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Prediction of Qualitative Properties and Maturity Classification of Fig Fruits using Vis/SWNIR Spectroscopy

Reza Saiad Haghshomar[1], Reza Mohammadigol[2]*, Babak Valizadehkaji[1]

1 Department of Horticulture Engineering, Agriculture Collage, Arak University, Arak, Iran
2 Department of Biosystems Engineering, Agriculture Collage, Arak University, Arak, Iran

*Corresponding author's email: r-mohammadigol@araku.ac.ir

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ABSTRACT

Fruit quality is crucial at various stages of the supply chain, including harvest, packaging, processing, grading, transportation, storage, and shelf life. This study investigates the potential of the Vis/SWNIR spectral region (425–950 nm) combined with chemometrics to predict anthocyanin content, taste index (SSC/TA), and flesh firmness in fig fruit. Additionally, we compare the effectiveness of artificial neural networks (ANN), k-nearest neighbors (KNN), and discriminant analysis (DA) classifiers in categorizing figs as ripe, semi-ripe, or unripe. A total of 167 fig fruits were used for model calibration and validation. We evaluated the performance of regression ANN and classifiers (KNN, ANN, and DA) using common pretreatments, such as moving average (MA), standard normal variate (SNV), and multiplicative scatter correction (MSC), as well as their combinations. The results indicated that the combination of MA + D1 + SG preprocessing yielded the highest mean relative prediction deviation (RPD) of 1.55 for predicting flesh firmness (RMSEP = 1.83, r_p = 0.76), while the model performances for predicting anthocyanin content and taste index were deemed inadequate. For classification accuracy, ANN and DA achieved mean accuracies of 89.86% and 89.52%, respectively, using MA + SNV and MA + MSC pretreatments. This study provides valuable insights into the application of spectroscopy (425–950 nm) for assessing the quality attributes of fig fruit.

Abbreviations: Artificial Neural Networks (ANN), First Derivative (D1), Discriminant Analysis (DA), k-Nearest Neighbors (KNN), Moving Average (MA), Multiplicative Scatter Correction (MSC), Near Infra-Red (NIR), Number of the test set samples (n_p), Principle Component (PC), First Principle Component (PC1), Second Principle Component (PC2), Third Principle Component (PC3), Principle Components Analysis (PCA), Partial Least Squares (PLS), Light reflection percentage (R), Ripe (R), Coefficient of determination (R), Light intensity of the ambient (R_D), Random Forest (RF), Root Mean Square Error of Prediction (RMSEP), Prediction correlation coefficient (r_p), Residual Prediction Deviation (RPD), Light intensity of the white reference material (R_R), Light intensity of the sample (R_S), Standard Deviation (SD), Savitzky-Golay (SG), Standard Normal Variate (SNV), Semi-ripe (SR), Soluble Solids Content (SSC), Short Wave Near Infrared (SWNIR), Titratable Acidity (TA), Number of samples that are correctly classified (TC), Unripe (UR), Measured value of sample I (X_i), Average value of measurements ($\bar{X}$), Predicted value of sample I (Y_i), Average value of predictions ($\bar{Y}$)

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Introduction

Fig fruit (*Ficus carica* L.) is renowned for its appealing flavor, vibrant color, and medicinal properties. According to Lama et al. (2020), anthocyanins play a key role in the fruit's color and contribute significantly to its antioxidant content. Taste, an important quality attribute for fresh fruits and vegetables, is determined by a combination of sourness and sweetness, which correlate with titratable acidity (TA) and soluble solids content (SSC), respectively. Thus, the ratio of SSC to TA serves as an index of fruit taste acceptability (Abasi et al., 2018). Additionally, flesh firmness is crucial for detecting mechanical damage and determining shelf life (Sun et al., 2021). It is also a key measure of ripeness in the non-destructive grading of certain fruits (Matteoli et al., 2015; Torkashvand et al., 2017).

