Differentiation of storage time of wheat seed based on near infrared hyperspectral imaging

Dong Gao[1,2,3], Guo Jian[2], Wang Cheng[3], Liang Kehong[1], Lu Lingang[1], Wang Jing[1], Zhu Dazhou[1,3*]

(1. *Institute of Food and Nutrition Development, Ministry of Agriculture, Beijing 100081, China*;
2. *Faculty of Physics and Optoelectronic Engineering, Xiangtan University, Xiangtan 411105, China*;
3. *Beijing Research Center for Information Technology in Agriculture, Beijing 100097, China*)

Abstract: Seed aging during storage is one of the main factors that influence the quality of wheat seed. Current detection methods based on NIR spectra were mostly for group seeds, they had poor stability for single seed detection because of sample uniformity. In this study, the characteristic changes of single wheat seed during storage procedure were measured through hyperspectral imaging technology. Firstly, hyperspectral imaging data of wheat grain including six years from 2007 to 2012 had been collected. The original spectra showed clear difference in the band of 1400-1600 nm, which may be caused by the decreasing of moisture and protein content during storage; principal component analysis (PCA) was applied to analyze the spectral data of wheat grain including six years, the clustering chart of the principal components indicated that the grain between same or similar year have an clustering characteristic, and the characteristic difference would become obviously with the increasing of storage time; soft independent modeling of class analogy (SIMCA) was applied to classify the grain of different years, results showed that the classification accuracy of the dichotomy between adjacent years could reach 97.05%, and the accuracy of the mixed classification of six years could also reach 82.5%. These results indicated that hyperspectral imaging technology could be used to differentiate the quality change of wheat seed during different storage time, which could provide support for the intelligent monitoring of stored wheat seeds.

Keywords: hyperspectral image, wheat seed, storage, intelligent monitoring, single seed
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1 Introduction

During the storage procedure of wheat, the unsaturated fatty acid and toxic substance (alcohols, aldehydes, ketone, and acids) will increase, and the nutrient content of protein, starch and soluble sugar will reduce year by year[1], which will greatly affect the eating quality. The physiological deterioration of seeds during storage and seed priming is closely associated with germination, and thus contributes to plant growth and subsequent grain yields[2]. As germplasm resources, the seed vigor of wheat will gradually lose with the increase of the term for storage, the qualified seeding percent will reduce, the quality of seeding will become weaker and thus result in the severe reduction of output[3]. At present, some sellers sell the mixture of wheat stored for years and the newly harvested wheat, which not only damage the farmers' benefits, but also cause damage to the national

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Biographies: Dong Gao, Master student, research interest: agricultural informatization, Email: donggaohb89@163.com; **Guo Jian**, Professor, research interest: optoelectronic technology, Email: guojian@xtu.edu.cn; **Wang Cheng**, PhD, Researcher, research interest: agricultural informatization, Email: wangc@nercita.org.cn; **Liang Kehong**, PhD, research interest: agricultural product detection, Email: wuqiong0615@sina.com; **Lu Lingang**, PhD, research interest: food nutrition, Email: lulingang@caas.cn; **Wang jing**, PhD, research interest: food nutrition, Email: wangjing07@caas.cn.
***Corresponding author: Zhu Dazhou**, PhD, Associate Researcher, research interest: agricultural product detection, No.12 Zhongguancun South Street, Haidian District, Beijing 100081. Tel: +86-10-82105482, Email: zhudazhou@caas.cn.

food security. So, the monitoring of the wheat during storage is of key significance.

The traditional methods for the quality identification of wheat mainly depend on the color, smell and the taste of the finished product, which have strong subjective consciousness. And as for the test for seed vigor, it mainly conducts identification of the seeding growth, test for conductivity, accelerated aging test, ATP assaying[4], etc. These methods have weaknesses such as long-term test, high destructive effect, inconvenience operation. And it's hard to effectively apply these methods in the test for wheat. Hence, a quick and non-damaging method to test the quality change of wheat seed is urgently necessary.

