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ORIGINAL ARTICLE

Pre-dispersive near-infrared light sensing in non-destructively classifying the brix of intact pineapples

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Abstract Exported fresh intact pineapples must fulfill the minimum internal quality requirement of 12 degree brix. Even though near-infrared (NIR) spectroscopic approaches are promising to non-destructively and rapidly assess the internal quality of intact pineapples, these approaches involve expensive and complex NIR spectroscopic instrumentation. Thus, this research evaluates the performance of a proposed pre-dispersive NIR light sensing approach in non-destructively classifying the Brix of pineapples using K-fold cross-validation, holdout validation, and sensitive analysis. First, the proposed pre-dispersive NIR sensing device that consisted of a light sensing element and five NIR light emitting diodes with peak wavelengths of 780, 850, 870, 910, and 940 nm, respectively, was developed. After that, the diffuse reflectance NIR light of intact pineapples was non-destructively acquired using the developed NIR sensing device before their Brix values were conventionally measured using a digital refractometer. Next, an artificial neural network (ANN) was trained and optimized to classify the Brix values of pineapples using the acquired NIR light. The results of the sensitivity analysis showed that either one wavelength that was near to the water absorbance or chlorophyll band was redundant in the classification. The performance of the trained ANN was tested using new pineapples with the optimal classification accuracy of 80.56%. This indicates that the proposed pre-dispersive NIR light sensing approach coupled with the ANN is promising to be an alternative to non-destructively classifying the internal quality of fruits.

Keywords Pre-dispersive Near-infrared · Non-destructive measurement · Brix, Artificial neural network · Pineapples

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Introduction

The total world pineapple (Ananas Comosus) production that was approximately 24.8 million tons contributed to more than 20% of the world's tropical fruits production in 2017 (Records The Daily 2017). Pre- and post-harvesting knowledge is paramount to prevent or minimize unnecessary wastes and losses by managing the ripening process and the optimal harvest date of fruits (Li and Li 2018). Intensive global transportation of high-quality fruits stresses the need for innovative and sustainable postharvest technologies. However, inadequate extension services and limited researches in fulfilling the export quality standards are the major challenges for pineapple farmers (Jaji et al. 2018).

Pineapple is a non-climacteric fruit that does not change its internal quality once it has been harvested (Paull et al. 2017). For instance, pineapples that are harvested prematurely will not continue to ripen in sweetness because pineapples do not reserve starch to be converted to sugar (Moyle et al. 2005). This implies that the determination of the optimal harvest day is crucial to meet the worldwide

Codex Alimentarius Standard for the minimum export Brix requirement i.e. 12 degree Brix. Ultrasonic technologies might be able to non-destructively predict the mechanical properties of pineapples e.g. firmness and apparent elastic modulus (Vasighi-Shojae et al. 2018). The conventional method of measuring the Brix of pineapples using a refractometer, however, is destructive and infeasible to ensure each exported pineapple fulfills the minimum Brix requirement. Consequently, these limitations cause unnecessary wastes and losses when low quality fruits have been exported. Thus, a non-destructive measurement alternative is needed to ensure all exported pineapples fulfill the minimum Brix requirement for marketing and commercial quality control (Unit United Nations. Economic Commission for Europe 2013).

