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Prediction of secondary components in sugarcane brandy by application of artificial neural network

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Abstract

This study aimed to use artificial neural networks to predict the secondary components of sugarcane brandy. We got data on the characteristics of sugarcane brandy from the literature. We divided this data into input data and output data. Secondary components in sugarcane brandy were the output data. The architecture used for artificial neural networking was the multilayer feed-forward network, which features a hidden layer. These hidden neurons have the role of intervening between the input and output layers of the network. We separated the data into 70% for training and 30% for tests. The artificial neural network transfer function was Relu, with Adam as the training algorithm for weight change with a constant learning rate. The number of neurons in the hidden layer was determined using the mean square error. Twenty neurons in the hidden layer were analyzed and considered appropriate, since in the artificial neural network with a greater number of neurons, we observed no significant variation in the reduction of error.

Keywords: Artificial intelligence; ANN; Feed-forward; Sugarcane spirits

1. Introduction

Sugarcane brandy is a centuries-old alcoholic beverage made from the fermentation and distillation of sugar cane broth or must [1]. Fermented beverages represent mainly the market for alcoholic beverages in Brazil, such as beer and wine, and by distilled yeast drinks such as "cachaça", whiskey, and vodka. The total production capacity of the country is 14.9 billion liters, with the highest share of beer with 88.9%, followed by distillates with 7.5% and the rest of the market for other beverages with 3.6% [2].

According to Brazil (2005), sugarcane brandy is the alcoholic beverage from 38 to 54% v/v to 20 °C, got from the simple alcoholic distillate of sugarcane or by distillation of fermented must of sugarcane juice, and can be added sugars up to 6 g L^{-1}, expressed in sucrose. If produced only in Brazil and attend an alcoholic graduation of 38% to 48% to 20 °C, this product can be called "cachaça".

The production method of sugarcane brandy so far has not been standardized in terms of sugarcane varieties, fermentation conditions and distillation equipment. These variations can lead to the production of different aromatic compounds during the fermentation and distillation process, which consequently may affect the sensory profile of the beverage [3].

Throughout the sugarcane brandy production process, several volatile compounds can occur that directly influence the sensory quality of the product, such as organic acids, methanol, esters, aldehydes, and superior alcohols [4].

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We know these volatile compounds as secondary components, charged with forming the characteristic bouquet of each beverage [5]. However, the analysis of the components is complicated and require sophisticated equipment and to enable producers to verify the quality of their product, it is proposed to use artificial neural networks to predict the composition of the secondary components of sugarcane brandy from routine analyses of sugarcane brandy.

Artificial neural network, which involve a connectionism structure, can predict these secondary components of sugarcane brandy in which several small densely interconnected units distribute processing [6].

This method seeks to understand and simulate the properties resulting from high proportion and connectivity of biological systems. Many processor elements, neurons, widely interconnected by connections with a value that determines connectivity between them, called connection weight or synapse, formed the Artificial Neural Network (ANN) [6]. The aim of this work is to use artificial neural network to predict the secondary components of sugarcane brandy.

2. Material and methods

Data from 7 scientific articles [7, 8, 9, 10, 11, 12, 13] were collected presenting results of routine analyses and secondary components of sugarcane brandy totaling 35 products. The collected data was tabulated in a spreadsheet.

The architecture employed for ANN was a multilayer feed-forward network that features a hidden layer. These hidden neurons have the role of intervening between the input layers and the output layers of the network. According to Furtado [6], this network better maps the most complex problems because of the addition of one or more layers.

We separated the data into 70% for training and 30% for ANN testing. We standardized these data with mean zero and standard deviation equal to 1.0. ANN architecture was developed using python software version 3.7. The variables, alcoholic degree, volatile acidity and aged or not aged drink, defined the number of neurons in the input layer. The variable aging was transformed from a categorical to numerical variable (Label Encoding). The output layer corresponds to the prediction of the following components: n-propyl alcohol, iso-butyl alcohol, isoamyl alcohol, higher alcohols, aldehyde, esters, and methanol.

Trial and error defined the number of neurons in the hidden layer using the lowest mean quadratic error parameter given by Equation 1:

$$\text{MSE} = \frac{1}{Q}\sum_{1}^{Q}(t(k) - a(k))^2 \qquad (1)$$

Where t(k) is the actual value and a (k) is the value predicted by ANN and Q regarding the number of samples.

A second parameter used to evaluate ANN performance was the coefficient of determination between the actual data and the data predicted by the artificial neural network for the training and test data. Graphs presenting the errors between the actual and predicted data, the difference between the values, were plotted.

