Nondestructive estimation of three apple fruit properties at various ripening levels with optimal Vis-NIR spectral wavelength regression data

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Highlights

- Automatic and accurate regression infrared spectral imaging system for nondestructive estimation of physicochemical properties in Fuji apple fruit
- Tissue firmness (kgf/cm), acidity (pH) and starch content (%) fruit properties estimated
- Hardware used includes: spectrophotometer, photo-detector, light source, and optical fiber
- System comprises both variable wavelength Vis-NIR ranges and fixed optimal NIR wavelength windows
- Numerical simulation results include: linear regression plots, regression (R) and determination (R^2) coefficient boxplots, and true versus mean estimated property value graphs
- Given accuracy in apple fruit property estimation, system could be adapted to real food industry environment conditions

Abstract

Nondestructive estimation of fruit properties during their ripening stages ensures the best value for producers and vendors. Among common quality measurement methods, spectroscopy is popular and enables physicochemical properties to be nondestructively estimated. The current study aims to nondestructively predict tissue firmness (kgf/cm), acidity (pH level) and starch content index (%) in apples (*Malus M. pumila*) samples (Fuji var.) at various ripening stages using visible/near infrared (Vis-NIR) spectral data in 400–1000 nm wavelength range. Results show that non-linear regression done by an artificial neural network-cultural algorithm (ANN-CA) was able to properly estimate the investigated fruit properties. Moreover, the performance of the proposed method was evaluated for Vis-NIR data based on optimal NIR wavelength values selected by a genetic optimization tool. Regression coefficients (R) in estimated acidity, tissue firmness, and starch content properties were $\mathrm{R} = 0.930 \pm 0.014$, $\mathrm{R} = 0.851 \pm 0.014$, and $\mathrm{R} = 0.974 \pm 0.006$, respectively, using only the three most effective wavelengths from the acquired spectra.

keywords: acidity, apple, artificial neural network, firmness, fruit, physicochemical properties, starch

1. Introduction

Application of smart agricultural techniques to evaluate fruit ripening stages may help in management of their quality. Because physicochemical issues in fruits directly impact their final quality, nondestructive and early prediction of these properties is of high commercial significance. Features such as titratable acidity (TA), soluble solid content (SSC), SSC/TA ratio, pH, starch content, tissue firmness and internal features such as shape, size, color, and appearance, are commonly used by the fruit industry to determine quality of apples (Mesa et al, 2016). Unfortunately, most of these parameters result in sample destruction and are time consuming to assess.

Among the widely used nondestructive methods for measuring fruit quality, Vis-NIR spectroscopy techniques are often the preferred ones (Pourdarbani et al, 2019). NIR spectroscopy applied to measure food quality has been presented by several researchers (Carames et al, 2017; Guo et al, 2016; Sirisomboon et al, 2018; Eisenstecken et al, 2016). Moreover, several investigations have been conducted to predict fruit quality. Soluble solid content, pH, total acidity, and ascorbic acid of apple fruits have been also estimated successfully using NIR technology (Pourdarbani et al, 2020; Nturambirwe et al 2019). Shah et al (2021) developed a Kensington Pride (KP) model for mango (Indigenous variety) ripening prediction using NIR spectra. They obtained promising results using partial least squares (PLS) regression. Nturambirwe et al (2019) considered three varieties of apples (Golden Delicious, Gala and Smith) from the viewpoint of predicting the SSC and TA using a genetic algorithm. In their study, mean error improved by 30% with the use of genetic algorithms. Bian et al (2021) studied the classification of apple juice based on variety and geographical origin. They applied PLS regression and fluorescent spectroscopy to analyze fluorescent spectra with two apple fruit varieties. Results proved that fluorescent spectroscopy combined with PLS method was successful in quality control of fruit juice. Subedi and Walsh (2020) introduced dry matter content (DMC) to evaluate the quality of avocado fruit using NIR spectroscopy. A PLS regression model was built for joint analysis of fruit in four locations and three growing seasons in a crop field. Zhang et al (2020) determined the maturity of Fuji apples. A total of 846 apples were classified into three maturation stages based on starch content. The results from different modeling methods were compared: the performance of the best proposed model had an accuracy of 89.05%. On the other hand, the accuracy of LDA models was the least with value ranges in 77.63%–80.95%. Uwadaira et al (2018) developed a spectroscopy (Vis-NIR) system for nondestructive analysis of peaches. Spectral data of samples were acquired by Vis-NIR spectroscopy and a determination coefficient of 0.8 was achieved for predicting the SSC. Tilahun et al (2018) predicted beta-carotene and lycopene in tomato cultivars by NIR and chromatography spectra. More than two hundred tomato fruit samples were used at three ripening levels. Spectral information was extracted and beta-carotene and lycopene were measured destructively in lab. Regression coefficients of carotene were found to be in the range of 0.52-0.98.

Based on the potential of NIR spectroscopy in predicting fruit quality, the aim of this study is set to accurately and nondestructively predict three physicochemical properties (starch, firmness and acidity) in Fuji apples in the 400-1000 nm range. The multi-dimensionality of the obtained spectra is to be reduced using artificial neural network-genetic (ANN-GA) algorithm so that a few selected wavelengths could potentially be used to further develop a simple and portable device for this apply quality prediction. The performance of prediction of a regression model based on a reduced (three) wavelengths with ANN-CA is investigated.

2. Materials and Methods

Figure 1 depicts the nondestructive proposed prediction system, comprising five steps needed to generate the input data, and to train and evaluate the system, which will be discussed in detail next.