Near-infrared (NIR) technology has been widely investigated as a non-destructive and rapid sensing technology in measuring the quality attributes of various fruits and vegetables, e.g. apples (Li et al. 2018), grapes (Yu et al. 2017), pineapples (Srivichien et al.2015), tomatoes (Torres et al. 2015), and spinach (Sánchez et al. 2018). This is because the amount of absorbed NIR radiation is related to the degree and ways in which the bonds between atoms of dissimilar mass are deformed (Abu-Khalaf et al. 2001). Additionally, the physical properties e.g. the solid density of cane stalk might be estimated using NIR technology (Sanseechan et al. 2018). Recently, several investigations have been conducted to reduce the financial barrier in utilizing NIR technology e.g. replacing a halogen lamp with a relatively low-cost NIR light emitting diode (LED); and replacing a high resolution NIR spectroscopy with a relatively low-cost sensing element that coupled with several bandpass filters for post-dispersive spectral acquisition. This may address the limitation of previous NIR pre-dispersive acquisition design that involved a concave holographic grating in which its maximum light transmission was 30% (Guthriea and Walshb 1999). Pre-dispersive spectral acquisition that uses a combination of a sensing element and NIR LEDs with specific different wavelengths, on the other hand, is promising to further reduce the financial barriers of NIR technology. This pre-dispersive spectral acquisition method is similar with the combination of a light source and monochromator that has been widely used to characterize liquid samples. For instance, a combination of seven NIR LEDs coupled with a webcam has been reported to be able to detect adulterations of hydrated ethyl alcohol fuel without visible spectrum (Dantas et al. 2017). For solid samples, this pre-dispersive sensing method was reported to be able to achieve a comparable predictive accuracy with a portable commercial visible-NIR spectrophotometer in testing the ripeness of white grapes (Giovenzana et al. 2015). Nevertheless, it is worthy to highlight that three of the four wavelengths that used in the study were from the visible spectrum (i.e. 630, 690, 750 and 850 nm) (Giovenzana et al. 2015). In other words, more studies are needed to evaluate the feasibility of the pre-dispersive NIR spectral acquisition in measuring the components of interest for solid samples e.g. the internal quality of intact fruits.

Previous pilot studies reported that the pre-dispersive acquired NIR spectral data from the top, middle and bottom of pineapples can be distinguished with 70% classification accuracy based on the fact that different parts of pineapples have different Brix values (Jam and Chia 2017a), and the accuracy of the Brix classification was 75.56% using K-fold cross-validation (Jam and Chia 2017b). However, an external validation has not been studied to evaluate the performance of the proposed method. Since this is crucial to justify the potential of the proposed method that might be further developed for pre- and post-harvesting applications, this study aims to evaluate the performance of the proposed pre-dispersive NIR spectral acquisition coupled with artificial neural network (ANN) in non-destructively classifying the Brix of pineapples using cross-validation and external holdout validation.

Materials and methods

Spectral data acquisition

13 Josephine-type pineapples that were freshly bought from a local market (Parit Raja, Johor, Malaysia) were used in this study. During the pre-dispersive NIR data collection, the three points of a pineapple (i.e. top, middle, and bottom) were scanned as each segment had different Brix values, as that depicted in a previous related study (Srivichien, Terdwongworakul, and Teerachaichayut 2015). The diffuse reflectance NIR data were non-destructively collected using the developed NIR sensing device (Fig. 1) that consisted of a photodiode detector and five NIR LEDs with different peak wavelengths of 780, 850, 870, 910, and 940 nm. These LEDs that were bought from Thorlabs.com had viewing half angles, spectral FWHM, and the maximum forward current of between 7 and 10 degree, 30 and 50 nm, and 75 and 100 mA, respectively. These wavelengths are at the third overtone NIR region (also known as shortwave NIR region) that contains the third overtone N–H stretching (775–850 nm) and the third overtone C–H stretching (850–950 nm) information (NIRSystems 2002). Besides, shortwave NIR region has better penetration into biological materials compare to NIR region that is above 1100 nm. Each NIR LED was allocated around the photodiode detector with the same radius and pointed to the same spot with 45 degree toward the spot.