3. Results and discussion

Data from the secondary components of sugarcane brandy showed the physical-chemical characteristics represented in Table 1.

We compared all data presented to Normative Instruction No. 13 of June 29, 2005 [14]. The alcoholic sugarcane spirits presented values ranging from 45.36% v/v to 76.99% v/v, so some data are outside the values (38% v/v to 54% v/v), established. However, through the literature studied, low alcohol graduation is a more common problem of "cachaça" standardization [15].

Regarding the concentration of volatile acidity, the mean value was 38.18 mg 100 mL^{-1} anhydrous alcohol. This result meets the maximum allowed limit of 150 mg 100 mL^{-1} of anhydrous alcohol. The maximum value was 175.43 mg 100 mL^{-1} anhydrous alcohol, this value is above the maximum allowed limit. Alves et al. [12] found that distillates produced from untreated broth presented higher levels of volatile acidity and esters, showing microorganisms distinct from the broth, which allowed the production of these compounds during alcoholic fermentation. Oliveira Filho et al. [16]

observed that the higher acidity of fermented mash from stored stems favored higher production of ethyl acetate at the end of the fifth fermentation cycle, providing low levels of volatile acidity in the distillate.

Table 1 Physical-chemical characteristics of sugarcane spirits samples

Parameter	Average	Minimal value	Maximum value	Standard deviation
Alcoholic grade (% v/v)	45.36	27.99	76.99	11.58
Volatile acidity (mg 100 mL^{-1})	38.18	3.63	175.43	40.89
N-propyl alcohol (mg 100 mL^{-1})	48.15	3.85	134.65	31.65
Iso-butyl alcohol (mg 100 mL^{-1})	56.84	11.98	151.61	28.32
Iso-amyl alcohol (mg 100 mL^{-1})	176.81	33.12	466.62	86.02
Higher alcohols (mg 100 mL^{-1})	281.65	49.28	572.60	108.71
Aldehyde (mg 100 mL^{-1})	16.99	0.00	65.51	17.54
Esters (mg 100 mL^{-1})	26.14	0.00	62.65	17.92
Methanol (mg 100 mL^{-1})	4.05	0.00	17.24	4.13

The mean concentration of higher alcohols of the data analyzed was 281.65 mg 100 mL^{-1} of anhydrous alcohol, while the legislation limits this compound to a maximum of 360 mg 100 mL^{-1} of anhydrous alcohol. Among the data analyzed from the upper alcohols, isoamyl alcohol was the only one that exceeded the established maximum limit of 466.62 mg 100 mL^{-1} anhydrous alcohol. Low concentrations of higher alcohols may be associated with sugarcane cutting care, as well as waiting time for grinding and fermentation [17]. According to Silva et al. [13], distillates with excessive amounts of superior alcohols usually show an unpleasant sensory aspect. The maximum value was 572.60 mg 100 mL^{-1} of anhydrous alcohol.

Oliveira Filho et al. [16] perceived that high concentrations of higher alcohols (n-propyl, iso-butyl, and iso-amyl) are intrinsic qualities provided by S*accharomyces cerevisiae* yeasts and state that certainly the reduction of these compounds during fermentation cycles is derived from the substitution of these yeasts by strains that develop during alcoholic fermentation.

The maximum limit of esters established by the legislation is 200 mg 100 mL^{-1} alcohol, the average value got from the data was 26.14 mg 100 mL^{-1} of anhydrous alcohol, among the data analyzed none exceeded the established limit, while the maximum value was 62.65 mg 100 mL-1 mL^{-1} anhydrous alcohol. The main ester present in spirits is ethyl acetate, followed by ethyl lactate, characterizing about 95% of the total amount of esters in the beverage. They linked this compound to the fruity odor, which in high concentrations becomes unpleasant. Distillation in stills favors a higher concentration of esters compared to spirits developed by distillation in continuous columns, because it catalyzed esterification reactions through copper in the heated distillation environment [13].

Silva et al. [13] found that aldehydes are of great relevance in the composition of spirits, because of acetaldehyde, furfural, and hydroxy-methyl furfural, of which they present penetrating odors, usually nauseated. The mean concentration of aldehydes was 16.99 mg 100 mL^{-1} of anhydrous alcohol and the maximum of 65.51 mg 100 mL^{-1}, this limit is above the maximum allowed of 30 mg 100 mL^{-1} of anhydrous alcohol, since low levels of aldehydes are expected in a good quality brandy. Acetaldehyde, when in low concentration, can give fruit aroma. However, in high concentration presents pungent odor [13].

