Application of NIR Spectroscopy to the quality control of citrus fruits and mango

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Introduction

NIR spectroscopy is a proved tool to measure the optical properties of the samples, which are related to their chemical and textural properties. This technology can be used for determining the internal and external quality of fruits. Accordingly, many studies have been reported for long time to assess the quality of different fresh fruits by using reflectance measurements acquired with visible-NIR spectroscopy. We have been working on the estimation of the quality of fruits using computer vision for more than twenty years, always focused on problems that affect the local industry. As the region of Valencia (Spain) is one of the main producers and exporters of citrus fruits worldwide, most of our research has been focused on this fruit, especially developing fast and reliable methods to detect defective fruit in quality control lines[1]. Nevertheless, our group have been carried out also other studies to determine the internal quality in other fruits with commercial interest for our region, such as, mangoes cv. 'Osteen', nectarines cv. 'Big Top' and cv. 'Magique', and persimmon cv. 'Rojo Brillante'.

Nowadays, the fruit producers demand automated systems to detect fruits with decay lesions that are not visible at early stages but that can spread the infection to other fruits during storage or shipping. In the case of citrus fruits, this is the most economically important postharvest disease of citrus worldwide. Detection of these diseases may considerably help to correctly discriminate and classify different fruit lots and take important decisions, based on fruit quality, about postharvest handling and final produce destination. However, the detection of rotten fruit in citrus packing-lines is performed manually, using the naked eye under ultraviolet (UV) light that induces visible fluorescence, what it is harmful for the workers. New automatic devices using UV or hyperspectral imaging[2] are being investigated as possible alternatives to manual inspections. However, industry's demands for innovative tools for rapid and cost-effective early detection have spurred considerable interest among researchers on the application of near-infrared spectroscopy (NIRS) on citrus fruit quality monitoring as stated in the review carried out by Magwaza et al.[3].

Moreover, Spain is the main European producer of subtropical fruits and in particular the south-west region has a large potential for the production of Mango fruit. In the past, external quality, related to the skin colour, fruit size and shape, free from defects and the absence of decay were the most common quality determinants, but nowadays other organoleptic characteristics related to the internal quality play an important role in the consumer's decision. Hence, another aim was to investigate the potential of visible and NIR to determine the internal quality of mango cv. 'Osteen', the main variety of mango grown in Spain.

NIR measurements

In all studies, the visible-near infrared (VIS-NIR) and NIR spectra were collected using a multichannel VIS-NIR spectrometer equipped with two detectors. The first detector (AvaSpec-ULS2048 StarLine, Avantes BV, The Netherlands) covering the VIS-NIR range from 595 nm to 1100 nm with a spectral sampling interval of 0.25 nm. The second one (AvaSpec-NIR256-1.7

NIRLine, Avantes BV, The Netherlands) covered the NIR range of 888 nm to 1795 nm with a sampling interval of 3.53 nm. A Y-shaped fibre-optic reflectance probe was configured with an illumination leg coupled to a stabilised 10 W tungsten halogen light source. A holder for positioning the sample properly over the probe and the reflectance probe delivered the light to the sample and collected the reflectance from the sample, which was carried by the fibre cable to the spectrometer in use. Figure 1 shows the equipment used to acquire the spectral measurements of the fruits. Equipment used for the spectral measurements The calibration was made using a 99% reflective white reference tile so that the maximum reflectance value over the wavelength range was around 90% of saturation. A commercial software (AvaSoft 7.2, Avantes, Inc.) was used for controlling both detectors and acquiring the spectra. The integration time was set to 90 to 120 ms, depending of the fruit, for the VIS-NIR detector and to 500 to 700 ms for the detector sensitive in the NIR region. For both detectors, each spectrum was obtained as the average of five scans to reduce the thermal noise. The average reflectance measurements of each sample (S) were then converted into relative reflectance values (R) with respect to the white reference using dark reflectance values (D) and the reflectance values of the white reference (W), as shown in equation (1):

