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Araştırma Makalesi/*Research Article (Original Paper)*

Prediction of Protein Content of Winter Wheat by Canopy of Near Infrared Spectroscopy (NIRS), Using Partial Least Squares Regression (PLSR) and Artificial Neural Network (ANN) Models

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Abstract: In this study to predict amount of protein in wheat, near infrared spectroscopy technique (NIRS) was used that is a non-destructive and fast observing method. Partial Least Squares Regression (PLSR) and Artificial Neural Network (ANN) methods were used to choose the spectral bands and the best models, respectively. To compare the efficiency of models Root-mean-square error (RMSE) and R^2 were applied. The finest consequence by cascade forward back propagation (CFBP) was related to network structure of 8-8-1 with Levenberg-Marquardt (LM), and function of TANSIG-TANSIG-PURELIN (TANSIG-TANSIG-PURELIN (RMSE=0.0289 and R^2=0.9881 at 14 epochs). The consequences of estimation for ANN model (R^2=0.9881) was better than the PLSR model (R^2=0.9783). Therefore, according to the results, it can be said that NIRS has a high potential for predicting the amount of protein in wheat.

Keywords: ANN, NIRS, PLSR, Wheat protein content

Kısmi En Küçük Kareler Regresyonu (KEKKR) ve Yapay Sinir Ağı (YSA) Modelleri Kullanarak, Kanopi Kızılötesi Spektroskopisi (KS) ile Kış Buğdayında Protein İçeriğinin Tahmini

Öz: Bu çalışmada, buğdaydaki protein miktarını tahmin etmek için, tahribatsız ve hızlı bir gözlem yöntemi olan yakın kızılötesi spektroskopi (KS) tekniği kullanılmıştır. Sırasıyla spektral bantları ve en iyi modelleri seçmek için Kısmi En Küçük Kareler Regresyonu (KEKKR) ve Yapay Sinir Ağı (YSA) yöntemleri kullanılmıştır. Modellerin verimliliğini karşılaştırmak için Kök-ortalama-kare hata (KOKH) ve R^2 uygulanmıştır. Cascade ileri geri yayılımının (CİGY) en iyi sonucu, Levenberg-Marquardt (LM) ile 8-8-1 ağ yapısı ve TANSIG-TANSIG-PURELIN (TANSIG-TANSIG-PURELIN (RMSE = 0.0289 ve R2) 'nin işlevi ile ilgilidir. YSA modeli için tahmin sonuçları (R2 = 0.9881), KEKKR modelinden (R^2 = 0.9783) daha iyi bulunmuştur. Bu nedenle, sonuçlara göre, buğdaydaki protein miktarının belirlenmesinde KS'nin tahmin etme potansiyeli yüksek olduğu söylenebilir.

Anahtar kelimeler: ANN, NIRS, PLSR, Buğday protein içeriği

Introduction

Protein content (PC) of winter wheat is essential for nutrition and food (Tang et al. 2004; Rasooli et al. 2013; Mabood et al. 2017). Precise and appropriate prediction of the winter wheat PC can aid agriculturists create correct choices about manure application, winter wheat diversity choice, and crop assortment (Diker et al. 2003; Wang et al. 2004; Rasooli et al. 2014). There are typical calculation techniques for protein content (Diker et al. 2003; Galasso et al. 2017). These techniques are usually hard and lengthy, and cannot be applied to quickly evaluate the quality features. NIRS protects the integrity of samples, reduces the common costs as a non-destructive method and is appropriate for experiments with high amount of samples (Bagchi et al. 2016; Magwaza et al. 2016; Galosso et al. 2017; Mabood et al. 2017). Therefore, it has been applied as a replacement for chemical methods and it is extensively used in food industries (Magwaza et al. 2016; Bagchi et al. 2016). Choosing modeling techniques performs a vital function and quantitative analysis. PLSR is a common technique that has been derivative from PCA (principle component analyzing) in the spectroscopy (Moreira et al. 2015), and it has considerable consequences to predict dependent variables from a huge number of independent variables (Shetty et al. 2011; Nouri et al. 2017).