Vis/NIR spectroscopy enables rapid, accurate, and non-destructive qualitative evaluations without requiring preliminary sample preparation. Advances in optical technology have resulted in compact spectrometers that are lightweight, cost-effective, and high-performing, meeting the demand for quick and accurate measurements (Cortés et al., 2019; Abasi et al., 2020). The Vis/SWNIR region (310–1100 nm) is particularly useful due to the prevalence of water absorption bands, with significant wavelengths reported at 970, 1200, 1450, 1950, and 2250 nm (Magwaza et al., 2012). Given that fruits and vegetables contain 80-90% water, this spectral region reduces the influence of water on the acquired spectra, making it favorable for studies of fruit quality attributes.

While the application of Vis/NIR spectroscopy for quantitative and qualitative measurements of various fruits and vegetables has been documented (Wang et al., 2015; Beghi et al., 2017; Cortés et al., 2019), research specifically focused on predicting fig fruit quality attributes remains limited. This study aims to address this gap by evaluating Vis/SWNIR reflectance spectroscopy in the 425–950 nm range to non-destructively predict qualitative attributes of fig fruit, including anthocyanin content, firmness, and taste index. Additionally, we investigated the effectiveness of ANN, KNN, and DA classifiers, along with common pretreatments, to classify figs as ripe, semi-ripe, or unripe.

Materials and Methods

Fruits

A total of 180 fig fruits, from the “Siahe Hazaveh” genotype, were harvested in July 2021 from a 15-year-old tree in an orchard located in Hezaveh village, Markazi province, Iran. The fruits were collected at three ripeness stages: ripe (dark purple), semi-ripe (pale purple), and unripe (green), with 60 samples per stage. They were then transported to the postharvest laboratory at Arak University. This region experiences moderate rainfall and relative humidity, alongside relatively high temperatures. The “Siahe Hazaveh” genotype is noted for its favorable taste, high productivity, attractive appearance, high juice content, and elevated levels of total soluble solids and anthocyanins.

Spectroscopy setup and measurements

The spectroscopy system used in this study comprised a portable spectrometer (Ocean Optics Flame series, USA) with dimensions of 88.9 × 63.5 × 31.9 mm and a weight of 265 g. It operates within a wavelength range of 350-1000 nm, featuring 2048 pixels, a signal-to-noise ratio of 250:1, and an optical resolution of 0.1 to 10 nm. A 12-Volt halogen bulb served as the light source, complemented by Qp400 optical fibers, a sample holder, and an interactance probe. Light reflection at each wavelength was recorded using Eq. 1 (Cavaco et al., 2009).

$$\mathrm{R}\ (\%) = 100(R_S - R_D)/(R_R - R_D) \qquad (1)$$

R is the light reflection percentage, RS is the light intensity of the sample, RD is the light intensity of the ambient, and RR is the light intensity of the white reference material. Spectroscopy of each sample was performed in its three central positions (along the equator line) at approximately 120 degrees from each other, and 12 scans per position were acquired using Spectra Suite software. The mean value of scans was considered to reduce any possible noises from the detector temperature during the spectra acquisition (Nicolai et al., 2007). Hereafter, the mean of 36 scans was considered as the spectrum of each fig sample. After acquiring the spectrum of each sample, reference measurements were performed in the laboratory.

Fruit quality attributes

Anthocyanin

The content of total anthocyanin was determined according to the pH differential method (Kim et al., 2003). Absorbance was measured at 520 and 700 nm and expressed as cyanidin-3-glycoside (molecular weight of 449.2) equivalents per 100 g of fresh fruit weight.

Flesh firmness

Flesh firmness of figs was recorded using a penetrometer (STEP SYSTEM, Germany) with an 8 mm diameter plunger. After removing the epidermis at two equatorial positions, a 5 mm plunger measured the fruits flesh firmness as kg cm^{-2}.

SSC/TA

The soluble solids content was determined in the juice of fig fruits with a refractometer (Atago, PAL-1, Japan) at 20 ± 1 °C and results expressed as the means of % (°Brix). The pH of the juice was recorded using a pH meter (Az 86502, Taiwan). The titratable acidity (TA) was determined by titration with 0.1 N NaOH up to pH 8.1, using 1 mL of diluted juice in 25 mL distilled water, and the results were expressed as % citric acid. Taste index was calculated by dividing SSC by TA % (Saki et al., 2019).

