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Classification of food vegetable oils by fluorimetry and artificial neural networks

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ABSTRACT

There is a large variety and trademarks of vegetable oils in Brazil. Vegetable oils have characteristics quite similar to each other and often cannot be distinguished by only observing the color, odor or taste. Methods for classification of these oils are often costly and time consuming and they usually take advantage of techniques from analytical chemistry and mathematical methods such as PCA (Principal Component Analysis), PCR (Principal Components Regression) or PLS (Properties of Partial Least Squares) and ANN (Artificial Neural Networks) to increase their efficiency. Due to the wide variety of products, more efficient methods are needed to qualify, characterize and classify these substances, because the final price should reflect the excellence of the product that reaches the consumer. This paper proposes a methodology to classify vegetable oils like: Canola, Sunflower, Corn and Soybean from different manufacturers. The method used is characterized by a simple mathematical treatment, a light emission diode and CCD array sensor to capture the spectra of the induced fluorescence in diluted oil samples. An ANN that has three layers, each one with 4 neurons is responsible to perform the spectra classifications. The methodology is capable of classifying vegetable oil and allows fast network training using very few mathematical manipulations in the spectra data with 72% a rate of success.

1. Introduction

Rapid and nondestructive measurements of quality-related parameters in foods are advancing due to progress in spectroscopy and development of new sensor technology including cameras and spectrophotometers (Skjervold et al., 2003). Advances in spectroscopy now enable researchers to obtain information about chemical and physical components in food or biological materials at the molecular level. Various spectroscopic techniques (e.g., atomic absorption spectroscopy, Raman and Fourier-transform infrared spectroscopy, near infrared spectroscopy, nuclear magnetic resonance spectroscopy, mass spectroscopy, X-ray fluorescence spectroscopy, ultra-violet spectroscopy) have been used to study structure-function relationships in foods (both liquid and solid) to improve overall food quality, safety and sensorial characteristics; to investigate fungal infections in plant materials (e.g., fruits, seeds); or to study the mobility of different chemical components in food materials. Processing, analyzing, and displaying these data can often be difficult, time-consuming, and problem-specific. Chemometrics is well established for calibrating the spectral data to predict concentrations of constituents of interest (Ghosh & Jayas, 2009). The fluorescence signals are complex data with fluorophore fingerprints that overlap themselves. Their processing take a long time and require powerful hardware and software (Vasilscu, Marmureanu, & Carstea, 2011). Fluorescence spectroscopy has been investigated among other uses as a tool for quantification of components of meat (Wold, Lundby, & Egelandsdal, 1999), and also related to structural properties of meat and cheese (Dufour, Devaux, Fortier, & Herbert, 2001; Dufour & Frencia, 2001; Lopez & Dufour, 2001), polyphenolic content in beverages (Andreu-Navarro, Fernandez-Romero, & et al., 2012) and to differentiate yeast and bacterial cells (Bhatta, Goldys, & Learmonth, 2006).

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Chemometrics is related to all those processes which transform analytical signals and complex data into useful information (Mujica-Ascencio, Moreno-Garcia, Stolik-Isakina, & de la Rosa-Vazquez, 2010). Traditional analysis of fluorescence spectroscopy is either uni- or multi-variate. Univariate analysis focuses in finding a pair of excitation-emission wavelengths where there is only one or a few known components giving rise to the signal. Wold et al. (1999) introduced the advantages of combining fluorescent images with fluorescence spectra.

During the last years, the Artificial Neural Networks and Channels Relationships methods have been frequently used to process spectral signals (Almhdi, Valigi, Gulbinas, Westphal, & Reuter, 2007). Artificial Neural Networks (ANNs) for modeling and simulating have become popular in energy sources, chemical engineering, water treatment, and control domain, among others (Jaafarzadeh, Ahmadi, Amiri, Yassin, & Martinez, 2012). ANN and their application in food chemistry and food science are described by Goyal (2013) and Marini (2009). ANN can be described as a mathematical model of a specific structure, consisting of a number of the single processing elements (nodes, neurons), arranged in inter-connected layers. An active neuron multiplies each input vector by its weight, sums the products and passes the sum through a transfer function to produce the output (Bieroza, Baker, & Bridgeman, 2011). The ANN is made up of a group of interconnected artificial neurons. It consists of an input, hidden and an output layers. Each layer is also composed of neurons. Each neuron transforms input and sends outputs to other neurons to which it is connected. Weights and bias are determined from the receiving neurons. The network is trained with a subset or dataset of observations and optimized based on its ability to predict a set of known outcomes (Klaypradit, Kerdpiboon, & Singh, 2011).

