17 Calibration transfer methods

17.1 Introduction

A situation is often encountered in the process of spectral analysis, when the model established on one spectrometer (master, master, primary, parent instrument) is used on another spectrometer (slave, slave, child instrument), the model cannot give correct prediction results due to the difference in spectra measured by different instruments [1, 2]. The first thing to solve this problem, is to improve the standardization of instrument hardware processing, improve the level of processing technology, and reduce the differences between the master and the slaves in terms of devices. Instrument standardization makes the spectra from the same samples measured by different instruments as consistent as possible. There have been many reports on the standardization of spectroscopic instrument hardware such as calibrating the wavelength accuracy, absorbance accuracy, resolution, spectral response line type and symmetry of the spectrometer through sharp-line emission light source, standard materials, etc [3-9]. As well, there have been developments on instruments by optimizing optical components, assembly processes, and control strategies with performance indicators within the allowable range of variation [10, 11]. This is called the First Principle of instrument calibration, which is the most fundamental basis of modern spectroscopic analysis technology [12, 13].

For Fourier instruments of the same or even different types, it is basically possible to directly transfer the spectra through the instrument calibration method ^[14-19]. In recent years, some portable instruments can also transfer spectra between the same type ^[20, 21]. Surely, different applications have various requirements for the consistency of instruments ^[22-24]. Calibration models established by different methods and different systems also have different tolerances for divergence between instruments ^[25-29]. Due to the sharp peaks of spectrum, Raman spectrometers can better solve the problem of consistency between instruments via hardwares ^[30-33].

Besides spectroscopic instruments, other instruments like mass spectrometers have also encountered similar problems, but most of which can be solved by simple peak calibration [34, 35].

Although there has been a development for decades, differences between different brands of instrumentsstill exist, e. g. the difference between a grating type and a Fourier transform type spectrometers. Due to these differences, the inapplicability of the multivariate models would produce unacceptable systematic prediction bias [36-38]. Thus, the solution to this prediction bias is called Calibraion Transfer or Instrument Transfer [39-42]. In the area of machine learning, the relevant keywords are Transfer Learning, Domain Adaptation, and Multi-Task Learning, etc [43]

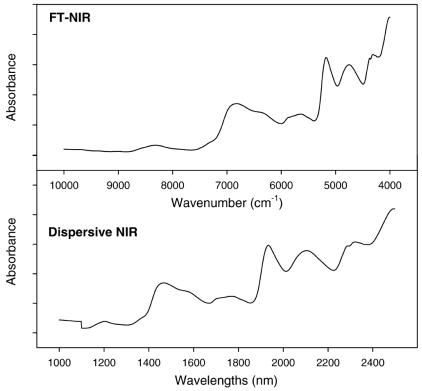


Figure 17-1 Near-infrared spectra of barley samples on dispersive and Fourier transform instruments

Calibration transfer mainly includes the following three catagories of solutions [43-46]

(1) Transfer in spectra

Transfer between the spectra establishes the functional relationship between the spectra measured by the master and slave through a mathematical method. There are

two ways of spectral transfer. One is to convert the master's calibration spectra, and then re-establish a calibration model suitable for the slave spectra, that is called Reverse Standardization in the literatures [47-49]. The other is to convert the slave spectra, and directly use the master model to predict the result. Algorithm of two ways is essentially the same and needs to be selected according to different applications.

(2) Regression coefficient conversion

Regression coefficient conversion is conducted to the master model so as to make it suitable for the slave spectra ^[50]. Also, prediction results of the master model can be corrected, such as the Slope/Bias Correction (SBC) method, etc., to eliminate the systematic deviation of the prediction results ^[51,52].

(3) Robust Calibration

A robust calibration is established through the preprocessing, wavelength variable screening algorithms, etc. Or the master calibration set is expanded by adding spectra under different test conditions, spectra from slave, etc., to establish a global calibration, or hybrid calibration [53, 54]. In some cases, this method is also called Model Updating or Calibration Maintenance. For instance, with the aging of the electronic components, detectors, and optical components of the instrument, as well as changes in the instrument hardware caused by the environment, these inevitable changes in the instrument will lead to changes in the spectra [55]. In practices, the most commonly used methods are the first and third ones [55, 56], the second is rarely used. This chapter mainly introduces the first and third types of calibration transfer methods.