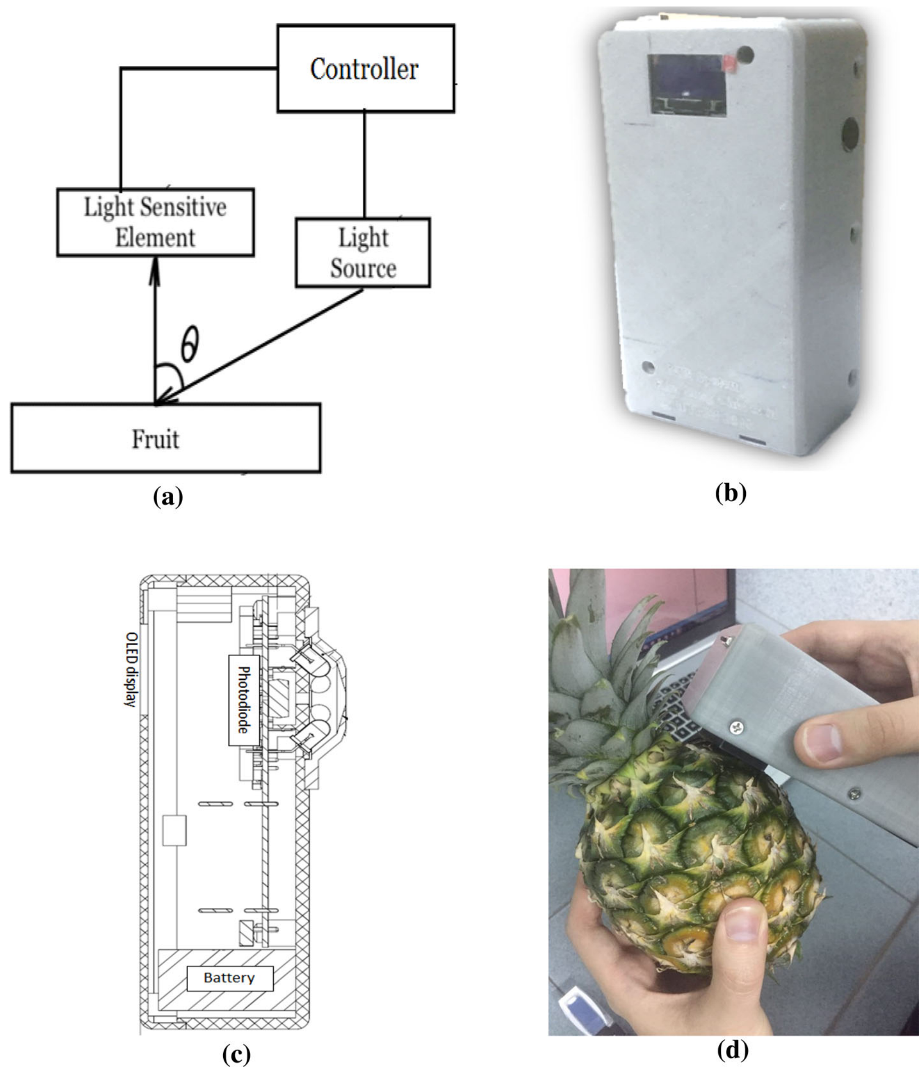

Fig. 1 The designed sensing device: **a** the framework of the design, **b** the front view of the developed NIR sensing device, **c** the sensing design (side view), and **d** NIR data acquisition

An OPT101 monolithic photodiode (Texas Instruments) was used as the photodiode detector because it has an on-chip transimpedance amplifier that eliminates common challenges e.g. noise pick-up, leakage current errors, and gain peaking during the data acquisition. The output voltage of the photodiode detector is proportional to the detected light intensity. The photodiode detector was allocated perpendicular to the spot. The spot was the scanned area of a pineapple. Next, a diffuse reflectance standard (PTFE Ocean Optics) was used to calibrate the developed NIR sensing device as follows. First, the intensities of all LEDs were maximized by minimizing their respective variable resistors' values. After that, the amplifier gain of the OPT101 was reduced until only one of the five LEDs was slightly below the saturation intensity. Lastly, the intensities of the rest of LEDs were reduced by increasing their respective variable resistors' values until each of the signal was slightly below the saturation intensity. For each NIR wavelength, an average of five scans were performed at each scanned area. This scanning process was repeated from one LED to another LED until all the five wavelengths had been scanned once. A microcontroller was used to automate this data acquisition and to transfer the acquired data in a laptop computer using an Universal Serial Bus (USB) cable for offline calibration and analysis. A 7.4 V 1000 mAh Li-poly rechargeable battery was used to supply electrical power to the developed NIR sensing device. An organic light-emitting diode (OLED) screen was used to display the predicted results.