Chemo-metrics

Pretreatment

Various pretreatment methods have been developed, each tailored for specific purposes. However, identifying the best pretreatment can be challenging, as different researchers often use varied samples and experimental conditions. In this study, after acquiring the spectra, commonly used pretreatments were applied (Nicolai et al., 2007). The moving average (MA) was utilized as one of the most common smoothing methods, incorporating five neighborhood points and quadratic polynomials to mitigate noise amplification. Additionally, normalization, standard normal variate (SNV), and mean scattering correction (MSC) were employed to address light scattering effects in the acquired spectra. The first derivative combined with a Savitzky-Golay (SG) filter was applied to enhance spectral properties and eliminate baseline shifts (Tiecher et al., 2020). Furthermore, Hotelling's T-squared distribution method was used to identify outliers (Maniwara et al., 2019; Mouazen et al., 2010).

Principle components analysis (PCA)

Principal Component Analysis (PCA) is a technique for extracting useful information from data, allowing for exploration of data and variables, their relationships, and the overall correlation between them (Beghi et al., 2017). PCA generates new variables that are linear combinations of the original variables. The first principal component captures the most variance, while the second principal component contains information not represented by the first, with the same principle applying to subsequent components (Callao and Ruisánchez, 2018). In this study, the first four principal components were used as inputs for regression analysis and classification with ANN.

Artificial neural networks (ANN) and classifiers

ANN are robust nonlinear methods for data analysis, capable of detecting and modeling complex relationships between inputs and outputs (Guo et al., 2016). An ANN typically consists of three layers: an input layer, hidden layers, and an output layer (Wang et al., 2015). In this study, the ANN topology included an input layer with four neurons representing the first four principal components, an output layer with three neurons corresponding to anthocyanin, flesh firmness, and taste index, and hidden layers with an optimal number of neurons determined automatically by the software. The application of classifiers for the qualitative analysis of fruits has been explored in various studies (Amuah et al., 2019; Kaiyan et al., 2020). Here, we compared the performance of commonly used classifiers—ANN, KNN, and DA—for classifying ripe, semi-ripe, and unripe fig fruits.

Validation

The evaluation of the models was performed using random subsampling while knowing that "hold out" was repeated ten times (Han et al., 2011). In this method, the acquired spectra were randomly partitioned into two independent sets, a training set and a validation set (20%). In each iteration, the training set was used to derive regression ANN and classifiers. The average of the overall accuracy and prediction index obtained from the ten validation sets, were reported. In this method, there is no problem regarding unrealistic prediction and classification results. The predictive ability of regression ANN was evaluated using the root mean square error of prediction (RMSEP), the prediction correlation coefficient (rp), and the residual prediction deviation (RPD), Eqs. 2-4 (Beghi et al., 2017; Guo et al., 2016; Theanjumpol et al., 2019; Wang et al., 2015). Meanwhile, the mean overall accuracy measure was used to evaluate the classifiers in validation sets Eq. 5.

$$\mathrm{RMSEP}=\sqrt{\sum_{i=1}^{n}(Y_i-X_i)^2 \Big/ n_p} \qquad (2)$$

$$r_p = \sum_{i=1}^{n}(X_i-\bar{X})(Y_i-\bar{Y}) \Big/ \left(\sqrt{\sum_{i=1}^{n}(X_i-\bar{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i-\bar{Y})^2}\right)$$

(3)

$$\text{RPD}=\sqrt{\sum_{i=1}^{n}(X_i-\bar{X})^2 \Big/ n_p-1} \Big/ \text{RMSEP}=\text{SD}/\text{RMSEP} \quad (4)$$

$$\%\text{Accuracy}=(\text{TC}/n_p)\times 100 \quad (5)$$

Where X_i is the measured value of sample i, Y_i is the predicted value of sample i, n_p is the number of the test set samples, $\bar{X}$ is the average value of measurements, $\bar{Y}$ is the average value of predictions, SD is the standard deviation of measurements in the test set, TC is the number of samples that are correctly classified. The Unscrambler X 10.4 software was applied for spectra pretreatments and PCA. Calibration and validation of classifiers and predictive model were done by IBM SPSS Modeler v18.0 software.

