

**Modeling thermal properties of exotic fruits pulps: an artificial neural networks
approach**

**Modelagem de propriedades térmicas de polpas de frutas exóticas: uma abordagem de
redes neurais artificiais**

**Modelado de propiedades térmicas de pulpas de frutas exóticas: un enfoque de redes
neuronales artificiales**

Received: 11/15/2020 | Reviewed: 11/21/2020 | Accept: 11/29/2020 | Published: 12/02/2020

Leandro Soares Santos

ORCID: <https://orcid.org/0000-0001-7431-318X>

State University of Southwest of Bahia, Brazil

E-mail: leandrosantos@uesb.edu.br

Moysés Naves de Moraes

ORCID: <https://orcid.org/0000-0002-9847-8971>

Federal University of São Carlos, Brazil

E-mail: moysessevan@gmail.com

Júlia Dos Santos Lopes

ORCID: <https://orcid.org/0000-0001-5544-9399>

State University of Southwest of Bahia, Brazil

E-mail: 2019m0128@uesb.edu.br

Luciana Carolina Bauer

ORCID: <https://orcid.org/0000-0001-8780-9440>

State University of Southwest of Bahia, Brazil

E-mail: luciana.carolina.bauer@gmail.com

Paulo Bonomo

ORCID: <https://orcid.org/0000-0002-1892-0185>

State University of Southwest of Bahia, Brazil

E-mail: paulobonomo@uesb.edu.br

Renata Cristina Ferreira Bonomo

ORCID: <https://orcid.org/0000-0002-9896-4099>

State University of Southwest of Bahia, Brazil

E-mail: rbonomo@uesb.edu.br

Abstract

Thermophysical properties are important in design, simulation, optimization, and control of food processing. Its prediction is very important but theoretical basis is difficult and empirical models were commonly used. In this work, the modeling of neural networks was applied as an alternative to predict density, thermal conductivity and thermal diffusivity from the temperature and moisture content of jackfruit, genipap and umbu. Data sets from literature were used, combined and individually, to obtain four networks. Supervised multilayer perceptron networks were developed, using the back-propagation algorithm. Several configurations of artificial neural networks (ANNs) were evaluated with one or two hidden layers and a maximum of 21 and 12 neurons in each one, respectively. Data sets were divided to learning (60%) and verification (40%) steps. Best ANNs were chosen based on correlation coefficient and root mean square errors (RMSE), and compared with polynomial models using average absolute deviations (AADs). From total disposable data set, the best ANN developed presents one hidden layer with 15 neurons and shows the same predictive ability of ANNs created from individual fruits data sets, presenting close RMSE and correlation coefficient. The ANNs developed presents AADs near to polynomial models and appears as alternative to conventional modeling. Results indicate that the ANN created from total data set can replace nine polynomial models to predict the thermophysical properties of jackfruit, genipap and umbu pulps.

Keywords: Density; Thermal conductivity; Thermal diffusivity; Back propagation; Moisture content; Temperature.

Resumo

As propriedades termofísicas são importantes no projeto, simulação, otimização e controle do processamento de alimentos. Sua previsão é muito importante, mas a base teórica é difícil e modelos empíricos eram comumente usados. Neste trabalho, a modelagem de redes neurais foi aplicada como alternativa para prever densidade, condutividade térmica e difusividade térmica a partir da temperatura e teor de umidade de jaca, jenipapo e umbu. Conjuntos de dados da literatura foram usados, combinados e individualmente, para obter quatro redes. Redes perceptron supervisionadas multicamadas foram desenvolvidas, utilizando o algoritmo de retropropagação. Diversas configurações de redes neurais artificiais (RNAs) foram avaliadas com uma ou duas camadas ocultas e no máximo 21 e 12 neurônios em cada uma, respectivamente. Os conjuntos de dados foram divididos em etapas de aprendizagem (60%) e verificação (40%). As melhores RNAs foram escolhidas com base no coeficiente de

correlação e erro quadrático médio (RMSE), e comparadas com modelos polinomiais usando desvios absolutos médios (AADs). Do conjunto de dados descartáveis totais, a melhor RNA desenvolvida apresenta uma camada oculta com 15 neurônios e mostra a mesma capacidade preditiva das RNAs criadas a partir de conjuntos de dados de frutas individuais, apresentando RMSE próximo e coeficiente de correlação. As RNAs desenvolvidas apresentam AADs próximos a modelos polinomiais e aplicativos como alternativa à modelagem convencional. Os resultados indicam que a RNA criada a partir do conjunto total de dados pode substituir nove modelos polinomiais para prever as propriedades termofísicas das polpas de jaca, jenipapo e umbu.