Regarding methanol, the average contents were 4.05 mg 100 mL^{-1} and the maximum content of 17,24 mg 100 mL^{-1} anhydrous alcohol, not exceeding the allowed limit of 20 mg 100 mL^{-1} of anhydrous alcohol. However, even at low concentrations, methanol is undesirable in spirits because of its toxicity characteristics. The presence of this alcohol is related to the degradation of pectin, a polysaccharide that is usually present in sugarcane, despite low levels of occurrence [8]. However, out-of-the-box values are extremely important for improving the prediction of the artificial neural network.

The transfer function of the artificial neural network was Relu, and Adam was the training algorithm for weight change with a constant learning rate. For the construction of the ANN architecture, of the 35 data analyzed were randomly divided into 70% for training and 30% for testing. Figure 1 shows the multi-layer feed network architecture.

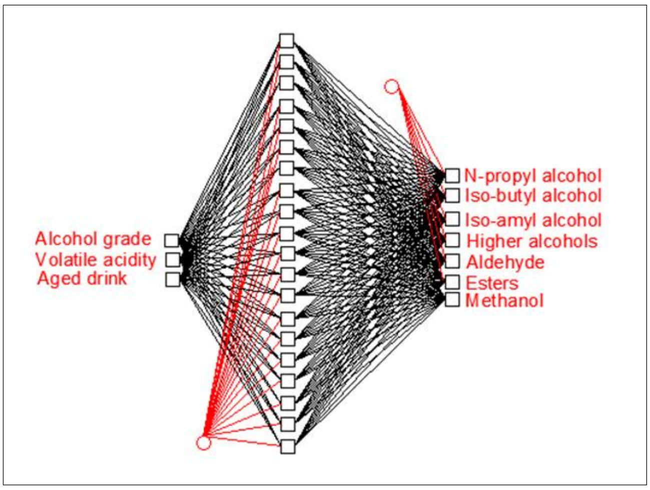

Figure 1 Representation of ANN architecture

The number of neurons in the hidden layer was determined by mean quadratic error (MSE), in which it was analyzed that 20 neurons in the hidden layer would be appropriate, since in the artificial neural network with a greater number of neurons a significant variation in error reduction (MSE) was not observed, as shown in Figure 2. In this work, we used 20 neurons in the hidden layer, and the ability to predict the artificial neural network for training and test data was verified by the coefficient of determination.

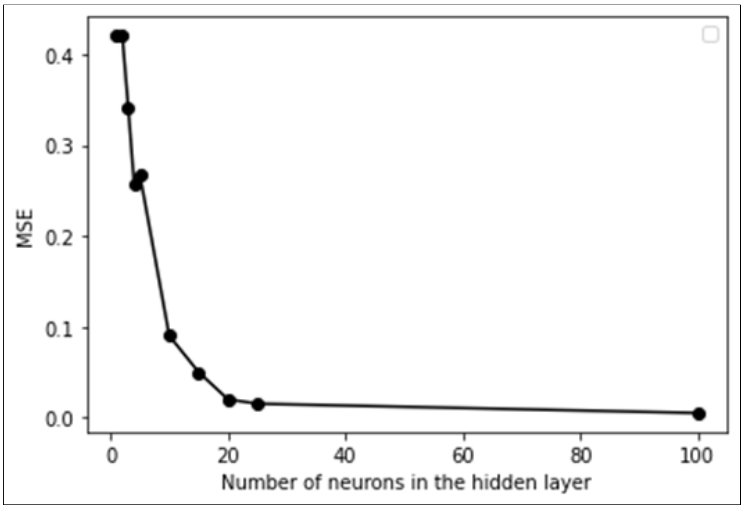

Figure 2 MSE as a function of the number of neurons in the hidden layer

Soares et al. [18] observed that, for the trained architectures, the values of mean quadratic error and the average relative were low. Therefore, the increase in the number of neurons in the intermediate layer and the number of variables in the input layer were equivalent to the lowest values for the errors. Maciel et al. [19] observed that with the increase in the number of neurons, the capacity of the network increased, but its performance desists.

According to Cerqueira et al. [20] in certain situations, artificial neural network, even after being trained, demonstrate low calibration errors and high prediction errors, i.e., over-fitting, because of the excessive number of neurons used in the intermediate layer. In view of this, to avoid over-fitting, i.e., small calibration errors and high prediction errors, it is necessary to optimize the number of neurons in the intermediate layer.