Results

Statistics of the samples

After eliminating the outliers, the statistical characteristics of the fig fruit samples was presented in the Table 1. As shown, with the completion of the ripening process of fig fruit, the mean anthocyanin content increased (0.11-0.86 mg $100g^{-1}$) as well as the sugar content and the mean of taste index (16.65-26.40). However, the mean firmness value decreased (8.97-3.83 Kg cm-2).

Table 1. Statistical characteristics of the samples for anthocyanin, flesh firmness, and taste index.

	Anthocyanin (mg 100 g^{-1})				Flesh firmness (Kg cm^{-2})				SSC/TA			
	Min	Max	Mean	SD	Min	Max	Mean	SD	Min	Max	Mean	SD
Ripe (56)	0.12	2.00	0.86	0.46	2.17	6.87	3.83	1.05	5.83	72.67	26.40	14.78
Semi-ripe (54)	0.04	1.70	0.76	0.31	2.63	9.70	4.98	1.65	4.56	56.67	19.49	10.45
Unripe (57)	0.02	0.89	0.11	0.15	4.17	15.03	8.97	2.65	1.75	35.00	16.65	5.75

SSC: Soluble Solids Content, TA: Titratable Acidity.

Spectra

Figures 1a and 1b display the spectra and the mean reflectance spectra of ripe, semi-ripe, and unripe fig samples within the range of 425-950 nm. The initial and final wavelengths were excluded due to significant noise. Notably, unripe figs exhibited a higher percentage of mean light reflection across all wavelengths compared to the other groups (Fig. 1b)

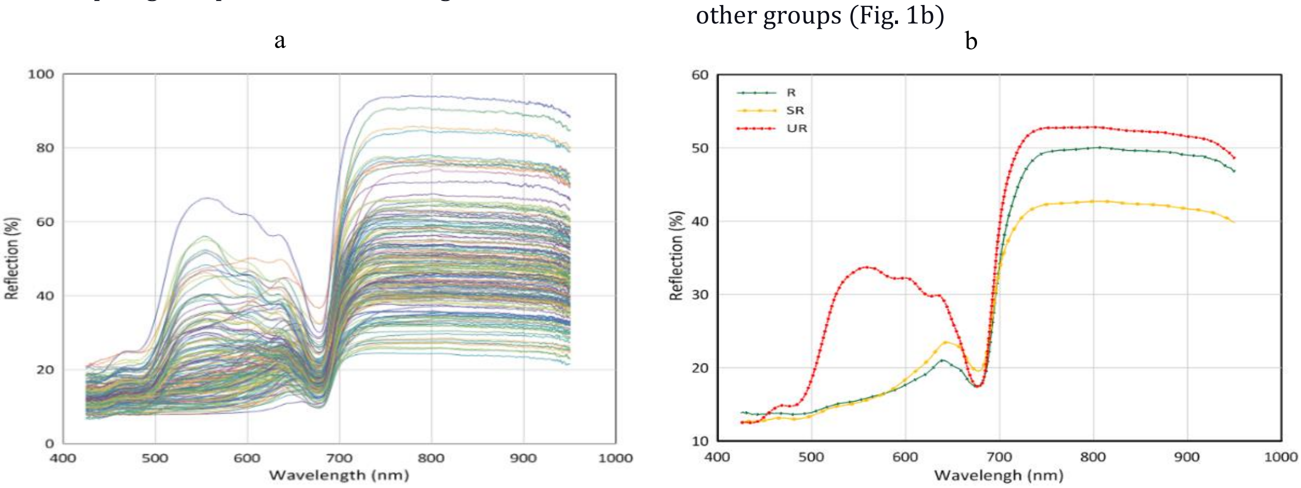
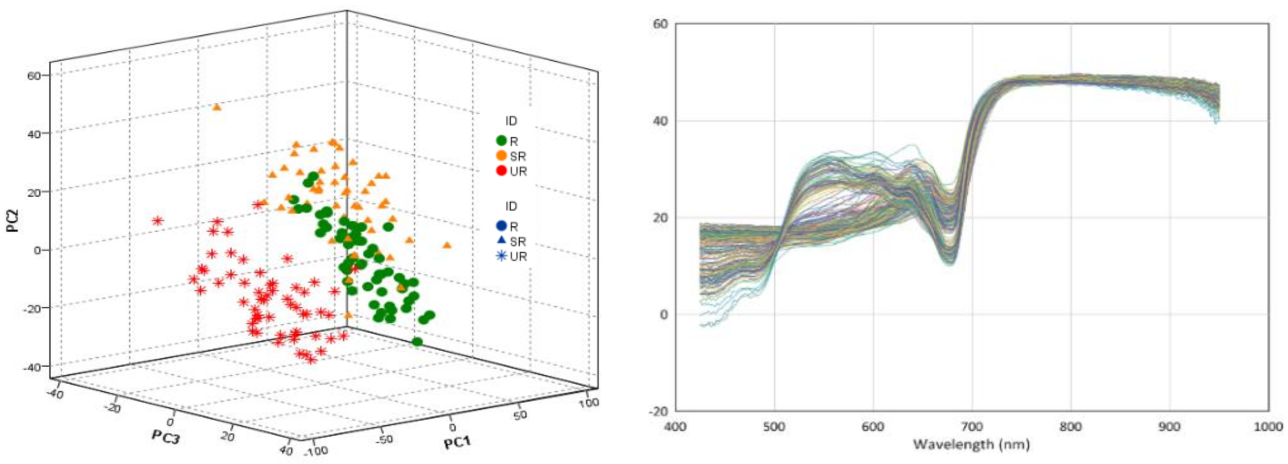