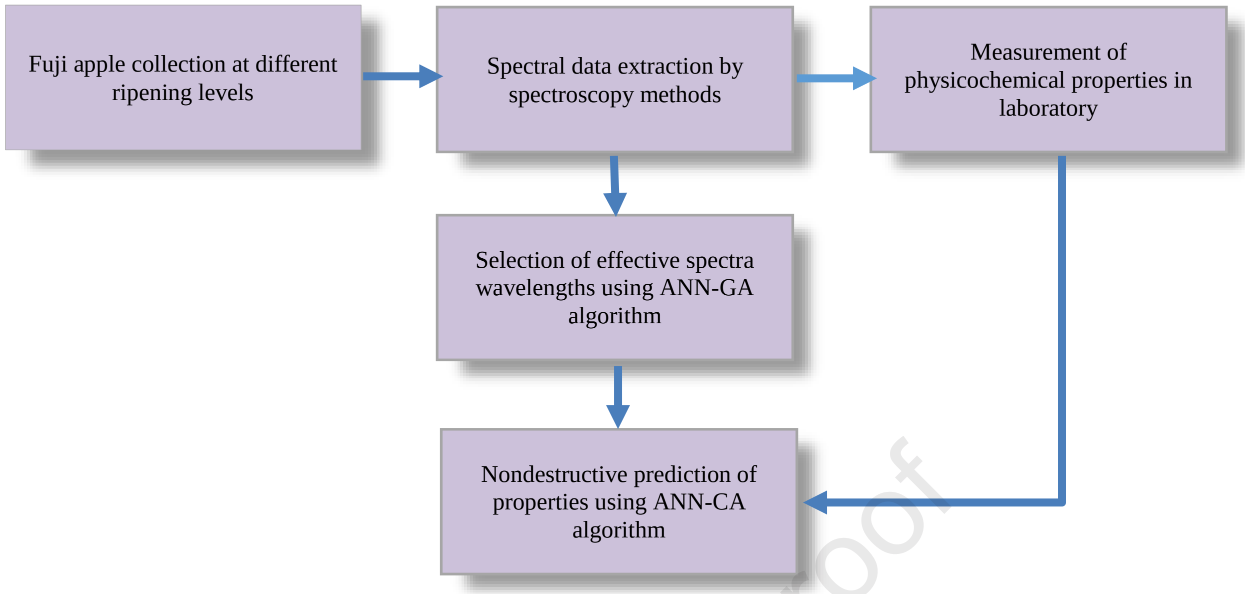


Figure 1. System flowchart for the nondestructive prediction of three physicochemical properties in apple (*Malus M. pumila*) fruits under various ripening stages with optimal Vis-NIR wavelengths: firmness (kgf/cm), acidity (pH) and starch content (%).

2.1. Sample collection

The collection of various samples was the first step for establishing the proposed prediction system: the approximate harvest time of Fuji apples was determined by human experts. A total of 160 samples were selected and classified in four growth stages by the human expert panel: 20 days before the optimal harvest date, 10 days before optimal, exact optimal harvesting time and 10 days after optimal harvesting date. Each ripening stage consisted of 40 samples. Immediately after collecting the fruit samples, they were scanned, and spectral data collected.

2.2. Extraction of spectral data

2.2.1. Vis-NIR Instrumentation

A Vis-NIR spectrophotometer (EPP200NIR, StellarNet, Tampa, FL) equipped with an indium-gallium-arsenide (InGaAs) photo-detector was used to acquire the spectral information in reflectance mode (Fig. 2). Illumination was done using a 20W. tungsten lamp (StellarNet, FL). To further process the acquired data, it was transferred to a laptop PC (Corei5, 500M at 2.13GHz, 4GB of RAM, Windows 10, MatLab).

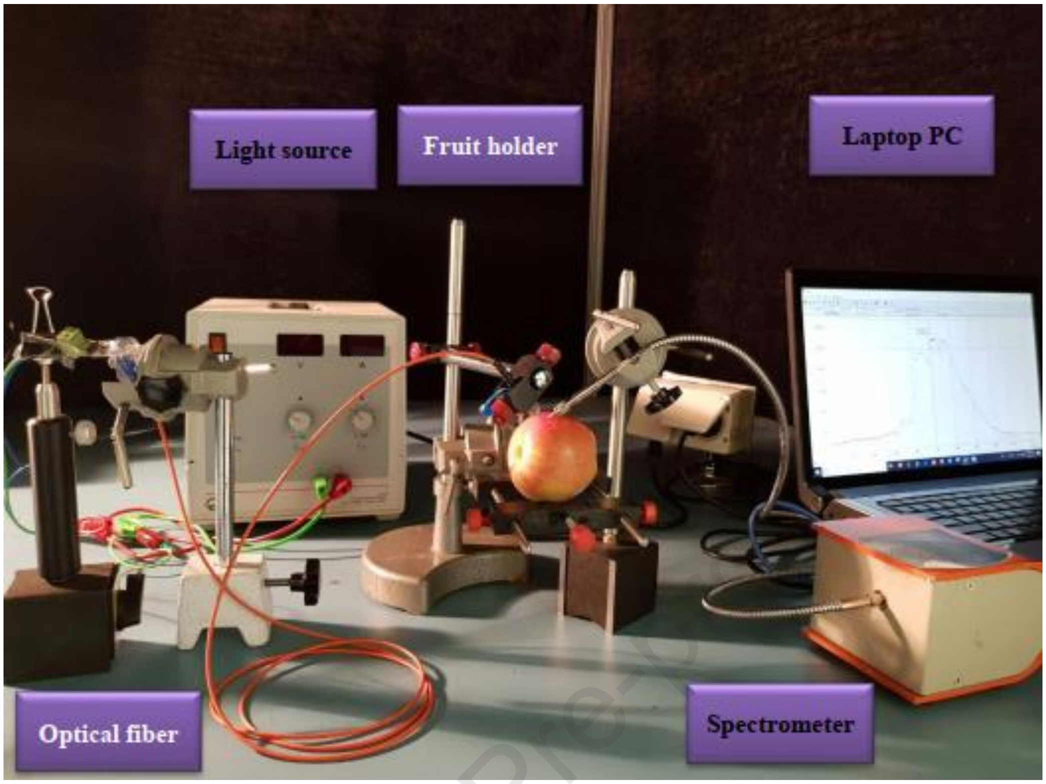
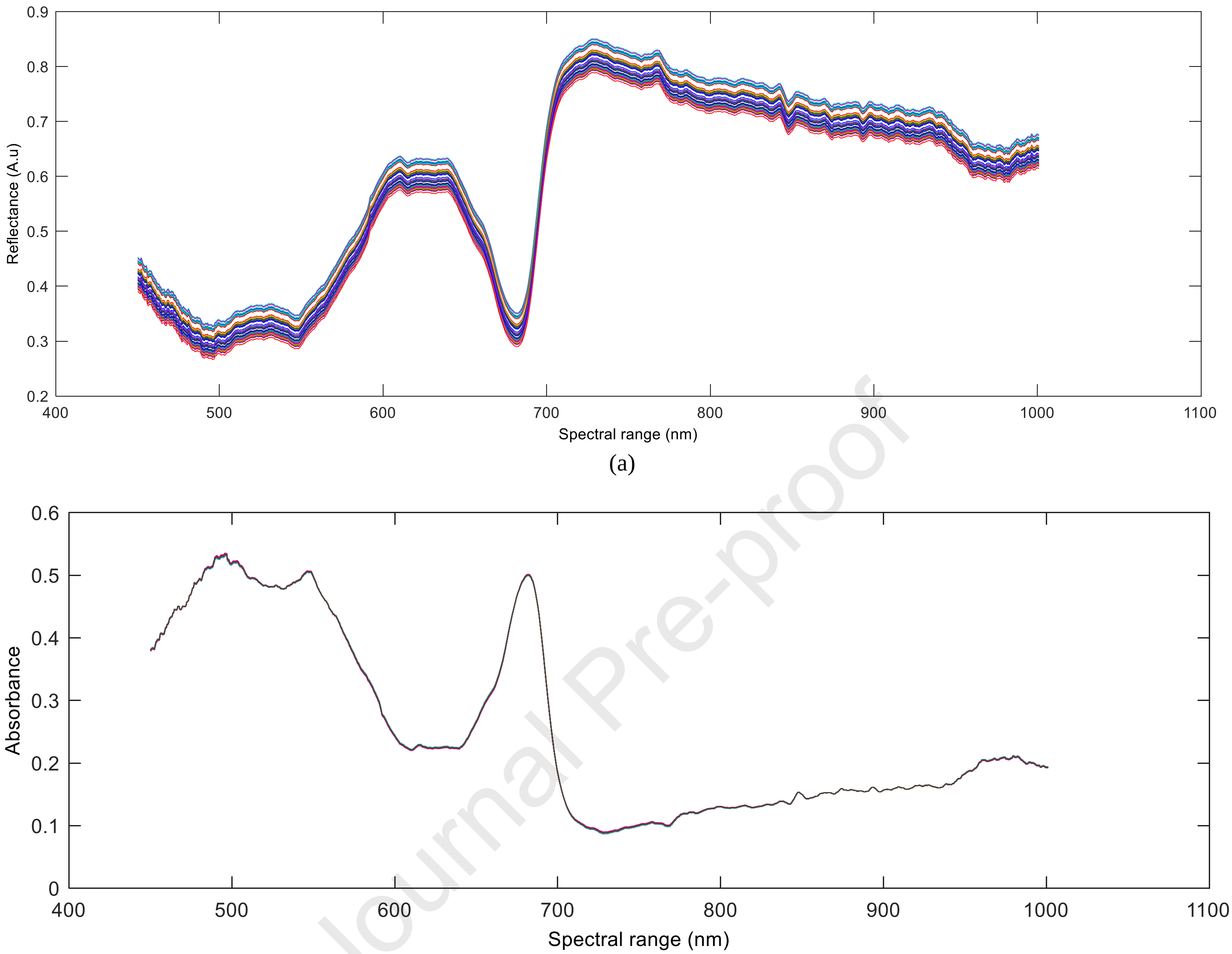


