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Applicability of model updating method to different detection indexes of cold fresh pork

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Abstract. Model updating method is used to maintain the hyperspectral models established to predict water content, pH value, and TVB-N content of cold fresh pork. After adding 11 slave variety samples to the calibration set of the master variety samples, the prediction results of the updated model of water content for the slave variety samples were $R_p^2=0.8224$ and $RPD=1.94$. After adding 45 slave variety samples, the prediction results of the updated model of pH value for the slave variety samples were $R_p^2=0.6160$ and $RPD=1.34$. After adding 9 slave variety samples, the results of the updated model of TVB-N content for the slave variety samples were $R_p^2=0.9073$ and $RPD=3.04$. The findings show that the model updating method can well maintain the TVB-N content model but shows poor maintenance ability for water content model, and it cannot be used to maintain the pH value model. Therefore, the applicability of the model updating method varies in different detection index models for cold fresh pork.

Keywords: model updating method, water content, pH value, TVB-N content

1 Introduction

Multivariate calibration models are of critical importance in analytical measurements when adopting spectroscopy technique for quantitative detection of the components of agriculture and livestock products. However, calibration models cannot be applied in all instances. The performance of multivariate calibration models can be affected by changes in instruments, samples, and surroundings, among others. To guarantee the effectiveness of multivariate calibration models, we should maintain them when their prediction performance drops [1, 2]. Model updating is the most commonly used method for model maintenance [3, 4, 5, 6]. It is usually used to address the issues that invalidate a model caused by changes in samples (such as the use of different varieties, the use of samples obtained from different places or at different times, and the use of samples stored under different conditions), environment for sample measurement (such as changes in temperature and humidity), and some other factors.

Most surveys have shown that the predictability of samples at different temperature, when using different instruments, and under some other situations improved when a model is maintained using the model updating method [7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. However, these surveys did not study the improvement degree for the new sample predictability and the influence degree for the prediction precision

of original samples. To eliminate the effects of the difference in varieties on calibration models, we used the model updating method to maintain the calibration model of three indexes (water content, pH, and TVB-N) of cold fresh pork in this study. The prediction performance of the TVB-N content model for predicting the master variety and the slave variety pork samples before and after using the model updating method was compared, and so done for pH value and water content models. Then we can ascertain the explicabilities of the model updating method in maintaining the models for different indexes of cold fresh pork.

2 Materials and Methods

2.1 Materials

The cold fresh pork samples used in our experiments were purchased from local supermarkets in Hongshan District, Wuhan City, Hubei province. To study the effects of different varieties, we selected the Enshi mountain pigs and the No.0 indigenous pigs as detection objects when determining the water content and pH value of cold fresh pork. The Enshi mountain pigs and the Jiakiang pigs were used as detection objects when determining the TVB-N content of cold fresh pork. We prepared samples consisting of back tenderloin of 82 Enshi mountain pigs and 79 No.0 indigenous pigs for water content and pH value detection. We prepared samples consisting of back tenderloin of 96 Enshi mountain pigs and 96 Jiakiang pigs to determine the TVB-N content.

2.2 Acquisition of Spectral Data

After preparing the experimental samples, we first adopted HyperSIS hyperspectral imaging system which was purchased from Beijing Zhuo-li-han-guang Instrument Co.Ltd to obtain the hyperspectral data of each pork sample. The ENVI4.7 software was subsequently used to extract spectral data from the hyperspectral data.

2.3 Measurement of Physicochemical Reference Values

Immediately after we collected the hyperspectral data of the pork samples, we conducted the experiments to determine the physicochemical reference value of all the samples.

The reference value for water content of cold fresh pork was measured using vacuum drying method, in accordance with the national standard of the People's Republic of China GB5009.3-2010 [17].

The reference value for pH value of cold fresh pork was measured using a pH meter in accordance with the standard of agriculture ministry of the People's Republic of China NY/T 821-2004 [18].

The reference value for TVB-N content of cold fresh pork was measured by micro-diffusion method in accordance with the national standard of the People's Republic of China GB/T 5009.44-2003[19].

