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Passive reflectance sensing using regression and multivariate analysis to estimate biochemical parameters of different fruits kinds

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ABSTRACT

Food quality control monitoring is crucial in food processing, due to the potential of adverse effects on the health of entire populations. The traditional biochemical measurements are based on chemical analysis techniques in the laboratory, which, despite being effective, are expensive, laborious, and time consuming, making them infeasible to obtain information on biochemical measurements in time and at large scales. In this study, the performance of non-contactless high throughput passive sensing was evaluated to estimate the biochemical parameters as well as to discriminate between fruit kinds via the application of chemometric techniques based on principle component regression (PCR), partial least square regression (PLSR) as well as simple regressions. Models of PCR or PLSR included data of the (i) spectral reflectance reading from 400 to 1000 nm and (ii) selected sixteen spectral indices that were calibrated and cross-validated for biochemical parameters prediction. Results show that the selected spectral indices showed close and highly significant associations with all measured parameters of guava, mandarin and orange fruits at three different ripening degrees with coefficient of determination (R^2) reach up to ($R^2 = 0.87$; $p \leq 0.001$, $R^2 = 0.86$; $p \leq 0.001$, $R^2 = 0.86$; $p \leq 0.001$, $R^2 = 0.80$; $p \leq 0.001$ and $R^2 = 0.42$; $p \leq 0.001$) for Chlorophyll *a* (Chl *a*), Chlorophyll *b* (Chl *b*), Chlorophyll t (Chl t), soluble solids content (SSC) and titratable acidity (T. Acidity), respectively. Multivariate analysis of PCR and PLSR models showed a good prediction performance of the measured parameters. For example, the PCR based on the selected sixteen spectral indices showed that a good prediction performance was obtained with coefficient of determination (R^2) of 0.85, 0.85, 84, 0.76 and 0.39, and root mean square errors of prediction of 0.052 (μg cm^{-2}), 0.099 (μg cm^{-2}), 0.152 (μg cm^{-2}), 0.683 (%) and 0.0485 (%) for Chl *a*, Chl *b*, and Chl t, SSC and T. Acidity for guava fruits, respectively. As well as the PLSR based on selected sixteen spectral indices showed that a good prediction performance was obtained with coefficient of determination (R^2) of 0.80, 81, 82, 0.73 and 0.22, and root mean square errors of prediction of 0.100 (μg cm^{-2}), 0.202 (μg cm^{-2}), 0.290 (μg cm^{-2}), 0.457 (%) and 0.0822 (%) for Chl *a*, Chl *b*, and Chl t, SSC and T. Acidity for orange fruits, respectively. The overall results demonstrate that passive reflectance sensing can be used to evaluate the quality of different fruit types via the application of chemometric techniques as well as simple regression.

1. Introduction

Food quality control has become a serious issue. Food quality control monitoring is crucial in food processing, due to the potential for adverse effects on the health of entire populations. Modern techniques of fruit quality have been developed in recent years. Someof them are based on the destructive measurements and others are non-contactless to the fruits. The global trend is currently to develop non-contactless techniques to measure the quality parameters of different fruits and vegetables kinds. Non-destructive techniques are rapid proceed, require only few samples and are easy to use in process control (Lammertyn et al., 2000). Passive reflectance sensor has spectral bands which includes the spectrum range from 380 to 2500 nm at visible and near infrared (Vis/NIR). It enables to obtain the spectral information of fruits, with the advantages of high spectral resolution. (McClure, 1994). Remotely estimating fruits´ spectral reflectance by passive reflectance sensing has the potential for detecting reflected radiation with the field view of a sensor, rendering evaluations more cost-effective and credible. Fruit spectal reflectance, calculated as the ratio of the reflected light to the incident solar radiation, is closely related to the physiological status. Changes in fruit color and cell structure, photosynthetic activity can alter the spectral reflectance of fruits in the Vis and NIR of

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Table 1
Spectral indices, spectral index abbreviation and references of the spectral indices used in this study.