As a fast high efficiency and non-destructive technique, Near Infrared (NIR) Spectroscopy has been widely used and developed quickly in recent decades. Combined with chemometrics method, NIR have been used to differentiate the inauthenticity and traceability of cereals[5]. Zhao et al.[6] analyzed the seeds of 10 wheat varieties harvested from three origins and found that origins and production year, along with genetic factor, greatly affect the NIR spectra of wheat. Fourier transform infrared (FTIR) spectroscopy was used to study red kidney beans and wheat of different storage times. The results showed that the spectral features of the same species of different storage times are similar, only with intensity differences of several peaks[7]. A prediction model of paddy storage time was established based on near infrared reflectance and chemometrics[8]. The effects of varieties, producing areas, ears, and ear positions of maize on NIR spectra were investigated to determine the factors causing the differences in NIR fingerprints of maize varieties[9]. However, the NIR spectra were generally collected from certain point of the sample, thus the test result is easily affected by the homogeneity of samples and determination conditions.

Hyperspectral imaging is a newly developed technology, it integrates the advantages of spectrum technology and image technology. It obtains the outside feature information of the sample, and also can provide the spectral information that reflecting the internal physical structure and the chemical components of the samples, thus realizing 'combination of image and spectrum'. Currently, the hyperspectral imaging has been widely applied in the non-destructive testing in agriculture, such as the information diagnosis of the crops[10,11], quality identification of agricultural products[12,13], determination of pesticide residues[14]. As for the seed detection, Zhu et al collected the average spectral information of the einkorn by hyperspectral imaging, and build the identification models of six varieties by SIMCA, the recognition rate can reach 93%[15]. Xing et al.[16] estimated the activity of the α amylase by hyperspectral image and partial least squares, and the precision reached over 80%. The researches of Wu et al.[17] showed that the hyperspectral imaging can create better effect in the predictive modeling of the wheat grain protein. Vermeulen et al.[18] applied near-infrared hyperspectral imaging for the detection and quantification of ergot bodies in cereals, and the correlation between the predicted values obtained by NIR hyperspectral imaging and those supplied by the stereo-microscopic method was higher than 0.94. Hyperspectral imaging technology was also applied for the identification of Fusarium head blight wheat[19]. NIR hyperspectral imaging has proved its suitability for quality and safety control in the cereal sector by allowing spectroscopic images to be collected at single-kernel level, which is of great interest to cereal control laboratories[20]. Wu et al.[21] introduced a method to predict single wheat grain protein content based on hyperspectral image.

All the researches above showed the potential ability of the hyperspectral imaging in exploring the feature change of the storage of wheat. This article selects the wheat grain stored for different years as the research subject, applies the hyperspectral imaging to acquire the spectrum information, and analyzes the spectrum difference caused by the period for storage by means of PCA and SIMCA. It aims to differentiate the quality change of wheat seed during storage by hyperspectral imaging, thus provide reference for the non-destructive monitoring of wheat quality.

2 Materials and methods

2.1 Sample preparation

Wheat samples of Jingdong 24 were cultivated by

Beijing Hybrid Wheat Engineering and Technological Research Center, and the period for storage covers six years, from 2007 to 2012. The moldy and shriveled grains shall be manually removed during the sampling. And 60 grains were select each year, totally 360 samples were measured. Each grain were put into the closed bags with serial number, and stored in the refrigeration storage at 4ºC. During the experiment, the grains were taken out at the normal temperature for 24 h before hyperspectral image collection.