Palavras-chave: Densidade; Condutividade térmica; Difusividade térmica; Retropropagação; Teor de umidade; Temperatura.

Resumen

Las propiedades termofísicas son importantes en el diseño, simulación, optimización y control del procesamiento de alimentos. Su predicción es muy importante pero la base teórica es difícil y los modelos empíricos se usaban comúnmente. En este trabajo se aplicó el modelado de redes neuronales como una alternativa para predecir la densidad, conductividad térmica y difusividad térmica a partir de la temperatura y contenido de humedad de la yaca, genipap y umbu. Se utilizaron conjuntos de datos de la literatura, combinados e individualmente, para obtener cuatro redes. Se desarrollaron redes de perceptrones multicapa supervisadas, utilizando el algoritmo de retropropagación. Se evaluaron varias configuraciones de redes neuronales artificiales (ANN) con una o dos capas ocultas y un máximo de 21 y 12 neuronas en cada una, respectivamente. Los conjuntos de datos se dividieron en pasos de aprendizaje (60%) y verificación (40%). Las mejores ANN se eligieron en función del coeficiente de correlación y los errores cuadráticos medios (RMSE), y se compararon con modelos polinomiales utilizando desviaciones absolutas promedio (AAD). A partir del conjunto de datos desechables total, la mejor ANN desarrollada presenta una capa oculta con 15 neuronas y muestra la misma capacidad predictiva de las ANN creadas a partir de conjuntos de datos de frutas individuales, presentando un RMSE cercano y un coeficiente de correlación. Los ANN desarrollados presentan AAD cercanos a modelos polinomiales y aparecen como alternativa al modelado convencional. Los resultados indican que la ANN creada a partir del conjunto de datos total puede reemplazar nueve modelos polinomiales para predecir las propiedades termofísicas de las pulpas de yaca, genipap y umbu.

Palabras clave: Densidad; Conductividad térmica; Difusividad térmica; Retropropagación; Contenido de humedad; Temperatura.

1. Introduction

Design, simulation, optimization and control of food processing, such as evaporation, heat exchange, spray drying and mixing are important tools for reducing costs and improving quality within industries. In addition, food products are constantly changing, being included in an interconnected, global and very complex manufacturing system. In this context, food properties are extremely important to understand and strengthen the production chain (Massood & Trujilo, 2016). Modeling this process requires the knowledge of reliable data, for example, on thermophysical properties such as density, thermal conductivity, thermal diffusivity, specific heat, among others. These data are essential for estimating operational parameters, such as friction losses in tubes, the total area of a heat exchanger and the maximum operating temperature.

Thermophysical properties values of fruits available in the literature are typically obtained in subtropical and cold areas (Fontan, et al., 2009; Ewetumo, et al., 2017), information about these properties for tropical or exotic fruits is still scarce. Tropical fruits, such as other foodstuffs, are also exposed to heating and cooling in their processing and the lack of information about their thermal properties represents a major problem for product development, especially for developing countries that have these fruits in abundance (Ewetumo, et al., 2017). Thermal treatments are needed to eliminate pathogenic and deteriorating microorganisms, to inactivate enzymes and retard metabolic and microbiological processes in storage conditions. Cooling or freezing also used when foods are not immediately consumed (Tavman, et al., 2019).

The effect of temperature and solids (or moisture) content on thermophysical properties of juices and fruit pulps are important in industrial systems. Water makes extensive hydrogen bonds what take to specific properties. Its characteristics take to a strong dependence of their properties with the temperature. Besides, when a food system receive (or give) energy due to a temperature gradient the molecules changes its energy levels (vibrational, rotational, ...) upset the Brownian and flow motions. So the distance among molecules changes as well as the total energy of the system, changing completely its flow and heat properties (Walstra, 2003). Thermophysical properties as density, viscosity, thermal conductivity, thermal diffusivity and specific heat of different fruits had been extensively

studied by Choi & Okos (1986), Constenla, Lozano & Crapiste (1989), Cepeda & Villarán (1999), Zuritz, et al. (2005), Azoubel, et al. (2005), Shamsudin, Mohamed & Yaman (2005), Souza, et al. (2009), Silva, et al. (2010), Souza, et al. (2010), Castilhos, et al. (2018), Silva, et al. (2020) among others.

