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Employing artificial neural networks and fluorescence spectrum for food vegetable oils identification

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Abstract

Vegetable oils (VOs) come in a wide range of flavors and trademarks. VOs are very similar in appearance, flavor, and taste, and it's frequently difficult to tell them from just by looking at them. Approaches for classifying these oils are sometimes expensive and time-intensive, and they frequently include analytical chemical techniques as well as mathematical algorithms like as Artificial Neural Networks (ANNs), Properties of Partial Least Squares (PLS), Principal Components Regression (PCR), and Principal Component Analysis (PCA) to enhance their effectiveness. Because of the large range of goods available, more productive techniques for qualifying, characterizing, and classifying these substances are required, as the ultimate cost should indicate the quality of the commodity that reaches the user. This study provides a technique for classifying VOs such as different manufacturers' soybean, corn, sunflower, and canola. This method utilized a Charge-Coupled Device (CCD) array sensor, a light emission diode, and a straightforward mathematical approach to capture the generated fluorescence spectrum (FS) in diluted oil. The spectrum classifications are performed using an ANN with three layers, each having four neurons. The approach can categorize VO and enables rapid network training with a 72% success rate utilizing only a few mathematical changes in the spectra data.

Keywords: vegetable oils quality; spectrometry; food; mathematical treatment.

Practical Application: Food vegetable oils identification using artificial neural networks and fluorescence spectrum.

1 Introduction

Because of advances in spectroscopy and the development of novel sensor technologies such as spectrophotometers and cameras, non-destructive and rapid assessments of quality-related factors in foods are becoming more common (Groß et al., 2019; Kucha et al., 2018). Researchers may now acquire data at the molecular level regarding physical and chemical components in food or biological materials because of advancements in spectroscopy (Abasi et al., 2018). Spectroscopic methods (e.g., ultra-violet spectroscopy, X-ray fluorescence spectroscopy (FS), mass spectroscopy, nuclear magnetic resonance spectroscopy, near-infrared spectroscopy, Fourier and Raman-transform infrared spectroscopy, atomic absorption spectroscopy) have been used to analyze infections caused by fungi in plant materials (e.g., seeds, fruits), to enhance the overall quality of food, safety, and sensory qualities, to explore structure-function connections in foods (both solid and liquid), and to study the movement of various chemical constituents in food ingredients (Boyaci et al., 2015; Esteki et al., 2018; Franca & Nollet, 2017; McQueen et al., 1995; Nawrocka & Lamorska, 2013; Petersen et al., 2021; Pignataro et al., 2020; Shi et al., 2012; Szmatoła et al., 2018; Wang et al., 2017). It's typically complicated, problem-specific, and time-consuming to process, analyze, and show this data. Chemometrics is a well-established method for adjusting spectral data (Andre & Soukoulis, 2020; Granato et al., 2018; Xu et al., 2020). Fluorescence signals are multi-dimensional data with overlapping fluorophore fingerprints (Yıldız et al., 2017). Their processing is time-consuming and necessitates the use of sophisticated gear and software (Nishi et al., 2015; Ren et al., 2014). FS has been studied for a variety of applications, including the measurement of meat components, structural characteristics of cheese and meat, polyphenolic concentration in drinks, and yeast and bacterial cell differentiation, among others (Hassoun et al., 2019; Karoui & Blecker, 2011; Sahar et al., 2016; Sikorska et al., 2005).

Chemometrics refers to all of the procedures that convert complicated data and analytical signals into usable knowledge. FS is usually analyzed in one of two ways: univariate or

