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Artificial neural networks to authenticate Virgin Coconut Oil adulterants using FTIR spectral data

[1]USHA RANI D, [2]PANDURANGAN M K, [3]M.RADHA MADHAVI
[1,3] DEPARTMENT OF MATHEMATICS, AGNI COLLEGE OF TECHNOLOGY, THALAMBUR, CHENNAI-130
[2]DEPARTMENT OF MATHEMATICS, PACHAIYAPPA'S COLLEGE, CHENNAI-30, Tamil Nadu
Email: usharani.sh@act.edu.in, kannappan.pandurangan@gmail.com

ABSTRACT
The present study the experimental validation of FTIR spectroscopy for the detection of adulteration in edible oil. The variation in blends in the spectral data from different proportions of adulterated oil were used for developing the to detect the adulteration. The adulteration of 5% palm oil of the virgin coconut oil does not reveal any significant, whereas, an adulteration form of adulteration in the mustard oil 15% reveal 65.90% virgin coconut oil and palm oil 15% reveal 62.8% virgin coconut oil.

KEYWORDS:

FTIR spectroscopy, artificial neural network, adulterants.

1.0 Introduction

Adulteration in food products means the addition of prohibited substance either partly or wholly in the state of financial gain or lack of hygienic conditions of processing and storing which leads to the consumer being cheated. Ignorance of this fact is, not fair since this may endanger consumer health. For most of the vegetable oil, the adulteration detection method is based on conventional chemical tests.

In the last decades important researches in the area of artificial intelligence were developed. One of the main objectives of the science is the implementation of new technology capacities approaching the human being, and even better. Artificial intelligence is a powerful accomplishment in various fields, since it can supplement the human being in various activities, both easy to perform, how complex and even impossible to make as it is carrying out an activity without interruption for long periods of time and where knowledge is required. In the search on the nature of intelligent mechanisms to try to develop machines that perform complex tasks, it is important to observe certain characteristics of human brain that can be considered crucial to the development of artificial neural networks (ANN).

Artificial neural networks are control systems necessary to solve problems in which the analytical methods are difficult to apply and their results have to be in a specific interval.

An ANN is the development of mathematical algorithms that will enable ANNs to learn by mimicking information processing and knowledge acquisition in the human brain. ANN models contain layers of simple computing nodes that operate nonlinear summing devices. These nodes are richly interconnected by weighted connection lines, and the weights are adjusted when data are presented to the network during a "training" process. Successful training can result in artificial neural networks that perform tasks such as predicting an output value, classifying an object, approximating a function, recognizing a pattern in multifactorial data, and completing a known pattern (Basheer and Hajmeer, 2000; Jimenez *et al*., 2009). In the present investigation to detect virgin coconut oil adulterants using FTIR spectral data.

2.0 Materials and methods

2.1. Sample preparation

Virgin Coconut Oil (VCO) adulterated with cheap oil (easily miscible with VCO varying from 5% to 15%) is used for this study. We have used palm oil and mustard oil as adulterant in this study and performed the experiment by maintaining constant room temperature 30°C.

2.2 FTIR spectra measurement

FTIR spectra of analyzed oil samples were recorded using Nicolet 6700 FTIR spectrometer (Thermo Nicolet Corp, Madison, WI) equipped with deuterated triglycine sulphate (DTGS) as a detector and potassium bromide (KBr)/Germanium as a beam splitter, and connected to software on the OMNIC operating system (Version 7.0 Thermo Nicolet). FTIR spectra were collected from 32 scans at a resolution of 4 cm^{-1} with strong apodization throughout the mid infrared region (4000–650 cm^{-1}). These spectra were subtracted against background air spectrum. After every scan, a background of the new reference air spectrum was taken. These spectra were recorded as absorbance values at each data point in triplicate.

2.3 Neural Networks

To improve the accuracy, we developed ANN based algorithm also. ANN is a model free estimator and learning highly non-linear input-output relationship through a process called learning (Haykin, 1999; Bai and Alex, 2009). Back propagation neural network is used to detect the percentage of adulteration in the VCO. The artificial neural network analysis was done by using SPSS 17.0. The spectra were area- normalized and baseline-corrected before data processing.

3.0 Results and Discussion

Nowadays, the evolution of computer science (software and hardware) has allowed the development of many computational methods used to understand and simulate the behaviour of complex systems. In this way, the integration of technological and scientific innovation has helped the treatment of large databases of chemical compounds in order to identify possible patterns. However, people who can use computational techniques must be prepared to understand the limits of applicability of any computational method and to distinguish between those opportunities which are appropriate to apply ANN methodologies to solve chemical problems.

