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► **To cite this version:**

Hao Ma, Haiyan Ji, Xue Liang, Zhenhong Rao. Study of Quantitative Analysis for Moisture Content in Winter Wheat Leaves Using MSC-ANN Algorithm. 5th Computer and Computing Technologies in Agriculture (CCTA), Oct 2011, Beijing, China. pp.17-23, 10.1007/978-3-642-27278-3_3. hal-01360959

HAL Id: hal-01360959

<https://inria.hal.science/hal-01360959v1>

Submitted on 6 Sep 2016

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Study of quantitative analysis for moisture content in winter wheat leaves using MSC-ANN algorithm

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Abstract. Reflectance spectra of winter wheat leaves specimens was acquired with portable spectroradiometer and integral sphere, after pretreatment with the method of multiplicative scatter correction(MSC), the principal components calculated were used as the inputs of artificial neural networks to build the Back--Propagation artificial neural networks model(BP-ANN), which can be used to predict moisture content of winter wheat leaves very well. In the article we made a study of quantitative analysis for moisture content of winter wheat leaves in booting and milk stage. The correlation coefficient(r) of predicted set in booting stage was 0.918, the standard deviation(SD) was 0.995 and the relative standard deviation(RSD) was 1.35%. And in milk stage $r = 0.922$, SD = 2.24, RSD = 3.37%. The model can truly predict the content of water in winter wheat leaves. Compared with the classical method, the artificial neural networks can build much better predicted model.

Keywords: MSC; ANN ; Moisture Content; Reflectance spectrum; Quantitative analysis¹

¹ **ACKNOWLEDGMENT.** This work was supported by 863 National High-Tech Research and Development Plan (No. 2007AA10Z211).

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1 Instruction

The moisture content is one of the most important factors to effect photosynthesis, respiration and biomass in plant[1-3]. Shortage of moisture would effect the physiological process, biochemical process and morphostucture of plant, and further effect the growing, output and quality of crops[4]. For the past few years there are many flood and drought disasters arising, which make the crop cutting into large area. Therefore, the scientific management of moisture content in crops increasingly becomes one of the most important measures in crop production.

Presently, the moisture content of large area crops has been researched by means of remote sensing, which indicates the deficit of moisture by measuring the temperature of plant canopy[5]. Another common method is to establish an inverse model about reflectance of leaves and moisture content, which bases on the characteristic of moisture absorbing infrared light. From the 80's, many famous scholars have proved that: the spectral reflectance of plant be used to detect status of moisture content is feasible[6-11]. In this paper we would investigate the mehtod of processing spectrum to promote the result of modeling.

Multiplicative scatter correction(MSC) is a very effective spectrum preprocessing method of dealing with living leaves of plant. It is a multi-variable scatter correction technique[12]. The original spectrum processed with the method can effectively eliminate the scattng caused by the physical factors, enhance the spectral information related to the tested ingredients, reduce the impact of baseline translation and drift between samples caused by the scattng, and can greatly improve the signal-to-noise ratio of correlative spectra.

In this paper we gathered the reflectance spectra of a new collection of winter wheat leaves, then analyzed the spectral data with the method of principal component analysis after the spectra preprocessed with the method of MSC, and finally made study of the model with the training system of artificial neural network. From the result of modeling, we can get the better result by the model of MSC-ANN, especially dealing with the living leaves in the field.

2 The algorithm

2.1 The algorithm of MSC

The use of MSC firstly requires to create a “ideal spectrum” of the tested samples, which is used to correct the others as a standard spectrum[13]. Actually, we usually calculate the average spectrum of all the samples as the standard spectrum, operate each sample spectrum with the method of unary linear regression to get their regression constant and regression coefficients, and then correct the original spectra of each sample to improve the signal-to-noise ratio. The concrete process of arithmetic is as follow:

(1) The average spectrum:

$$\overline{\mathbf{A}}_{i,j} = \frac{\sum_{i=1}^n \mathbf{A}_{i,j}}{n}$$

(2) Unary linear regression:

$$\mathbf{A}_i = \overline{\mathbf{A}}_i m_i + b_i$$

(3) MSC:

$$\mathbf{A}_{i(MSC)} = \frac{(\mathbf{A}_i - b_i)}{m_i}$$

In the formula, i is the number of samples, j is the number of wavelength.