2.2 Hyperspectral imaging system and images collection

The hyperspectral imaging system used in the experiment is shown as Figure 1. This system mainly contains the pushbroom imaging spectrometer (HELIOS NIR, Elektronisch Visualisieren Klassifizieren, Germany), two optical halogen lamp of 75 W, control platform moving horizontally, and a set of specialized computer system. The detailed composition refers to the reference[13]. The spectral resolution is 2.7 nm, spatial resolution is 0.25 mm, and the collected scope of spectral band is 850-1700 nm. Before collecting the data, the matching between the time of exposure of the spectrograph and the luminance of light source shall be confirmed to acquire the optimal spectrum energy value, and the speed of the push and pull of the moving platform shall be adjusted to the point to avoid image distortion. Through many times of debugging and optimizing of preliminary experiments, the final confirmed acquisition parameters are time of exposure of 24 ms, moving speed of 1.6 mm/s and object distance of 91 mm.

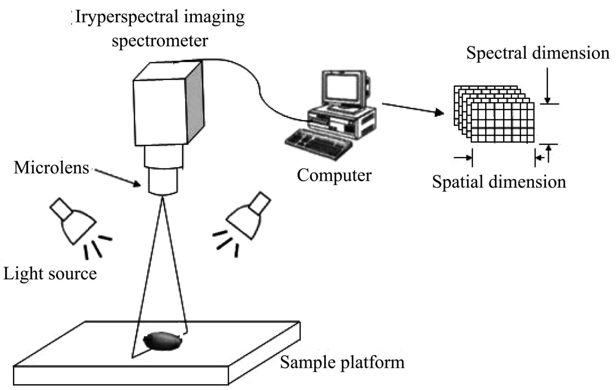


Figure 1 Hyperspectral imaging system

In order to reduce the spectrum error brought by the baseline drift, the optical spectrum instrument shall be pre-heated for 30 min before the experiment. In the experiment, the whole spectral imaging system shall be covered under the shading cloth to avoid the interference of the external lights. When collecting the data, the abdominal groove of grains shall be put adown on the platform, and the direction shall be consistent with the moving direction of the platform. The whole scanning process shall be finished under the control of ScanView software. In the meantime, in order to reduce the influence of the change of light source and the system noise, the images of standard white board and black image shall be collected every 15 min during the experiment for black-and-white correction of the spectrum images.

2.3 Data processing and analysis methods

2.3.1 Spectroscopic data extraction

The hyperspectral data used in the following analysis subjects to the average spectroscopic data of the whole grain area. The direct extraction of the spectroscopic data from the whole original image (Figure 2) shall generate spectrum errors caused by the interference of the background, so we need to use the picture segmentation to establish the mask (Figure 3) of the whole area and then use the mask to obtain the spectrums of the grain parts in batch.

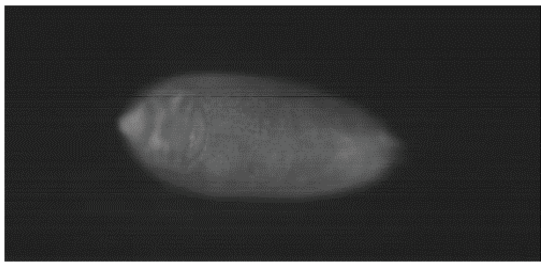


Figure 2 Original picture

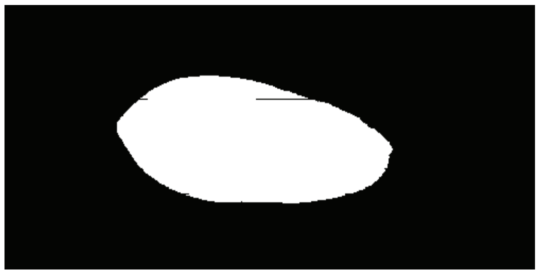


Figure 3 Mask of the seed

The original hyperspectral data extracted from the mask are the values of the light intensity of reflection of each pixel. We need to compare them with the white board spectrum tested synchronously, so as to calculate the spectral reflectance of the target area. The computing method is as below:

$$\mathrm{Re}\, f_{Target} = \frac{Rad_{Target}}{Rad_{White\ Board}} \times \mathrm{Re}\, f_{White\ Board} \times 100\% \qquad (1)$$

where, $\mathrm{R}ef_{Target}$ is the spectral reflectance; Rad_{Target} is the light intensity of the target object tested by the spectrograph; $Rad_{White\ Board}$ is the light intensity of the white board tested by the spectrograph; $\mathrm{R}ef_{White\ Board}$ is the standard reflectance value of the white board.

