of features to the model output, respectively.

As shown in Figure 9, the main features whose negative contributions to the predicted value were substantial included leaf temperature (SHAP = -0.045), reflectance at 723 nm (SHAP = -0.035), relative humidity (SHAP = -0.028), and reflectance at 685 nm (SHAP = -0.021). The leaf temperature of this sample was 38.5°C during measurement, indicating a high-temperature condition. This result was consistent with the SHAP analysis, in which temperature was identified as the dominant negative driving factor. Photoinhibition and photorespiration may be intensified by high temperature, whereby high temperature was identified as a key factor contributing to the decrease in F_v/F_m . The negative contribution of relative humidity (RH) to the predicted F_v/F_m value for this sample warrants further physiological consideration. RH is not only a direct environmental factor but is also physically coupled with leaf temperature through evaporative cooling effects. Under the high-temperature condition observed for this sample ($T_l = 38.5^{\circ}\text{C}$), the relatively low ambient RH (42%) would enhance the leaf-to-air vapor pressure deficit, thereby promoting stomatal closure and reducing transpirational cooling [38]. This stomatal response can further exacerbate leaf warming and restrict CO_2 uptake, ultimately aggravating photoinhibition and reducing PSII photochemical efficiency [39]. Furthermore, changes in leaf water status associated with humidity conditions may influence near-infrared optical responses by affecting internal scattering properties of leaf tissues [40]. Therefore, the negative SHAP value for RH in this local explanation likely reflects a synergistic effect in which low humidity amplifies the thermal stress already imposed by high leaf temperature, rather than an independent causal factor. This interpretation is consistent with the well-documented interactive effects of temperature and humidity on plant photosynthetic performance under stress conditions [41].

Meanwhile, chlorophyll degradation or changes in cellular structure caused by water stress may be indicated by the relatively high reflectance at 723 nm (0.38), and an association was also observed between the elevated reflectance at 685 nm and weakened chlorophyll absorption. In contrast, PAR for this sample was $820 \mu\text{mol m}^{-2}\cdot\text{s}^{-1}$, representing a moderate light condition. Its SHAP value was $+0.008$, by which a weak positive contribution was provided, suggesting that the light condition was relatively favorable and stress was not further aggravated. Overall, it was quantitatively demonstrated by the local attribution

results how elevated leaf temperature, red-edge reflectance, humidity, and chlorophyll absorption-related wavelengths jointly contributed to the reduction in the predicted Fv/Fm value, whereby the physiological interpretability of the model was improved.

3.6. Model Applicability and Limitations

Although the proposed framework showed promising prediction performance under the experimental conditions, its practical applicability and several limitations should be carefully considered. From the perspective of practical vineyard management, the proposed framework provides a potential approach for rapid physiological monitoring of grape leaves. In practical applications, spectral information and environmental parameters could be collected using portable sensing devices or proximal sensing platforms, and the trained model could then be used to estimate Fv/Fm values for evaluating photosynthetic performance and identifying potential stress conditions. Such information may support precision irrigation and stress management decisions.

However, this study was conducted at a single protected cultivation site during one growing season using a single grape cultivar. Therefore, the established model mainly reflects the relationships among spectral characteristics, environmental variables, and Fv/Fm variation under the investigated conditions. Its generalizability to different vineyards, cultivation systems, climatic conditions, and grape cultivars requires further validation using independent multi-site, multi-year, and field datasets. In addition, although SHAP analysis provided quantitative insights into the contributions of important spectral and environmental features, the physiological mechanisms underlying these relationships were not directly validated because biochemical and structural measurements, such as chlorophyll concentration, leaf water status, and anatomical characteristics, were not included in the present study. Therefore, the identified important wavelengths should be regarded as model-associated spectral indicators rather than direct evidence of specific physiological mechanisms. Future studies should focus on expanding the experimental dataset, integrating spectral data with physiological and biochemical measurements, and evaluating model transferability across diverse production environments to further improve the robustness, interpretability, and practical applicability of the proposed framework.