2.4 Model Updating Method

Model updating method used in this paper aimed to eliminate the influence of variety difference on the hyperspectral models of cold fresh pork. No.0 indigenous pigs and Enshi mountain pigs were selected as the master variety and slave variety, respectively, to predict the water content and pH value of cold fresh pork. In addition, Enshi mountain pigs and Jiajiakang pigs were chosen as the master variety and slave variety, respectively, to predict the TVB-N content of cold fresh pork. Firstly, the sample set of the master variety were divided into calibration set and test set, and the PLSR models for predicting the TVB-N content, pH value, water content were established with the calibration set of the master variety. Then a small amount of representative slave variety samples were selected and added to the calibration set of the master variety by using SPXY algorithm [20] to establish the updating models. The rest samples of the slave variety were used as test set to validate the results of model updating.

2.5 Method to Evaluate the Updating Model

The results of the updating model was evaluated according to the foundation of the model performance by using 5 parameters such as the cross validation coefficient of determination R_{cv}^2 , the root mean square error of cross validation (RMSECV), the prediction coefficient of determination R_p^2 , the root mean square error of prediction (RMSEP), and residual prediction deviation (RPD).

The foundation of the model performance can be assessed as follows [21]: when $R^2 \leq 0.50$ (R^2 stands for R_{cv}^2 and R_p^2) and $RPD \leq 1.5$, the model established is not available. When $0.50 < R^2 \leq 0.65$ and $1.5 < RPD < 2.0$, the model established can identify the high or low value of the measurement. When $0.65 < R^2 < 0.81$ and $2.0 < RPD \leq 2.5$, the model can be used in approximate quantitative calculation. When $0.81 < R^2 \leq 0.90$ and $2.5 < RPD \leq 3.0$, the model performance is good. When $R^2 > 0.90$ and $RPD > 3.0$, the model shows excellent performance. The larger the R^2 and RPD, the smaller the RMSECV and RMSEP, the better the model performance will be.

3 Results and Analysis

3.1 PLSR Model of Each Index of the Master Variety

After eliminating 5 abnormal No.0 indigenous pork samples and 8 abnormal Enshi mountain pork samples found by using the Monte Carlo method [22], we obtained 74 normal No.0 indigenous pork samples and 74 normal Enshi mountain pork samples for predicting water content of cold fresh pork. The No.0 indigenous pork was selected as master variety and the Enshi mountain pork was selected as slave variety.

By using CG algorithm [23], we divided the 74 master variety samples into calibration set and test set at 3:1 ratio. The calibration set was used to establish the PLSR model called the master variety PLSR model for predicting water content of cold fresh pork.

After eliminating 6 abnormal No.0 indigenous pork samples and 6 abnormal Enshi mountain pork samples found by using the Monte Carlo method, we obtained 73 normal No.0 indigenous pork samples and 76 normal Enshi mountain pork samples for predicting pH value of cold fresh pork. The No.0 indigenous pork and Enshi mountain pork were selected as the master and slave varieties, respectively. By using SPXY algorithm, we divided the 73 master variety samples into calibration set and test set at 3:1 ratio. The calibration set was used to establish the PLSR model for predicting pH value of cold fresh pork.

After eliminating 9 abnormal Enshi mountain pork samples and 6 abnormal Jiajiakang pork samples by using the Monte Carlo method, we obtained 87 normal Enshi mountain pork samples and 90 normal Jiajiakang pork samples for predicting TVB-N content of cold fresh pork. Enshi mountain pork and Jiajiakang pork were selected as the master and slave varieties, respectively. By using CG algorithm, we divided the 87 master variety samples into calibration set and test set at 3:1 ratio. The calibration set was used to establish the PLSR model for predicting TVB-N content of cold fresh pork.

Table 1 shows the performance parameters of the PLSR model of master variety pork for predicting water content, pH value, and TVB-N content.