Since prediction of thermal properties based on theoretical fundamentals is difficult, experimental measurements have been fitted by polynomial regression. It is difficult to know previously functional relationships of thermal properties, especially of more complex foods. A preliminary choice could be an obstacle to an adequate estimation of these properties. A usual solution consists in presenting these relationships as empirical polynomial equations, with a degree sufficiently high to explain the properties variations for an specific case (Varela, et al., 2017).

When any satisfactory analytical model exists or a low-order empirical polynomial model is inappropriate, artificial neural networks modeling could be an efficient alternative (Chegini, et al., 2008). The motivation for the development of neural networks technology stemmed from the desire to develop an artificial system that could perform “intelligent” tasks similar to those performed by the human brain. The great advantage of neural networks is the ability to learn the relationships directly from the experimental data representing both linear and nonlinear behaviors (Rai, et al., 2005).

According to Hayken (1999) a neural network is a complex processor (like the brain) made up of simple processing units (the neurons), with a natural capacity for storing experimental knowledge and making it available for use. The knowledge is acquired through a learning process and the synaptic weights between neurons are used to store the acquired knowledge.

Artificial neural networks (ANN) can be used to solve several different problems in food processing, such as prediction of food properties, analysis and prediction of food quality and safety, as well as other fields of food engineering (Nayak, et al., 2020). ANN have been used successfully by researchers to predict a large number of food properties and process parameters. Torkashvand, et al. (2017) used the ANN to estimate the firmness of kiwifruit having as inputs the concentrations of different nutrients in the fruits (N, K, Ca and Mg), while Sartori, et al. (2017) proposed models of artificial neural networks to predict the effects of different operational variables (peroxidation time, temperature, pH, peroxide dosage and initial ° Brix) on the removal of color and sucrose content of sugarcane juice clarified. Mutlu, et al. (2011) predicted 10 different quality properties of wheat flours combining near infrared reflectance spectroscopy (NIR) with the artificial neural network and Sucipto, et al. (2019)

were able to classify wheat flour as hard, medium and soft, relating bioelectric properties to protein content.

Choi & Okos (1986) propose multiple linear models to describe some thermophysical properties of foods in general, based only on their composition and temperature. This work had a similar objective, use ANN modeling to obtain just one network able to predict density, thermal conductivity and thermal diffusivity of exotic tropical fruits pulps in general as a function of temperature and moisture content.

2. Materials and Methods

In section 2.1 a description of used database is presented and in section 2.2 information about development and evaluation of the ANN models used in this work were given.

2.1 Data acquisition

Data for density, thermal conductivity and thermal diffusivity of exotic tropical fruits were obtained from literature to this study. It were used density, thermal conductivity and thermal diffusivity data of Genipap (Silva, et al., 2010), Uumbu (Souza, et al., 2010) and Jackfruit pulps (Souza, et al., 2009) at different temperatures and moisture contents. The size of data sets and the ranges of input and output variables to each fruit pulp are shown in Table 1.

Table 1. Ranges of input and output variables and number of available data by fruit pulp.

	Genipap ^a	Jackfruit ^b	Uumbu ^c	Total
Data set	42	63	45	150
Temperature (°C)	5 - 80	5 - 85	5 - 85	5 - 85
Moisture content (%)	76 - 94	75 - 95	65 - 95	65 - 95
ρ (kg·m ⁻³)	976,13 – 1092,26	966,40 – 1140,72	956,11 – 1102,35	956,11 – 1140,72
κ (10 ³ W·m ⁻¹ ·K ⁻¹)	0,56 – 2,17	0,36 – 1,87	0,59 – 2,51	0,36 – 2,51
α (10 ⁷ m ² ·s ⁻¹)	1,58 – 5,48	1,04 – 4,95	1,44 – 6,26	1,04 – 6,26

^a data from Silva, et al. (2010). ^b data from Souza, et al. (2009). ^c data from Souza, et al. (2010)
 Source: Authors.

2.2 ANN development

A neural network is an array of neurons in layers connected themselves. Each neuron receives an input signal and sends an output signal like brain neurons. The strength of the connections depends of the weights applied to each one during the learning step. Multilayer perceptrons (MLPs) neural networks are the most of widely used of the class of supervised neural networks, had been choice to be evaluated in this work. MLPs networks have one or more hidden layers between input and output layers fully connected or not. The input signal propagates through on a forward direction, on a layer-by-layer basis, being popular the back-propagation algorithm to train itself (Hayken, 1999, Rai, et al., 2005).