Ye et al. (2018), applied PLSR to make a model based on the spectral data measured to predict the PC in wheat, and suggested a new method, global search method, to select PLSR components. The consequences represented that the combination of ISA-SPA realized the reduction of the number of variables from 100 to 14 and decrease of SEP value from 0.0716 to 0.0528 compared to full-dimensionality variables. In the study, PC and canopy spectra in rice were measured based on rice field experiment. Key spectral bands were selected by principal component analysis (PCA) method, and the predicted models were built by multiple linear regressions (MLR), ANN and PLSR. The results showed that there is a significant correlation between CPC content and key spectral bands. The results of prediction for the three models were in order of PLSR > ANN > MLR with correlation values of 0.96, 0.92 and 0.90, respectively, for the validation data (Zhang et al. 2012). Gatius et al. (2004) used NIRS to analyse the PC of dried and milled samples of wheat and to discriminate samples according to their stage of growth. Kahriman et al. (2016) developed and validated qualitative and quantitative models to discriminate different types of maize and estimate biochemical constituents. Quantitative models with full spectral data gave more robust prediction than the others. The best prediction result (RMSEC= 222.4 µg g-1, R2 for Cal= 0.739, SEP= 213.3 µg g-1; RPD= 2.04 and r= 0.877) was obtained from the SVMR-FS model developed for chlorophyll content.

ANN is known as fine implement for dynamic modeling since it does not need factors of physical models (Amiri and Kaveh, 2014; Yousefi et al. 2014; Mohebbi et al. 2011). Zhang et al. (2012) studied three prediction methods calls PLS, MLR and ANN. Eventually they found out that the predictive power in PLS was highest. The outcomes of estimation for the models were respectively PLSR > ANN > MLR. Chen and Jing (2017) investigate the yield estimation technique with NIRS. To propose a suitable model, the generally applied ANN and PLSR yield estimation techniques were chosen and contrasted in this work. In another work, the anticipation of quality parameters in winter wheat under canopy NIRS with the use of PLSR Models and Artificial Neural Networks was investigated. The results showed that simultaneous use of NIR with ANN could be proper to estimate the qualitative properties of agricultural products (Mutlu et all. 2011; Akkol et all. 2017). In the other research by Mehmet ODABAS et al. (2015) Artificial Neural Network (ANN) model was developed based on the RGB (red, green, and blue) components of the color image captured with a digital camera for estimating the chlorophyll concentration. According to the obtained results, the neural network model is capable of estimating the St. John's wort leaf chlorophyll concentration with a reasonable accuracy. The coefficient of determination (R2) was 0.99 and mean square error (MSE) was obtained 0.005 from validation. To assess the procedures available in the current paper, the relevance between PC and spectral data in samples was investigated by PLS multivariable regression modeling and ANN. For this purpose, firstly, outlier samples were recognized and removed in terms of spectral data using the PCA technique. In addition, several pretreatment methods were applied such as SNV, D1, and D2 with Savitzky–Golay algorithm to remove unwanted variations in spectral data. For prediction of PC, nonlinear models are applied because of suppleness and nonlinear behavior of natural crops.

Materials and Methods

Field reference and spectral data was obtained from the farm lands of Ardabil province, Iran. A common type of winter wheat in Ardabil "Pishgam" was cultivated in two continuous years from 2015 to 2016. Dimensions of experimental field were 40 × 120 m^2. The land was separated into 8 blocks (four fertilizing level by two repetitions). Reflectance data were attained using a Spectroradiometer FieldSpec3 (FS3) (Analytical Spectral Devices, Inc. USA). Spectral reflection can be measured in domains between 350-2500 nm (Zhang et al. 2011; Zhang et al. 2017). In this study, all information of wavelengths after 1350 nm band were emitted because of noises due to water absorption phenomena. The specification of Spectroradiometer (FS3) was shown in the table 1. The samples for measuring of protein content of wheat grains were taken from 40 target points (5 points in each block) as the same area which reference data was randomly set in the field in each year. Then, the PC was determined by Kjeldahl method based on the standard of GB/T 5009.5-1985 (Rasooli et al. 2014).