$$R = \frac{S-D}{W-D} \tag{1}$$

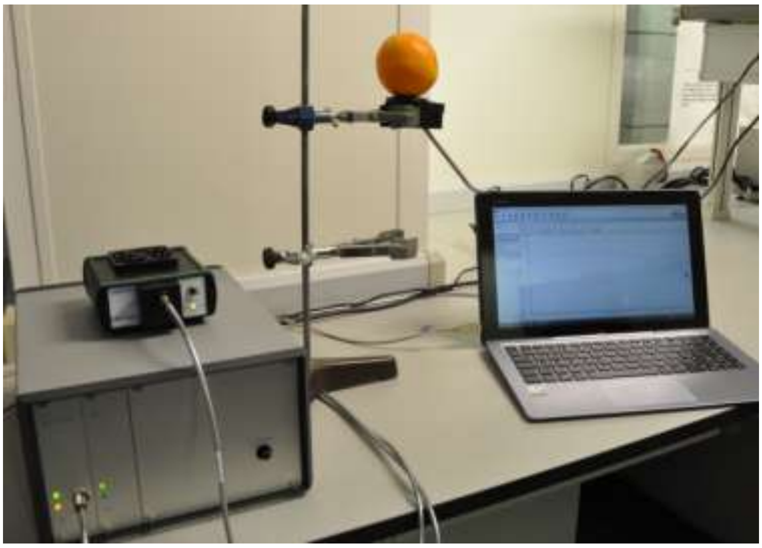

Figure 1. Equipment used for the spectral measurements

Experiments on citrus fruits

For the experiments with citrus fruits for early detection of rotten fruit, a total of 117 mandarins cv. 'Clemenvilla' (*Citrus reticulata* Hort. ex Tanaka) were used: 67 fruits were superficially punctured on the rind and inoculated with spores of *P. digitatum* fungus and the other 50 were injured in the same way but treated with sterilised water for control purposes[4]. After inoculation, the fruits were stored until decay lesions with diameters equal to or higher than 10 mm appeared on all the infected fruits. The control fruits inoculated with just water were used to evaluate how the physical changes produced in the rind by the inoculation procedure influenced the spectral measurements. In addition, spectra from sound skin were also acquired from 50 fruits. Therefore, a total of 167 skin samples were analysed in this work: 100 sound skin samples (50 samples of sound skin and 50 control samples inoculated with water) and 67 decaying skin samples. Figure 2 shows examples of a sound and a decayed fruit.

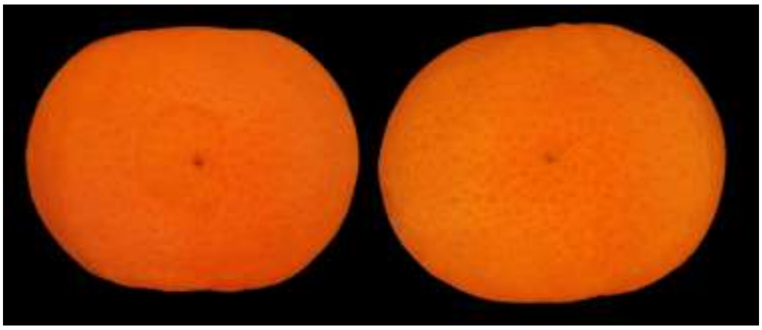

Figure 2. A rotten fruit showing symptoms of a hardly visible decay lesion in the centre (left), and a control sample inoculated with water (right).

The raw spectra acquired with both spectrophotometers were pre-processed using multiplicative scatter correction (MSC) and standard normal variate (SNV) to reduce spectral variability. In addition, due to the underlying nature of most of the techniques used in this work, such as principal component analysis (PCA), spectra were mean centred by subtracting the mean spectrum of each data set from each spectrum. The intrinsic dimensionality of the data is defined as the minimum number of parameters needed to describe all the information in the data. To estimate this, four different approaches were employed in this work: eigenvalue-based estimator (EB), maximum likelihood estimator (ML), correlation dimension estimator (CD) and geodesic minimum spanning tree estimator (GMST). Finally, three popular unsupervised learning methods were investigated to reduce the dimensionality, as PCA, factor analysis (FA) and Sammon mapping. The data transformation is linear in PCA and FA, while Sammon mapping is a non-linear method, thus being capable of handling more complex data with non-linear relationships. Finally, the low-dimensional data were used as input feature vectors to classify samples of mandarin skin into sound and decaying using a supervised classifier based on linear discriminant analysis (LDA).