Conventional brix measurement

Immediately after the non-destructive NIR data acquisition of an intact pineapple was completed, the pineapple was cut using a stainless-steel apple corer to obtain the flesh under each scanned area. The Brix value of the obtained flesh was conventionally measured using a digital refractometer (PAL-1, Atago, Tokyo, Japan). Both reflected NIR light and Brix data acquisition process was repeated for the rest of pineapples.

Data arrangement

The acquired samples from the first 10 pineapples were used as training dataset to study and identify the optimal architecture of the artificial neural network (ANN) using the K-fold cross-validation. The samples from the rest of three pineapples were reserved as an independent testing dataset to evaluate the robustness of the optimal ANN. Both training and testing datasets were pineapples that harvested on different days. During the K-fold cross-validation, the best architecture of an ANN (i.e. the optimal number of hidden neurons) was determined. After that, all the training data were used to produce the optimal ANN that would be tested using the independent samples as that depicted in Fig. 2.

Classification

All pineapple samples were categorized into Class A and Class B according to their Brix values. Pineapple samples that had Brix values equivalent to or more than 12 degrees Brix would be categorized as Class A, while the rest would be categorized as Class B. This Brix value classification was based on the minimal Brix requirement of 12 degrees Brix for exported intact fresh pineapples (Unit United Nations. Economic Commission for Europe 2013). The training samples selection was carried out using a boxplot and leave-one-out cross-validation analysis from the training dataset.

An artificial neural network (ANN) was developed to classify the Brix values of pineapples as either Class A or Class B. The architecture of the ANN consisted of an input layer, a hidden layer, and an output layer (Fig. 3). The acquired diffuse reflected NIR lights of 780, 850, 870, 910, and 940 nm were used as the inputs of the ANN. The classification training algorithm of the ANN was the Scaled Conjugate Gradient (SCG). Unlike other conjugate training algorithms, SCG uses a step size structure instead of a line search, which reduces the computation cost of an ANN (Garg and Bansal 2015). The performance of the ANN was studied when its hidden neuron number and the random seed value were varied during the training process. In general, the complexity of an ANN is proportional to the number of its hidden neuron. The random seed value is another important parameter that affects the initial weights of an ANN, and consequently that affects the performance of an ANN. An ANN with the optimal hidden neurons number and the best random seeds will achieve the optimal accuracy without both under- and over-fitting issues.

Performance analysis

K-fold cross-validation was used to identify the best hidden neuron number of the ANN. K-fold cross-validation with higher K value has more computational time, while that with lower K will lead to an increase in the variance value (Behroozi-Khazaei and Nasirahmadi 2017). The ANN was optimized using a fivefold cross-validation. All the training data were randomly divided into five sub-datasets i.e. each sub-dataset had the samples from two of the ten pineapples. The number of hidden neurons was adjusted to find the best ANN. The effects of the hidden neuron number and the random seed value of the ANN were studied.

To evaluate the robustness of the proposed method, the ANN with the best architecture was re-trained using the training dataset, and then the trained ANN was evaluated using the independent testing dataset. The independent data were tested without any sample selection. The performance of the ANN was evaluated by computing the classification accuracy rate i.e. the ratio of the number of correctly classified samples to that of total samples (Zhang et al. 2020).

