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Full Length Research Paper

Estimation of *Pinus brutia* Ten. wood density from Fourier Transform Infrared (FTIR) spectroscopic bands by Artificial Neural Network (ANN)

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In this study, the rapid Fourier transform infrared (FTIR) spectroscopic method was used to indirectly measure the wood density of *Pinus brutia* Ten. samples. A model was constructed to relate FTIR data to wood density determined by laboratory analysis, through the application of artificial neural network (ANN) modelling approach to a set of calibration observations. The proposed model with two hidden neurons performed very good to estimate the wood density with high correlation R^2 values of 0.9833 for training and 0.9814 for testing, respectively, and with a low prediction error of 0.71% in the validation. This analysis showed that ANN coupled with FTIR spectroscopy could be used to accurately predict the density of wood samples.

Key words: Wood density, Fourier transform infrared (FTIR) spectroscopy, Artificial neural network (ANN), *Pinus brutia*.

INTRODUCTION

The structure of wood has been subjected in many studies based on vibrational spectroscopic methods. All of these techniques provide information on the molecular structure of wood and, in many cases; solid or ground wood samples can be analyzed directly without tiresome preparation. Hence, it is possible to get information on the molecular level interactions between wood polymer components in their native condition. Moreover, these methods are both time-saving and nondestructive (Rodrigues et al., 1998; Silva et al., 1999; Meder et al., 1999; Haukson et al., 2001; Rodrigues et al., 2001; Kelley et al., 2004; Yasar, 2010)

In most of the published studies addressing the assessment of solid wood properties by spectroscopic methods, the chemical properties (Rodrigues et al., 1998; Silva et al., 1999; Meder et al., 1999; Rodrigues et al., 2001; Kelley et al., 2004; Yasar, 2010) and density (Meder et al., 1999; Haukson et al., 2001) of solid wood samples have been determined from the spectral data combined with multivariate data analysis methods.

Fourier transform infrared (FTIR) spectroscopy can be used rapidly and it is costly effective in analyzing some wood properties. There are several publications on the application of the FTIR spectroscopy to determine extractives, lignin and carbohydrate contents of *Pinus radiata* using Partial Least Squares (PLS) (Meder et al., 1999), lignin content of *Picea sitchensis* (Bong.) Carr. using Principal Component Regression (PCR) (Silva et al. 1999), residual lignin content of holocellulose (*Pinus brutia* Ten.) using Artificial Neural Network (ANN) (Yasar, 2010), monosaccharide composition of *Eucalyptus globulus* using PLS data analysis method (Rodrigues et al., 2001). However, the density is related to chemical constituents of wood (Diaz-vaz et al., 2009). Therefore, density of wood is also estimated from FTIR spectrum using PLS data analysis technique (Meder et al., 1999).

The standard paradigm for ANN classification comprises a pre-processing stage of feature extraction and normalization, a classification stage using an 'optimum' network architecture and weights set, and a post-processing stage to resolve any discrepancies between

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the classifications of complexes detected across more than one channel. Within this paradigm, the optimum network architecture and weights set is determined during a learning phase in conjunction with a criterion for when to stop learning – namely the number of passes through the training set that minimizes the error between the desired and network output values. Multiple training runs are performed for each network architecture using a different random initialization of the weights on each run. Once the training is completed, the optimum network structure is selected using selection criteria – namely the network that has the smallest error rate. The classification performance of this network is then evaluated on an independent test set whose data are not included in the training. After testing phase, the network that presents best estimation performance is used for predicting the external data set (Zupan and Gasteiger, 1993; Zhang et al., 1998; Boozarjomehry and Svrcek, 2001)

This paper describes the building of an empirical density of *P. brutia* Ten. wood of model using ANN; with the model, the density value of a wood sample may be predicted by the FTIR spectrum measured on it.

MATERIALS AND METHODS

Materials

The samples were wood discs taken at 1.30 m height from *P. brutia* Ten. trees harvested 30 - 35 year-old plantations from Asagı Gokdere-Isparta and Kas-Antalya in Turkey.

Methods

Blocks cut from wood discs were 2 × 2 × 3 cm. Wood density was then calculated as the sample oven dry weight is divided by the dry sample volume (Haygreen and Bowyer, 1996). Volume dimensions were measured with electronic calipers. Determination of wood density was carried out in 5 measurements for each sample.