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multivariate. The goal of the univariate analysis is to discover a couple of excitation-emission wavelengths in which the signal is produced by just one or a few known components (Ali et al., 2018; Christensen et al., 2005; Sádecká & TóthoVá, 2007; Sikorska et al., 2019). Artificial Neural Network (ANN) and Channel Relationships techniques have been widely utilized to handle spectral data in recent years (Silva et al., 2015; Vasilescu et al., 2011). ANNs for simulation and modeling have gained popularity in various fields, including control, water treatment, chemical engineering, and energy (Molajou et al., 2021; Nourani et al., 2019a, b). The use of ANN in food chemistry and research is investigated (Gonzalez-Fernandez et al., 2019; Haroni et al., 2018; Zhou et al., 2019). ANN is a mathematical model of a certain structure made up of several single processing components (neurons, nodes) stacked in interconnected layers (Sharghi et al., 2018; Sharghi et al., 2019; Nourani et al., 2019c). Each input vector is multiplied using its weight, the products are added, and the sum is sent through a transfer function to generate the output (Bisgin et al., 2018). An ANN is made up of a collection of artificial neurons that are linked together. It has three layers: one for input, one for hiding, and one for output. Neurons can be found in each stratum. Each neuron receives information and changes it before sending it to other neurons with whom it is linked (Hernández, 2009; Pouladzadeh et al., 2016). The receiving neurons are used to calculate weights and biases. The network is tuned based on its capability to forecast a set of known outcomes using a subset or dataset of observations (Dash et al., 2020; Goñi et al., 2008).

Marine et al. (2007) used a mixture of two distinct neural network architectures to resolve simulated binary mixes of olive oils from various cultivars. Cámara et al. (2012) concluded that the Radial Basis Network (RBN) mathematical method proposed may be considered a reliable approach to monitor the stability of lycopene in tomato products (ketchups, sauces, and juices, etc.) during their shelf life and maybe a useful approach for monitoring lycopene degradation kinetics in tomato-based products using RBN with a mean prediction error lower than 2.62% and a correlation coefficient (CC) higher than 0.983. Also, artificial neural networks were used to recognize patterns in the FS of olive oil (Gonzalez-Fernandez et al., 2019).

Food safety issues are major concerns in the food business that are linked to social and health advancement on a global scale (King et al., 2017; Olaimat et al., 2020). Consumers are increasingly searching for trustworthy food brands, and producers and merchants are expected to deliver high-quality goods (Fung et al., 2018). Food product authentication has become more complex as customer knowledge of food safety and quality problems has grown. However, the majority of these procedures are time intensive and need significant sample preparation, dangerous chemicals, and experienced and professional personnel (Ashurst & Dennis, 2013; Danezis et al., 2016). Because of these drawbacks, new and easier techniques, such as fluorimetry, have been developed.

According to the vast number of trademarks for vegetable oils (VOs) on the Marketplace, it's usual to have doubts about whether the purchased material is truly pure. VOs have a lot of similarities in terms of color, smell, and flavor, and it's frequently impossible to tell them from just by looking at them. In this paper, based on a few mathematical manipulations and the use of ANN to distinguish the FS of VOs, we present a technique for their classification.

2 Material and methods

The data was collected using a spectrofluorometer type CCD/LED created at the Federal University of Bahia (UFBA) in Brazil's Laboratory of Optical Properties (LAPO). FS between 350 and 1050 nm may be obtained using this apparatus. This apparatus was patented in 2012 and is listed in the QUIMIS catalog as Q-798FIL (Meira et al., 2014, 2015; Tomazzoni et al., 2014). Figure 1 indicates a schematic diagram of a spectrofluorometer. A Light Emitting Diode (LED) is utilized as the source of