Figure 2. Vis-NIR spectroscopy system setup, depicting: apple sample, holder, laptop PC, light source, spectrometer, and optical fiber.

2.2.2. Spectral data pre-processing

Multiplicative scatter correction (MSC) functions were used to preprocess the spectral data obtained from the spectroscopy system (Rossel, 2008). This operation is needed to correct variations in spectra arising from sample size, surface sample roughness and type of spectrometer, among others. Equation (1) was used to convert reflectance to absorbance spectra (see Fig. 3) for each input sample:

$$\text{absorbance spectra} = log\left({}^{1}/_{\text{reflectance spectra}}\right) \tag{1}$$



(a)

(b)

Figure 3. Spectral graphs of different apple input samples. (a) reflectance spectra of different samples; (b) pre-processed spectral absorbance spectra, as done in three steps: 1) conversion of reflectance to absorbance spectra with equation (1), 2) light scatter and baseline correction by MSC, and 3) smoothing of spectral peaks by median filtering.

2.3 Measurement of actual (true) physicochemical properties from apple samples using laboratory (destructive) methods: firmness (kgf/cm), acidity (pH) and starch content (%)

Table 1 provides the statistical summary of actual (measured) value of firmness, acidity and starch content of Fuji apple samples. According to the Table 1, the *relative* standard deviation, also known as the Coefficient of Variation (CV = std. dev./mean) of starch content is higher than those in acidity and firmness properties.

Table 1: Statistical evaluation of actual value of three physicochemical properties in Fuji apple fruit samples: maximum (max.), minimum (min.), mean, standard deviation (std. dev.) and CV (std. dev./mean) values shown, for firmness (kgf/cm), acidity (pH), and starch (%).

	max.	min.	mean	std. dev.	CV = std. dev./mean
firmness (kgf/cm)	15.8	11	13.11	1.18	0.090
acidity (pH)	4.36	3.8	4.10	0.16	0.039
starch content (%)	85	2	52.63	24.71	0.470

2.3.1 Firmness

The method used by De Belie et al (2000) was applied to measure fruit firmness, on hand. In brief, the different steps taken are as follows: a handheld penetrometer with a special probe (diameter of 11 mm and a height of 8 mm) was used and the probes were placed on both sides of the apple. The probes were pushed into the samples to record the amount of force applied, measured in kgf/cm units. The average force applied on both sides of the apple was considered as firmness measure.

2.3.2 Starch content (%)

The method used by Martínez-Valdivieso et al (2014) was used to measure starch content: the middle part of the apple was pealed and a slice weighing 0.5 g was isolated. The slice was crushed in the mortar and apple juice extracted. A phosphate solution was prepared and the resulting sediment was mixed with 1.5 ml of the buffer solution. Centrifugation was performed at 12,000 rpm for twenty minutes to completely separate the mixed sediment. The resulting emulsion was mixed with iodine-hydrochloric acid (1:5) and samples absorbance was measured (in mg/g) with a spectrophotometer (Optizen 2120 UVplus, Mecasys, Korea) working at a wavelength of 600 nm. Standard starch emulsion was prepared using specified starch concentrations (0 to 100 mg/l). With the help of the absorbance numbers of standard starch solutions, a scatter graph was plotted using Excel and a linear curve fitting, as well as the equation of conversion of the absorption number to starch value in g/ml was obtained. The curve was used to determine starch values.

2.3.3 Acidity (pH)

A general purpose pH-meter was employed to measure acidity of fruit samples.

2.4 Selection of effective (relevant) spectral data wavelengths in Vis-NIR spectrum: ANN-GA optimization algorithm

As mentioned above, development of portable nondestructive devices requires as little as possible number of wavelengths, therefore from the entire spectral data a subset of the most effective wavelengths must be selected. In this paper, ANN-GA algorithm was applied to select optimal wavelength values in the Vis-NIR range. A genetic algorithm is a special type of evolutionary optimization algorithm that uses biology parameters such as inheritance, biological mutation probability, and Darwin's theory of natural selection to seek the optimal formulae for predicting a certain property in regression problems. Then potential optimal solutions are evaluated as candidates by a fitness function, and if a pre-defined exit condition is met, the algorithm ends. In general terms, the whole spectra is organized in a vector formulation first. Different size vectors are selected as input to the NN by the GA algorithm. In our problem, the output of the neural network (NN) are the fruit properties under consideration. Data is split intro tree disjoint data sets: 70% training, 15% validation, and 15% test set. The ANN (multilayer perceptron (MLP) type) hidden layers' structure is given in Table 2. Mean squared error (MSE) is computed and saved, and lower MSE value vector is chosen as the winner, with the wavelength values within that vector selected as the optimal Vis-NIR wavelengths.