Fig. 1. (a) All spectra, and (b) mean spectra of R, SR, and UR figs in the 425-950 nm band. R: Ripe, SR: Semi-ripe, UR: Unripe.

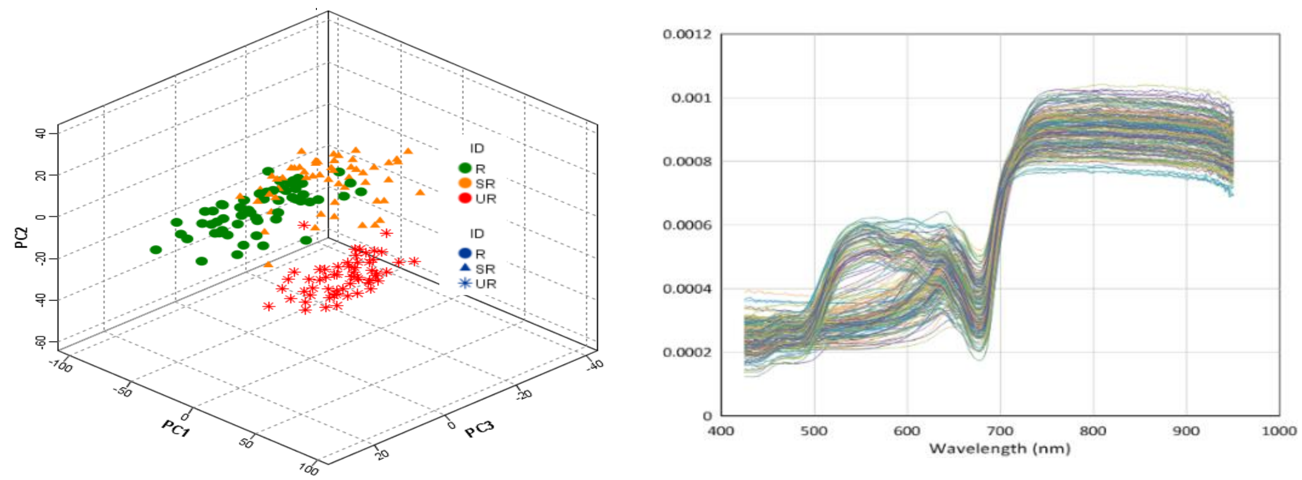
Pretreatment

Scatter plots for various pretreatments and the shapes of the pretreated spectra are shown in Figures 2a-d. The reflectance patterns varied within the 450-670 nm range, while they remained quite similar outside this band. Most pretreatments resulted in relatively effective separation in the PC1-PC3 coordinates. This can be attributed to the ability of mean scattering correction (MSC), standard normal variate (SNV), and normalization methods to mitigate light scattering effects.