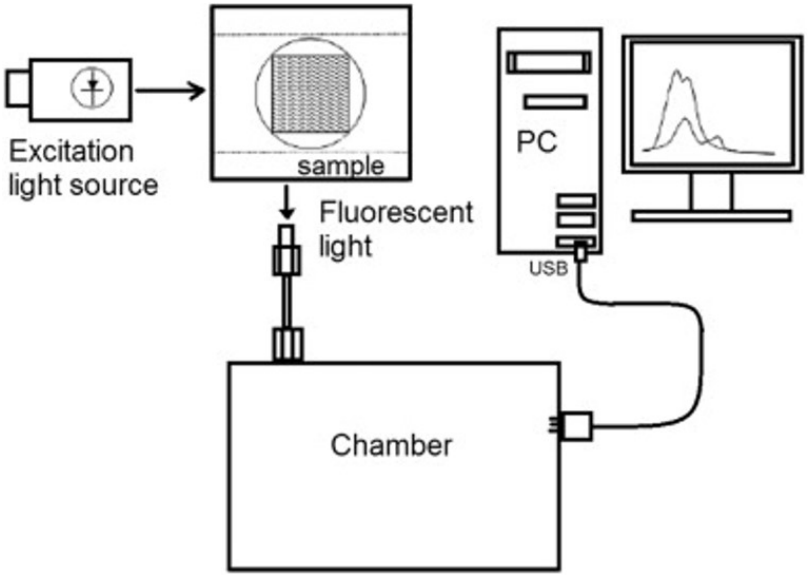

Figure 1. The LED/CCD spectrofluorimeter Q-798FIL.

excitation light. Standard 3.5 mL cuvettes, microscope slides, or micro cuvettes may all be placed in the sample container. The LED emits short-wavelength light on the sample, which is then converted into fluorescent light of a different wavelength. The detector captures both fluorescence light from the sample and dispersed light from the LED optical system.

There are ten different VO brands available at local shops in Salvador. Several of them make several different types of VO (Soybean, Corn, Sunflower, and Canola). Using four distinct VOs, they may be categorized into six separate brands. Each oil was divided into twenty dilutions, yielding 480 samples in total. The neural network was trained using them. We created 158 additional samples from another batch, using two brands for each oil, to construct the validation set employing the same technique. Every sample was made by diluting the VO in heptane in a volume of 30 mL and varying the amount of the VO from 5% to 100% in 5% increments. Oils of the same labels used during training but from various production batches were utilized to validate the network and the categorization technique created.

2.1 Data collection and analysis

A 382 nm light-emitting diode was used as the excitation source for the FS. The CCD was maintained active for 1000 ms during the fluorescence light collecting. This time is referred to as integration time, and it is used to charge the metal–oxide–semiconductor (MOS) structure of each CCD pixel. The electrons from the CCD's active outer layer, where the photoelectric effect occurs, charge the CCD like an "almost capacitor." The data carried by the fluorescence photons is accumulated in the form of electrical charge as a result. The apparatus is cleared of its content at the conclusion of the integration time. An analog to digital converter receives the voltage gathered in each pixel and converts it to digital, resulting in wavelength data and light intensity in a two-dimensional array. To obtain spectral data, each sample was exposed to light for 15 seconds. It was necessary to conduct certain mathematical calculations:

1) The LED spectrum A was first subtracted from the overall spectrum to get the sample fluorescence known as FLU.
2) Following that, a constant C was used to split the FLU.

The maximum fluorescence intensity observed for the sum of 640 samples was C = 10,422.95 in this research (100% corn oil). This division facilitates comparisons by obtaining normalized spectra (NOR).

2.2 Ann training

The number of neurons in the hidden layer of the ANN was changed from 3 to 13 to get the best possible classification results. The number of successful examples in the hidden layer dwindled as the number of neurons increased. In the buried layer, there were four neurons with the most effective instances. The best efficiency was found between 1 and 4000 nm across a wide range of weights. The network mistakes were considerably different while utilizing shorter gaps for the weights. The feedforward supervised approach was utilized for training the ANN in this study, as shown in Figure 2. Each layer of the ANN has four neurons. The material to be categorized is described as follows in the output layer. Each neuron's output has a binary value of false (0) or true (1), and there are no combinations with more than one true neuron. As a result, the scenarios that may occur are as follows: for Soybean [0 0 0 1], for Corn [0 0 1 0], for Sunflower [0 1 0 0], and for Canola [1 0 0 0].

MATLAB® was used to create the neural network. As previously stated, several alternative layouts and network parameters were explored, with the configuration with four neurons in each layer providing the best results.