Formula	Index abbreviation	References
$(R_{780} - R_{670})/(R_{780} + R_{670})$	$NDVI_{780,\ 670}$	Raun et al., 2001
$(R_{780} - R_{550})/(R_{780} + R_{550})$	$NDVI_{780,\ 550}$	Gutierrez et al., 2010
$(R_{780} - R_{710})/(R_{780} + R_{710})$	$NDVI_{780,710}$	Jiang and Carrow, 2007
$(R_{780} - R_{570})/(R_{780} + R_{570})$	$NDVI_{780,570}$	Rutkowski et al., 2008
$(R_{820} - R_{694})/(R_{820} + R_{694})$	$NDI_{820,\ 694}$	This work
$(R_{750} - R_{678})/R_{480}$	CRMI	Nagy et al., 2016
$R_{750} - R_{678})/R_{550}$	PRMI	Nagy et al., 2016
$(R_{750} - R_{678})/(R_{750} + R_{678})$	NCI	Nagy et al., 2016
$(R_{828} - R_{700})/(R_{828} + R_{700})$	$NDI_{828,\ 700}$	This work
$(R_{826} - R_{670})/(R_{826} + R_{670})$	$NDI_{826,\ 670}$	This work
$(R_{850} - R_{680})/(R_{850} + R_{680})$	$NDI_{850,\ 680}$	This work
$(R_{800} - R_{620})/(R_{800} + R_{620})$	$NDI_{800,\ 620}$	This work
$(R_{800} - R_{640})/(R_{800} + R_{640})$	$NDI_{800,\ 640}$	This work
$(R_{900} - R_{670})/(R_{900} + R_{670})$	$NDI_{900,\ 670}$	This work
$(R_{970} - R_{670})/(R_{970} + R_{670})$	$NDI_{970,\ 670}$	This work
$(R_{760} - R_{720})/(R_{760} + R_{720})$	NAI	Rouse et al., 1974

the spectrum (Elsayed et al., 2016; Nagy et al., 2016).

The traditional biochemical measurements are based on chemical analysis techniques in the laboratory, which, despite being effective, are expensive, laborious, and time consuming, making them infeasible to obtain information on biochemical measurements in time and at large scales. For that, Laboratory techniques cannot easily account for rapid changes in biochemical parameters arising from changes in environmental conditions (Elsayed et al., 2016).

Currently, destructive measurements of biochemical parameters normally depend on fruits sampling from the field followed by chemical estimate under laboratory conditions. Thus, real-time and accurate estimating of the biochemical parameters of different fruits by high-throughput passive reflectance sensor is thus of great significant importance for food processing and harvest time, which could be economically and environmentally beneficial. In this study Chl, SCC and T. acidity used as indicators of fruits quality. The Chl concentration is the most important indicator of fruit maturation or ripening and it is responsible for changing the color, when additional pigments are formed (Svanberg, 2004; Maxwell and Johnson, 2000). As well as SSC, acidity is considering taste parameters of the fruit.

Some studies estimated the biochemical parameters of different fruit kinds by using non-destructive high throughput passive reflectance and spectroscopic measurements (Merzlyak et al., 2003; Solovchenko et al., 2005; Zude et al., 2006; Rutkowski et al., 2008; Slaughter et al., 2013; Elsayed et al., 2016; Nagy et al., 2016). For examples, Merzlyak et al. (2003) reported that spectral indices, R_{800} /R_{700} and R_{800} /R_{640}, were positively relate to the total Chl content at range from 0.4 to 11 nmol/cm^2 (R^2 > 0.93) and the spectral index $(R_{678}$ - $R_{500})/R_{800}$ index allowed reliable assessment of the carotenoid to chlorophyll ratio (R^2 = 0.88) in a wide range of its changes in anthocyanin-free fruits. As well as Nagy et al. (2016) found that the reflectance at 678 nm wavelength is sensitive for distinguishing a low chlorophyll content and as well as the reflectance at 700 nm presented more variability for high chlorophyll content and can be used for detecting the ripening early stage and the pigment content changes.

An alternative approach is to use chemometric methods such (PCR) and (PLSR), is applied multi-analysis and regression methodology in spectroscopy to obtain information concerning the object attributes. In chemometric methods as PCR and PLSR orthogonal components are unaffected by collinearity and are derived from all variables (Wold et al., 2001). Generally, multicollinearity and over-fitting are common problems that are inherent to target hyperspectral reflectance dataset, and these problems usually occur when one or more of the spectral wavelengths (independent variables) are highly correlated with one or more of the other spectral wavelengths (Mirzaie et al., 2014). For that these two methods were tested in this study.