Table 2: Structure of a NN-MLP architecture applied in selecting the most relevant Vis-NIR wavelengths: MatLab software.

Layers	2
Neurons	11, 21
Transfer Function	tribas, tribas
Backpropagation Weight/Bias Function	learnos
Backpropagation Network Training Function	trainnr

2.5 Prediction of three physicochemical properties in apples by ANN-CA regression algorithm

Cultural Algorithms (CA) are the socio-cultural counterparts of genetic algorithms (GA), and instead of biological evolution, socio-cultural evolution is considered the lifeblood in optimization. CA algorithms are focused on knowledge-based data structure.

2.6 Performance evaluation of neural networks to estimate fruit properties

We used well-known performance indices: mean square error (MSE), root-mean-square error (RMSE) and mean absolute error (MAE). We also computed common regression (R) and determination (R^2) coefficients (Pourdarbani et al, 2020; Sabzi et al, 2020).

3 Results and Discussion

Three most effective (optimal) wavelengths in the acquired spectral range (i.e. 400 to 1000 nm) were identified using ANN-GA for each fruit property, as listed next: for firmness**,** wavelengths of 869, 798 and 902 nm were selected as optimal wavelengths; acidity (pH) could be best estimated using the wavelengths of 842, 867 and 881nm; for starch content, 799, 864 and 900 nm were selected as optima wavelengths.

3.2 Prediction of fruit properties using reflectance spectra at 400 to 1000 nm: regressions

3.2.1 Firmness (kgf/cm)

Figure 4 illustrates the scatter plot of regression analysis between estimated (mean) and true firmness values in apple samples from the whole spectrum data inside 400 to 1000 nm over the entire test set. Given that each iteration includes forty-eight test samples, there were a total of 5472 samples in 114 repeated uniform random trials (iterations) to choose different combinations of training, validation and test sets. Since we had a total of 158 samples, there were around 34 estimated firmness values on average, per test set sample. A regression coefficient of 0.829 was reached. Observing Figure 4 scatter plot, one can see a relatively low regression coefficient, at least lower than that observed for other apple fruit properties, which could be due to the fact that firmness was harder to estimate using spectral information alone.

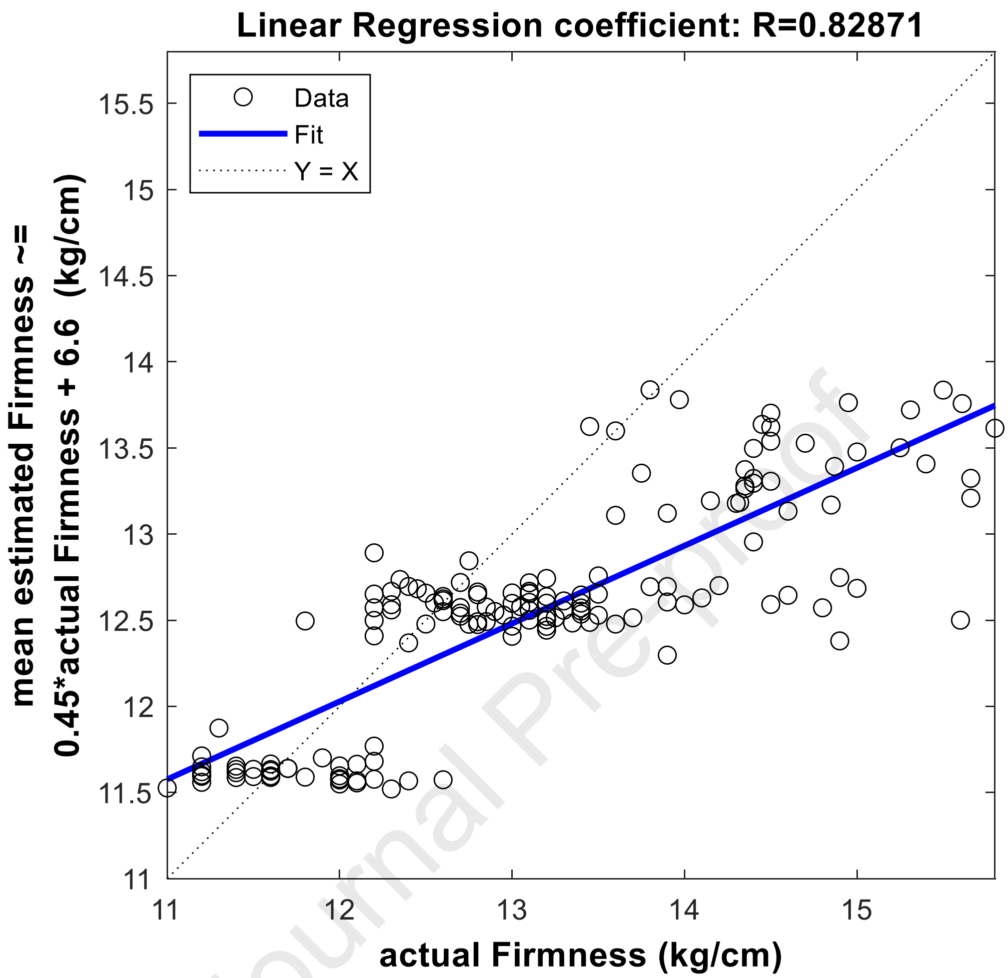
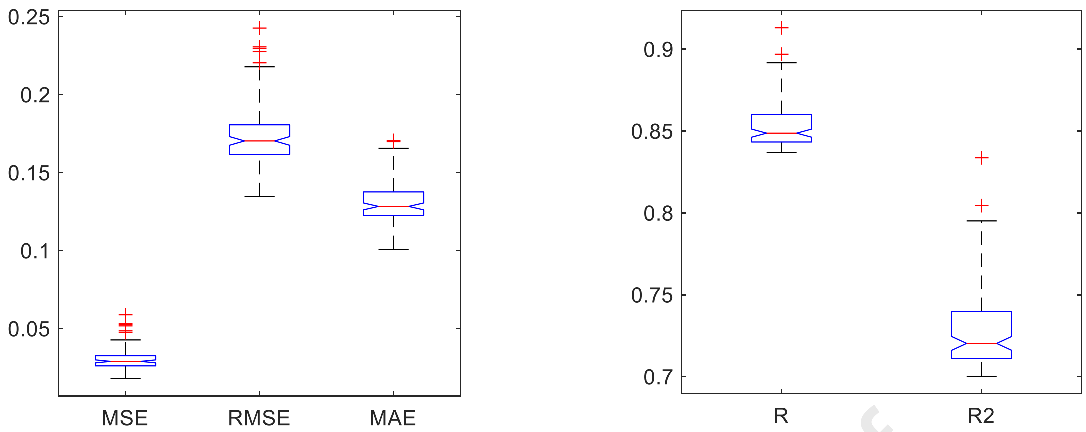


Figure 4. Regression analysis (ANN-CA) between mean estimated and true firmness (kgf/cm) values in apple fruit from whole spectral data at 400 to 1000 nm: test set.