Based on the sum of square error convergence the number of used in the present study is 4. In the present study, we find that our network is activated by training time. The case processing summary shows that 71 cases were assigned to the training sample, 24 cases in the testing sample and no cases were holdout and excluded from the analysis.

The final three-layer 6-4-1-feed-forward, back propagation ANN model with variables consisting of palm oil 5%, palm oil 10%, palm oil 15%, mustard oil 5%, mustard oil 10% and mustard oil 15%, is developed and trained in 95 spectral data (Fig.1).

The network information table displays information about the neural network and it is useful for ensuring that the specifications are correct. The number of variables in the input layer is the number of covariates plus the total number of factor levels; a separate variable is created for each category of adulterants namely palm oil 5%, palm oil 10%, palm oil 15%, mustard oil 5%, mustard oil 10%, mustard oil 15% and none of the categories are considered “redundant” units as is typical in modeling procedures. Likewise, a separate variable has been created for each category of virgin coconut oil. Thus, the output layer will have only one variable, which is a pre-requisite for any modeling procedure. Covariates are rescaled using the adjusted normalized method. Automatic architecture selection has chosen 4 units in the hidden layer.

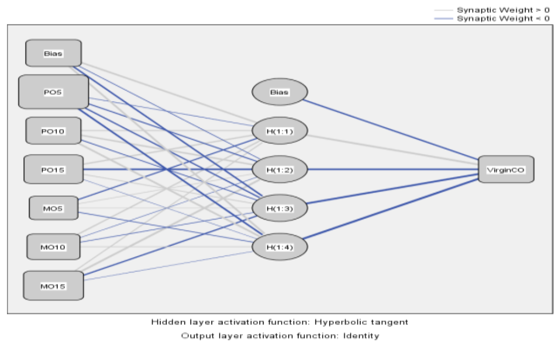

Fig.1 A neural network for the prediction of adulterants in virgin coconut oil consisting of six inputs, variable (excluding–bias node), a hidden layer with three nodes (excluding –bias node) and one output variable.

Table.1 Dependent variable

Model Summary

Training	Sum of Squares Error	.049
	Relative Error	.001
	Stopping Rule Used	1 consecutive step(s) with no decrease in error[a]
	Training Time	00:00:00.005
Testing	Sum of Squares Error	.015
	Relative Error	.001

Dependent Variable: Virgin coconut oil

a. Error computations are based on the testing sample.

This structure is known as a feed forward architecture because the connections in the network flow forward from the input layer to the output layer without any feedback loops. The input layer contains the predictors with six variable (i.e.) covariates with one bias. The hidden layer contains unobservable nodes, or units. The value of each hidden unit is some function of the predictors; the exact form of the function depends in part upon the network type and in part upon user-controllable specifications. The improvement procedure has been discussed. The number of hidden layers is decided with the help of least sum of square error (Table.1). In the current model, the optimum level was reached with two hidden layers with a sum of square error values of 0.001 (Table.4). The output layer contains the responses. Since the history of default is a categorical variable with a single category, namely virgin coconut oil, it is recoded as an indicator variable. Each output unit is some function of the hidden units. Again, the exact form of the function depends, in part, on the network type and, in part, on user-controllable specifications. The MLP (multiple perception layer) network allows a two hidden layer; in that case, each unit of the second hidden layer is a function of the units in the first hidden layer, and each response is a function of the units in the second hidden layer (Table.2).

Table.2 Hidden layer parameters

Predictor		Predicted				
		Hidden Layer 1				Output Layer
		H(1:1)	H(1:2)	H(1:3)	H(1:4)	VirginCO
Input Layer	(Bias)	.324	-.118	-.272	.300	
	PO5	-.107	-.221	-.250	-.285	
	PO10	.237	.312	-.153	.334	
	PO15	.281	-.573	.208	-.041	
	MO5	-.246	.143	.086	-.143	
	MO10	.260	-.082	-.118	.166	
	MO15	.185	.382	-.264	-.075	
Hidden Layer 1	(Bias)					-.272
	H(1:1)					.772
	H(1:2)					-.472
	H(1:3)					-.913
	H(1:4)					-.949

Table.3 Independent variable importance

	Importance	Normalized Importance
Palm oil 5%	.289	100.0%
Palm oil 10%	.141	48.8%
Palm oil 15%	.182	62.8%
Mustard oil 5%	.077	26.5%
Mustard oil 10%	.121	41.8%
Mustard oil 15%	.191	65.9%