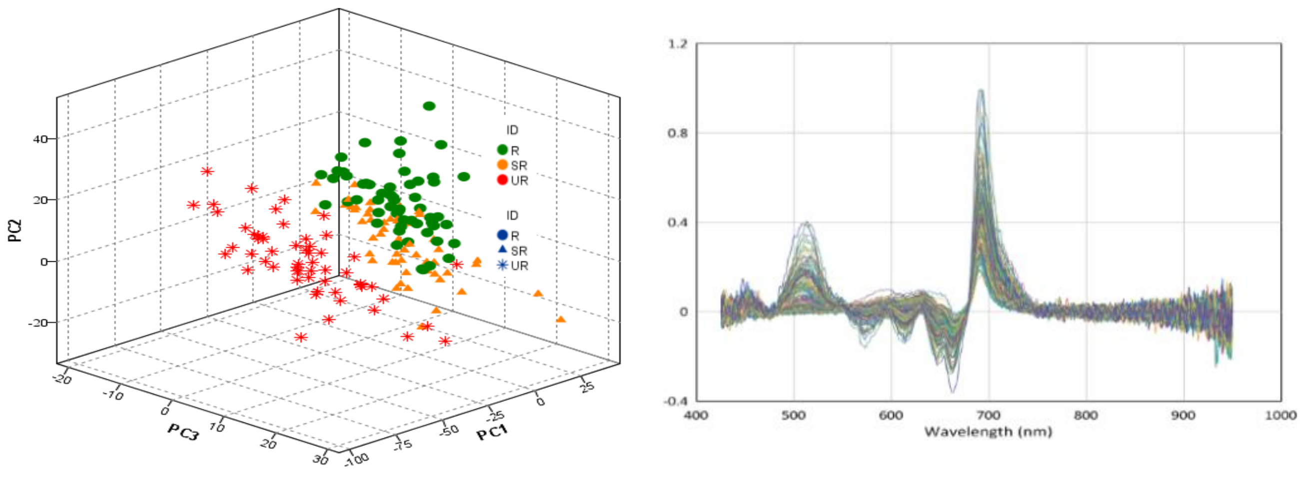
a


PC2
PC3
PC1
ID
R
SR
UR
ID
R
SR
UR
Wavelength (nm)

b


PC2
PC1
PC3
ID
R
SR
UR
ID
R
SR
UR
Wavelength (nm)

c


PC2
PC3
PC1
ID
R
SR
UR
ID
R
SR
UR
Wavelength (nm)