Table 1. The performance parameters of the master variety PLSR model for predicting water content, pH value, and TVB-N content

The master variety PLSR model	Cross validation results			Prediction results of master varieties			Prediction results of slave varieties		
	R_{cv}^2	RMSECV	RPD	R_p^2	RMSEP	RPD	R_p^2	RMSEP	RPD
Water content	0.9593	0.2091	4.99	0.9301	0.2521	3.53	0.2678	1.0300	0.87
pH value	0.8726	0.0817	2.80	0.7426	0.0710	2.02	0.3492	0.1509	0.86
TVB-N content	0.9706	1.1324	5.88	0.9503	1.5190	4.25	0.6992	3.0513	1.58

We can draw the following conclusions from Table 1. The prediction results of the master variety PLSR model for predicting water content of the master variety are $R_p^2=0.9301>0.90$ and $RPD=3.53>3.0$, and that for predicting water content of the slave variety are $R_p^2=0.2687<0.50$ and $RPD=0.87<1.5$. The prediction results of the master variety PLSR model for predicting pH value of the master variety are $0.65<R_p^2=0.7426<0.81$ and $2.0<RPD=2.02<2.5$, and that for predicting pH value of the slave variety are $R_p^2=0.3492<0.50$ and $RPD=0.86<1.5$. The prediction results of the master variety PLSR model for predicting TVB-N content of the master variety are $R_p^2=0.9503>0.90$ and $RPD=4.25>3.0$, and that for predicting TVB-N content of the slave variety are $0.65<R_p^2=0.6992$ and $1.5<RPD=1.58<2.0$.

According to the assessment foundation of model performance, we have obtained the following conclusions. The master variety PLSR model for predicting the water content of cold fresh pork is good for the master variety samples, although it is unworkable for the slave variety samples. The master variety PLSR model for

predicting the pH value of cold fresh pork can be used in approximate quantitative calculation for the master variety samples, but it is unworkable for the slave variety samples. The master variety PLSR model for predicting the TVB-N content of cold fresh pork is good for the master variety samples, but it can only be used to assess the high or low values of the slave variety samples. Therefore, the master variety models for predicting the water content, pH value, TVB-N content of cold fresh pork should be maintained before they were used to predict the corresponding values of the slave variety samples.

3.2 Model Updating Results of the PLSR Model of Water Content

Table 2 shows the cross-validation results and the prediction results for the test set of the slave variety which were obtained by using the updating models of water content established by adding different numbers of representative slave variety (Enshi mountain pork) samples to the calibration set of the master variety (N0.0 indigenous pork).

Table 2. The results of the water content models updated by adding different numbers of slave variety samples

Number of samples added	number of principal components	Calibration set			Test set of the slave variety		
		R_{cv}^2	RMSECV /%	RPD	R_p^2	RMSEP /%	RPD
0	13	0.9593	0.2091	4.99	0.2678	1.0300	0.87
1	10	0.8720	0.4062	2.81	0.6895	0.7241	1.23
2	10	0.8943	0.3725	3.08	0.7004	0.7276	1.23
3	14	0.8787	0.4124	2.88	0.8019	0.6348	1.41
4	14	0.8717	0.4194	2.80	0.8064	0.6480	1.38
5	14	0.8921	0.3836	3.05	0.8128	0.6435	1.39
6	15	0.9041	0.3701	3.23	0.8233	0.6418	1.39
7	15	0.9062	0.3673	3.26	0.8156	0.6504	1.37
8	14	0.8758	0.4184	2.85	0.8266	0.5576	1.60
9	14	0.8539	0.4504	2.63	0.8163	0.5345	1.67
10	14	0.8671	0.4393	2.76	0.8175	0.4791	1.87
11	15	0.8741	0.4290	2.83	0.8224	0.4613	1.94
12	15	0.8833	0.4147	2.94	0.8098	0.4723	1.89
13	14	0.8848	0.4096	2.96	0.8104	0.4808	1.86
15	14	0.8921	0.3958	3.06	0.8079	0.4837	1.85
20	13	0.8964	0.3867	3.12	0.8167	0.4821	1.85

We can conclude from Table 2 that after adding 11 slave variety Enshi mountain pork samples to the master variety No.0 indigenous pork samples, the performance of updating model for predicting water content of cold fresh pork tends to stabilize, and the prediction performance of the updated water content model for slave variety samples are $0.81 < R_p^2 = 0.8224 < 0.90$, and $1.5 < RPD = 1.94 < 2.0$. According to the assessment foundation of model performance, we can conclude that the PLSR updating model for predicting water content can be used to identify the high or low

values to be measured in the slave variety samples. In addition, the prediction results of the water content PLSR updating model for the master variety could be calculated and that are $0.81 < R_p^2 = 0.8179 < 0.90$, and $2.0 < RPD = 2.1 < 2.5$. Obviously, the updating model can be used for approximate quantitative calculation of water content of the master variety samples.