Table 1. The specification of Spectroradiometer FieldSpec3 (FS3)

Spectral Range	350-2500 nm
Spectral Resolution	3 nm @ 700 nm
	10 nm @ 1400/2100 nm
Sampling Interval	1.4 nm @ 350-1050 nm
	2 nm @ 1000-2500 nm
Scanning Time	100 milliseconds
Noise Equivalent	UV/VNIR 1.1 x 10-9 W/cm2/nm/sr @700 nm
Radiance (NEdL)	NIR 2.4 x 10-9 W/cm2/nm/sr @ 1400 nm
	NIR 4.7 x 10-9 W/cm2/nm/sr @ 2100 nm
Weight	12 lbs (5.2 kg)

Data analysis

Firstly, to establish a dataset from two years sampling, the average of common targets was calculated for samples of spectral data and PC. Then one matrix of dataset included 40 rows (averaged samples) and 1001 column (one column of PC and 1000 column of spectral data) were upload to Unscramble x10 software (CAMO Software, Oslo, Norway). And 4 outliers samples which having a harmful effect on modelling were determined and eliminated (Heise and Winzen, 2006). For this purpose, PCA was used to evaluate the variation in spectral data of all the samples (Zhang et al. 2013; Nicolai et al. 2007). After eliminating the outliers (4 samples, No. 7, No. 15, No. 24 and No. 39), all the 36 remnant samples were prepared in order to evaluation of their protein content. Then, to create the validation and calibration sets, samples were divided into two groups. Validation and calibration sets consist of the 30% and 70% of all samples, respectively. Then the anticipated models were constructed by PLSR model with Unscramble x10 software. The accuracy of regression model was calculated by RMSE and coefficient of determination (R^2).

Artificial neural networks modeling

In order to compare the result of prediction model using PLSR with the ANN the same dataset was imported in MATLAB R2017 software environment. The structure of ANN is presented in Figure 1. The variables of wavelengths were contemplated as the inputs, whereas one parameter of protein was applied as the outputs. The hidden layer's neurons are selected using the training, and testing data sets. Each dataset was comprised of two categories, including 30% test and 70% training.

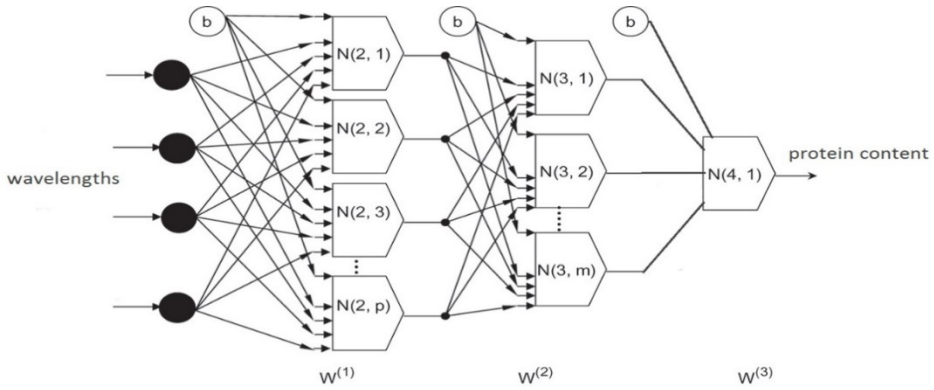

Figure 1. ANN structure.

In present study, there were two kinds of multilayer perceptron (MLP), called FFBP and CFBP that were applied to predict the protein content. Also BFGS Quasi-Newton and LM were applied to finalize ANN. The important diversity between CFBP and FFBP is in the relationship of between neurons (Amiri et al. 2012). To reach the enhanced network arrangement, transfer functions were engaged, which are defined in the next equations (Aghajani et al. 2012; Kaveh and Amiri, 2015):

$$\text{PURELIN}: Y_j = X_j \quad (1)$$

$$\text{TANSIG}: Y_j = \frac{2}{(1 + \exp(2X_j)) - 1} \quad (2)$$

$$\text{LOGSIG}: Y_j = \frac{1}{1 + \exp(-X_j)} \quad (3)$$

where:
Y_j is j^{th} neuron output
X_j is sum of weighed inputs for each neuron in j^{th} layer and computed according to Eq. (4):

$$X_j = \sum_{i=1}^{m} W_{ij} * Y_i + b_j \quad (4)$$

where:
m is the number of output layer neurons
W_{ij} is weight coefficient between i^{th} and j^{th} layers
Y_i is i^{th} neuron output
b_j is bias of j^{th} neuron for FFBP and CFBP networks

Results and Discussion

The averaged protein for 40 rows of winter wheat samples (No. 1 to No. 40) ranged between 7.9 to 11.5 % was of significant importance for this study; the amount of PC is demonstrated in Table 2.

Table 2. The PC for 40 rows of winter wheat samples.