Table 2 Weight matrix between the input and hidden layers (W1) and weights between the hidden and output layers (W2) for the final structure f the ANN

W_1* (weights)			Bias*	W_2*(weights)							
Input				Neuron	Output						
Alcohol grade	Volatile acidity	Aged drink		Hidden layer	N-propyl	Isobutyl	Iso-amyl	Higher alcohols	Aldehyde	Esters	Methanol
-1.12731	0.23618	-1.51492	1.49830	1	-1.23330	5.96111	0.10017	1.26780	4.48718	3.61805	5.35957
-1.54842	-0.89323	-0.08179	-1.23697	2	3.66080	-2.76038	-0.85332	-0.32975	1.31792	-1.01458	-2.50879
-2.59626	2.83574	0.78989	0.64816	3	1.60423	-1.36296	-2.78086	-2.12205	0.59659	-0.31775	1.00701
$-1.5\cdot10^{-306}$	$-3.8\cdot10^{-305}$	$1.9\cdot10^{-274}$	- 0.23452	4	$-1.9\cdot10^{-270}$	$2.3\cdot10^{--286}$	$-3.6\cdot10^{-259}$	$-3.3\cdot10^{-270}$	$8.2\cdot10^{-306}$	$-4.1\cdot10^{-260}$	$-1.8\cdot10^{-298}$
-1.30192	1.62805	1.72532	- 2.56200	5	-3.43327	2.50704	-0.40449	-0.68373	-5.00720	3.23370	3.19536
2.13760	1.27888	0.36118	0.12981	6	2.85953	3.03469	-0.77269	0.95098	2.64466959	-1.22083	2.07558
$-1.2\cdot10^{-288}$	$-2.5\cdot10^{-304}$	$-3.1\cdot10^{-304}$	- 0.37227	7	$1.8\cdot10^{-303}$	$-4.9\cdot10^{-241}$	$2.0\cdot10^{-284}$	$-2.3\cdot10^{-305}$	$-2.9\cdot10^{-301}$	$-1.2\cdot10^{-252}$	$-5.2\cdot10^{-283}$
-3.87345	0.79131	-1.76019	1.49400	8	-0.58088	-1.34290	0.60132	-0.01993	-2.30717	-2.56395	-2.02879
1.40801	-3.97908	-0.09910	- 0.38894	9	-0.23970	2.78542	4.24826	4.02191	-0.22255	-0.64021	0.09440
1.71778	-1.80686	0.21437	- 1.60846	10	-0.11037	-2.09348	-0.49246	-1.03464	3.10079	0.87053	1.59838
2.86870	1.41600	-0.82765	0.52065	11	-3.76492	2.81841	-0.65687	-0.77004	-1.85942	3.04885	-0.47975
0.90945	2.14366	-0.03615	0.83165	12	-0.74608	-2.77728	1.66892	0.35071	-0.16235	0.89268	-0.87016
0.35377	-3.17249	-0.40476	- 1.44341	13	0.45131	-1.35269	-3.13068	-2.64122	-1.41367	2.62703	-2.55739
-2.41041	1.35132	1.58968	- 2.50148	14	-1.54658	4.55035	3.43829	3.55631	3.51511	0.20800	-0.73859
1.21691	2.27926	0.89439	- 1.38484	15	1.85336	-3.41616	1.74327	1.00219	0.80441	-2.34558	-0.97322
0.29841	1.53680	-0.68531	1.00096	16	1.90784	-0.16192	-0.54758	0.06741	-0.49474	-0.20981	-2.01665
-0.93909	-3.55622	0.55786	- 1.46025	17	0.26893	-0.94311	-3.97919	-3.34796	0.95783	-1.93450	2.64270
2.43720	0.52655	-0.65306	1.98765	18	-0.38930	2.18734	3.76246	3.44809	-0.02136	0.11474	0.88889
3.05811	-1.25353	-2.56471	1.98231	19	1.68057	-4.19191	-3.35631	-3.30994	-0.20248	-1.80573	-0.55975
-2.33769	-1.06927	0.01283	1.19986	20	0.30628	-0.89990	1.77088	1.24066	-0.77111	1.91827	-1.06021
				Bias*	-2.20055	-0.52992	-1.20477	-1.62573	-0.99564	-0.37392	-3.10489

*Rounded data for five decimal places, except for values close to zero

Table 2 shows the coefficients of determination (R^2), between the experimental and predicted values for the secondary components of the brandy using ANN for all data used for training and testing. The coefficients of determination are close to one, showing that ANN is a suitable tool for predicting secondary components from the input data, alcohol degree, volatile acidity, and aging drink.