Figure 5 shows boxplots of different evaluation criteria of ANN-CA method to estimate firmness using the whole spectral data at 400 to 1000 nm after 114 uniform random test samples iterations. In general words, compact diagrams imply the closeness of the results in various repetitions indicating high reliability (robustness) of the prediction. It is also observed that the graph of the mean squared error is also compact.



(a) (b)

Figure 5. Boxplot diagram of different performance evaluation criteria: a) Error indices, b) Regression (R) and determination (R^2) coefficients ANN-CA method in estimating firmness (kgf/cm) on the 400 to 1000 nm spectral data (test set)

Figure 6 illustrates graphs showing the performance of ANN-CA method in fruit tissue firmness estimation using the whole spectral data in 400 to 1000 nm, displaying true and estimated (mean) values after over 100 experiments. Whenever true and mean estimated value are close to each other, they overlap in the graph, which is a common case shown in Figure 6. However, there are several outliers. The presence of these outliers indicates that there are some input fruit samples for which the performance of the regression was poor, thus reducing total system robustness.

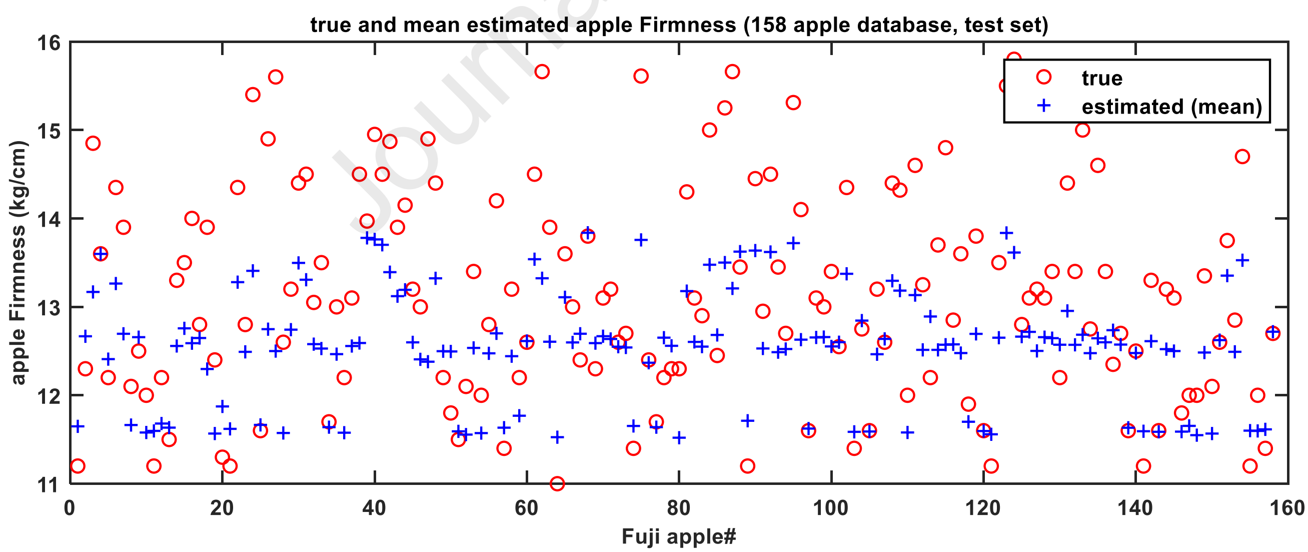


Figure 6. Boxplot of actual and mean estimated value of 158 Fuji Apples in predicting firmness (kgf/cm) by wavelength data of 400 to 1000 nm: test set.

3.2.2 Acidity (pH)

Figure 7 illustrates the regression analysis between mean estimated and true acidity (pH) values in apple fruit from the whole spectral data inside the 400 to 1000 nm range, with about 34 (on average) estimated property values for each test set sample, reaching a regression value of R=0.948. The linear regression coefficient for acidity is significantly higher than that shown in the estimation of firmness property before, as remains also clear after observing graph circular samples.