2.2 The algorithm of ANN

The neural network developed in recent years is a very active interdisciplinary, which refers to many disciplines such as biology, electronics, computers, mathematics, physics and so on, and it has a extensive future[14]. Artificial neural network is an effective means of researching spectroscopy, which is widely applied in the study of spectrum and NMR. Currently the most active model is the back propagation(BP) algorithm model, proposed by Rumelhart[15], which involves parallel distributed processing theory and multi-layer network. BP neural network model is a powerful learning system to achieve the nonlinear mapping between input and output in high degree[16], and it has proved the model can approximate to any continuous nonlinear curves[17]. The preprocessor spectra is operated with the method of principal component analysis to get appropriate principal components, which are used as the input of multi-layer feedforward neural network, and finally establishing the training model of BP neural network.

3. Experiment

3.1 Test method and instrument

we collected respectively 40 leaves as the samples in booting and milk stages of winter wheat, and then measured their reflectance spectra by using the FieldSpec@Pro FR portable spectrometer, which produced by the U.S. ASD company, and 1800 integrating sphere that produced by LI-COR company. The true values of moisture content were gathered by drying method[18]. We first surveyed the fresh weight of the leaves with AB104N precision electronic balance, and put the leaves in 105°C to dry until their weight were constant, the moisture content is as follow:

$$\text{Moisture content (\%)} = (\text{fresh weight} - \text{dry weight}) / \text{fresh weight} \times 100\%$$

3.2 The information of sample spectra

Scanned range is from 400nm to 2100nm, the data are collected in each nanometer of the spectral region, so we can get 1700 data points from each spectrum. Actually, each sample was scanned 5 times, the average spectrum is calculated to be used as the true spectrum of sample. That in figure 1 is three spectrograms choosed. From the figure we can see there are three characteristic peaks in each spectrum, 1160nm, 1440nm and 1930nm, especially the peak point of the 1440nm is the most notable.

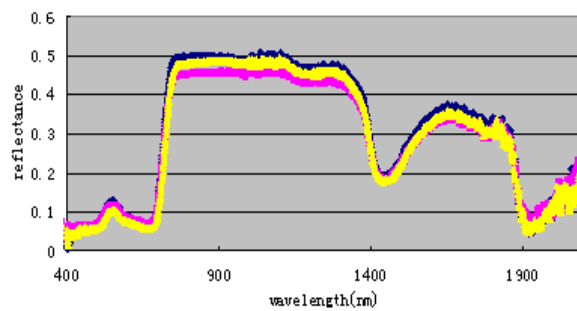


Fig.1 Reflectance spectra of winter wheat leaves

4. The results of experiment and analysis

4.1 Modeling for winter wheat leaves in booting stage and prediction results

The reflectance spectrum is used for modeling ranging from 1431nm to 1470nm. Two distinct different samples are removed from the 40 samples collected and the remaining 38 samples are divided into two parts, 30 samples are put into calibration set and the others into test set. The number of principle component is setted to 5. The parameters of neural network model are as follows:

```
net.trainParam.lr=0.04; % the learning rate of training is setted to 0.04.  
net.trainParam.mc=0.2; % the momentum coefficient is setted to 0.2.  
net.trainParam.epochs=20; % the training epochs is setted to 20.  
net.trainParam.goal=0.4; % the error of training objective is setted to  
0.4.
```

After several rounds of training, we can get a better prediction network. Modeling for the calibration set, we can get the relationships between predicted and true values of moisture content of winter wheat leaves in booting stage from figure 2. The correlation coefficient $r = 0.958$, the standard deviation of forecast $SD = 0.337$, the relative standard deviation $RSD = 0.45\%$. Detecting the data of test set, we can get the relationships between predicted and true values of moisture content in the model of test set from figure 3. $r = 0.918$, $SD = 0.995$, $RSD = 1.35\%$.