Basically, back-propagation algorithm consists of two passes. In the forward pass an input vector is applied and its effect propagates through the network layer-by-layer, until an output set be produced. At this point the connection weights (or synaptic weights) are all fixed. Then, in the backward pass the synaptic weights are all adjusted according to an error correction rule (Hayken, 1999). Back-propagation is used to training supervised feed-forward networks (Rai, et al., 2005). The architecture of the networks tested is presented on Table 2. Below are discussed some parameter in details.

Table 2. Architecture of tested networks.

Network used	Back propagation neural network
Learning	Supervised
Activation function	hyperbolic tangent (tanh)
n° of input variables	2
n° of hidden layers	2
n° of neurons on 1 st hidden layer	3 to 21
n° of neurons on 2 nd hidden layer	0 to 12
n° of output variables	3
Learning rule	Extended delta-bar-delta
Initial learning rate	0.3
Momentum	0.4
Iterations	30000

Source: Authors.

To activate a neuron (transfer a signal), some activation functions are used, as sigmoid or hyperbolic tangent functions. The last one is preferred when biological or more complex systems are studied (Rai, et al., 2005). The activation function used was a hyperbolic function type:

$$\varphi = \tanh(\nu_k) \quad (1)$$

Where ν_k is the activation potential of the k^{th} neuron (the sum of the input signals pondered by synaptic weights and the biases).

They were tested two hidden layers, sufficient to approximate any mathematical function (Hayken, 1999). The choice of the neurons number on each hidden layer was based on the minimization of RMSE and maximization of correlation coefficient, associated to predictive capacity of the network (Rai, et al., 2005). In the first hidden layer were tested 3 to 21 neurons and in second hidden layer 0 to 12 neurons were tested. A total of 23 configurations with different number of neurons on first and second hidden layers were tested until the choice of the best one. All tested networks had the neurons of a layer totally connected with the neurons of a neighbor layer.

Learning rate and momentum are also important in the development of a network. The learning rate indicates the rate of change of connection weights during training. A small learning rate turns too slow the training while large values accelerate the process. Typical values for the learning rate are numbers between 0.05 and 0.75 (Rai, et al., 2005).

To accelerate the learning step, modifications on back-propagation algorithm were used. One of them is the extended delta-bar-delta (EDBD) rule that use a momentum term to increase the learning speed and reducing the instability risks (Hayken, 1999, Braga, et al., 2011). The momentum term is added on the weights adjust function and helps to 'smooth' out the weight changes. Using the EDBD rule the learning rate is individually calculated to each connection (Braga, et al., 2011, NeuralWare, 2000). In this work was used an initial learning rate of 0.3 and a momentum value of 0.4.

The number of used iterations is also of great importance. A small number of iterations takes to large errors while a high number of iterations could demands too much computational time. To this work were used 30000 iterations in the learning step. This value was considerate satisfactory with a stable error obtained and short time to analysis.

To develop the artificial neural networks was employed the commercial software Neural Works Professional II/Plus® (Neuralware Inc., Pittsburg, USA) (Neuralware, 2000).

Training and validation

The total data set was divided into learning and verification sets to create a feed forward back-propagation neural network. Genipap, umbu and jackfruit were randomly divided in two sets. The first set, containing 60% of the data, was used to learning step and the second set, with 40% of the data, was used to verification step. There are two input variables, temperature ($X1$) and moisture content ($X2$), and three output variables, density (ρ), thermal conductivity (κ) and thermal diffusivity (α).

In order to verify its prediction capacity, the network obtained using the total data set, was compared with other three ANNs created from individual fruit pulps data sets (genipap, umbu and jackfruit), also using 60% of data reserved for learning step and 40% for verification step.

The input and output data were normalized automatically by used software using Eq. 2 and Eq. 3 (NeuralWare, 2000) respectively.

$$x_{i,norm} = \frac{x_i - \bar{x}_i}{R_{i,max}} \quad (2)$$

$$x_{i,norm} = \frac{x_i - x_{i,min}}{x_{i,max} - x_{i,min}} \quad (3)$$

Where $x_{i,norm}$ is the normalized data, x_i is the experimental data, \bar{x}_i is the average of data, $R_{i,max}$ is given by $R_{i,max} = \max[x_{i,max} - x_i, x_i - x_{i,min}]$, $x_{i,min}$ and $x_{i,max}$ are the minimum and maximum values of x_i respectively.

