JURNAL RONA TEKNIK PERTANIAN

ISSN : 2085-2614

JOURNAL HOMEPAGE : http://www.jurnal.unsyiah.ac.id/RTP

Rapid Classification Of Agricultural Products Based On Their Electro-Optic Properties Using Near Infrared Reflectance And Chemometrics

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Abstract

Near infrared technology have been widely applied in many fields, including agriculture especially in sorting and grading process. The advantage of this technology: simple sample preparation, rapid, effective and non-destructive. The main objective of this study is to evaluate the feasibility of NIR technology in classifying several agricultural products based on their electro-optic properties. NIR diffuse reflectance spectra of apples, bananas, mangoes, garlics, tomatoes, green grapes, red grapes and oranges were acquired in wavelength range of 1000-2500 nm with gradual increment of 2 nm. Chemometrics methods were applied in combination with NIR spectra data. Classification was performed by applying *principal component analysis* (PCA) followed by *non-iterative partial least square* (NIPALS) *cross validation*. The results showed that NIR and chemometrics was able to differentiate and classify these agricultural products with two latent variables (2 PCs) and total explained variance of 97% (88% PC1 and 9% PC2). Furthermore, it also showed that *multiplicative scatter correction* (MSC) was found to be effective spectra correction or enhancement method and increased classification accuracy and robustness. It may conclude that NIR technology combined with chemometrics was feasible to apply as a rapid and non-destructive method for sorting and grading agricultural products.

Keywords: NIR, chemometrics, classification, PCA

Rapid Classification Of Agricultural Products Based On Their Electro-Optic Properties Using Near Infrared Reflectance And Chemometrics

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Abstract

Aplikasi teknologi *near infra red* (NIR) telah digunakan dalam banyak bidang, termasuk untuk bidang pertanian terutama pada proses sortasi dan *grading*. Keunggulan metode ini antara lain : *rapid*, efektif, simultan dan tanpa merusak objek yang dikaji. Tujuan utama dari studi ini adalah untuk mengkaji potensi NIR dalam mengklasifikasi beberapa produk pertanian berdasarkan karakteristik sifat elektro-optik dari produk tersebut. Spektrum NIR pada panjang gelombang 1000 – 2500 nm dengan *increment* 2 nm diakuisisi untuk produk pertanian : apel, pisang, manga, bawang putih, tomat, anggur hijau, anggur merah dan jeruk. Metode chemo metrics digunakan dalam studi ini untuk dikombinasikan dengan spektrum NIR. Klasifikasi produk pertanian dilakukan dengan menerapkan metode *principal component analysis* (PCA) yang disertai dengan metode *non-iterative partial least square* (NIPALS) *cross validation*. Hasil studi menunjukkan bahwa kombinasi NIR dan *chemo metrics* mampu membedakan dan mengklasifikasi produk pertanian tersebut dengan menggunakan dua *latent variable* pada PCA (2 PCs) dengan *total explained variance* 97% (88% PC1 dan 9% PC2). Selain itu, dari studi ini juga didapatkan bahwa perbaikan data spectrum dengan metode *multiplicative scatter correction* (MSC) sebelum klasifikasi mampu meningkatkan akurasi hasil klasifikasi. Secara umum, dapat disimpulkan bahwa teknologi NIR dan *chemo metrics* dapat dijadikan sebagai metode yang efektif untuk sortasi dan atau grading produk pertanian.

Kata kunci: NIR, *chemometrics*, klasifikasi, PCA

INTRODUCTION

In foods and agricultural products processing, the quality evaluation of these products is an important issue. Consumers are gradually looking for quality seals and trust marks on food and agricultural products, and expect producers and retailers to provide products with high quality. In order to ensure and maintain the chain supply of acceptable agricultural products, it is important to sort and grade products based on their quality. Thus, quality control plays a major important role in in every phase of the agricultural products processing (Cen and He, 2007; Jha et al., 2012). To determine quality parameters in food and agricultural products, several methods are already widely used whereby most of them are based on solvent extraction followed by other laboratory procedures. However, these methods often require laborious and complicated processing for samples. Also, they are time consuming and destructive. Therefore, a rapid and non-destructive method is required as an alternative method in determining quality parameters of foods and agricultural products.