2.3.2 Data preprocessing

For the sake of eliminating the spectrum errors brought by the random noise with high frequency, and baseline drift, we need to conduct preprocessing to the original spectrum data, so as to highlight the effective spectrum information. This article firstly adopts the Savitkzy-Golay smoothing techniques to conduct noise elimination for the original spectrum data. Through the verification, the effect of noise elimination can be guaranteed when the smoothing dot selects at 9, it also will not cause excessive smoothing of the spectrum data to result in anamorphose. The baseline correction will be proceeded by the first derivation to the spectrum through smoothing process. And the method of derivation chooses Savitkzy-Golay and the window size selects 5. Meanwhile, the noise of the two ends of the spectrum is big due to the weak response of the detector, so only the spectrum range of 920-1620 nm was selected for analysis.

2.3.3 Principal Component Analysis

The principal component analysis is a kind of technology of data mining in the multivariate statistics. The main target is to synthesize and simplify the multiple information. Under the precondition of keeping the main spectrum information, it uses less variables to replace the more variables originally, so as to exclude the overlapping information coexisting in the plenty chemical information[22]. After the principal component transformation, each sample corresponding to each principal component has a score value. The score value can reflect the similarity and independence between different samples[23]. In this article the principal component transformation is conducted to all the grains' spectrum. Then the first two principal components of each sample was selected and constitute the score value chart of the principal components. And thus the clustering feature and internal information of the grain samples at different years can be analyzed through the score value chart of the principal components of the samples. At the same time, it also provides the information of the principal components for the establishment of the SIMCA disaggregated model.

2.3.4 Methods of classification modeling

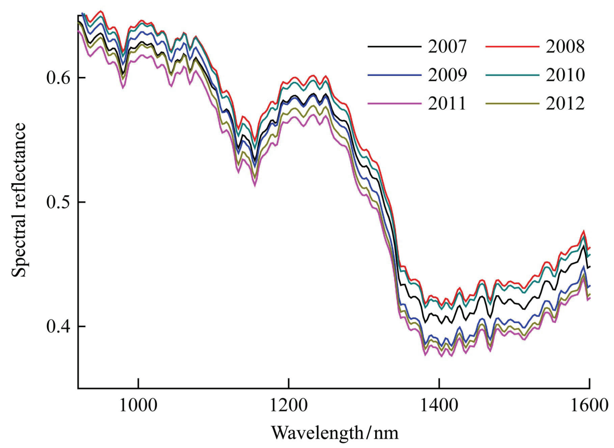
SIMCA is the discrimination model established based on the PCA analysis of each types of training set. It confirms the classification of the sample through calculating and judging the distance between the unknown sample point and the PCA model of the training set. When using the SIMCA to classify, this article uses the spectrum data of the wave band of 920-1620 nm as the input data. The optimal number of the principal component of each classification model is confirmed through mutual verification, that is, to choose the predictive remaining square and the corresponding number of the principal component not at the obvious reduction.

The samples are divided into training set and prediction set when modeling. The training set is used for establishing disaggregated model and the prediction set is used to test the effect of classification of the models. About the composition of the training set and prediction set, the samples of different types will be randomly selected from the total samples at ratio of 2:1. Finally, the correct recognition rate will be calculated to evaluate the classification performance.