The wood samples used for wood density determination were separately milled to pass 40 - 100 mesh in Retsch SK 1 mill. The milled chips were then pulverized with agate mortar and pestle to have particle size from 20 - 45 µm. The FTIR pellets were prepared by mixing 10 mg of the each pulverized sample with 1000 mg KBr and further by compression of 8 t. The spectra were recorded in a Perkin Elmer BX FTIR Spectrometer in the wave number range 4000 - 400 cm^{-1}. Five scans per sample were collected.

However, the region between 2000 and 550 cm^{-1} of FTIR spectra was generally found to be informative for rapid determination of chemical and physical wood properties (Silva et al., 1999; Meder et al., 1999; Rodrigues et al., 2001). Therefore, we used the region 1876 - 832 cm^{-1} for estimating the wood density, and corrected the baseline of spectra to zero absorbance at 1876 cm^{-1} prior to ANN analysis.

Neural networks are a general technique of modeling non-linear systems, and were employed using MATLAB software in this study. They composed of simple computational elements (that is, neurons) operating in parallel. Each neuron produced one output through an activation function, typically a sigmoid function, which takes the weighted sum of the input arguments. Multiple neurons were combined into a layer, and a network contained a hidden layer. In the constructed neural networks, 25, 5 and 4 data pairs were used randomly for training, testing and validation sets, respectively. In a data pair (inputs-output), inputs consisted of 522 points (absorbance values) between 1876 -832 cm^{-1} from FTIR spectrum of each sample as neurons in the input layer and output was wood density (oven dry basis, g/cm^3) as a neuron in the output layer. Neural networks were trained with different number of neurons in the hidden layer (Figure 1).

We used the logistic function as activation function in the network construction. Therefore, before presenting to ANN, all data were normalized into a range 0.1 - 0.9 by the equation below:

$$X_N = 0.1 + \frac{0.8(X - X_{\min})}{(X_{\max} - X_{\min})} \quad (1)$$

X_N: The normalized value of the input or the output data
X: Original value of the data
X_{max} and X_{min}: The maximum and the minimum original values of the data

After training, the classification performance of network model is then evaluated on an introducing test set. The overall accuracy of the models was measured by root mean square (RMS) error using following equation:

$$RMS = \sqrt{N^{-1} \sum_{i=1}^{N} (X_i' - X_i)^2} \quad (2)$$

N: The number of data
X'i :The target value
Xi : The output value produced by the network

RESULTS AND DISCUSSION

The bands from FTIR spectrum, absorbance values between 1876 and 832 cm^{-1}, are demonstrated in Figure 2, and were used as input variables for the network models.

The density values of wood samples, which were output variables for the network models, and data sets (training, testing and validation), are indicated in Table 1. The values of density varied between 0.457 and 0.597 g/cm^3.

For estimating the wood density, neural networks were trained and tested using FTIR spectral data. ANNs were evaluated in terms of RMS error and NN2 model was chosen to predict the external data (validation) with RMS error value of 0.017574 in training and 0.024658 in testing (Table 2). Calibrations of NN2 model produced good correlation between actual and predicted data by the network. Correlation coefficient (R^2) was generally high and 0.9833 for training and 0.9814 for testing of NN2 model, respectively (Figure 3).

Four data pairs were used as an external data set for validation of the NN2 model, which was chosen as best model for predicting the wood density in the training and testing phases. The validation results shown in Table 3, developed good average percent relative standard error between the predicted and the actual values (0.71%).