The performances of the various ANN configurations were compared using the correlation coefficient (R) between experimental and predicted output data and root mean square error (RMSE), expressed by Eq. 4. RMSE and correlation in learning and verification steps of the ANNs created were calculated from normalized data.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_d - x_p)^2} \quad (4)$$

Where n is the number of data points, and x_d and x_p are the experimental and predicted values of thermophysical properties, respectively.

Testing and comparison polynomial models

To verify the prediction ability of the ANN created, some comparisons were made. The network obtained from total data set was used to predict density, thermal conductivity and thermal diffusivity values for some conditions of temperature and moisture content. The same conditions were used to predict these properties with the polynomial models proposed by Souza, et al. (2009, 2010) and Silva, et al. (2010). The results were compared with experimental data to each fruit pulp and the average absolute deviation (AAD), calculated by Eq. 5, was used to evaluate each one.

$$AAD = \frac{1}{n} \sum_{i=1}^n \frac{|Y_{exp} - Y_{mod}|}{Y_{exp}} \quad (5)$$

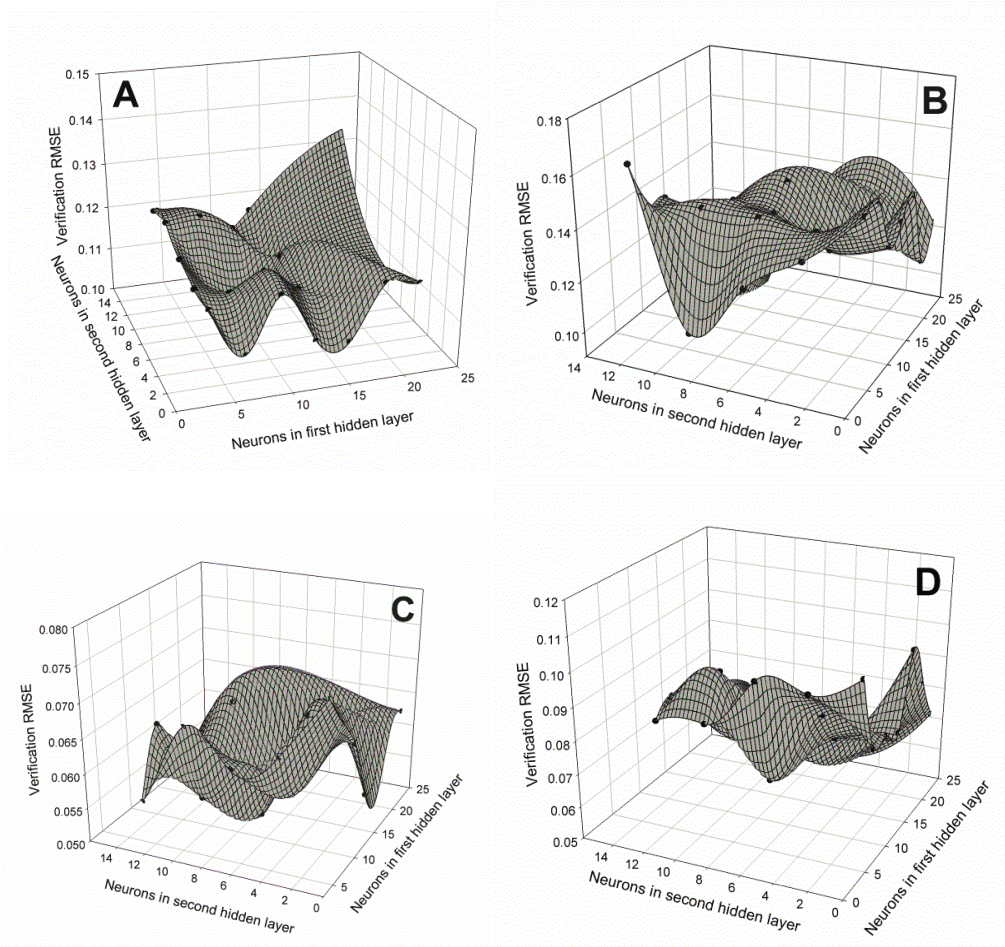
Where: n is the number of data, Y_{exp} is the experimentally observed value of desired thermal property and Y_{mod} is the predicted value by ANN model.