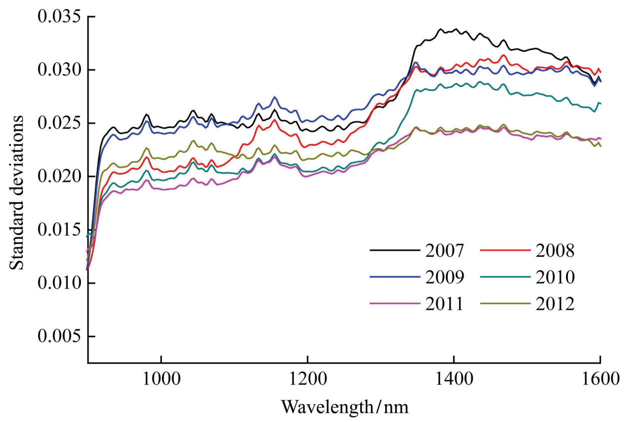
3 Results and discussion

3.1 Curve analysis of the spectral reflectance of the grains stored for different years

The curve chart of the spectrum of the grains stored for six different years from 2007 to 2012 were shown in Figure 4a. From the figure, we can see that there exist big differences between the seeds stored for these six years, especially at the region between 1400-1600 nm, the spectral reflectance of 2007 and 2008 is obviously higher than that of 2011 and 2012. Figure 4b shows the standard deviations of each year's spectral reflectance, which indicating a clearer tendency that the standard deviation is higher when the storage time is long. And the standard deviation of year 2007 nearly achieved 0.0325 at 1450 nm, which also showed a greater change of the substance inside the seed.



a



b

Figure 4 (a) Spectral reflectance of the grains stored for different years; (b) Standard deviations of spectral reflectance of the grains stored for different years

With the increase of storage time, the content of the dry matter inside the wheat grain will gradually become bigger, the corresponding water content will reduce year by year and the presentation in the spectrum curve is that the spectral reflectance of the segment focusing on water absorption will tend to increase. The wave band around 1450 nm is one of the bands with strong water absorption, and the difference of water content of the seeds stored for different years will become more obvious in the spectrum near this wave band. Meanwhile, this is the reason why the spectral reflectance of this wave band in 2007 and 2008 is higher than that in 2011 and 2012.

During the process of storage, with the deduction of the water content, the proteins component including catalase will also gradually degrade with the storage period increases, which results in the constant reduction trend of the total protein content [1]. The reduction of the protein content brings about the enhancement of the reflectivity of the grain with protein as the main absorption band. The band of 1470-1500 nm is the band with strong absorption of protein, and the spectral reflectance of this band in 2007 and 2008 is higher that in 2011 and 2012, which is consistent with the practice.

3.2 Principal component analysis of the spectrum of the wheat stored for different years

Conduct transformation of the principal component of the spectrum data of 920-1620 nm, and the clustering chart (Figure 5) of the principal component of the grain of the six years can be gotten. The abscissa axis represents the score of the principal component 1 (PC1) of the sample, and the vertical axis represents the principal component 2 (PC2). The accelerating contribution rate of the former two principal components reaches 81%, it can almost represent the main spectral variance and effective information of the sample.

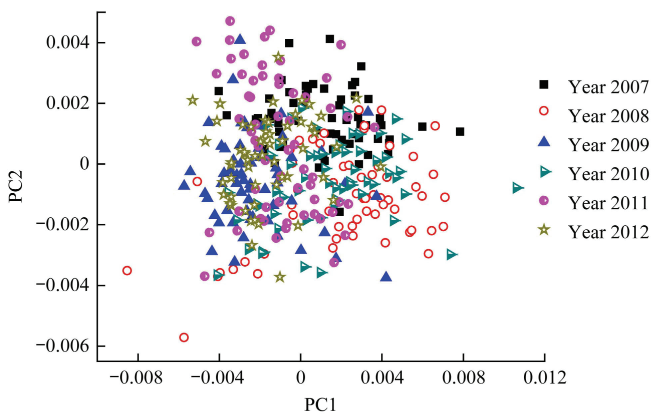


Figure 5 Clustering chart of the principal component of the grain of six years

Figure 5 can roughly show the distributions of the grains of 2007, 2008 and 2012 have certain clustering feature, they are distributed in three separated areas. However, the whole clustering figure for six groups of wheat seems quite disorder due to the influence of the grains of the middle transition years (for example 2010, 2011). This figure indicated that wheat seeds in different storage time have some spectral difference, but also have some extent of overlap. More principal components may be needed to be selected to reflect the distributions of the differences in the multi-dimensional space.