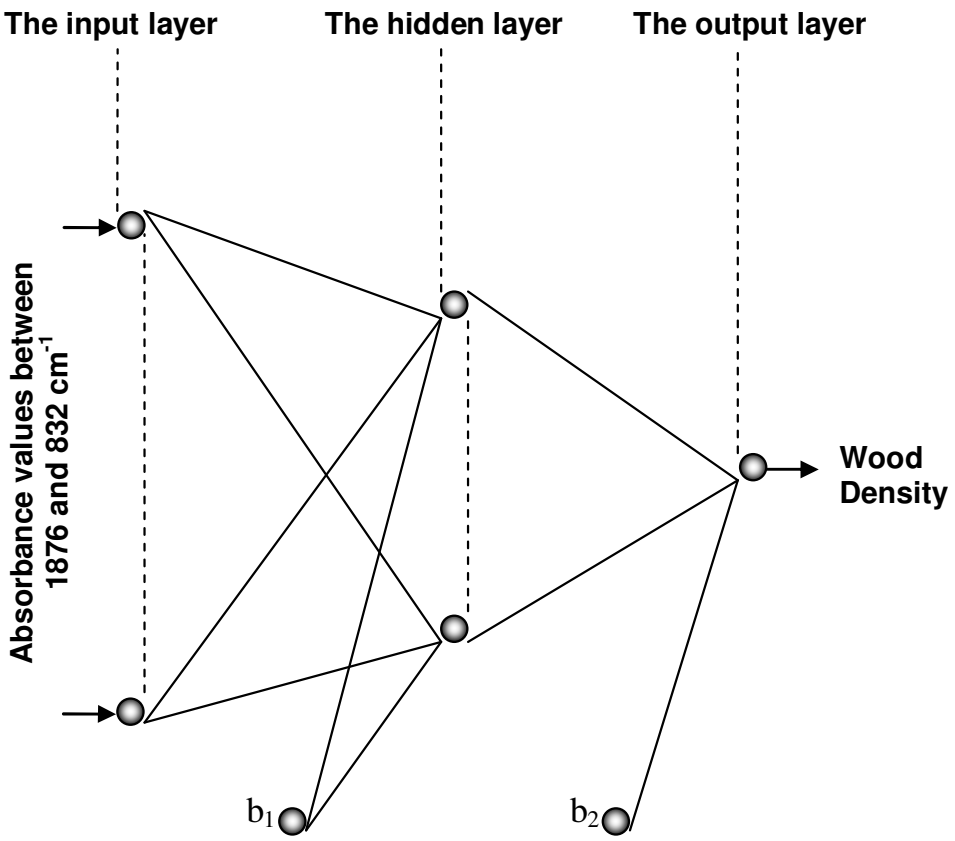

Figure 1. Network architecture used for prediction of wood density of *P. brutia* Ten. samples from FTIR spectral data.

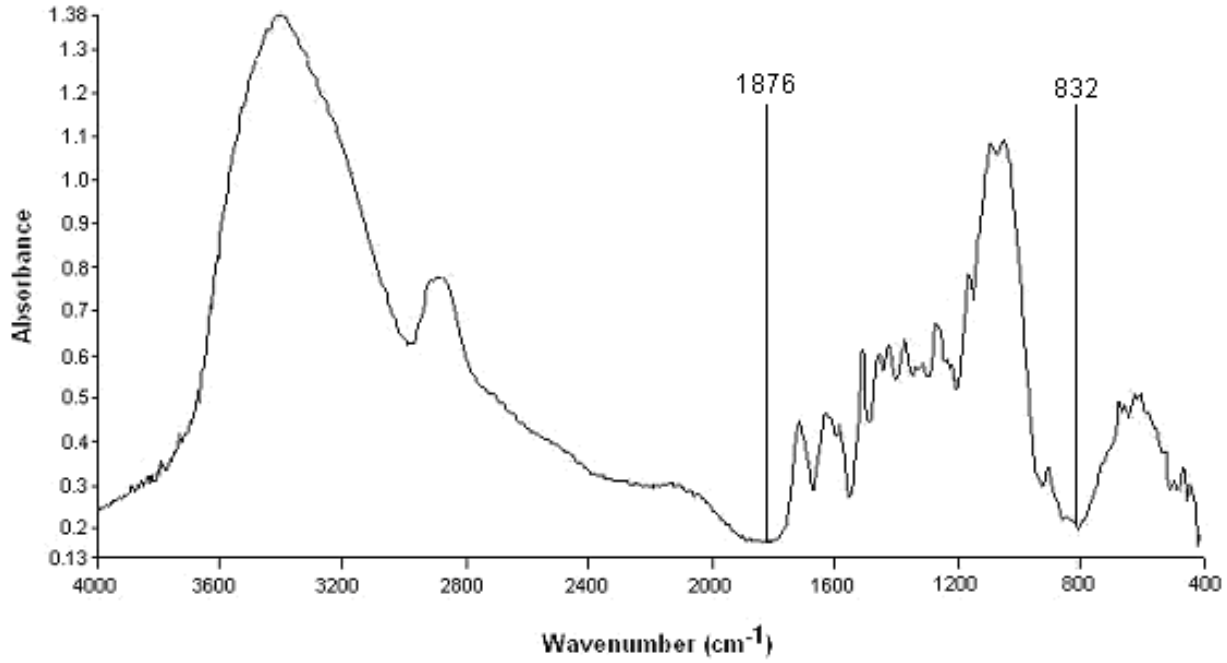

Figure 2. Typical FTIR spectrum of *P. brutia* Ten. wood sample.

Table 1. Wood density of *P. brutia* Ten. samples and data sets for ANN.