Row number	Protein content/%	Row number	Protein content/%
1	8.7	21	7.9
2	10.1	22	8.3
3	11.2	23	11.5
4	10.6	24	11.0
5	10.5	25	10.8
6	11.2	26	11.3
7	11.5	27	8.2
8	9.95	28	12.4
9	9.3	29	8.6
10	10.2	30	12.3
11	10.7	31	8.5
12	11.3	32	10.1
13	10.2	33	11.4
14	10.8	34	10.6
15	10.0	35	11.0
16	9.1	36	10.5
17	10.7	37	11.3
18	11.6	38	11.4
19	13.3	39	11.7
20	9.95	40	9.8

Evaluation of PLSR Model

The canopy in winter wheat showed a diverse raw reflectance in the 510–690 nm and 730–1050 nm (Figure 2). The consequences presented in the current study that there were two clear band ranges amid 510–690 nm and 730–1050 nm (Figure 2). Alike consequences were reported in earlier papers (He et al. 2006; Li et al. 2006; Yi et al. 2007). Since unnecessary spectra influence accuracy of model, PCA technique was applied to decrease main input factors. Then, the anticipated model was constructed by partial least squares regression (PLSR) technique. For this purpose, various preprocessing methods include SNV, D1, D2, based on the Savitzky–Golay algorithm and their combinations were used. In order to investigate the impact of these divers' methods on the precision of the developed models, a multivariate modeling for spectra was performed without any pre-processing. After development of PLS models, the evaluation of the models was done by a full cross-validation method (Haddad et al. 2013; Farzad AZADSHAHRAKI et al. 2018).

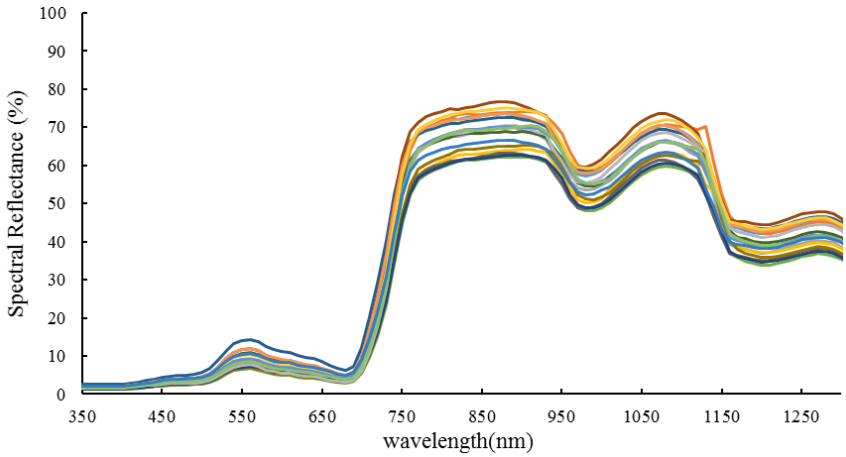

Figure 2. Spectral reflectance & wavelength.

In order to determine the best predictive model for protein content, regression coefficients and standard error predictions of models were calculated and compared. The values of R^2 and RMSE by removing the uncertain sample were obtained, then these values were calculated without removing the uncertain sample and finally, the values were compared with each other (Table 3). The amounts of R^2 and RMSE for No. 7, No. 15, No. 24 and No. 39 were 0.977, 0.975, 0.981, 0.983 and 0.2194, 0.2223, 0.2010, 0.1899, respectively. Other researchers also found similar results in their research (Ye et al. 2018; He et al. 2006; Li et al. 2006; Yi et al. 2007).

Table 3. The impacts of No. 7, 15, 24 and 39 samples on models

removed samples	R^2	RMSE
No deleting	0.974	0.2384
No. 7	0.977	0.2194
No. 15	0.975	0.2223
No. 24	0.981	0.2010
No. 39	0.983	0.1899
No. 24, No. 39	0.988	0.1590
No. 15, No. 39	0.984	0.1856
No. 15, No. 24	0.983	0.1905
No. 7, No. 39	0.986	0.1726
No. 7, No. 24	0.984	0.1845
No. 7, No. 15	0.978	0.2155
No. 7, No. 15, No. 39	0.986	0.1704
No. 7, No. 15, No. 24	0.985	0.1746
No. 7, No. 24, No. 39	0.990	0.1458
No. 15, No. 24, No. 39	0.989	0.1501
No. 7, No. 15, No. 24, No. 39	0.991	0.1374

The amount of R^2 and RMSE for PC are displayed in Table 4. The value of R^2 varied between 0.959–0.979 and the RMSE values were from 0.4333 to 0.1457. Study of the results showed that, simultaneously usage of the three preprocessing methods formed outstanding consequences.