Separately analyze the clustering chart (Figure 6) of the principal components from 2010 to 2012. It can be concluded that the grains of 2010 and 2012 present obvious clustering distribution. Although there is partial superposition between them, there is still certain discreteness. As the transition year, in 2011, the grain distribution has certain randomness, indicating that the grains will reflect obvious difference in the figure of principal components as long as the grains accumulate for certain period with the increase of the storage time. Further analyzing the clustering chart (Figure 7) of the principal components from 2007 to 2009, the distributions of the grains in the three years all indicate evident clustering feature, and the discreteness between them seems more obvious. As the transition year, in 2008, the grain distribution is relatively regular. The above two conclusions showed that the quality change of the grains with the change of year may be a process from the slow speed to fast. With the storage time increase, the difference between the grains of different years become more distinct, and the feature of clustering distribution of the grains in the space diagram of the principal components become more notable. This is similar with the research of Liu et al.[7], they found that the absorption ratios of A1653/A1023, A15 38/A1023, A1080/A1023, A1155/A1023 and A1538/A1653 of wheat increase with the increase of storage time, and these spectral change may reflect the structure change of protein and amylose.

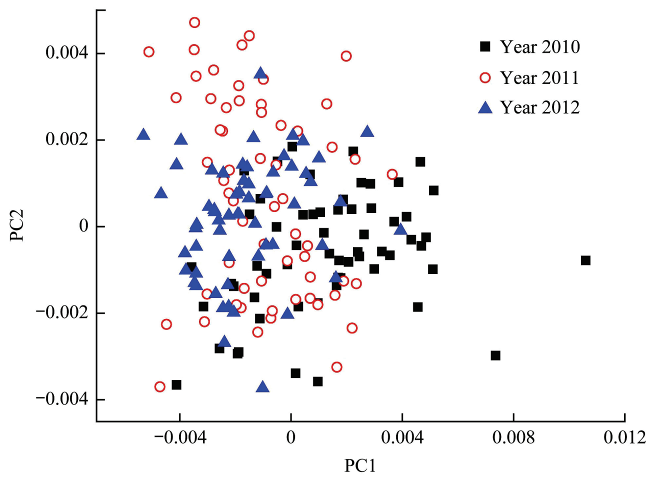


Figure 6 Clustering chart of the principal components

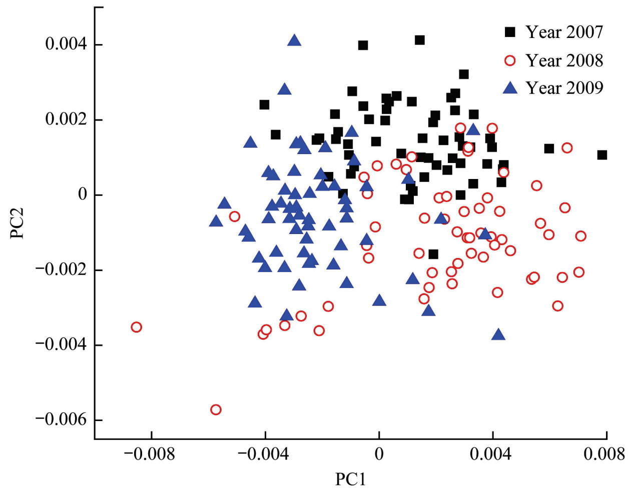


Figure 7 Clustering chart of the principal components of the grain from 2010 to 2012 of the grain from 2007 to 2009

3.3 Discriminant analysis of the seeds of different storage time

To further study the quantified difference between the seeds of different storage time, this article conducts qualitative identification through modeling of the wheat grains of different storage time by SIMCA.