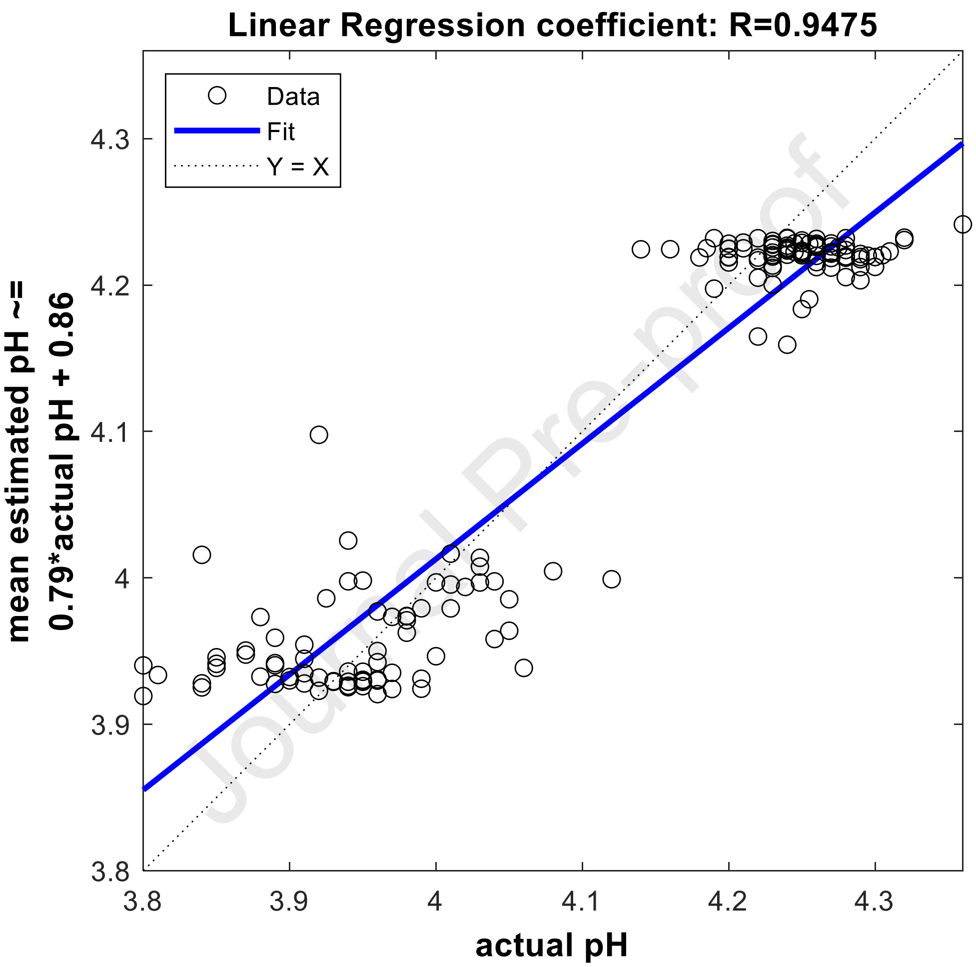
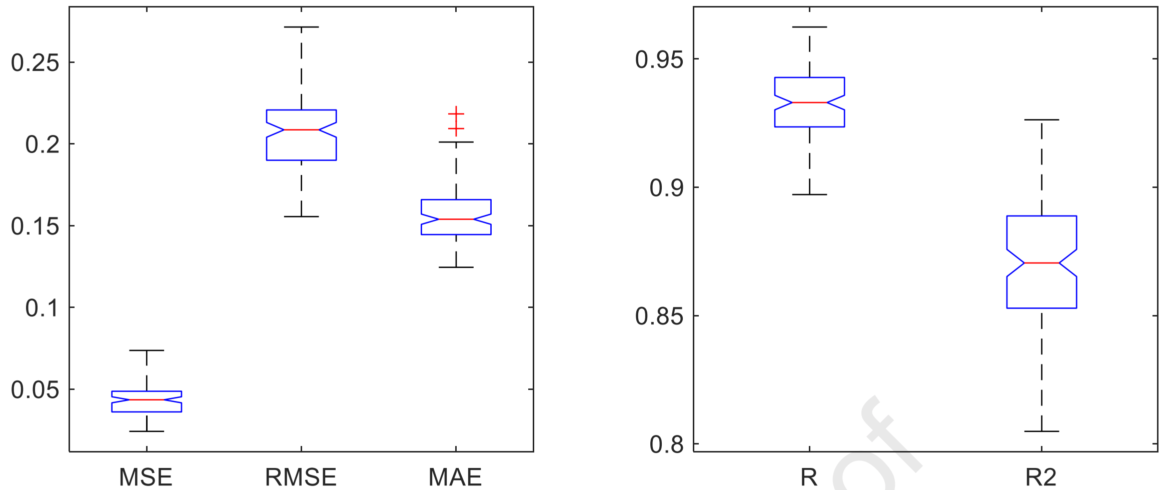


Figure 7. Linear regression plot between estimated (mean) and true acidity (pH) apple fruit values from spectral data of 400 to 1000 nm: test set.

Figure 8 shows the boxplot of error criteria, regression (R) and determination (R^2) coefficients of ANN-CA in estimating acidity in the whole range of 400 to 1000 nm after over 100 iterations. It can be observed that most regression coefficient values (median value) are above 0.9.



(a) (b)

Figure 8. Box diagram of different performance evaluation criteria: a) Error indices, b) Regression (R) and determination (R^2) coefficients) ANN-CA method in estimating acidity (pH) on 400 to 1000 nm (test set).

Figure 9 illustrates the performance of ANN-CA regression in estimating pH values of apple samples. It can be observed how estimated values in different iterations are close together and often true and mean estimated pH values are really close and overlapping. The number of observed outliers here is rather low.

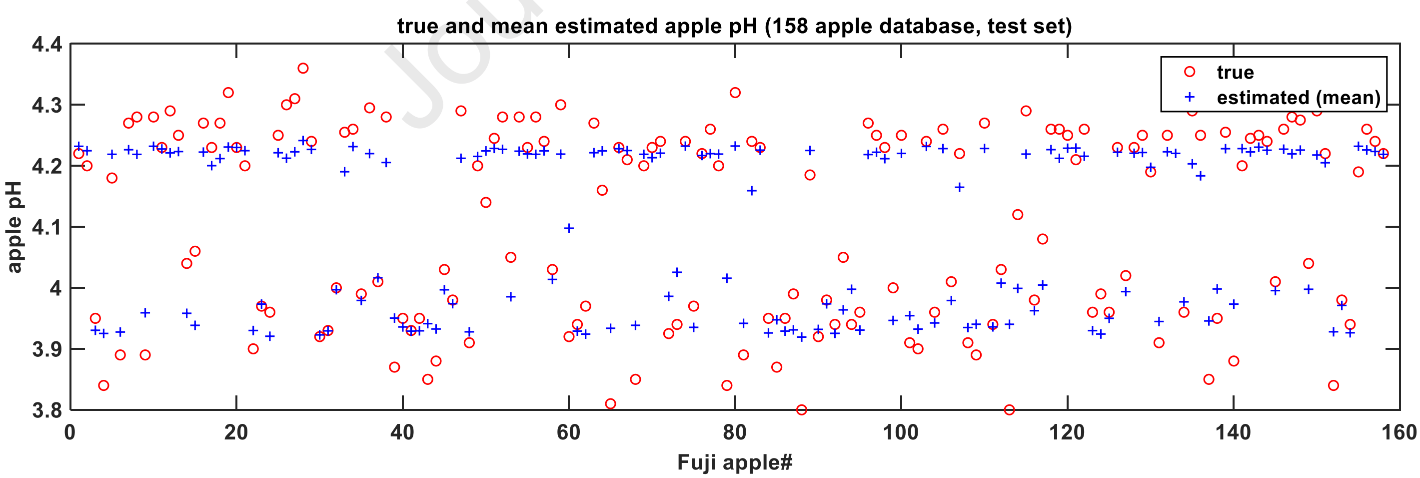


Figure 9. Boxplot of actual and mean estimated value of 158 Fuji apples in predicting acidity (pH) value at whole 400-1000 nm spectral range: test set.

3.2.3 Starch content index (%)

Figure 10 depicts the regression analysis of estimated and true starch content values (%) in apple samples within the entire 400 to 1000 nm spectral range. Again, to predict the starch content values more than 100 uniform random experiments (random sampling) were executed, reaching a rather high regression coefficient value of R=0.973. Starch content (%) linear regression coefficient was highest among the three fruit properties estimated, which is clearly indicated in Figure 10.