Tests were aimed at evaluating and comparing the scatter-correction methods (raw data, MSC and SNV), the intrinsic dimensionality estimators (EB, ML, CD and GMST) and the dimensionality reduction techniques (PCA, FA and Sammon mapping) in terms of their classification performance. In particular, the main interest of this work lies on finding out what combination of spectral range, pre-processing technique, estimator of intrinsic dimensionality and dimensionality reduction method provided the best classification performance for decay detection in citrus fruits.

A five-fold cross-validation procedure was used to evaluate the performance of the classification models, dividing the data randomly into five folds (subsets) of equal size to use four as the calibration set and the remaining one for validation to assess classifier performance. This process was repeated five times leaving one different fold each time. The whole five-fold cross-validation process was repeated 100 times to reduce variability and obtain reliable performance estimations, resulting in a total of 500 iterations for each model. The validation results were finally averaged over all the iterations, thus obtaining a mean confusion matrix. The results achieved are shown in Table 1.

Table 1. Overall classifier accuracies using the different scatter-correction methods, intrinsic dimensionality estimators and dimensionality reduction techniques

		VIS-NIR				NIR			
		Intrinsic dimension	PCA (%)	FA (%)	Sammon (%)	Intrinsic dimension	PCA (%)	FA (%)	Sammon (%)
Raw data	EB	1	89.68	89.70	88.89	1	92.47	92.51	92.87
	ML	3	95.07	95.05	88.68	3	97.69	97.76	96.63
	CD	1	89.68	89.70	89.66	2	94.90	96.72	95.20

	GMST	2	89.16	89.07	88.61	3	97.69	97.76	97.59
MSC	EB	3	56.90	54.46	59.69	2	88.56	89.01	89.07
	ML	15	73.12	83.44	69.05	3	93.92	92.61	94.42
	CD	1	62.01	61.90	52.67	2	88.56	89.01	89.06
	GMST	11	70.27	80.80	62.84	3	93.92	94.26	93.72
SNV	EB	4	75.93	72.47	61.13	2	88.56	88.96	89.05
	ML	14	78.02	84.84	71.29	3	93.95	94.04	93.44
	CD	2	59.09	57.26	61.10	2	88.56	88.96	89.05
	GMST	12	79.41	83.17	71.50	3	93.95	94.04	94.32

Experiments on mango

The main biochemical (total soluble solids and titratable acidity) and physical properties (firmness and flesh colour) of 140 mangoes (*Mangifera indica* L., cv. 'Osteen') where analysed destructively after NIR data acquisition. The overall internal quality of the fruit was determined using two indices, a ripening index (RPI) and an internal quality index (IQI) calculated using equations 2 and 3[5]. The main difference between them is that IQI does not need the TA analysis, which is more complex and expensive for the industry than colour parameters included in IQI.

$$RPI = ln\,(100 \cdot F \cdot TA \cdot TSS^{-1}) \qquad (2)$$

$$IQI = ln\left(100 \cdot F \cdot L^{*} \cdot {h_{ab}}^{*} \cdot TSS^{-1} \cdot {C_{ab}}^{*-1}\right) \qquad (3)$$

where F is firmness (N), TA is titratable acidity (grams citric acid equivalent/100 g sample), TSS is total soluble solids (°Brix) and L^*, h_{ab}^* and C_{ab}^* are the colour attributes of the flesh colour.

Different pre-treatments and multivariate analyses were performed in order to establish the relationship between the spectral measurements and the internal quality of mango. In order to reduce the influence of light scattering and the baseline drift various pre-processing methods were applied to the spectra. Savitzky-Golay smoothing with a gap of three data points combined with extended multiplicative scatter correction (EMSC) were considered the best methods for the VIS-NIR spectra, and these two together with the second derivative with Gap-Segment (2.3) obtained the best results for the NIR spectra. Figure 3 shows the apparent absorbance spectra of mangoes at different ripening stages after pretreatments.