During the last few decades, near infrared spectroscopy (NIRS) has become one of the most promising and used non-destructive methods of analysis in many field areas including in agriculture due to its advantage; simple sample preparation, rapid, and environmental friendly since no chemicals are used. More importantly, it has the potential ability to determine multiple quality parameters simultaneously (Liu et al., 2010). Numerous studies have been carried out to investigate and apply NIRS in quality assessment of foods and agricultural products (Vesela et al., 2007; Gomez et al., 2006; Jaiswal et al., 2012; Liu et al., 2008; Curda and Kukackova, 2004; Kavdir et al., 2007; Liu et al., 2007; Cen et al., 2007; Chen et al., 2011; Fan et al., 2009; Bobelyn et al., 2010; Penchaiya et al., 2009). The increasing importance of NIRS in agriculture is obvious from the recent increase in numbers of publications, as well as from the fact that many manufacturers and agricultural industries (e.g., grains, beverage, milk and dairy, and fruits and vegetables) have now implemented NIRS systems to measure and determine various quality parameters (Nicolai et al., 2007; Cozzolino et al., 2011).

The NIRS is a technique or method which uses near infrared radiation (780 – 2500 nm) of the electromagnetic spectrum to analyze the chemical composition of organic matter. It provides information through spectra signatures and patterns, regarding with the intrinsic organic bonds of the molecules and thus the primary chemical constituents of the object can be determined (Strang, 2004; Workman and Shenk, 2004; Nicolai et al., 2007). The term spectroscopy as defined by Clark (1999) is the study of electromagnetic radiation as a function of wavelength, which has been reflected, absorbed or transmitted from a solid, liquid or gas material. Spectroscopy generates a unique spectral pattern of the material monitored. Each biological object has its own special optical properties, which means it has a different spectra pattern or signatures indicated its chemical compositions. The spectral patterns of different matter are defined by their reflectance or absorbance as a function of wavelength (Siesler et al., 2002). These special signatures were then used to describe and predict the chemical constituents of biological matter.

Since NIRS itself cannot reveal chemical information in the spectra, chemometrics is required to extract the information about quality attributes buried on NIR spectra through a process called multivariate calibration from which a mathematical relationship between NIR spectra and the measured quality parameter will be revealed to determine desired quality attributes.According to Naes et al. (2004) chemometrics is the use of statistical and mathematical procedures to extract information from chemical and physical data. It has been used to extend and improve the potential application of NIRS technique in many fields including food and agricultural industries. In NIRS analysis, this method is includes three facets: (1) spectral data pre-processing to eliminate noise and enhance spectra prior to models development, (2) building calibration models for quantitative and qualitative analysis and (3) model transfer for real-time and in-line prediction (Cen and He, 2007). Therefore, the main objective of this study is to evaluate the feasibility of NIRS method combined with chemometricsin classifying different agricultural products based on their electro-optics properties.

RESEARCH METHODS

1. Samples and instrumental setup

This study was performed at the laboratory of quality analysis, process engineering and electronic application, Georg-August University of Goettingen, Germany. Samples used in this study are several agricultural products: apples, bananas, red grapes, tomatoes, garlics, green grapes, mangos and oranges. These samples were selected and purchased randomly in local auction markets in Goettingen. Instrument used in work is a Fourier transform near infrared (FT-NIR) instrument (Thermo Nicolet, Antaris model MDS-method development sampling). The instrument was set in optical gain 8x and saved in three different files format (*.spa, *.csv and *.jdx) for further analysis.

2. Spectra acquisition of agricultural products

NIR spectra data of all samples were acquired using a benchtop FT-NIR instrument. High resolution (2 nm interval) sample measurement with integrating sphere was chosen as a basic measurement in this study. Background spectra correction was performed every hour automatically. Samples were placed manually upon the measurement window of the integrating sphere (1 cm of diameter) of the light source to ensure direct contact and eliminate noise. Diffuse reflectance (Log 1/R) spectra in wavelength range of 1000 – 2500 nm with 2 nm resolution were acquired 64 times and averaged.

3. Spectra data pre-processing

The spectra data acquired from NIR instrument may contain spectra background information and noises which are interfered desired relevant quality attributes information. Thus, spectra pre-processing was performed prior to further chemometrics analysis. Multiplicative scatter correction (MSC) and standard normal variate (SNV) were used for this purposes. MSC is used to compensate for additive (baseline shift) and multiplicative effects in the spectral data, whilst SNV is normalized to zero mean and unit variance (Naes et al., 2004; Nicolai et al., 2007; Cen and He, 2007).

4. Classification using principal component analysis (PCA)

Corrected and enhanced NIR spectra data were subjected to PCA in order to identify and classify samples based on their similarities. These similarity was based on electro-optic properties buried in the spectra for each individual samples. PCAemploys a mathematical procedure that transforms a set of possibly correlated response variables into a new set of non-correlated variables. During classification by PCA, a non-iterative partial least square (NIPALS) cross validation was applied to verify classification accuracy (Cozzolino et al., 2011; Reich, 2005).