Table 1 is the result of classification of the wheat grains of every two adjacent storage times of the six years. It can be made out that the recognition rate of the dichotomy between the two adjacent years is relatively high. And the recognition rate of 2009 and 2010 reaches 97.44% while the recognition rate of 2011 and 2012 only reaches 89.74%. That's maybe because the aging change of the seeds during the storage is a process of 'slow-fast-slow'. We can use a reversed 'S' curve to roughly describe it[24]. The seeds of 2011 and 2012 are relatively fresh, and the change of the inner matters may be slow with the change of the storage time. Thus, the wheat seeds from different years may have some similarities, which make the recognition rate low. And, the seeds before 2010 may just at the stage of fast change, and the recognition rate is slightly higher than 2011 and 2012.

Table 1 Classification results of the grains of every two adjacent years

Datasets (Different storage time)	Number of latent variables	Correct recognition rate	
		Training set	Prediction set
Year 2007 and 2008	3, 4	100%	97.05%
Year 2008 and 2009	4, 3	97.50%	92.31%
Year 2009 and 2010	4, 3	98.75%	97.44%
Year 2010 and 2011	3, 5	97.53%	94.87%
Year 2011 and 2012	5, 3	97.53%	89.74%

Table 2 shows the result of the six classification after mixing the grain six years and the three classification after dividing the every two adjacent years as a group. The table indicates that the results of these two classification methods are roughly close to each other. The recognition rate of the mixed classification of the six years is 82.50%, and that of the three classifications is 81.67%, which shows that the hyperspectral imaging data can present the differences of the seeds stored for different years to some extent. Compared to the effect of the classification of the two adjacent years in Table 1, it can be seen that the effect of recognition reduces while it edgewise reflects the change of the seeds with in change of storage time advances gradually, and between the seeds of the adjacent storage times, there is no absolute boundary of distinction. Classify the seeds of six years strictly with one year as the interval, the recognition rate of classification will inevitably be disturbed by the similarity between the seeds of two adjacent years and will reduce the effect.

Table 2 Results of the six classification and three classification after dividing every two adjacent years as a group

Datasets (Different storage time)	Classification pattern	Number of latent variables	Correct recognition rate	
			Training set	Prediction set
2007-2008, 2009-2010, 2011-2012	Three classification	5, 3, 4	85.50%	81.67%
2007, 2008, 2009, 2010, 2011, 2012	Six classification	4, 3, 4, 5, 4, 3	92.53%	82.50%

On the other side, the reduction of the recognition may also caused by the fact that when using SIMCA to build classification models, it only conduct separate PCA analysis for each category and selects different principal components for each category to build models, while it ignores the influence of other categories, which results in the limited resolving ability in multi-classification.

4 Conclusions

This article acquires the near infrared spectrum imaging data of single wheat seeds of each year from 2007 to 2012 through the hyperspectral imaging system. The conclusions were as follows:

1) The differences of the spectral reflectance of the storage times of segment between 1400-1600 nm is greatly affected by the content of the water and protein inside the seeds. The loss of water and degradation of protein will make the reflectivity of the corresponding segment bigger.

2) The seeds of the same year may have some clustering features in PCA plots and the features will become more outstanding at some stage with the storage period extending.

3) The classification results indicate that the hyperspectral data can reflect the difference change during the storage of the wheat seed, and shows the application of the hyperspectral imaging technology in the exploration of the wheat storage is feasible.

However, the wheat seeds used in this experiment are the same variety from the same place, while the changes of feature of the seeds during storage will be greatly affect by the variety and place of origin. In the following experiments, the seeds of different varieties from different places of origin shall be collected to validate the results.

Acknowledgements

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