3. Results and Discussion

3.1 Evaluation of the best ANN architectures

The best ANNs were choices based on number of neurons in hidden layers which gave a minimum RMSE on training and verification steps and presents good correlation. Variation of the RMSE in function of the number of neurons on hidden layers to ANNs tested using total and individual data sets are present in Figure 1. It could be observed that the error surfaces are complexes and irregulars, with points of lockup, edges and local minimum. A similar behavior was observed by Chegini, et al. (2008) studying the use of ANNs to predict product parameters in an orange juice spray dryer.

Figure 1. Effect of neurons number in hidden layers on neural networks performance on verification step. (A) using total data set, (B) jackfruit data set, (C) genipap data set, (D) umbu data set.



Source: Authors.

Table 3 presents the values of correlation coefficients and RMSE for learning and verification steps of networks chosen. Other tested configurations presents higher RMSE and lower correlation which happens when the number of neurons on hidden layers are lacking or in excess. In the first case ANN is not able to do relationships between input and output variables. On the other hand, when there are many neurons, the network can incorporate data noise, reducing the generalization capacity and increasing the memorization instead of learning.

Table 3. Artificial neural networks generated with respectively RMSE and correlation coefficient values.

Data set	n° of neurons on hidden layers		Learning step		Verification step	
	First	Second	RMSE	Correlation	RMSE	Correlation
Total	15	0	0.1167	0.929	0.1095	0.920
Jackfruit pulps	3	9	0.0643	0.973	0.1017	0.948
Umbu pulps	18	0	0.0444	0.987	0.0905	0.975
Genipap pulps	15	0	0.0551	0.979	0.0777	0.933

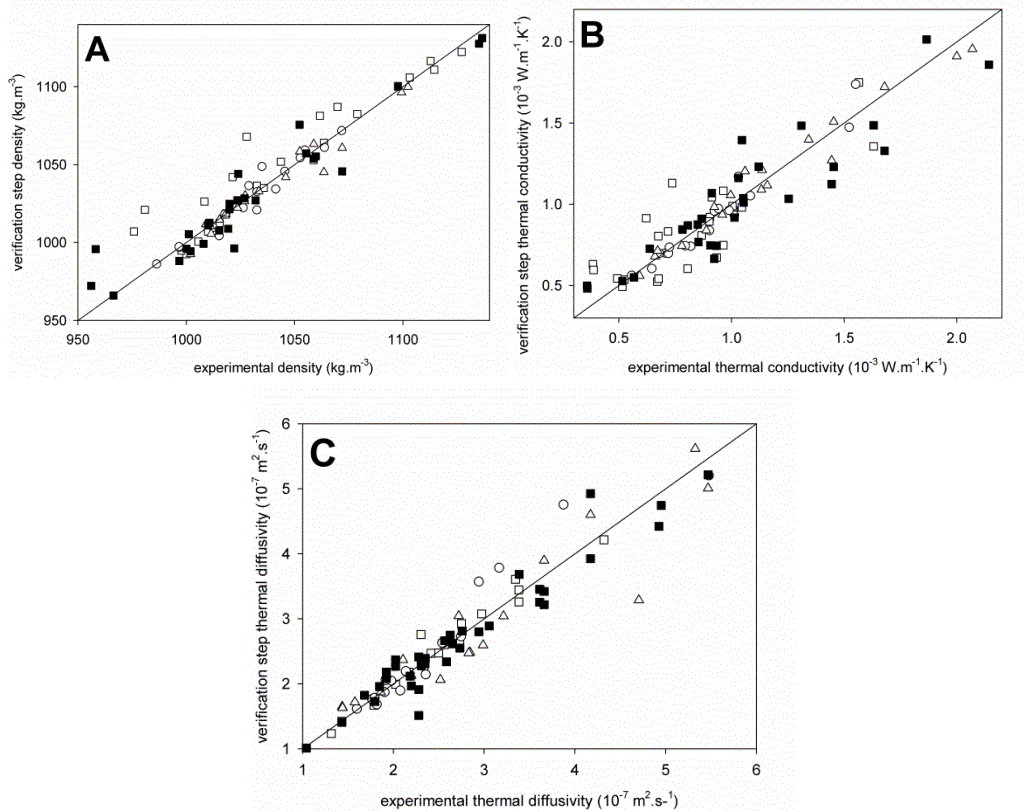
Source: Authors.