RESULTS AND DISCUSSION

In NIRS, the object is irradiated with near infrared radiation and the reaction (reflection, absorption or transmission) is captured. While the radiation penetrates the object, its spectral characteristics changes through wavelength dependent scattering and absorption process. The contribution of each reaction depends on the chemical composition, cell structure and physical properties of the object. A captured NIR spectra of biological object consists the response of the molecular bonds O-H, C-H, C-O and N-H. These bonds are subject to vibrational energy changes when irradiated by NIR frequencies.

The primary information that can be gathered from the interaction of the near-infrared radiation with the biological object is its physical, optical and chemical properties. Fruit, grain and forage material have shown to have identifiable C-H, N-H, and O-H absorption bands in the near-infrared region whereas each have a specific vibrational frequency and it is different between one object and the others. Figure1 shows typical diffuse reflectance spectra of NIR for some selected agricultural products.

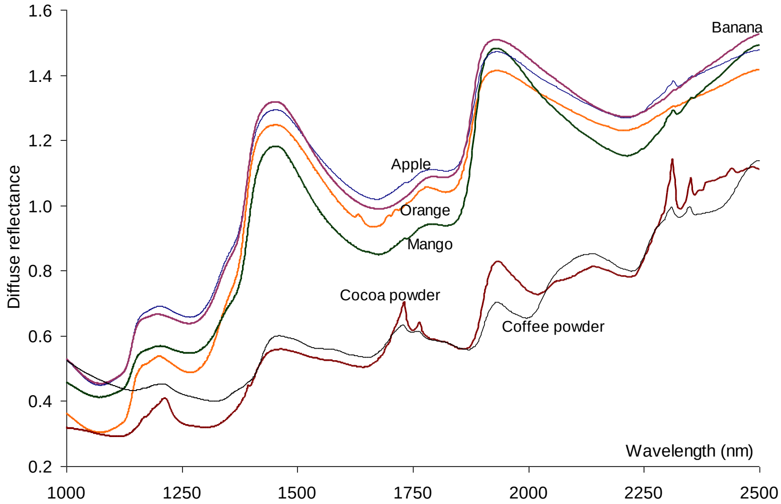

Figure 1. Typical diffuse reflectance spectra of some agricultural products. The near infrared reflectance spectra were acquired using a FT-NIR instrument.

NIR spectra of fruits and vegetables is essentially composed of a large set of overtones and combination bands and further may be complicated since the spectra is influenced by wavelength dependent scattering effects, tissue heterogeneities, instrumental noise, ambient effects and other source of variability. These factors may generate spectra noise and influence NIR prediction performance. Several methods are introduced as spectra pre-treatment to overcome these factor effects.

Multiplicative scatter correction (MSC) and standard normal variate (SNV) are the most popular normalization technique. MSC is used to compensate for additive and multiplicative effects in the spectral data, which are induced by physical effects, such as the non-uniform scattering throughout the spectrum. The degree of scattering is dependent on the wavelength of the radiation, the particle size and the refractive index. This method attempts to remove the effects of scattering by linearizing each spectrum to an ‘ideal’ spectrum of the sample, which is normally corresponds to the average spectrum. On the other hand, in SNV each individual spectrum is normalized to zero mean and unit variance. Apart from the different scaling, the result is more-less similar to that of MSC.Figures2 shows a visual result after spectra pre-processing.