17.2 Tranditional algorithms

Commonly used methods for converting spectra among different instruments (or under different conditions) include: Spectral Substration Correction (SSC), Shenk's Algorithm, Direct Standardization (DS), and Piecewise Direct Standardization (PDS), etc. These methods usually require a representative set of standard samples (15-30 samples), which are called calibration transfer methods with standard samples.

17.2.1 Spectral Substration Correction

Calculate the average spectrum x_{ms} and x_{ss} of the master standard sample spectral matrix X_{ms} and slave matrix X_{ss} respectively, then calculate the difference between the average spectra of them $\Delta x = x_{ms} - x_{ss}$.

For the unknown spectrum $x_{s,un}$ from the slave spectroscopy, convert with formula $x_{s,un}^p = x_{s,un} + \Delta x$, acquire the spectrum $x_{s,un}^p$ consistent with $x_{m,un}$, the final result is calculated by the calibration model established by the master [57].

17.2.2 Shenk's algorithm

Shenk's algorithm consists of two main steps as wavelength correction and absorbance correction [58-60]. The following introduces this algorithm by taking the transfer of spectrum from the slave to master (slave \rightarrow master) as an example.

- (1) Wavelength correction
- **a**. Corresponding to $X_{ms,i}$, choose the spectral part $X_{ss,j+k+1}$ with window size of (k+j+1) from the matrix X_{ss} in the slave instrument, calculate the correlation coefficients of $X_{ms,i}$ and $X_{ss,i-j},R_{ss,i-j+1},\ldots,X_{ss,i+k-1},X_{ss,i+k}$, respectively. If the coefficient r_l of $X_{ms,l}(i-j \le l \le i+k)$ and $X_{ms,i}$ is max, it is indicated that the l wavelength from the slaveinstrument corresponds to the i wavelength from the master. To obtain more accurate results, wavelengths l-1, l, l+1 and their corresponding correlation coefficients r_{l-1} , r_l , r_{l+1} are selected to establish a univariate quadratic parabola model as $r=a_i+b_ii+c_ii^2$. The slave wavelength i^* corresponding to the master wavelength i would be obtained from this fitted parabola.
 - **b**. Loop i to find all corresponding i^* .
- **c**. Establish the one-dimensional quadratic parabola wavelength calibration model $i^*=A+Bi+Ci^2$ using the obtained i^* and i.
 - (2) Absorbance correction

After wavelength correction, calculate the absorbance matrix $X_{ss,i}^*$ of the slave

wavelength i^* by the interpolation method, then find the regression coefficients sa_i and sb_i using the linear equation $X_{ms,i}=sa_i+sb_iX_{ss,i}^*$.

For the unknown spectrum $\mathbf{x}_{s,un}$ from the slave instrument, wavelength fitting calibration curve $\mathbf{i}^* = A + B\mathbf{i} + C\mathbf{i}^2$ is used to calibrate the wavelength, calculate $\mathbf{x}_{s,un}^*$ by the interpolation method, and finally the spectral transfer result consistent with the master is obtained by $\mathbf{x}_{s,un}^p = sa_i + sb_i\mathbf{x}_{s,un}^*$.

17.2.3 Direct Standardization

DS algorithm uses the transfer matrix F to convert the unknown sample spectrum $x_{s,un}$ measured from the slave machine to $x_{s,un}^p$. Transfer matrix F is calculated by $X_{ms}=X_{ss}F$ through the least square as $F=X_{ss}^+X_{ms}^{-[61,62]}$, where X_{ss}^+ is the generalized inverse matrix of X_{ss} , F is a $m\times m$ -dimensional matrix (m is the number of wavelength variables).

For the spectrum $x_{s,un}$ measured from the slave machine, transfer is conducted by $x_{s,un}^p = x_{s,un} F$, the final result is calculated by the calibration model established by the master.

17.2.4 Piecewise Direct Standardization

In PDS algorithm, as shown in Figure 17-2, standard sample spectral matrix $X_{ss,j+k+1}$ with the window width (j+k+1)on both sides of the i-th wavelength point from the slaveinstrument((i-j)th to (i+k)th points) and standard sample spectral maxtrix $X_{ms,i}$ from the master i-th wavelength point are used to calculate the transfer coefficient F_i of the i-th wavelength point. Then, the transfer matrix F of all wavelengths is obtained by moving i point by point [63-66].