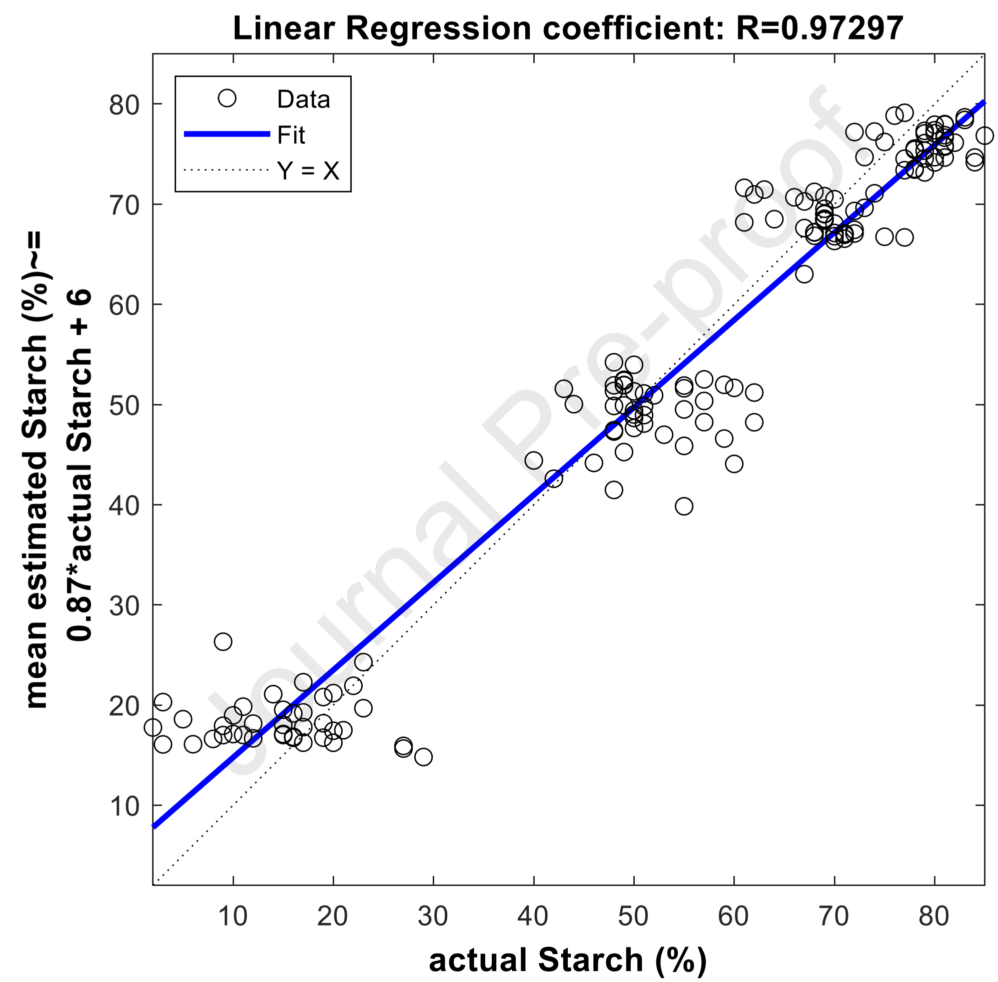
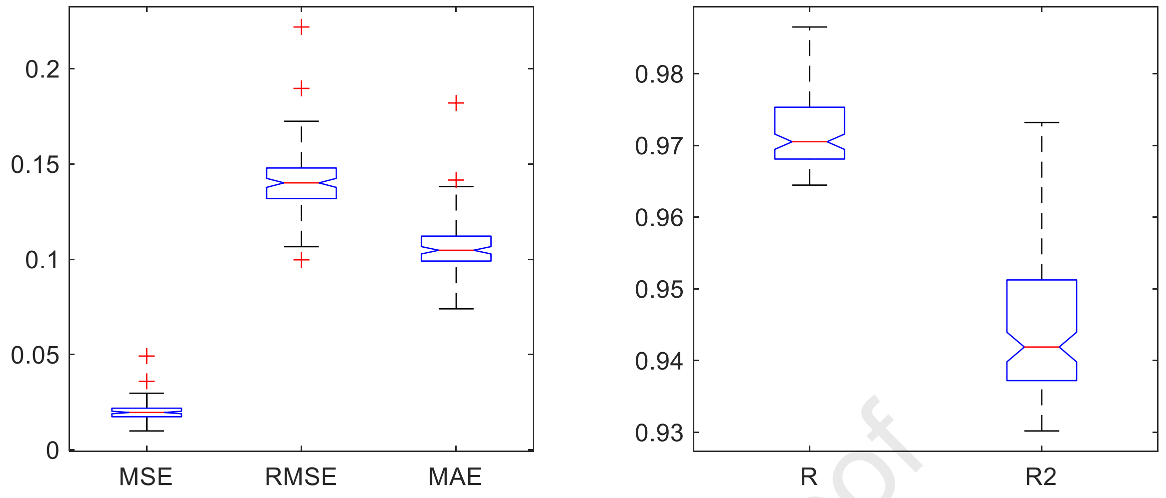


Figure 10. Linear regression analysis of mean and true apple fruit starch content index (%) at whole 400-1000 nm wavelength range: test set.

Figure 11 represents the performance evaluation criteria of ANN-CA method to predict starch content (%). These graphs show that R value for starch content (%) was greater than 0.97 (median value). Boxplots of error-based criteria are compact implying high and stable performance.



(a) (b)

Figure 11. Boxplot diagram of different performance evaluation criteria: a) Error indices, b) Regression (R) and determination (R^2) coefficients, ANN-CA method in estimation of starch content (%) at whole spectral range of 400 to 100 nm (test set)

Figure 12 shows the regression performance estimating starch content (%) of apple samples using true and mean estimated values. In most cases, there are either overlaps or closeness between true and mean estimated values indicating a remarkable performance of the proposed nondestructive regression method in predicting starch content (%) values. The number of observed outliers here is again rather low, implying a good estimation robustness.