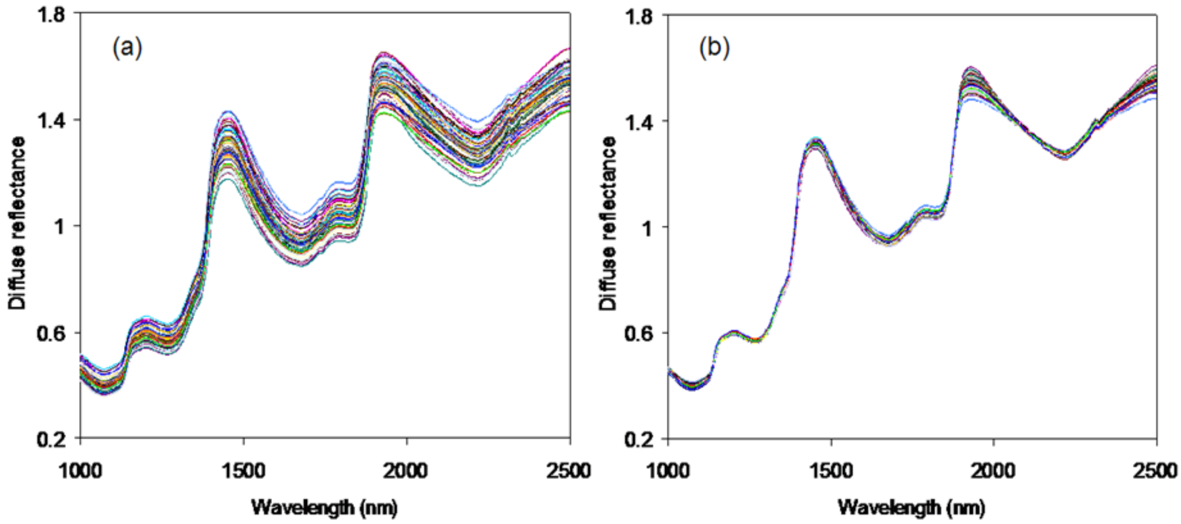

Figure 2.(a) Raw untreated near infrared spectra and (b) after multiplicative scatter correction

Enhanced spectra data were then subjected to PCA in order to obtain clear distinction of selected samples based on their electro-optic properties. Figure 3 shows the best PCA result derived from MSC spectra data.

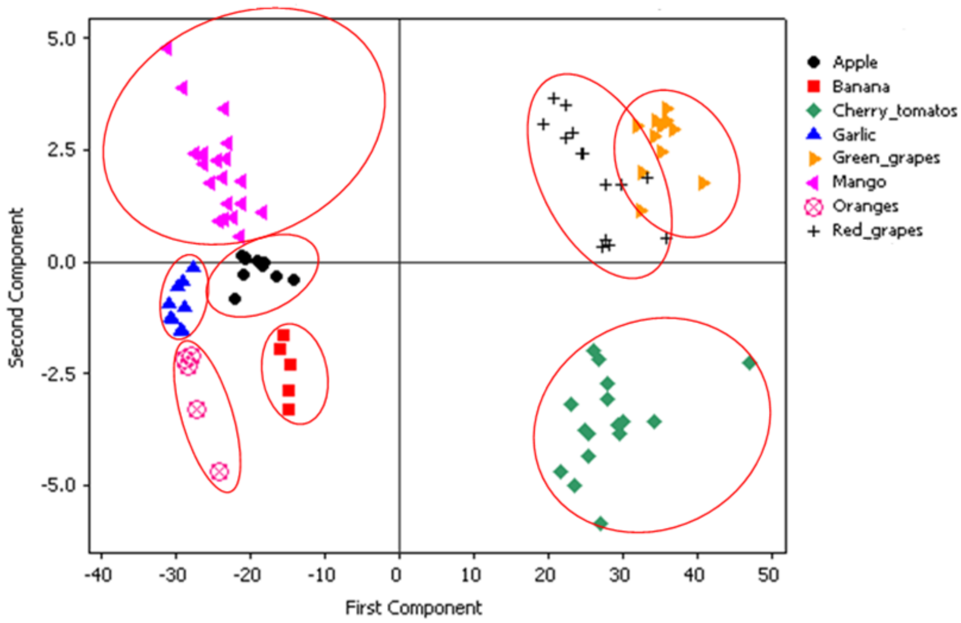

Figure 3. PCA classification of some agricultural products based on near infrared reflectance diffuse reflectance spectra data.

The first principal component accounts for as much of the variability in the data as possible, and each succeeding component accounts for as much of the remaining variability as possible. In this study, classification was successfully accomplished by using two principal components (PCs) with a total explained variance 97% (88% PC1 and 9% PC2). Red and green grapes clearly in the same region since they represent grapes 'family' and nearby to tomatoes. It is obvious since these mentioned samples are typically have a high amount of moisture contents. The remaining studied samples were mapped in another region. The loading analysis of PCA described the potential and relevant wavelength corresponded to PCA classification result. NIR wavelength of 1490 and 1920 are the most two relevance wavelength for the classification. These two wavelengths are corresponded to O-H vibration and related to moisture content of the biological object. This result was also in agreement with Cen and He (2007) from which they found the presence of strong water absorbance bands was observed at around 1460 nm and 1930 nm because of O-H tone combination and its first overtone. Absorption bands at around 1400 nm and 1900 nm were previously assigned to water absorption (Workman and Weyer, 2008).

The size of the coefficients founded in PCA loading analysis indicates which independent variables (wavelengths) significantly impact on the response variables (referred quality attributes). Wavelengths having higher absolute value of regression coefficient than others, located at the peaks or valleys of the spectrum, were noted as the important or effective wavelengths that contributed more to the models.

CONCLUSION

Based on our study, it may conclude that NIR technology combined with chemometrics are suitable and feasible to identify and classify several agricultural products based on their electro-optic properties. Further, these combination methods may be used as an online screening, sorting and grading of agricultural products.

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