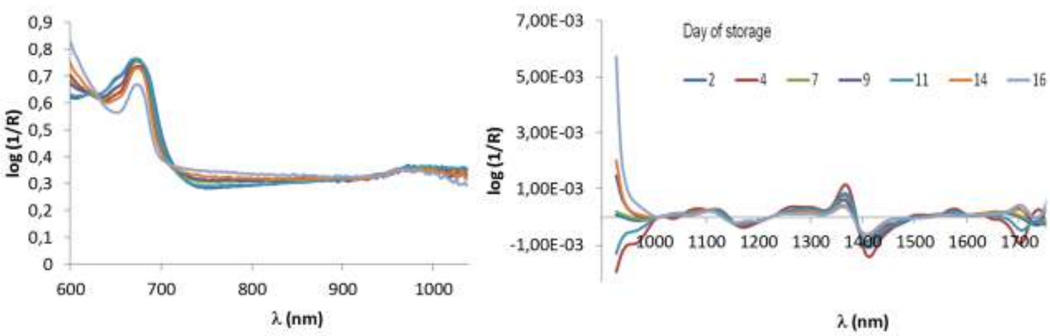

Figure 3. Apparent absorbance spectra of mangoes at different ripening stages for the VIS-NIR region (left) and the NIR (right) after pretreatments.

Each set (NIR and VIS-NIR) was divided randomly into two groups, a calibration set (75% of the samples) and a prediction set (25% of the samples). Partial least squares regression (PLS) was applied to the full range spectra to construct separate calibration models for RPI and IQI and each spectrum with segments of 20 objects. The performance of the calibration models was optimised by internal cross-validation and then externally validated using the prediction set. The relative performance of the constructed models was assessed by the required number of latent variables (LVs), the coefficient of determination (R_{CV}^2), and the root mean square error of leave-one-out cross-validation (RMSECV). The predictive ability of the models was evaluated using the coefficient of determination for prediction (R_P^2), the root mean square error of prediction (RMSEP) and the ratio of prediction to deviation (RPD=SD/RMSEP), where the SD was the standard deviation of the Y-variable in the prediction set. For RPD values above 2.5, the prediction is considered to be good to excellent. Table 2 shows the results achieved in this study. A strong performance in predicting the internal quality of mango for both detectors can be observed.

Table 2. Results of the PLS models for the calibration and prediction of IQI in mango samples by using the spectral data

Index	**Detector**	**#W**	**#LV**	**Cross validation**		**Prediction**		
				R_{CV}^2	**RMSECV**	**R_P^2**	**RMSEP**	**RPD**
IQI	VIS-NIR	285	4	0.891	0.421	0.877	0.435	2.691
	NIR	242	10	0.831	0.523	0.833	0.507	2.341
RPI	VIS-NIR	285	8	0.902	0.412	0.902	0.470	2.767
	NIR	242	10	0.868	0.478	0.845	0.592	2.340

Conclusions

In general, the results of the application of NIRS to develop tools for the non-destructive measurement of the internal quality in intact fruits that are important for our region are being promising. NIRS applied to the detection of invisible decay lesions in citrus fruits can represent an important advance in the creation of new automated methods to detect and eliminate infected fruit in postharvest. On the other hand, the non-destructive estimation of internal quality of mangoes (or other fruits such as nectarines or persimmons) based on this technology could serve as a decision tool for postharvest handling of these fruits. Other applications currently under study are also achieving good results including the creation of a fast in-line system for fruit sorting based on NIRS and the integration of NIRS system on a smart robotic hand for fruit handling.

Future trends

Similar studies are now being applied to develop fast, reliable and non-destructive tools to sort in-line other fruits by internal quality in order to decide, for instance, if the fruit should be stored or sent immediately to the market in the case of nectarines or if some residual astringency (soluble tannins) remains in persimmon after applying deastringency treatments. First results are being promising although in these cases more study is still required. The final aims are to create in-line systems to sort de fruit in real-time by internal quality in a sensor fusion approach together with a computer vision system, and also to incorporate a spectroscopic probe in a smart robotic hand so the internal quality can be measured while the fruit is being manipulated.

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