Table 3 Coefficient of determination between data provided by the ANN and data from the literature for the evaluated parameters.

Parameter	R^2 Training	R^2 Test	R^2 Total
N-propyl alcohol	0.98	0.74	0.96
Iso-butyl alcohol	0.95	0.90	0.93
Alcool Iso-amyl	0.99	0.92	0.99
Higher alcohol	0.99	0.98	0.99
Aldehyde	0.94	0.81	0.89
Esters	0.97	0.96	0.97
Methanol	0.97	0.94	0.95

The weights of connections in the constructed ANN are shown in Table 3.

Figure 3 shows the error obtained for each physical-chemical parameter evaluated for the secondary components of the sugarcane brandy, the error was calculated by the difference between the actual value and the value predicted by ANN.

It can be observed that in Figure 3A, the error between real values and predicted by ANN for the n-propyl alcohol component was close to zero, with a predominant variation of 20 mg 100 mL^{-1} of anhydrous alcohol. There was a larger variation of two data for composition that ranged from 3.85 to 134.65 mg 100 mL^{-1} anhydrous alcohol. In Figure 3B, the error between the actual values predicted by ANN for the iso-butyl component was close to zero with a difference of 10 mg 100 mL^{-1} of anhydrous alcohol. For three data there was a greater variation of 25 mg 100 mL-1 of anhydrous alcohol. The composition ranged from 11.98 to 151.61 mg 100 mL^{-1} of anhydrous alcohol.

The error represented in Figure 3C for the iso-amyl alcohol component showed a predominant variation of 25 mg 100 mL^{-1} of anhydrous alcohol. There was a greater variation for a data for the composition that ranged from 33.12 to 466.62 mg 100 mL-1 of anhydrous alcohol. In figure 3D it is possible to observe that the error between the values predicted by ANN for the upper alcohols presented a difference of 20 mg 100 mL^{-1} of anhydrous alcohol. The composition ranged from 49.28 to 572.60 mg 100 mL^{-1} of anhydrous alcohol.

The error presented in Figure 3E for aldehyde was close to zero, ranging from 10 mg 100 mL^{-1} of anhydrous alcohol. There was a greater variation between one data of 20 mg 100 mL^{-1} of anhydrous alcohol the composition ranged from 0.00 to 65.51 mg 100 mL^{-1} of anhydrous alcohol. In figure 3F it is possible to verify that the error between the values predicted by ANN for esters was close to zero with variation of 10 mg 100 mL^{-1} of anhydrous alcohol. The composition ranged from 0.00 to 62.65 mg 100 mL^{-1} of anhydrous alcohol.

Figure 3G shows that the error between the predicted values for methanol was close to zero, ranging from 2 mg 100 mL^{-1} of anhydrous alcohol. The composition ranged from 0.00 to 17.24 mg 100 mL^{-1} of anhydrous alcohol.

Several researchers have been developing applications of Artificial Neural Network to the processes of the food industry, Pereira [21] applied the artificial neural network technique to investigate beer styles, although it did not identify a pattern among the recipes tested, it achieved a good performance by correctly setting the other styles. It was also observed that, to further improve neural network training; it is workable to place a greater number of beer styles to train them, thus decreasing the network error rate.