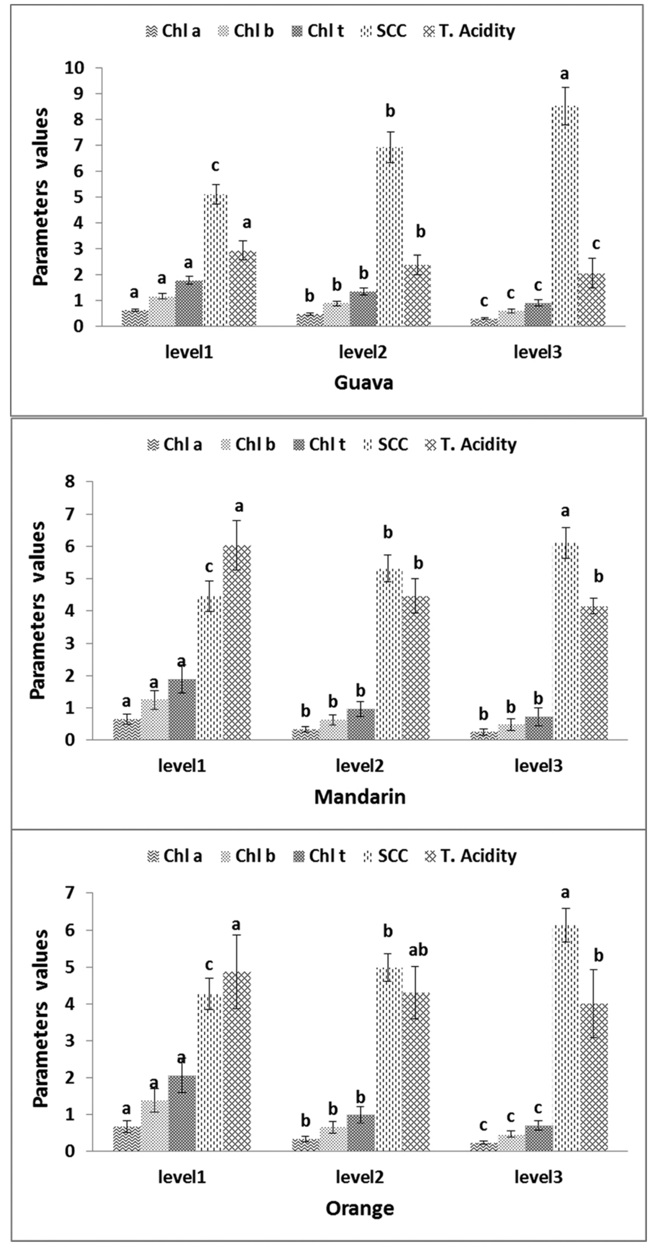

Fig. 1. Results indicating mean values of Chl *a* (μg cm^{-2}), Chl *b* (μg cm^{-2}), chlorophyll t (μg cm^{-2}), soluble solids content (%) and titratable acidity (%) of guava, mandarin and orange fruits at three ripening degrees. The same letters indicate no statistical difference (P ≤ 0.05) between the ripening degrees.

The scientific hypothesis raised in this study investigates whether changes in biochemical parameters and discrimination between fruit kinds can be assessed from changes in spectral reflectance measurements based on the change in color of skin fruits, physical attribute and chemical constitution of guava, mandarin and orange fruits. To the best of our knowledge, there is little data available about performance of high throughput passive sensing systems for assessing the biochemical parameters of guava and mandarin fruits via the application of chemometric techniques based on PCR, PLSR and simple linear or quadratic regression. As well as most of studies to estimate biochemical parameters of orange used spectroscopy techniques.

The purpose of this work was: (i) to establish correlation matrices (contour maps) for selecting the best spectral indices to estimate the biochemical parameters and discriminating between fruit kinds (ii) to study the stability of spectral indices for estimating the biochemical parameters of different fruit kinds and (iii) to compare the performance