3 Results and discussion

An empty bucket was put in the sample container in order to get the spectrum A mentioned before. To put it another way, it's a device that doesn't contain any samples. Figure 3 shows the spectrum of LED excitation. Light dispersed by the bucket walls reaches the detecting fiber. The spectrofluorimeter employed can measure fluorescence light between 350 and 1050 nanometres, as seen in this diagram. The existence of LED light (382 nm) was obviously reliant on the quantity of dispersed excitation light

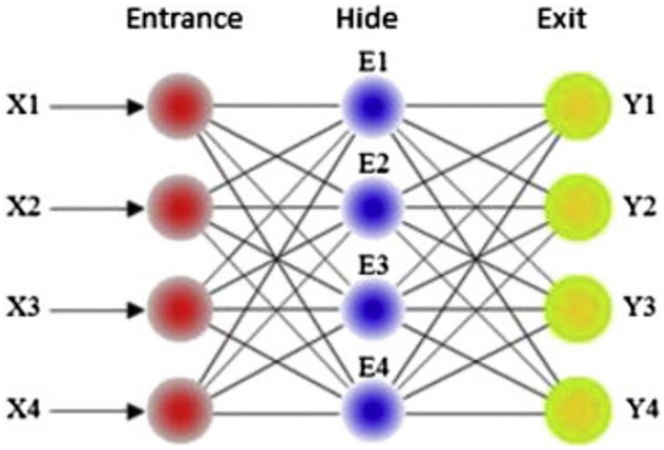

Figure 2. ANN model.

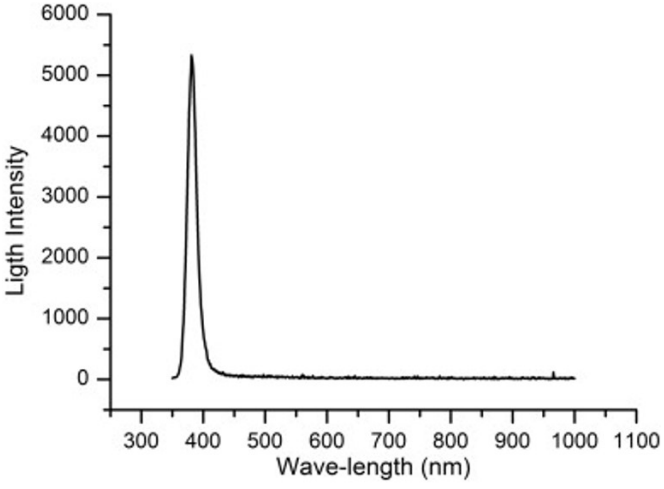

Figure 3. The empty fluorimeter/ LED spectrum's light spectrum.

that did not interact with the fluorescent medium in certain samples, as shown by the measured spectra. The dispersed light from the LED was more prominent for tiny quantities of the oils at various dilutions. Spectra of canola oil (Bom Preço brand) samples at various dilutions ranging from 5 to 100% are shown in Figure 4.

Figure 5 shows the spectra of all VOs (soybean, corn, sunflower, and canola) utilized at a concentration of 100% for the excitation light (LED) centered at 382 nm. Although the spectra were comparable, having peaks that were extremely near to one another, the intensity of light was very different. The numerical separation of even extremely close peaks was possible. As a result, the FS were highly distinctive and could be utilized to determine the oil type.

Nikolova et al. (2012) discovered similar spectra as well. When the network training time was compared to the training time for the previous approach in all spectra (Silva et al., 2015), the network training was determined to be 1.2 times quicker. As previously stated, The LED spectrum was removed from the total spectrum as the only mathematical treatment of the spectra and the result was divided by 10.42295. The spectra for the various VOs utilized in ANN training are given in Figure 6, resulting from this mathematical method.

In the validation tests, the ANN's responses are shown in Table 1. The approach was successful in 2 situations, and the best effects may be seen in soybean (brand Liza) and corn (brand Mazola) oils. Only 5 of the Sunflower oil (brand Bom Preço) samples were accurately identified, which was the poorest