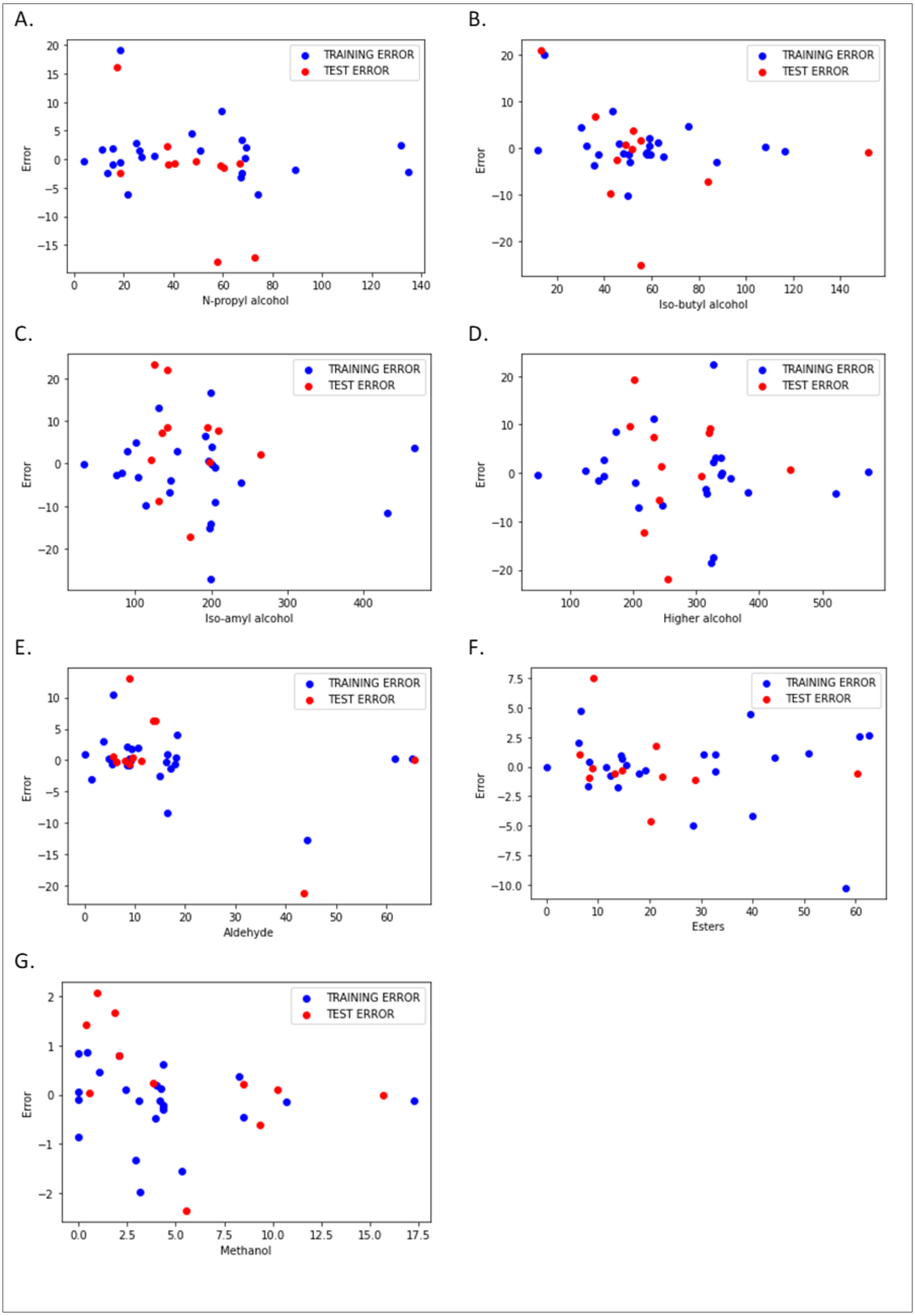

Figure 3 Error between the actual values and predicted by ANN for the secondary components of the sugarcane brandy

Morelle et al. [22] published work with the use of ANN to detect and predict the evolution of foam during bottling of non-carbonated beverages, comprising 12 different commercial juices. Using image data had as the advantage of noninvasive acquisition and no supplemental sensor hardware with direct contact with the product should be installed. From the filling speed, viscosity, surface tension and density, they used the foaming behavior during the filling process with the recurrent neural network. The neural network could predict the evolution of foam height with average errors below five millimeters. Both models are easily transferable to new use cases through training.

Dias et al. [23], in using neural networks for classification of honey type, used 25 samples and applied to test the parameters of entry pH, reducing sugars and ash and, for the output parameters, the floral honey or honey melon. The amount of samples used for network training was 70% and for tests 30%. For the data of the 25 samples tested, the developed system showed better results as a neural model containing 4 neurons in the intermediate layer. The learning rate was equal to 0.9. Through the developed model, it was possible to classify 100% of the tested samples, which confirms their efficiency and shows their speed and low cost.

4. Conclusion

Using the multilayer artificial neural network allowed the prediction of the secondary components of sugarcane brandy through the results of routine analyses. The results found present a great potential of ANN application for prediction of secondary components of sugarcane brandy with sophisticated equipment. The development of applications for smartphones may allow producers of sugarcane brandy to have a practical way of controlling and standardizing the characteristics of beverages.

Compliance with ethical standards

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To the Federal Institute of Education, Science and Technology of Southeastern Minas Gerais, Barbacena, Brazil.

Disclosure of conflict of interest

The authors declare that there is no conflict of interest.

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