4. Conclusions

An explainable multi-source information fusion framework for the rapid and non-destructive estimation of the chlorophyll fluorescence parameter Fv/Fm in grape leaves under protected cultivation was proposed in this study. To overcome the limitations of single-source spectral modeling, static model inputs, and insufficient interpretability in existing Fv/Fm estimation methods, VIS–NIR reflectance spectra, measured Fv/Fm values, and key environmental variables—including PAR, air temperature, leaf temperature, and relative humidity—were synchronously collected under different water-stress conditions. The MSC-CARS-SPA method was employed for spectral preprocessing and feature wavelength selection; an XGBoost-based multi-source information fusion model was constructed; and SHAP was introduced to interpret the model. The main conclusions are as follows.

First, spectral dimensionality was effectively reduced and sensitive wavelengths related to Fv/Fm were extracted by the combination of MSC preprocessing and CARS-SPA feature selection. A total of 12 wavelengths were selected from the 1339 original spectral bands, including key physiologically relevant regions such as the red-edge band at 723 nm, the chlorophyll absorption band at 685 nm, and the NIR water absorption band at 940 nm. A validation R^2 of 0.868, an RMSE of 0.0510, and an MAE of 0.0418 were achieved by the XGBoost model constructed using these selected spectral features, whereby PLSR and other conventional machine learning models, including BP, ELM, and SVR, were outperformed.

The effectiveness of feature wavelength selection combined with nonlinear modeling for Fv/Fm prediction is demonstrated by these results.

Second, model performance was further improved by the integration of real-time environmental variables. A validation R^2 of 0.906, an RMSE of 0.0432, and an MAE of 0.0352 were achieved by the proposed XGBoost-EF model. Compared with the spectral-only XGBoost model, an increase of 4.4% in R^2 was observed, while decreases of 15.3% and 15.8% were recorded in RMSE and MAE, respectively. Data augmentation using spectral shift and Gaussian noise was further applied to simulate instrument drift and random noise under field measurement conditions. Under the shift-augmented dataset, the decrease in the R^2 of XGBoost-EF was only 1.9%, whereas that of XGBoost was 3.1%; under the Gaussian-noise-augmented dataset, the decrease in the R^2 of XGBoost-EF was 2.5%, which was substantially lower than the 3.9% decrease observed for XGBoost. It is indicated by these results that stress-related physiological information was provided by the incorporation of environmental variables, the tolerance of the model to spectral disturbances was improved, and more effective modeling of the dynamic environment–spectrum–physiology relationship was enabled.

Third, the decision-making mechanisms of the multi-source prediction model were revealed by the SHAP-based interpretability analysis. As shown by the global feature importance ranking, the red-edge wavelength at 723 nm, the chlorophyll absorption-related wavelength at 685 nm, and the NIR water absorption wavelength at 940 nm were the most important spectral features. Among the environmental variables, the fourth and sixth ranks were held by leaf temperature and PAR, respectively, and their contributions were greater than those of air temperature and relative humidity. These findings were consistent with the established physiological roles of leaf thermal stress and light-driven photosynthetic regulation. It was further demonstrated by local attribution analysis of a representative drought-stressed sample how elevated leaf temperature and increased reflectance at 723 nm jointly contributed to the decrease in the predicted Fv/Fm value, whereby the physiological transparency of the model was improved.

Overall, a grape leaf Fv/Fm estimation model was developed in this study, by which multi-source information is integrated with XGBoost and SHAP, whereby accurate, robust, and interpretable non-destructive monitoring is achieved. A methodological reference for early crop stress diagnosis and intelligent decision-making in precision agriculture is provided by the proposed framework. Since this study was conducted under a protected cultivation environment using a single grape cultivar, the model performance may be affected by variations in climate conditions, cultivation systems, and genetic backgrounds. Therefore, multi-site and multi-season field validation is necessary to evaluate the transferability of the proposed framework. Furthermore, because the proposed framework integrates spectral characteristics, environmental information, and explainable machine learning techniques, it has the potential to be extended to the physiological monitoring of other crops after appropriate calibration and validation using crop-specific datasets. Future studies should further evaluate its applicability across different crop species, stress types, and spatiotemporal scales, and explore its deployment in lightweight and embedded systems for real-time field monitoring.

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(Boyan Zhang); supervision, H.L. and Q.Z.; project administration, H.L.; funding acquisition, H.L. All authors have read and agreed to the published version of the manuscript.

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