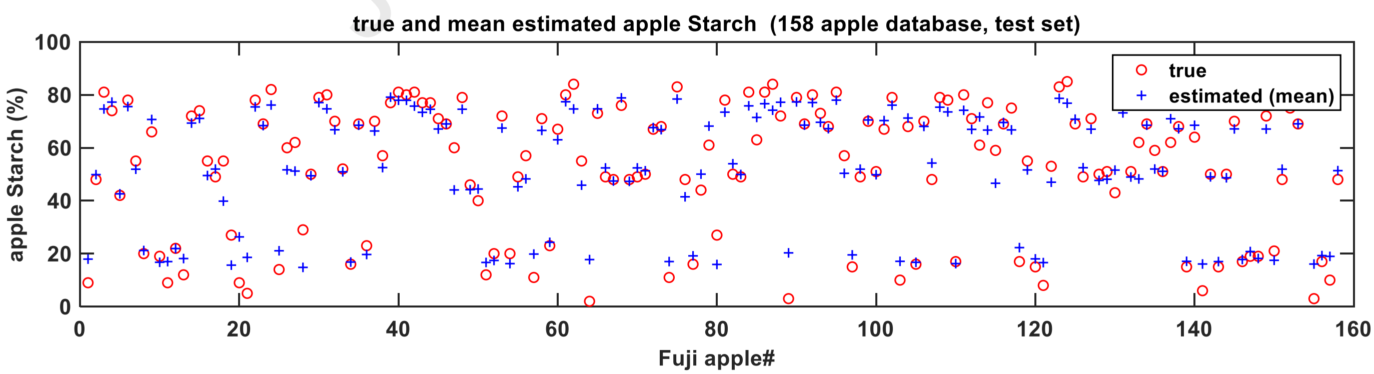


Figure 12. Boxplot of actual and mean estimated value of 158 Fuji Apples in starch content (%) prediction at whole spectral 400-1000 nm range: test set.

3.3 Comparison of regression performance using either entire spectral data or the three most effective (optimal) wavelengths: three error indices and regression (R) and determination (R^2) coefficients

3.3.1 Firmness (kgf/cm)

Table 3 provides mean ± standard deviation (std. dev.) values of regression method in predicting fruit firmness (kgf/cm) after 114 uniform random iterations, as well as the results using the entire spectra data and the three most effective (optimal) wavelengths. The standard deviation values in most criteria remain low implying a highly reliable (stable, reduced variance) estimation. Moreover, since the performance of the proposed method when comparing entire Vis-NIR spectra versus three effective wavelengths is almost identical, the use of spectral data based on optimized wavelengths is preferred in order to save cost and computation time.

Table 3: Mean ± standard deviation (std. dev.) performance of various criteria and regression (R) and determination (R^2) coefficients with ANN-CA method in estimating firmness (kgf/cm) using either whole spectral data at 400 to 1000 nm or using only optimized spectral wavelength data: 114 iterations, test set.

performance indices		MSE	RMSE	MAE	R	R^2
Whole spectral data at 400 to 1000 nm	mean ± std. dev.	0.033 ± 0.007	0.173 ± 0.019	0.130 ± 0.013	0.853 ± 0.014	0.728 ± 0.024
	best case	0.018	0.134	0.101	0.913	0.833
Three most effective wavelengths data	mean ± std. dev.	0.034 ± 0.005	0.174 ± 0.016	0.131 ± 0.010	0.851 ± 0.014	0.727 ± 0.026
	best case	0.022	0.142	0.112	0.911	0.827

3.3.2 Acidity (pH)

Table 4 compares performance criteria according to two types of data: whole Vis-NIR spectra and the three most effective wavelengths, when estimating acidity (pH) values after 114 random iterations. The regression coefficients (R) of both types are almost the same, implying that acidity (pH) value may be predicted using only data based on optimal wavelengths alone.

Table 4: Mean ± standard deviation (std. dev.) of performance of several criteria and regression (R) and determination (R^2) coefficients with ANN-CA method in estimating acidity (pH) using either whole Vis-NIR spectral data at 400 to 1000 nm or optimal wavelength data: 114 iterations, test set.

performance indices		MSE	RMSE	MAE	R	R^2
Whole spectral data at 400 to 1000 nm	mean ± std. dev.	0.043 ± 0.009	0.208 ± 0.023	0.155 ± 0.018	0.932 ± 0.013	0.869 ± 0.025
	best case	0.027	0.165	0.127	0.962	0.926
Three most effective wavelength data	mean ± std. dev.	0.045 ± 0.02	0.211 ± 0.024	0.158 ± 0.017	0.930 ± 0.014	0.862 ± 0.028
	best case	0.024	0.157	0.128	0.962	0.923

3.3.3 Starch content index (%)

Table 5 displays regression analysis of ANN-CA method using different criteria based on either whole Vis-NIR 400-1000 nm spectral range or only the three more relevant spectral data wavelengths. According to regression coefficient values shown in table, it can be concluded that starch content (%) can be properly predicted using only data from optimal wavelength values.

Table 5: Mean ± standard deviation (std. dev.) of several performance criteria and regression (R) and determination (R^2) coefficients with ANN-CA method in estimating starch content (%) using either whole Vis-NIR 400 to 1000 nm spectral data range or only three more relevant wavelength spectral data:114 iterations, test set.

performance indices		MSE	RMSE	MAE	R	R^2
Whole spectral data at 400 to 1000 nm	mean ± std. dev.	0.020 ± 0.004	0.140 ± 0.016	0.106 ± 0.013	0.972 ± 0.005	0.944 ± 0.009
	best case	0.018	0.137	0.106	0.971	0.943
Three most effective wavelength data	mean ± std. dev.	0.022 ± 0.006	0.145 ± 0.019	0.110 ± 0.012	0.974 ± 0.006	0.941 ± 0.012
	best case	0.017	0.134	0.105	0.978	0.949

Results also show that the effective wavelengths for predicting firmness, acidity and starch content were selected in the following NIR spectral wavelength ranges: 798 to 902, 842 to 881, 799 to 900 nm, respectively. This implies that it is not possible to predict properties in the visible light region non-destructively and thus prediction operations must be performed in the NIR region. The reason for this might be due to the molecular structure of fruits. Given that the spectral properties depend on the amount of radiation absorbed by the fruit, it might be possible to predict different physicochemical properties at certain optimal wavelengths, Nicolai et al (2007), Zhang et al (2021). We also verified that using only spectral data coming from the three most discriminant wavelengths, fruit properties under study are estimated with regression coefficients (R) comparable to those from total Vis-NIR spectral data in the 400 to 1000 nm range, implying that optimized wavelength values generated valid results for the potential development of portable devices to accurately and nondestructively predict apple fruit properties.

4 Conclusion

Physicochemical degradation of fruits can cause a loss of quality. Therefore, a rapid, non-destructive method of estimating these properties could help improve industrial quality control of horticultural products. In this study, nondestructive prediction of three Fuji apple (*Malus M. pumila*) fruit physicochemical properties, i.e. firmness, acidity and starch, were accomplished using ANN-CA regression method. Based on our results, mean correlation coefficients (R^2) of firmness (kgf/cm), acidity (pH) and starch content (%) were $R^2 = 0.727 \pm 0.026$, $R^2 = 0.862 \pm 0.028$, and $R^2 = 0.941 \pm 0.012$, respectively, using only the three most effective wavelength spectral data, over the test set.

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