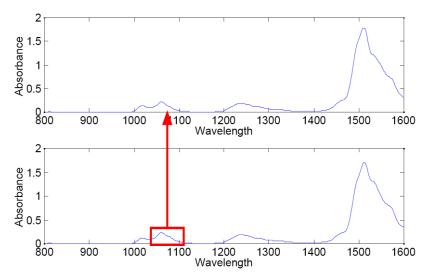


Figure 17-2 PDS algorithm scheme

When calculating the transfer matrix F, besides PLS method, as shown in Figure 17-3, methods such as artificial neural networks can also be used $^{[67, 68]}$. Moreover, spectra can also be transferred and transmitted in the Fourier transform domain or the wavelet domain, etc $^{[69, 70]}$.

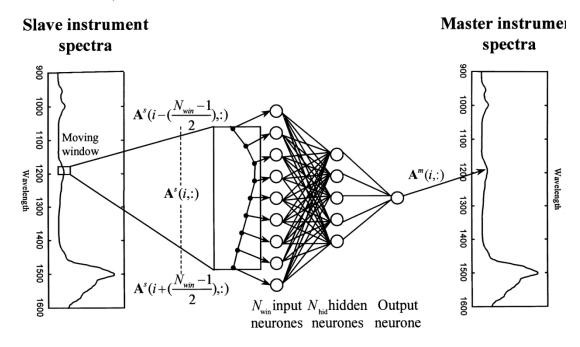


Figure 17-3 Schematic diagram of PDS algorithm based on artificial neural network

17.2.5 Procrustes Analysis

Statistically, Procrustes analysis is used to compare two matrices $X_1(m \times p_1)$ and $X_2(m \times p_2)$, and to find the transfer matrix F between the matrices X_1 and X_2 , where m

is the samples numbe, p_1 and p_2 are the variables number.

Detailed algorithm is as follows [71,72].

- (1) Perform singular value decomposition on the matrices X_1 and X_2 respectively, $X_1=U_1S_1V_1^{\text{t}}$, $X_2=U_2S_2V_2^{\text{t}}$, where X_1 and X_2 represent the spectral matrix measured by the master and slave (after averaging or standardization pretreatment), U is score matrix, V is loading matrix, and U and V matrices contain the rotation information between the spectral matrices, S matrix contains the stretching information between the spectral matrices.
- (2) Calculate $\mathbf{Z}_1 = \mathbf{U}_{1g}\mathbf{S}_{1g}$ and $\mathbf{Z}_2 = \mathbf{U}_{2h}\mathbf{S}_{2h}$, separately, where g and h represent the number of PCs used to find \mathbf{Z}_1 and \mathbf{Z}_2 respectively.
- (3) Calculate transfer matrix F between \mathbf{Z}_1 and \mathbf{Z}_2 by $F = \mathbf{Z}_2^+ \mathbf{Z}_1$, where \mathbf{Z}_2^+ is the generalized inverse matrix calculated by $\mathbf{Z}_2^+ = \mathbf{S}_{2g}^{-1} \mathbf{U}_{2g}^{t}$.
- (4) A spectrum x_{un} measured from a slave can be transferred into spectrum x_{un}^p consistent with the master through the transfer matrix F and the loading matrix V.

17.2.6 Target Transformation Factor Analysis

Target transformation factor analysis (TTFA) is also a transfer method based on PCA. Its core concept is to use the target transfer method to make the principal component score (virtual component concentration) of slave equal to that of master. Main steps are as follows ^[73]:

- (1) Perform PCA on the standard sample spectral matrix of the master to obtain the load and score matrix $\mathbf{X}_m = \mathbf{T}_m \mathbf{P}_m^{\ t}$
- (2) Perform PCA on the standard sample spectralmatrix of the slave to obtain the load and score matrix $X_s = T_s P_s^{t}$
 - (3) Establish the mathematical relationship between master and slave $T_m = TT_s$ Solve the transformation matrix by generalized inverse operation

$$\boldsymbol{T} = \boldsymbol{T}_m \boldsymbol{T}_s^{\ t} (\boldsymbol{T}_s \boldsymbol{T}_s^{\ t})^{-1}$$

(4) Transfer of spectrum from master to slave can be expressed as $X_s^P = X_m P_m T^+ P_s^{\ t}$

Where, the transfer matrix $\mathbf{F} = \mathbf{P}_m \mathbf{T}^+ \mathbf{P}_s^{t}$

17.2.7 Maximum Likelihood Principal Component Analysis

Maximum likelihood principal component analysis (MLPCA) treats calibration transfer as an issue of missing data ^[74].