d

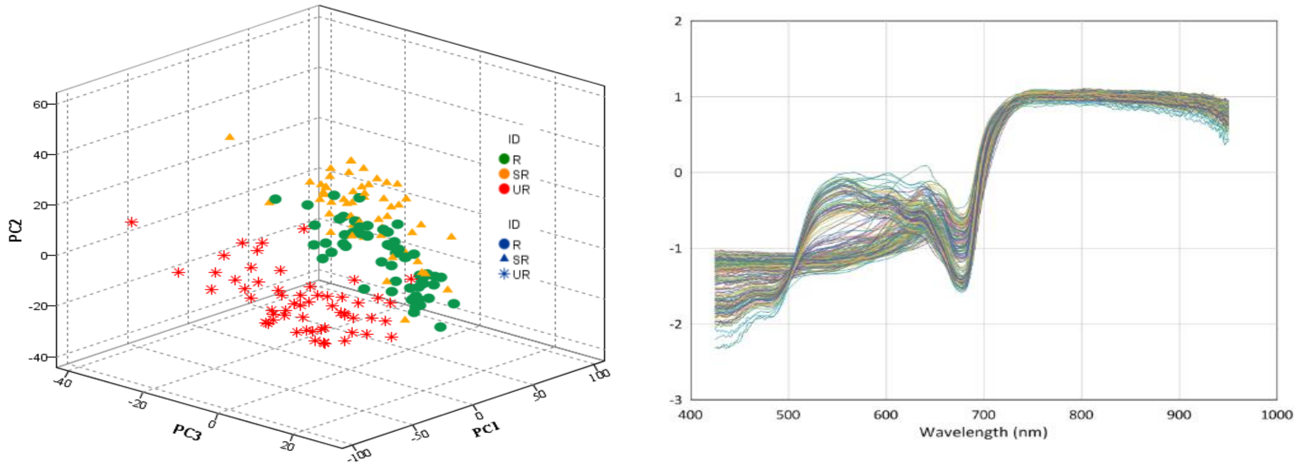


Fig. 2. Scatter plots of R, SR, and UR figs spectra along with the shape of the spectra for the pretreatments of (a) MA + MSC, (b) MA + Normalize, (c) MA + D1 + SG, (d) MA + SNV. R: Ripe, SR: Semi-ripe, UR: Unripe. MA: Moving Average, MSC: Multiplicative Scatter Correction, D1: First Derivative, SG: Savitzky-Golay, SNV: Standard Normal Variate.

Predictive ANN and classifiers

The results of ANN and the developed classifiers validation are summarized in Table 2 and 3.

The maximum mean value of RPD for anthocyanin prediction in MA + D1 + SG pretreatments was 1.38 (r_p = 0.69 and RMSEP = 0.31), which indicated the weakness of the developed ANN in the prediction of anthocyanin. The maximum mean value of RPD in the prediction of flesh firmness was 1.55 in MA + D1 + SG pretreatment (r_p = 0.76 and RMSEP = 1.83). The maximum mean value of RPD in the prediction of SSC/TA was also 1.07 in MA + D1+ SG pretreatment (r_p = 0.37 and RMSEP = 11.53) (Table 2). The results of the validation set classification by ANN, KNN, and DA classifiers were 89.86, 87.02, and 89.52, which resulted from MA + SNV, MA + MSC, and MA + MSC pretreatments, respectively. Thus, ANN and DA provided higher overall accuracy for validating the samples (Table 3).

Table 2. Mean evaluation indices of ANN developed to predict of anthocyanin, flesh firmness, and taste index based on the different pretreatments.

Pretreatments		Anthocyanin (mg 100 g^{-1})			Flesh firmness (Kg cm^{-2})			SSC/TA		
		RMSEP	r_p	RPD	RMSEP	r_p	RPD	RMSEP	r_p	RPD
No preprocessing		0.32	0.68	1.32	1.84	0.75	1.54	12.15	0.26	1.01
Smoothing (MA)	**SNV**	0.32	0.66	1.32	1.99	0.72	1.42	12.21	0.23	1.01
	MSC	0.31	0.70	1.37	1.94	0.73	1.45	12.26	0.26	1.01
	Normalize	0.33	0.66	1.29	1.93	0.73	1.47	11.97	0.26	1.03
	D1 + SG	0.31	0.69	**1.38**	1.83	0.76	**1.55**	11.53	0.37	**1.07**

Bold values indicate the best results for each attribute or index. ANN: Artificial Neural Networks, SSC: Soluble Solids Content, TA: Titratable Acidity, RMSEP: Root Mean Square Error of Prediction, r_p: Prediction correlation coefficient, RPD: Residual Prediction Deviation, MA: Moving Average, MSC: Multiplicative Scatter Correction, D1: First Derivative, SG: Savitzky-Golay, SNV: Standard Normal Variate.

Discussion

According to our results, riper fig fruit exhibited higher mean anthocyanin content, sugar content, and taste index; however, its firmness decreased due to changes in cell wall composition and water content. This reduction in firmness can be attributed to the degradation of pectin and hemicellulose by specific enzymes in ripe fruits, leading to changes in the cell wall, softening, increased fruit transparency, deeper light penetration, and a consequently reduced percentage of light reflection (Cavaco et al., 2009; Pourdarbani et al., 2020).