Table 4. Anticipated results for PC

Pre-processing	R^2	RMSE	components
Raw	0.972	0.2670	7
D_1	0.969	0.3185	5
D_2	0.966	0.3488	5
SNV	0.959	0.4304	6
S-G	0.972	0.2676	7
D_1+SNV	0.978	0.1486	5
D_2+SNV	0.973	0.2637	4
S-G+SNV	0.959	0.4333	6
S-G+D_1	0.969	0.3120	5
S-G+D_2	0.970	0.2957	8
S-G+D_1+SNV	0.979	0.1457	5
S-G+D_2+SNV	0.975	0.2206	4

For this state RMSE value reduced importantly from 0.2670 to 0.1457 in contrast with the state without using preprocessing methods. In addition, the R^2 was 0.979 for this state. Figure 3 shows the investigational data of PC against the anticipated values of PC. Many researchers have achieved better results in predicting of crop characteristics using different preprocessing methods (Chen et al. 2017; Porfire et al. 2017). Millar, (2003) informed higher R^2 for PC from whole grain that was obtained here. Delwiche et al. (1998) informed R^2 values for estimating PC that were similar to those reported here. Wentzell (2003) contrasted the PCR and PLSR, and introduced the PLSR needs less hidden variables than PCR. Zhang et al. (2012) selected spectral bands by PCA technique, and made the anticipated models by ANN, PLSR, and MLR.

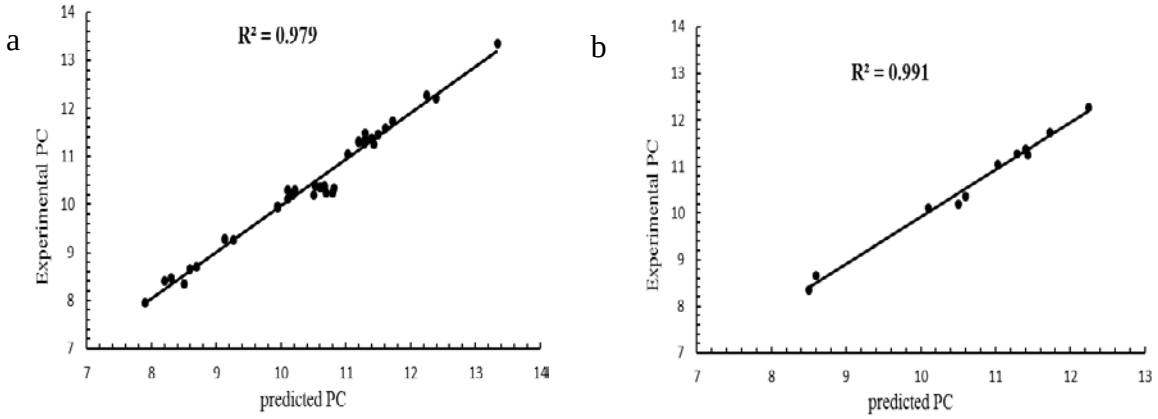

Figure 3. Predicted PC & experimental PC by PLSR. a) All data b) Validation.

Evaluation of ANN Model

The predicted PC with different methods has shown in Table 5. To train FFBP and CFBP networks, LM and BFGS were applied. Some structures were chosen the finest consequences. Consequences of models performance indices ($R2$ and RMSE) are shown in Table 5.