The obtained RMSE and correlation values are in agree with information reported by many authors. Chegini, et al. (2008) found RMSE values of 0.037 and 0.042 and correlation of 0.89 and 0.99 for learning and verification steps respectively, to a network with 3-14-10-7 configuration (3 input neurons, 14 on first and 10 on second hidden layers and 7 outputs). Studying the prediction of moisture content and water activity of semi-finished cassava crackers using ANNs, Lertworasirikul & Tipsuwan (2008) concluded that the best one was the network with the 3-9-2 configuration, presenting RMSE of 0.0917 and correlation of 0.99. Sucipto et al. (2019), seeking to classify the protein content of wheat flour from its bioelectric properties (capacitance and resistance) found that the best RNA topology for classification between hard, medium and soft flour of protein content is 2-20-50-3, which produced RMSE values of 0.0097 and 0.0399 and a correlation of 0.99 and 0.98 for the learning and verification stages, respectively.

3.2 ANNs performance

In Figure 2 are presented the comparison between experimental and predicted values (on verification step) to each thermophysical property studied. The plots showed a predictive ability of the ANNs all properties, with data points located around the ideal unity-slope line. From Figure 2 and RMSE and correlation values in Table 3 it could be verified that the predictive ability of the ANN obtained from total data set didn't differ of the ANNs generated from individual data sets, being adequate to estimate density, thermal conductivity and thermal diffusivity values from temperature and moisture content data, inside trained ranges.

Figure 2. Correlation between experimental data and predicted values by ANNs generated on verification step. (A) density, (B) thermal conductivity, (C) thermal diffusivity. ■ total data set, □ jackfruit, ○ genipap and △ umbu data sets.



Source: Authors.

When compared to polynomial models fitted by Souza, et al. (2009, 2010) and Silva, et al. (2010), ANN models presented near AAD values, showed in Table 4. This suggests the use of ANNs to predict studied properties, once only one network (created from total data set) could replace nine polynomial models. Chegini, et al. (2008) concluded that the ANN obtained to predict seven performance indices of orange juice spray dryer from three input variables could replace polynomial models previously fitted.

Table 4. Average absolute deviations for created ANNs and reported polynomial models.

Experimental data set	Property	Network models		Polynomial models		
		Total ANN*	Individual ANNs**	Souza et al. (2009)	Silva et al. (2010)	Souza et al. (2010)
Jackfruit	ρ	0.0349	0.0356	0.0092	---	---
	κ	0.2346	0.1970	0.2379	---	---
	α	0.6341	0.3180	0.2354	---	---
Genipap	ρ	0.0268	0.0255	---	0.0730	---
	κ	0.1979	0.2744	---	0.7917	---
	α	0.3815	0.4401	---	0.0843	---
Umbu	ρ	0.0219	0.0250	---	---	0.0031
	κ	0.3423	0.2410	---	---	0.0705
	α	0.3423	0.1968	---	---	0.7434

* ANN created from total data set. ** ANNs created from data sets to each fruit.
Source: Authors.

ANNs still have the advantage of the ability to re-learn to improve their performance if new data are available. ANN models could improve their performance with results obtained from new experiments which provides the gradual possibility of establishment of a unique powerful model which can be of paramount importance in automatic control system (Chegini, et al., 2008).

The utilization of a unique ANN generated to predict thermal properties of other tropical fruits pulps is possible and had a great potential, being necessary more studies. The use of ANNs permit a fast modeling with the as same reliability polynomials models, besides to be a valuable tool in automation and equipment design.

4. Conclusions

Artificial neural network modeling presents as alternative to polynomial modeling of thermal properties, showing near reliability and predictive ability. A neural networks were created to predict three thermophysical properties from temperature and moisture content of

three exotic tropical fruit pulps. The best found ANN configuration from total disposable data set had one hidden layer with 15 neurons and presents RMSE and correlation close to networks generated from each fruit data sets. Compared to polynomial models developed networks presents similar average absolute deviations. The results suggests that only one ANN can replace nine polynomial models to predict thermophysical properties of jackfruit, genipap and umbu pulps. More studies are necessary to extended the results to other tropical fruit pulps.

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Percentage of contribution of each author in the manuscript

Leandro Soares Santos - 25%

Moisés Naves de Moraes – 25%

Júlia Dos Santos Lopes – 10%

Luciana Carolina Bauer – 15%

Paulo Bonomo – 10%

Renata Cristina Ferreira Bonomo – 25%