Combine the standard sample spectra of master and slave: $\mathbf{x}_{i,comb} = [\mathbf{x}_{i,m}, \mathbf{x}_{i,s}]$, i=1,2,...,n, where n is number of standard samples.

Besides, other samples of the calibration set on the master that have no corresponding spectra on the slave can be expressed as $\mathbf{x}_{i,comb}^{\#} = [\mathbf{x}_{i,m}, \mathbf{x}_{i,s}^{\#}]$, i=1,2,...,m, where m denotes the number of calibration set samples minus standard set samples, $\mathbf{x}_{i,s}^{\#}$ denotes the missing spectra from the slave.

 $x_{i,comb}$ and $x_{i,comb}^{\#}$ can be expressed as a matrix $X_{comb} = \begin{bmatrix} X^* \\ X^{\#} \end{bmatrix}$, where X^* represents combined spectral matrix without missing data in the standard sample set, $X^{\#}$ represents combined spectral matrix of other samples in calibration set with missing data in the slave.

Perform MLPCA on
$$X_{comb}$$
: $\begin{bmatrix} X^* \\ X^\# \end{bmatrix} = \begin{bmatrix} U^* \\ U^\# \end{bmatrix} DP^t$

Then, the spectrum $x_{i,m}$ collected on the master can be transferred into the spectrum on the slave according to the following formula:

$$\widehat{\mathbf{x}}_{i,s} = \mathbf{U}^{\#} (\mathbf{U}^{*t} \mathbf{U}^{*})^{-1} \mathbf{U}^{*t} \mathbf{x}_{i,m}$$
 (17-1)

Afterward, based on the MLPCA algorithm, Folch-Fortuny et al. ^[75] used the trimmed scores regression (TSR) method to deal with the issue of missing data, and proposed the TSR method for calibration transfer.

17.2.8 Slope/Bias correction

Different from the above methods that are based on the transfer between spectra, there is a method based on the transfer between the prediction results, that is, the functional relationship between the prediction results obtained by the master and slave is established, which is named Slope/Bias correction (SBC) algorithm [76-78].

Calibration model established on the masteris used to predict the analysis results y_{mp} and y_{sp} of the master and slave standard sample spectral arrays X_{ms} and X_{ss} , respectively. Assume that y_{mp} and y_{sp} have a relationship of $y_{mp}=a\times y_{sp}+b$, the least squares method can be used to obtain a and b.

As for the unknown spectrum $\mathbf{x}_{s,un}$ measured by the slave, firstly, the calibration model established by the master is used to calculate $\mathbf{y}_{sp, un}$, and then formula $\mathbf{y}_{sp,un}^{p}=b+a\times\mathbf{y}_{p,un}$ is used to calculate the corrected analysis result $\mathbf{y}_{sp, un}^{p}$.

Normally, the SBC algorithm is not recommended. Because if the spectral difference between instruments is significant, it would be difficult or even impossible to identify the outlier samples of the model.

17.3 Improvement of tranditional algorithms

In the process of calibration transfer, the selection of standard samples is particularly important ^[79]. For the model update problem, Capron et al. ^[80] compared the effects of the weighting of calibration samples and the selection of representative samples, and the results showed that the selection effect of representative samples is better. Siano et al. ^[81, 82] compared the influence of different transfer standard selection methods on the spectrum transfer effect of PDS, etc., and the results showed that the optimal K-dissimilarity selection (OptiSim) method is better than the K-S method. Li H. et al. ^[83] replaced the Euclidean distance in the K-S algorithm with the Mahalanobis distance, and selected the transfer standard sample through the improved K-S algorithm. In the PDS algorithm, the samples selected by the Mahalanobis distance are more representative, because the combination of concentration differences and spectral differences can better represent the differences between samples. Zhou Z. et al. ^[84] proposed a transfer standard set selection method based on Markov chain, and the result is better than the K-S method.