Table 5. Best selected topologies

Network	Training algorithm	Threshold function	Number of layers and neurons	RMSE	R^2	Epoch
FFBP	*LM*	TAN-TAN-TAN	5-5-1	0.0385	0.979	10
		LOG-TAN-TAN	10-5-1	0.0298	0.988	9
	BFG	TAN-TAN-TAN	5-5-1	0.0374	0.981	10
		TAN-TAN-PUR	8-8-1	0.0342	0.984	10
CFBP	LM	TAN-TAN-TAN	10-10-1	0.0361	0.983	12
		TAN-TAN-PUR	8-8-1	0.0289	0.988	14
	BFG	TAN-TAN-TAN	5-5-1	0.0319	0.987	10
		TAN-LOG-PUR	15-10-1	0.0322	0.986	12

The finest consequence attained by FFBP in prediction of PC was related to 10-5-1 topology and LOG-TAN-TAN threshold function with LM algorithm in the initial strategy. This structure produced RMSE=0.0298 and R^2=0.9879 with 9 epochs. The finest consequence for the next strategy of FFBP with BFG algorithm was assigned to 8-8-1 topology and threshold functions of TAN-TAN-PUR. This structure created RMSE=0.0342 and R2=0.9838 for PC. The finest consequence by CFBP was related to structure of 8-8-1 by LM, TAN-TAN-PUR and the initial strategy. The output of the arrangement was RMSE=0.0289 and R^2=0.9881 at 14 epochs. CFBP with the second strategy, BFG algorithm, topology of 5-5-1 and threshold functions of TAN-TAN-TAN introduced the output of RMSE=0.0319 and R^2=0.9874. Figure 4 displays the investigational data of PC versus the anticipated values PC. The qualitative models developed by Kahriman et al. (2016) had the potential to discriminate maize plants by their genotypic specialties (HOM, HPM or NORMAL). However it shows that spectral measurements can also be used for quantitative determination of protein content.

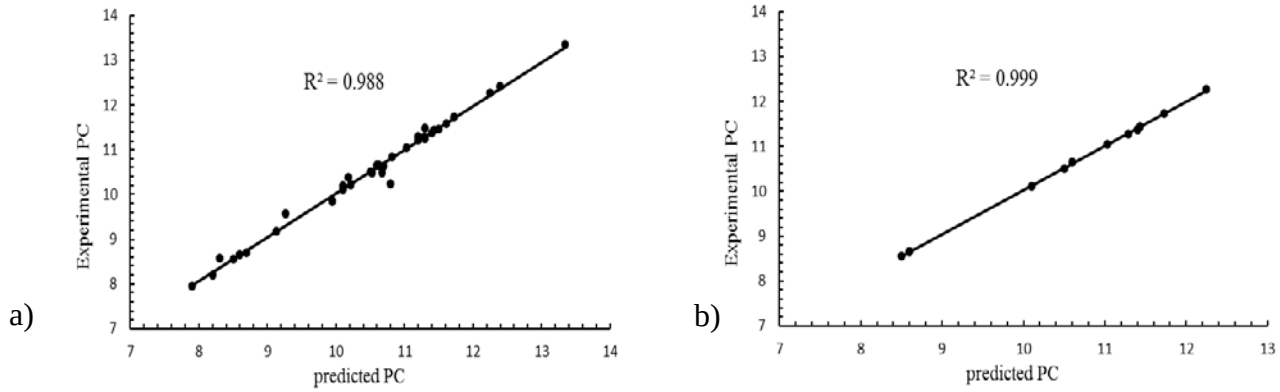

Figure 4. Predicted PC & experimental PC by ANN. a) All data b) Validation.

Conclusion

Prediction of PC in wheat has been an effective use of NIRS since it includes powerful absorbency bands in the near infrared area. Outcomes achieved in literatures to PC content in wheat were almost alike to those achieved in this work. The consequences presented an important correlation between PC and spectral data. The best consequences were obtained by PLSR. In this paper, numerous ANN models and PLSR models were established to predict protein of wheat. The consequences presented that the capability of advanced ANN models and PLSR models to calculate and estimate the protein content in winter wheat. The best result for PLSR model was obtained for state that, three preprocessing methods simultaneously used. For this state RMSE value reduced importantly from 0.2670 to 0.1457 in contrast with the state without using preprocessing methods. In addition, the R^2 was 0.9783 for this state. Also eliminating four variables gave us the best result. The finest consequences attained by FFBP in prediction of PC was related to 10-5-1 topology and LOG-TAN-TAN threshold function with LM algorithm in the initial strategy. This structure produced RMSE=0.0298 and R^2=0.9879 with 9 epochs. The finest consequence by CFBP was related to structure of 8-8-1 by LM, TAN-TAN-PUR and the initial strategy. This arrangement output was RMSE=0.0289 and R^2=0.9881 at 14 epochs. According to the results, it was found that using different models of artificial neural network provides better results in predicting the amount of winter wheat protein in comparison with partial least squares regression model.

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