Moreover, we can draw from Tables 1 and 2 the following conclusions. The model updating method caused limited improvement of the prediction precision of the water content PLSR model for the slave variety samples, and it only improves the model from being useless to being able to identify the high or low values of the slave variety samples. However, this updating model significantly influenced the prediction precision of the master variety samples and can reduce it from excellent prediction performance to approximate quantitative calculation. Therefore, the model updating method cannot be used to maintain the water content model of cold fresh pork.

3.3 Model Updating Results of the PLSR Model of pH Value

Table 3 shows the cross-validation results and the prediction results for the test set of the slave variety which were obtained by using the updating models of pH value established by adding different numbers of representative slave variety (Enshi mountain pork) samples to the calibration set of the master variety (N0.0 indigenous pork).

Table 3. The results of the pH value models updated by adding different numbers of slave variety samples

Number of samples added	number of principal components	Calibration set			Test set of the slave variety		
		R_{cv}^2	RMSECV /%	RPD	R_p^2	RMSEP /%	RPD
0	19	0.8726	0.0817	2.80	0.3492	0.1509	0.86
1	8	0.8601	0.0932	2.70	0.3201	0.1704	0.76
2	6	0.8618	0.0930	2.71	0.3188	0.1601	0.81
3	8	0.8788	0.0885	2.90	0.3057	0.1619	0.80
4	10	0.8747	0.0896	2.84	0.3182	0.1612	0.81
5	10	0.8854	0.0863	2.97	0.3248	0.1587	0.82
10	4	0.7972	0.1166	2.19	0.3332	0.1472	0.88
15	20	0.6690	0.1575	1.61	0.3461	0.1237	1.05
20	2	0.6295	0.1603	1.56	0.4390	0.1222	1.07
25	2	0.6877	0.1428	1.73	0.4635	0.1253	1.04
30	2	0.6953	0.1383	1.76	0.4507	0.1278	1.02
35	2	0.7085	0.1340	1.82	0.4996	0.1223	1.06
40	4	0.7172	0.1318	1.81	0.5579	0.1119	1.16
45	4	0.6530	0.1455	1.61	0.6160	0.0971	1.34

We can conclude from Table 3 that although 45 slave variety (Enshi mountain pork) samples were added into the calibration set of the master variety (No.0 indigenous pork), the updating model for predicting pH value of cold fresh pork remains unworkable to the slave variety samples. The prediction performances of the pH value updating model for the slave variety samples are $R_p^2 = 0.6160 < 0.65$ and

RPD=1.34<1.5. Therefore, the model updating method cannot be used to maintain the PLSR model for predicting pH value of cold fresh pork.

3.4 Model Updating Results of the PLSR Model of TVB-N Content

Table 4 shows the cross-validation results and the prediction results for the test set of the slave variety which were obtained by using the updating models of TVB-N content established by adding different numbers of representative slave variety (Jiajiakang pork) samples to the calibration set of the master variety (Enshi mountain pork).

Table 4. The results of TVB-N content models updated by adding different numbers of slave variety samples

Number of samples added	number of principal components	Calibration set			Test set of the slave variety		
		R_{cv}^2	RMSECV	RPD _{cv}	R_p^2	RMSEP	RPD _p
0	18	0.9706	1.1324	5.88	0.6992	3.0513	1.58
1	18	0.9711	1.1307	5.92	0.6996	3.0829	1.56
2	20	0.9483	1.5275	4.39	0.8568	2.1850	2.21
3	20	0.9519	1.4591	4.57	0.8524	2.2040	2.19
4	20	0.9468	1.5371	4.32	0.8836	1.9905	2.42
5	20	0.9485	1.5174	4.38	0.8730	2.0111	2.40
6	20	0.9425	1.6041	4.13	0.9038	1.7460	2.76
7	20	0.9430	1.5873	4.15	0.8973	1.7626	2.74
8	20	0.9444	1.5609	4.20	0.9049	1.6073	3.00
9	20	0.9446	1.5647	4.22	0.9073	1.5837	3.04
10	19	0.9076	2.0479	3.22	0.8901	1.8123	2.66