From the perspective of optimizing the selection method of the transfer standard set, Liang et al. [85] optimized the transfer matrix of the PDS algorithm and proposed

the Rank-KS-PDS calibration transfer algorithm. When Rank-KS selects the transfer standard sample set, it comprehensively considers the influence of sample spectral space and sample concentration space, overcomes the shortcomings of K-S algorithm insensitive to low concentration areas, and improves the accuracy of calibration transfer. Based on the idea of Backward Selection variables, Zheng et al. [86] proposed a backward selection iterative method to transfer the selection of the standard sample set. Through this method, the transfer effect of the standard sample set is better than the standard sample set selected by the KS algorithm. Aiming at the problem of difficulty in obtaining and storing standard samples of natural plant models, Ni Lijun et al. [87] proposed a method for preparing standard samples, this kind of standard sample is stable under normal temperature and pressure, similar to the color of various natural plants, with constant spectrum and good reproducibility, and can be used for a long time in the transfer process of the near-infrared model of a variety of natural plants.

Aiming at the limitations of the SBC algorithm in solving nonlinear problems, Xin X. et al. ^[88] established a linear function relationship between the prediction results of the master and the slave by introducing high powers, both Lagrange interpolation and Newton interpolation are used to find the parameters, and the nonlinear fitting of the two sets of data is realized. Cao Y. et al. ^[89] proposed a method for selecting PDS algorithm parameters (number of standard samples, number of PLS main factors, window width) based on the angle of the spectral space. Zhang et al. ^[90] used sampling error profile analysis (SEPA) to optimize the PDS algorithm's window width and PLS main factor number and other parameters, and proposed the SEPA-PDS method.

Blanco et al. ^[91, 92] used the spectral difference of a set of standard sample sets under different conditions combined with weighting to calculate a mutation matrix, and randomly added it to the calibration set spectrum, which solved the problem of the laboratory-prepared drug calibration samples used for production process analysis. On this basis, Wang J. et al. ^[93] improved the SSC algorithm, the spectrum compensation between the master and the slave does not use the average spectral

difference of the standard sample set spectrum array uniformly, but for each sample in the calibration set, select the most similar standard sample set to compensate for the spectral difference between the master and slave, and the compensation spectrum is weighted by the concentration ratio between the calibration set samples and the standard set samples. On the basis of the SSC algorithm, Li et al. [94] respectively compensated different correction vectors for different types of correction sets, and then through continuous model updates, the influence of different measurement environments on the identification of corn haploid grains by NIRS can be eliminated. Based on the traditional SBC algorithm, Wang et al. [95] proposed a dual-domain model delivery strategy. In this method, the master model is used to predict the spectra of the master and slave standard sample sets respectively, and the transfer model is established by using the ratio of the predicted value and the spectrum of the slave standard sample set. For the spectra collected by the slave, the initial value is calculated firstly using the master model, and then the ratio is calculated by the transfer model, and finally the final prediction result is obtained through the ratio. Li et al. [96] established a PLS model between the spectral difference and the predicted concentration difference between two NIRS instruments to achieve the correction of the predicted concentration from the slave machine. Tan et al. [97, 98] improved the finite impulse response (FIR) transfer algorithm without standard samples, which eliminated the peak problem caused by the FIR algorithm and improved the transfer effect of the FIR method. Bouveresse et al. [99] used the local weight regression algorithm for the correction between spectral absorbance and improved Shenk's algorithm.

Before performing DS and PDS operations, Wang et al. ^[100] used additive background correction to improve the effect of spectral transmission. In response to the nonlinear transfer between spectra in the tranditional PDS algorithm, and the appearance of discontinuities and even abnormal peaks ^[101], Wang H. et al. ^[102] replaced the PLS regression in the PDS algorithm with a radial basis function neural network, and obtained better results. Chen X. et al. ^[103] believe that the appearance of the peak in the PDS algorithm originates from the coefficient of the larger norm in the

PLS model, and its essence is an over-fitting problem, they used a linear regression method with coefficient norm penalty to establish a spectral transfer model, and the transferred spectra were smoother and more robust.