Marine, Dyer, and Jochemsen (2007) employed a combination of two different neural networks architectures for the resolution of simulated binary blends of olive oils from different cultivars. Cámara, Fernández-Ruiz, Redondo, Sánchez-Mata, and Torrecilla (2012) modeled Lycopene degradation kinetics in tomato-based products using a radial basis network (RBN) obtaining a mean prediction error lower than 2.62% and a correlation coefficient higher than 0.983, they concluded that the RBN mathematical approach proposed can be considered as a reliable tool to monitor the stability of lycopene in tomato products (juices, sauces and ketchups) during its shelf life and may be a useful tool for tomato industry. Scott, James, Ali, O'Hare, and Rowell (2003) used ANNs for pattern recognition of olive oil fluorescence spectra. Chen et al. (2012) used ANN to classify honeys by their near infrared spectra. Groselj, Vracko, Pierna, Baeten, and Novic (2008) studied olive oil adulteration with hazelnut oils using the Counter-propagation Artificial Neural Networks (CP-ANN) model. Torrecilla, Rojo, Oliet, Domínguez, and Rodríguez (2010) used self-organizing maps and learning vector quantization networks as tools to identify vegetable oils and detect adulterations of extra virgin olive oil.

In the food industry, food safety and quality are considered important issues worldwide that are directly related to health and social progress. Consumers are increasingly looking for trusted brands of food products, and expect manufacturers and retailers to provide high quality products (Gori, Cevoli, Fabbri, Caboni, & Losi, 2012).

Increased consumer awareness of food safety and quality issues has led to the development of new and increasingly sophisticated techniques for food product authentication. However, most of these techniques are time consuming, and require extensive sample preparation and hazardous chemicals as well as skilled and experienced operators (Gori et al., 2012). These disadvantages have prompted for the adoption of new and simpler methods such as fluorimetry.

Due to the large variety of brands and trademarks of vegetable oils in the Brazilian market, it is common not to know for sure if the substance that is being bought is really a product without adulteration. Vegetable oils have characteristics quite similar to each other and often cannot be distinguished by only observing of the color, odor or taste. In this work we propose a method to classify vegetable oils: Canola, Sunflower, Corn and Soybean using a very few mathematical manipulation and ANN – Artificial Neural Networks as a tool to differentiate the fluorescence spectrum of these oils.

2. Material and methods

2.1. Instrument developed

The instrument used in data acquisition is a spectrofluorometer type LED/CCD that has been developed in the Laboratory of Optical Properties (LAPO) at the Federal University of Bahia (UFBA)-Brazil. This equipment is able to obtain fluorescence spectra between 350 nm and 1050 nm. This equipment was patented in 2012 and can be found in the QUIMIS catalog under the ticker Q-798FIL.

The spectrofluorometer schematic diagram is shown in Fig. 1. As a source of excitation light, a LED (Light Emitting Diode) is used. The sample holder can receive standard cuvettes of 3.5 mL, micro cuvette or microscope slides. Fluorescence light collection is made at 90° from the light source excitation at a fixed distance. The LED emits light with short wavelength on the sample, which, in its turn, emits fluorescent light at another wavelength. The detector captures both the fluorescence light from the sample and the scattered light of the LED optical system.

The LED used as the excitation light source was manufactured by Nichia Corp. Am. (part number NSPu510CS) type ub9. The choice of this particular LED is due to its known ensured traceability (a nearly Gaussian emission profile centered at 382 nm, with a width of 13.054 nm) that guarantees the quality of the light source and ensure standard exchange for maintenance.

2.2. Samples

At local shops in the city of Salvador, one can find 10 trademarks of vegetable oils. Some of them produce more than one kind of vegetable oil. Choosing four vegetable oils (Canola, Sunflower, Corn and Soybean) they can be grouped at 6 different trademarks for each vegetable oil. Twenty dilutions were produced for each oil,

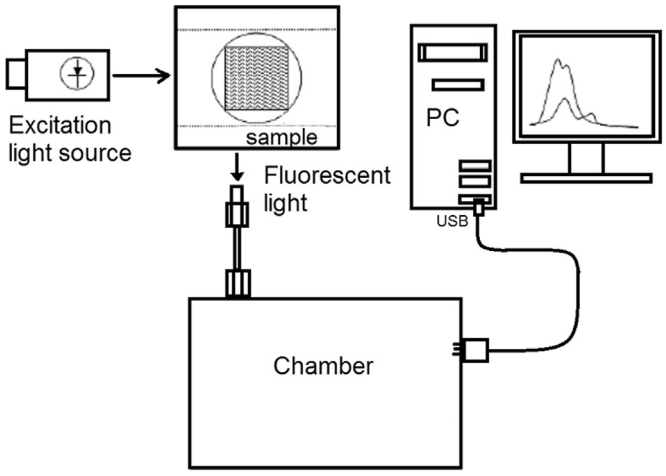

Fig. 1. Diagram of the spectrofluorimeter LED/CCD Q-798FIL.