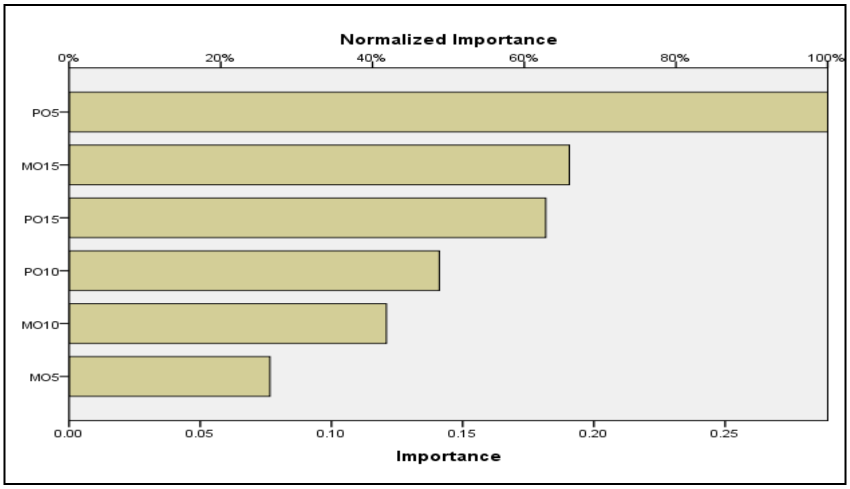

Fig.2 Sensitivity analysis of the input variables (The value shown for each input variable is a measure of its relative importance).

Table.4 Comparison of models

Size of Hidden Layer	Sum of Squares Error	Relative Error
2	0.067	0.004
3	1.071	0.113
4	0.015	0.001

The error computations are based on the testing sample. The model summary (Table.2) displays information about the results of training, testing, and application of the final network to the holdout sample. Sum of squares error is an error function that the network tries to minimize during training and testing (Table.4).

As shown in the normalized importance (Table.3; Fig.2), palm oil 5%, and mustard oil 15% and palm oil 15% were the most important predictors of persistent adulterants of sensitivity. As previously mentioned, each neural network input element has an associated synaptic value, which is represented by a numerical value that controls input; the higher the synaptic value, the more relevant is the input for the result that is generated from the neural network. Figure.2 represents a relevance chart for each input field to obtain fitting results, information that becomes available after the creation of the node corresponding to the model generated. Thus the adulteration of 5% palm oil with virgin coconut oil does not reveal any significant change, whereas, an adulteration form of adulteration in the mustard oil 15% reveal 65.90% virgin coconut oil and palm oil 15% reveal 62.8% virgin coconut oil. The other adulterant, have shown significant changes in the virgin oil at more than 5% level and those adulterants are not explained further.

Neural networks are beginning to play an important role in the daily life of all human activity, and thus industrial operations are gradually incorporating this technology into their work routines. Due to the robustness and efficacy of ANNs to solve complex problems, these methods have been widely employed in several research fields such as medicinal chemistry, pharmaceutical research, theoretical and computational chemistry, analytical chemistry, biochemistry, food research, etc. Therefore, ANN techniques can be considered valuable tools to understand the main mechanisms involved in chemical problems.

Conclusion

The ANN based FTIR spectroscopy to detect adulteration in coconut oil was investigated. The data sets were used to design, validate and test an artificial neural network, which allowed the detection of the adulteration in the VCO. The adulteration of 5% palm oil of the virgin coconut oil does not reveal any significant, whereas, an adulteration form of adulteration in the mustard oil 15% reveal 65.90% virgin coconut oil and palm oil 15% reveal 62.8% virgin coconut oil.

References

a) *Bai, D.G and Alex, Z.C. (2009). ANN technique for the evaluation of soil moisture over bare and vegetated fields from microwave radiometer data. Indian Journal of Radio & Space Physics, 38(5), pp.283-288.*
b) *Basheer, I.A and Hajmeer, M. (2000) Artificial Neural Networks: Fundamentals, Computing, Design, and Application. E. Funes et al. 40 Journal of Microbiological Methods, 43, pp.3-31.*
c) *Haykin, S. (1999). Neural networks: A comprehensive foundation (2nd ed.), Prentice-Hall, Inc.*
d) *Jiménez, A., Aguilera, M.P., Uceda, M and Beltrán, G. (2009) Neural Network as Tool for Virgin Olive Oil Elaboration Process Optimization. Journal of Food Engineering, 95, pp.135-141.*