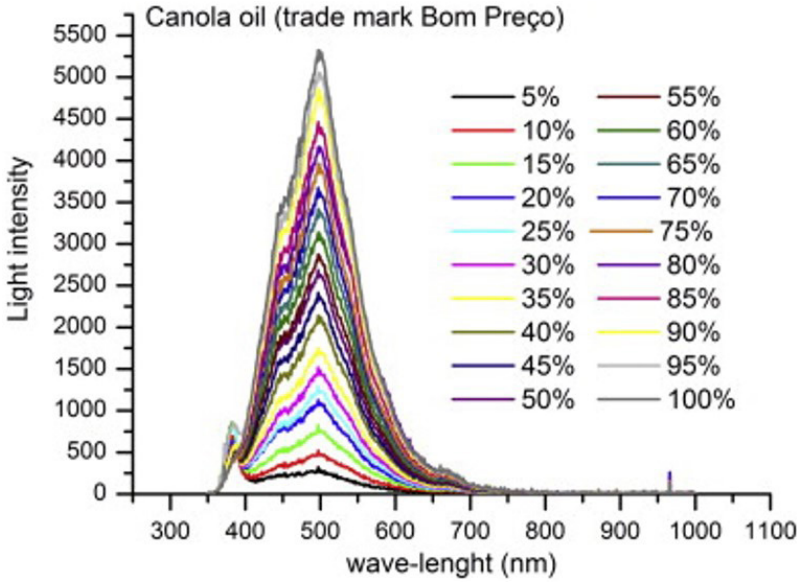

Figure 4. Canola oil light spectra at concentrations ranging from 5% to 100%.

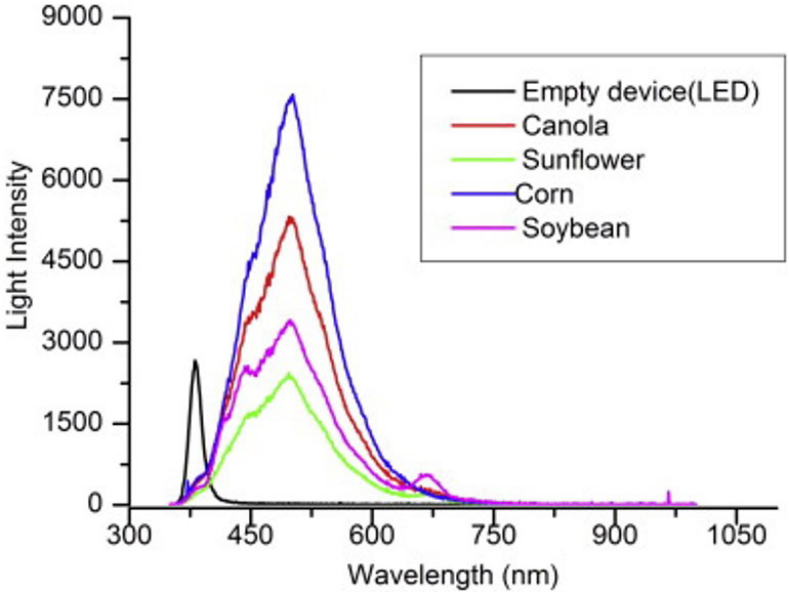

Figure 5. Four VOs' light spectra and an empty apparatus.