We can conclude from table 4 that after adding 9 slave variety (Jiajiakang pork) samples to the calibration set of the master variety (Enshi mountain pork), the performance of the updating model for predicting TVB-N content of cold fresh pork tends to stabilize, and the prediction performance of the updated TVB-N content model for slave variety samples are $R_p^2=0.9073>0.90$ and $RPD=3.04>3.0$. According to the assessment foundation of model performance, we can obviously conclude that the prediction performance of the updating model for predicting TVB-N content of the slave variety samples is excellent. In addition, the prediction results of the TVB-N content PLSR updating model for the master variety could be calculated and that are $R_p^2=0.9655>0.90$, $RPD=5.40>3.0$. Obviously, the updating model is excellent for the master variety samples too. We can draw from Tables 1 and 4 the following conclusions. The model updating method significantly improved the prediction precision of the PLSR model of TVB-N content for the slave variety samples, and it improved the performance of the model for the slave variety samples from being able to identify the high or low values to being excellent. Furthermore, the updating model slightly affected the prediction precision for the master variety samples, and it is still excellent for the master variety samples. Therefore, the model updating method can maintain the TVB-N content model of cold fresh pork well.

4 Conclusions

A survey was conducted to study the applicability of the model updating method to maintain the different index models of cold fresh pork. Maintaining the PLSR models for predicting water content, pH value, and TVB-N content of cold fresh pork by using model updating method, and we obtained the following conclusions.

1) The master variety model of water content of cold fresh pork shows a good prediction performance for the master variety samples ($R_p^2=0.9301>0.90$, $RPD=3.53>3.0$) but it is unworkable for the slave variety samples ($R_p^2=0.2687>0.50$, $RPD=0.87<1.5$). After adding 11 representative slave variety samples to the master variety calibration set, the performance of the updating model for predicting the water content of cold fresh pork is that the updating model can identify the high or low values of water content of the slave variety samples ($R_p^2=0.8224>0.81$, $RPD=1.94>1.5$), and it can perform approximate quantitative analysis for the master variety samples ($R_p^2=0.8179>0.81$, $RPD=2.1>2.0$). The results indicated that model updating method caused limited improvement for the prediction precision of the water content PLSR model for the slave variety samples, and it only improves the model from being useless to being able to identify the high or low values of the slave variety samples. However, this updating model significantly influenced the prediction precision of the master variety samples and can reduce it from excellent prediction performance to approximate quantitative calculation. Therefore, the model updating method cannot be used to maintain the water content model of cold fresh pork.

2) Although 45 slave variety (Enshi mountain pork) samples were added into the calibration set of the master variety (No.0 indigenous pork), the updating model for predicting pH value of cold fresh pork remains unworkable to the slave variety samples. The prediction performances of the pH value updating model for the slave variety samples are $R_p^2=0.6160<0.65$ and $RPD=1.34<1.5$. Therefore, the model updating method cannot be used to maintain the PLSR model for predicting pH value of cold fresh pork.

3) Before using the model updating method, the master variety PLSR model for predicting TVB-N content shows a good prediction performance to the master variety samples ($R_p^2=0.9503>0.90$, and $RPD=4.25<3.0$), but it shows a worse prediction performance to the slave variety samples and it only can identify the high or low values of TVB-N content ($0.65<R_p^2=0.6992<0.81$, $1.5<RPD=1.58<2.0$). The updating model was built by adding 9 representative slave variety samples to the master variety calibration set, and its prediction performance was good for both the master and slave variety samples (the prediction results for the master variety was $R_p^2=0.9655>0.90$ and $RPD=5.40.3>3.0$, the prediction results for the slave variety was $R_p^2=0.9073>0.90$ and $RPD=3.04>3.0$). The results indicated that the model updating method can well maintain the TVB-N content model of cold fresh pork.

4) By using model updating method, the maintenance results for the PLSR hyperspectral model of water content, pH value and TVB-N content of cold fresh pork vary greatly. The method can well maintain the TVB-N content model, but the maintenance result for the water content model is slightly worse, furthermore it cannot maintain the pH value model. The results indicated that the applicability of the model updating method varies in different detection index models for cold fresh pork. The model updating method can well maintain the hyperspectral model of TVB-N

content of cold fresh pork, but it cannot maintain the hyperspectral models of water content and pH value of cold fresh pork.

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