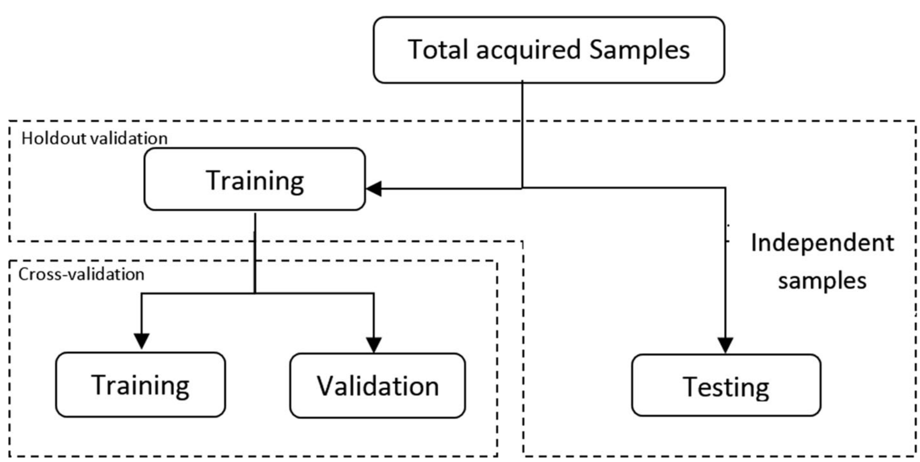

Fig. 2 The relationship between the data used for cross-validation and holdout validation. Independent samples from new pineapples were used as testing data to evaluate the robustness of the model

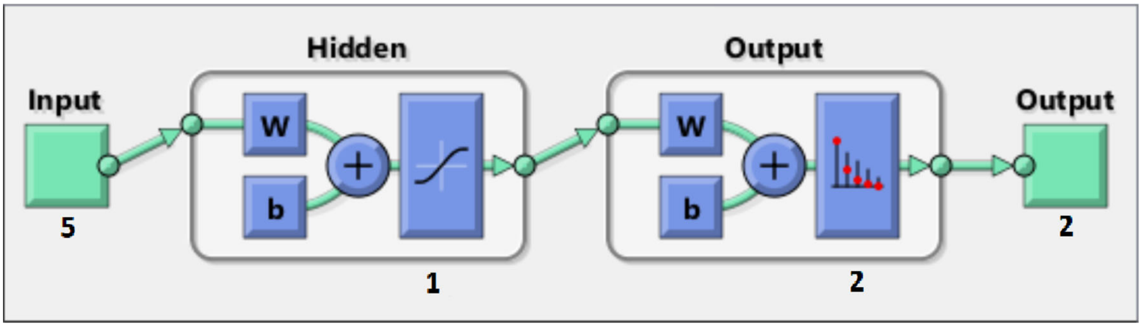

Fig. 3 The neural diagram of the neural network: the measured NIR intensities were the inputs, the hidden neurons were studied from one to 10, and the output was the predicted result (i.e. Class A or Class B)

Sensitivity analysis

The sensitivity analysis was used to study how the noise variation affects the behaviour of an ANN (Kapanova et al. 2017), and the uncertainty of the output performance (Li et al. 2016). This method was applied by removing some of the inputs of a predictive model (Olden et al. 2004). In this study, the effect of each NIR wavelength was studied and discussed using the sensitivity analysis in classifying the Brix values of pineapples. Reducing data dimension by identified the optimal region (also known as the optimal combination of inputs) would not degrade the performance of the predictive model (Islam et al. 2018).

Results and discussion

Table 1 summarizes the descriptive statistics of the acquired data for training and testing datasets. The training dataset consisted of a total of 108 pineapple samples i.e. 62 Class A and 46 Class B pineapple samples. The range of the Brix values was between 8.20 and 16.50 degree Brix. For testing analysis, the 36 pineapple samples that were acquired from new pineapples were used as the independent testing dataset, ranging from 9.80 to 14.50 degree Brix.

K-fold cross-validation

Figure 4 shows that the ANN with seven hidden neurons and the best random seed value achieved the most accurate classification result of 85.24% in the fivefold cross-validation. In other words, the presence of more than seven hidden neurons did not improve the performance of the ANN. This implies that the ANN might be overfitted because its performance was not significantly improved even though its complexity was increased. Different optimal initial weights were used for the ANN that had different hidden neuron number to achieve the optimal classification accuracies of between 81.43 and 85.24%. According to the principle of parsimony, the ANN that used one hidden neuron was selected as the best architecture with 82.8% classification accuracy to avoid potential over-fitting issue for the sensitivity analysis and the external holdout validation.