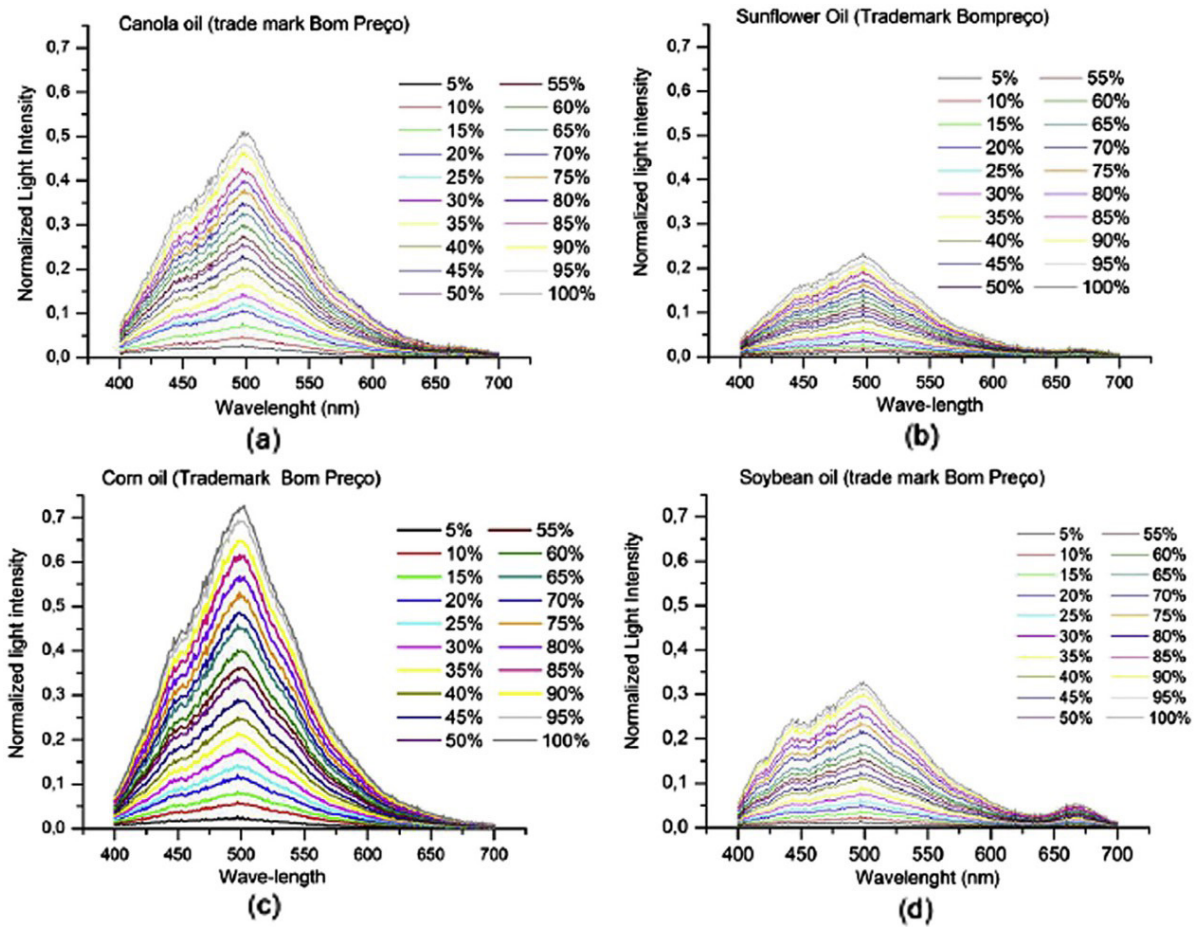

Figure 6. After the mathematical procedure, the spectra of soybean, corn, sunflower, and canola oils (Bom Preço brand) were obtained.

Table 1. The ANN's responses in 158 validation tests.

Oil	Trademark	Total success in 20 samples
Soybean	Soya	18
Corn	Salada	18
Canola	Qualitá	10
Corn	Mazola	20
Sunflower	Liza	18
Soybean	Liza	20
Canola	Bom Preço	17
Sunflower	Bom Preço	5

result of all. During earlier testing, it was discovered that some Sunflower samples' FS have been much more identical to those of canola oil samples, and the network was unable to differentiate between them.

A technical modification of fats and oils allows more flexibility in the selection of raw materials and helps to adjust the trends among local supply and demand in order to satisfy market demands and offer homogenous products from raw variables.

4 Conclusions

It was decided to create an approach based on artificial neural networks. This approach enables quick network training and only utilizes a few arithmetic operations on the spectra data. From the perspective of VO quality management, this is a promising technique that may be utilized to design future research focusing on the resolution of actual blends of oils from different cultivars, namely for soybean and corn oils. More research on canola and sunflower oils is needed to enhance categorization precision. The requirement for thorough research of the features that characterize the regions of interest across the FS is confirmed by this novel technique, which uses the most relevant characteristics of the FS as input data for ANN. Thus, interpreting the data from FS of VOs and other more sophisticated compounds requires first examining the fluorescence of the basic components that make up the samples to be examined.

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