Various studies have examined the scattering status of samples in principal component coordinates (Teye et al., 2019; Theanjumpol et al., 2019). The maximum RPD value for predicting flesh firmness was observed with the combination of MA, D1, and SG pretreatments. In developing a predictive model, an RPD value of less than 1.5 indicates that the model is not applicable; values between 1.5 and 2 suggest the model can estimate high and low values of the desired parameter; values between 2 and 2.5 indicate the model can quantify the parameter; and values above 2.5 or 3 signify good to excellent predictive accuracy (Beghi et al., 2017).

At lower RPD values (less than 2), slight differences were noted in model performance. For example, an RPD value of 1.4 to 1.8 was considered relatively appropriate, while an RPD of 1.8 to 2 indicated the model's ability to quantify parameters (Mouazen et al., 2010; Rossel et al., 2006). Based on these RPD values, the model can only predict low or high flesh firmness.

Table 3. Mean overall classification accuracy of R, SR, and UR samples by developed classifiers in the calibration and test sets based on a combination of different pretreatments.

Pretreatments		KNN (%)		ANN (%)		DA (%)	
		Training	Testing	Training	Testing	Training	Testing
No preprocessing		89.14	83.54	87.65	86.41	86.08	86.65
Smoothing (MA)	**SNV**	88.26	83.14	88.70	**89.86**	87.06	88.95
	MSC	89.09	**87.02**	89.66	89.78	88.26	**89.52**
	Normalize	87.96	86.09	86.22	85.63	83.63	84.68
	D1 + SG	86.92	84.86	88.58	90.12	87.28	88.54

Bold values indicate the best overall accuracy. R: Ripe, SR: Semi-ripe, UR: Unripe, ANN: Artificial Neural Networks, KNN: k-Nearest Neighbors, DA: Discriminant Analysis, MA: Moving Average, MSC: Multiplicative Scatter Correction, D1: First Derivative, SG: Savitzky-Golay, SNV: Standard Normal Variate.

The spectral signatures related to sugars, primarily associated with C-H fundamental vibrations and their overtones, are mainly found at wavelengths beyond the 425-950 nm range (Golic et al., 2003). This may explain the model's failure to predict the taste index, which heavily depends on sugar content.

In line with this study, Sun et al. (2021) developed RF and PLS models for predicting fig fruit hardness in the 950-1700 nm range and specific sub-bands. Their calibrated RF and PLS models yielded R2 values of 0.7355 and 0.7660, respectively. However, RF performed better than PLS overall in sub-band assessments. They concluded that RF can quickly and effectively predict fig hardness. Physiological changes after harvest affect the internal quality of figs during measurements.

The softening of the fruit causes the acquired spectra deviate from the original information, and as a result, this will effect on the performance of the models. These limitations must be overcome in the future. The pretreatments of MSC (KNN and DA) and SNV (ANN) after MA provided the most excellent effect on increasing the accuracy of classifiers.

Conclusions

The spectra of figs in the 425-950 nm range displayed few peaks, attributed to the absorption of light by overtones and the combination of fundamental bond vibrations of the fig's organic constituents. The reflection spectra showed similar patterns across many wavelengths, prompting an investigation into the effectiveness of pretreatments, including MSC, normalization, SNV, and the first derivative after smoothing with a moving average. The first four principal components obtained from PCA were used as inputs for the predictive ANN model, as well as for the ANN, KNN, and DA classifiers. The mean evaluation indices for the validation sets indicated that the regression ANN could not accurately predict anthocyanin content or the taste index. However, it was effective in predicting high and low values of fruit firmness. When the performance of predictive models is lacking, conducting qualitative analyses using classifiers is a beneficial approach, as classification models generally exhibit higher accuracy than predictive models. ANN and DA demonstrated the highest overall accuracy for validating samples, with rates of 89.86% and 89.52%, respectively, highlighting their potential for practical applications. Further research is warranted to explore the performance of other predictive and classification models across different fig cultivars.

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Conflict of Interest
The authors indicate no conflict of interest in this work.

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