Sensitivity analysis

Table 2 tabulates the classification accuracy of the ANN that used one hidden neuron in classifying the Brix of pineapples using K-fold cross-validation and external holdout validation. The external holdout validation consisted of both training and testing analysis, in which, training and independent testing datasets were used, respectively. When all of the five wavelengths were included as the inputs of the ANN, the ANN was able to

Table 1 The descriptive statistics of the training and testing datasets

Dataset	Maximum Brix	Minimum Brix	Mean (Brix)	Standard deviation (Brix)	Number of samples		
					Class A	Class B	Total
Training	8.20	16.50	12.0185	1.4019	62	46	108
Testing	9.80	14.50	12.6111	1.1966	28	8	36
Total	8.20	16.50	12.1667	1.3738	90	54	144

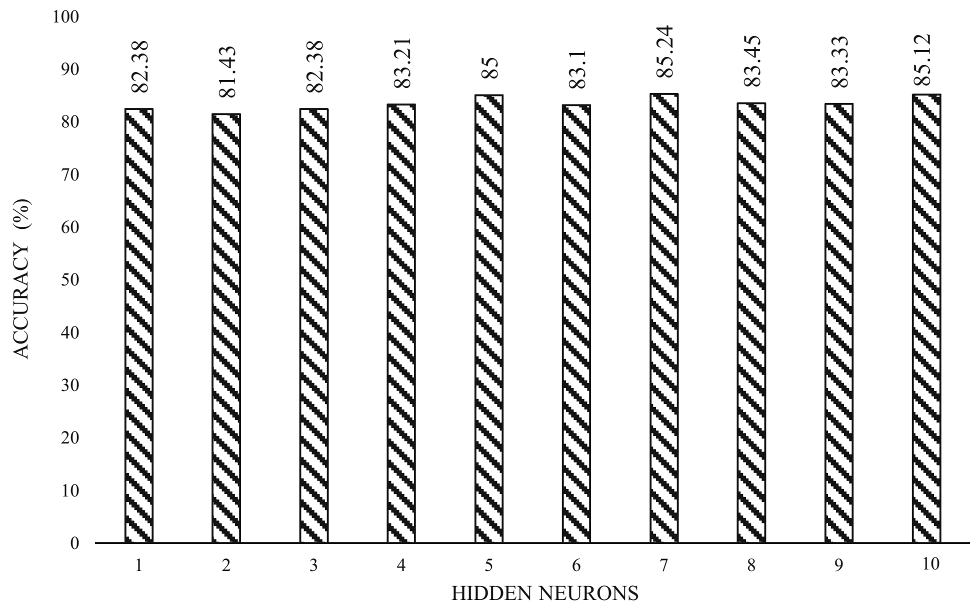

Fig. 4 The classification accuracy of K-fold validation when ANN used different hidden neurons

Table 2 The classification accuracy of ANN that used one hidden neuron in classifying the Brix of pineapples using K-fold cross-validation and holdout validation

Third overtone region (NIRSystems 2002)	Excluded wavelength (nm)	Accuracy		
		K-fold cross-validation accuracy (%)	Holdout validation accuracy (%)	
			Training	Testing
Both N–H and C–H stretching	None	82.38	76.85	75.00
N–H stretching (775–850 nm)	780	78.81	75.00	80.56
	850	82.38	79.63	72.22
C–H stretching (850–950 nm)	870	80.48	70.37	77.78
	910	77.74	74.07	77.78
	940	82.14	75.00	80.56

classify the Brix values of pineapples with a satisfying classification accuracy of 82.38, 76.85, and 75% for K-fold cross-validation, training, and testing analysis, respectively. This shows that the performance of cross-validation was more optimistic compared with the holdout validation.

Next, the performance of the ANN was re-evaluated when each wavelength was excluded once to investigate the effects of each wavelength. It is noticeable that the ANN achieved the lowest cross-validation accuracy when 910 nm was excluded. This implies that 910 nm was the most important wavelength among the five wavelengths. However, this finding disagrees with the previous study because the exclusion of 910 nm was reported to have a better classification accuracy (Jam and Chia 2017b). Next, the least important wavelength might be the 850 nm wavelength because the ANN that excluded and that included 850 nm achieved the same cross-validation accuracy. In short, the results of the K-fold cross-validation suggested that 850 nm was the least important wavelength, followed by 940, 870, 780, and 910 nm.