Sample	Wood density (g/cm^3)	Data set
1	0.457 (0.011)	Training
2	0.461 (0.009)	Testing
3	0.480 (0.008)	Validation
4	0.481 (0.008)	Training
5	0.482 (0.016)	Training
6	0.486 (0.006)	Training
7	0.503 (0.006)	Training
8	0.510 (0.013)	Testing
9	0.512 (0.010)	Training
10	0.520 (0.019)	Training
11	0.521 (0.010)	Validation
12	0.524 (0.020)	Training
13	0.526 (0.018)	Training
14	0.531 (0.013)	Testing
15	0.533 (0.008)	Training
16	0.536 (0.011)	Training
17	0.538 (0.012)	Training
18	0.543 (0.007)	Training
19	0.545 (0.015)	Training
20	0.546 (0.010)	Training
21	0.547 (0.010)	Training
22	0.548 (0.016)	Validation
23	0.550 (0.023)	Training
24	0.552 (0.028)	Training
25	0.553 (0.015)	Testing
26	0.554 (0.007)	Training
27	0.555 (0.002)	Training
28	0.557 (0.027)	Training
29	0.565 (0.012)	Training
30	0.570 (0.015)	Training
31	0.572 (0.015)	Training
32	0.579 (0.008)	Validation
33	0.586 (0.005)	Testing
34	0.597 (0.005)	Training

( ): Standard deviation.

Table 2. Performances of the neural network models for estimating the wood density of *P. brutia* Ten. samples.

Model	RMS error	
	Wood density	
	Training	Testing
NN1 522-1-1	0.026744	0.028531
NN2 522-2-1	0.017574	0.024658
NN3 522-3-1	0.028341	0.032378
NN4 522-4-1	0.029549	0.035770
NN5 522-5-1	0.030885	0.037444

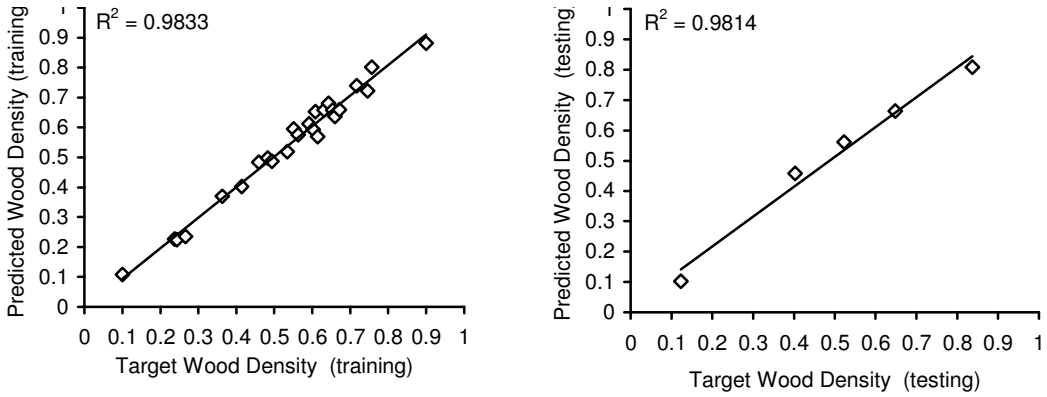

Figure 3. Relationship between the predicted and measured (target) values for wood density of *P. brutia* Ten. samples using FTIR spectroscopy via NN2 model.

Table 3. Validation of NN2 model for estimating the wood density of *P. brutia* Ten. samples.

Sample	Wood density (g/cm^3)		
	Actual	Predicted	RE %
3	0.480	0.483	0.63
11	0.521	0.525	0.77
22	0.548	0.552	0.73
32	0.579	0.583	0.69

The study showed that the application of ANN coupled with FTIR spectral data can improve the prediction level of wood density.

Conclusion

An artificial neural network model has been developed to predict wood density of *P. brutia* Ten. samples from FTIR spectral data. The model was composed of input, hidden and output layers. In this model, input variables consisted of absorbance values (522 points) between 1876 and 832 cm^{-1} from FTIR spectrum and output variables formed from wood density values. The model with two hidden neurons was performed fairly well. In the training and testing, the actual values was close the predicted values of wood density with high correlation coefficient (R^2) of 0.9833 and 0.9814, respectively. The proposed model estimated the wood density with a little prediction error of 0.71% in the validation. It was obtained that ANN is an affirmative way for predicting the wood density from FTIR spectral data.

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