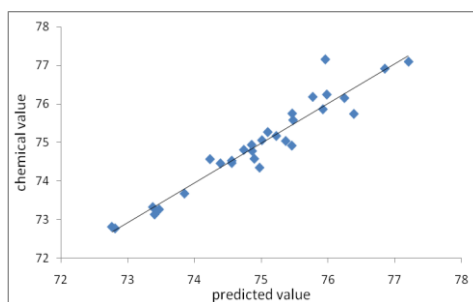


Fig.2 Relationships between predicted and true values of calibration set in booting stage

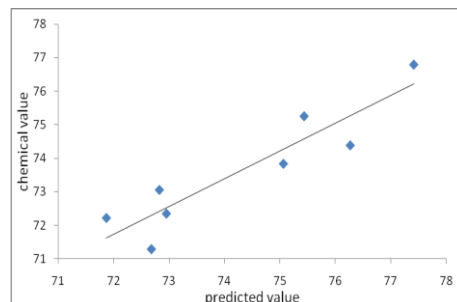


Fig.3 Relationships between predicted and true values of predicted set in booting stage

4.2 Modeling for winter wheat leaves in milk stage and prediction results

The reflectance spectrum is used for modeling ranging from 1411nm to 1480nm. The 40 samples are divided into two parts, 30 samples in calibration set and the others in test set. The number of principal component is setted to 5. The parameters of neural network model are as follow:

```
net.trainParam.lr=0.04; % the learning rate of training is setted to 0.04.  
net.trainParam.mc=0.2; % the momentum coefficient is setted to 0.2.  
net.trainParam.epochs=20; % the training epochs is setted to 20.  
net.trainParam.goal=1.0; % the error of training objective is setted to  
1.0.
```

After several rounds of training, we can get a better prediction network. Modeling for the calibration set, We can get the relationships between predicted and ture values of moisture content of winter wheat leaves in milk stage from figure 4, $r = 0.963$, $SD = 0.949$, $RSD = 1.43\%$. Detecting the data of test set, we can get the relationships between predicted and ture values of moisture content in the model of test set from figure 5. $r = 0.922$, $SD = 2.24$, $RSD = 3.37\%$.

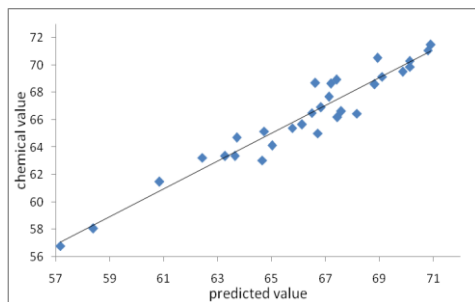


Fig.4 Relationships between predicted and ture values of calibration set in milk stage

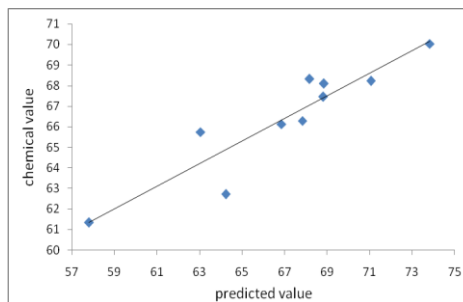


Fig.5 Relationships between predicted and ture values of calibration set in milk stage

4.3 Error Analysis and Model Evaluation

There are several factors in source of the error. The first reason is that the smoothness, cleanliness of leaves and the external environment changing make a

great influence on the reflectance spectra. And in addition, water lost in the process of measurement and hard to achieve constant weight in drying attribute to another reasons. These measurement errors accumulate eventually to cause differences in the results of the quantitative analysis. However, the artificial errors can be minimized by MSC-ANN algorithm. From the figure of prediction model, we can see that the prediction values are very close to the chemical values measured by standard method. So it is feasible to quickly determine the moisture content of winter wheat leaves by NIR reflectance spectroscopy and the model of MSC-ANN algorithm.

5. Conclusion

In this paper, a new modeling method for quantitative analysis moisture content in winter wheat leaves is studied: Multiplicative scatter correction - artificial neural network(MSC-ANN). In the research, we establish the quantitative analysis model of moisture content in different growing seasons of winter wheat leaves, and then make an analysis of the model. By analyzing the experimental data, MSC-ANN algorithm in dealing with chemical and biological living components is better than the traditional algorithm, according to the source of errors, the measurement errors mainly due to human factors, and another factors are influenced by the noise of instrument and background noise caused by environment changing. These errors can be effectively decreased by the re-training of the artificial neural network, which is better than other algorithm, so the MSC-ANN algorithm proved that it is reliable as a method of modeling.

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