On the other hand, the results of the holdout validation indicated that 850 nm was the most important wavelength, followed by 870 or 910 nm, and then 780 or 940 nm based on the testing accuracy. The 850 nm is closed to the third combination overtone of sugar O–H stretching at 840 nm i.e. the second harmonic of a combinational O–H stretching and bending vibration (Golic et al. 2003). 870 and 888 nm are corresponding with the absorbance band due to carbohydrate e.g. starch, sucrose, fructose and glucose (Suhandy 2009). The least important information were the wavelengths that near to the chlorophyll band of 680 nm and the water absorbance (O–H stretching vibration) of 960 nm, i.e. 780 and 940 nm, respectively. The trained ANN that was tested using the new pineapples achieved the best classification accuracy of 80.56% when either 780 or 940 nm was excluded during the holdout validation.

Previous researches reported the derivative of absorbance at 876 nm was important in pineapple Brix prediction (Guthriea and Walshb 1999). Nevertheless, different effective wavelengths were reported for Brix predictions e.g. 884 and 878 nm for tomato and mango, respectively (Suhandy 2009). This could be due to different fruits, NIR instruments, acquisition setups, and validation approaches were used in different researches. For instance (Islam et al. 2018) reported that different variable selection methods might suggest different sets of selected. Another possible reason could be due to the nature of NIR third overtone spectrum that is highly overlapping and correlated. Consequently, the use of adjacent wavelengths that are highly correlated with each other may achieve a comparative prediction performance. Nevertheless, more researches are needed to study the effectiveness of variable selection in NIR related researches.

The proposed method is a secondary measurement approach that can non-destructively classify the Brix values of intact pineapples. With the external holdout validation accuracy of 80.56%, the proposed method might help farmers to make a judgment about when they should harvest their pineapples and how they should sort their harvested pineapples. This is important because the internal quality of pineapples will have little change once it has been harvested. Pre-dispersive transmission spectral acquisition that fulfills Beer-Lambert law has been commonly used to characterize liquid samples. This is because the light travel path through a liquid sample can be fixed from a light emitter to a receiver. For the proposed pre-dispersive reflectance spectral acquisition, the geometrical effects were minimized by fixed the positions of the light emitters to the receiver. Nevertheless, the accuracy of the proposed method might be further improved by investigating the geometrical effects of the pre-dispersive reflectance spectral acquisition.

Conclusion

This study shows that the proposed pre-dispersive NIR light sensing approach (that consists of one sensing element and five NIR LEDs) could be an alternative to classify the internal quality of pineapples without an expensive NIR spectroscopy and a halogen lamp. The proposed method is a secondary measurement approach that correlated the non-destructively measured NIR data to the conventionally measured Brix values of pineapples using an ANN. The external holdout validation (i.e. training and testing analysis) was used to evaluate the robustness of the proposed method, in which, pineapples that harvested on different day were used as testing data to evaluate the classification accuracy. The ANN that used one hidden neuron and the five different NIR wavelengths (i.e. 780, 850, 870, 910, 940 nm) as its inputs achieved a classification accuracy of 82.38, 76.85, and 75% for K-fold cross-validation, training, and testing analysis, respectively. The classification accuracy of K-fold validation (i.e. between 77.74 and 82.38%) was comparable with the testing accuracy in the external holdout validation (i.e. between 72.22 and 80.56%). Next, the sensitivity analysis indicated that the exclusion of one wavelength that near to the water absorbance or chlorophyll band could potentially improve the classification accuracy. This implies that the use of fewer number of different NIR wavelengths as the inputs of an ANN could potentially achieve a better classification accuracy. Nonetheless, more studies are needed to study the related parameters using different algorithms so that the parsimonious principle can be complied by having a better understanding about the relationship between the acquired pre-dispersive reflectance NIR light and the component of interest in solid samples.

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Compliance with ethical standards

Conflict of interest The authors confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

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