Univariate correction is a special case where the PDS method takes a window width of 1. Yang H. et al. [104] proposed the Simple Linear Regression Direct Standardization (SLRDS) method, this univariate correction method is more suitable for the case where the spectrum has a small linear difference. Norgaard et al. [105] also used this method in fluorescence spectroscopy, which is called the single wavelength standardization (SWS). Galvao et al. [106] calculated the covariance matrix based on the univariate spectral correction using the spectral residuals transferred from the master and slave of the standard sample set, and then established the model through a robust regression method. This method has certain advantages in the case of fewer wavelength variables. Lu H. et al. [107] used the minimum angle regression to first select the characteristic wavelength variable, and then used the unary linear direct correction method to transfer the spectrum, which further improved the transfer effect. Wang W. et al. [108] used the dynamic time warping algorithm (DTW) in speech analysis to correct the spectral wavelengths on the two instruments, and then use the unary regression or multiple regression algorithm to correct the absorbance and obtain satisfactory results. In order to prevent excessive warping, Zou et al. [109] proposed a variable penalty dynamic time warping (VPdtw), which has a better transfer effect on the NIRS than the PDS algorithm.

Yan et al. ^[110] gave different weights to the wavelength variables in the moving window of the PDS algorithm, and proposed a windowed PDS algorithm (WPDS) based on ridge regression and penalty terms. The PDS, a special case of the WPDS algorithm, can be regarded as all wavelength variables assigned the same weight. The double window PDS algorithm (DWPDS) is an extension of the tranditional PDS algorithm, that is, a window of a certain width is taken from the master and slave spectra, and the spectrum transfer matrix is established window by window. Oliveri et al. ^[111] used the idea of the dual-window PDS algorithm to calculate the transfer coefficient between the average spectrum of the standard sample spectral matrix

transferred from the master and the slave, and the transfer coefficient was calculated using the least square method (Figure 17-4). Greensill et al. [112, 113] also used the dual-window PDS algorithm to transfer different array types of near-infrared spectra, but the best result is the wavelet transform combined with DS algorithm. Ottaway et al. [114] improved the DS and PDS algorithms by adding higher-order terms and derivative terms, which can solve the problem of nonlinear differences between different spectroscopic instruments to a certain extent.

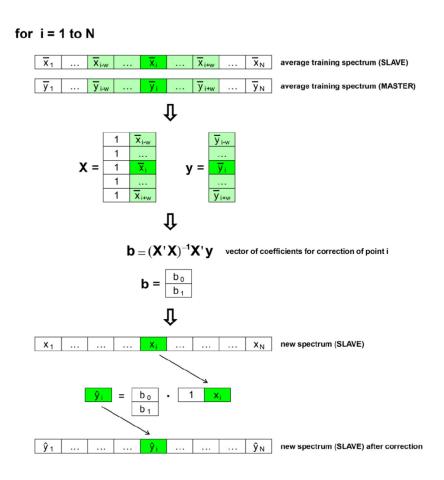


Figure 17-4 Spectral transfer method based on the concept of double-window PDS

On the basis of the DS algorithm, Chen et al. ^[115] used Extreme Learning Machine Auto-encoder to establish the relationship between the master and slave standard sample spectral matrixes, and obtained stable spectral transfer results through an integrated strategy. Laref et al. ^[116] used SVM for DS algorithm to obtain the signal transfer of different electronic nose instruments, and the standard set samples were obtained by the SPXY method. The stacked partial least squares

(VIP-SPLS) method improved by the variable importance in the projection proposed by Li X. et al. [117] rearranges the wavelengths and divides them into a series of non-overlapping spectral intervals, and then transfers them through the DS algorithm.

Tan et al. ^[118] used wavelet transform spectroscopy to denoise and compress the signal, then reconstructed spectral signals of different scales through inverse wavelet transform, and then carried out transfer operations on the spectral signals of different scales respectively, and proposed a wavelet hybrid direct standardization (WHDS). Chen D. et al. ^[119] also proposed a similar calibration transfer method. Yoon et al. ^[120] perform wavelet transform on the spectrum to obtain wavelet coefficients firstly, and then use the DS algorithm to transfer. For large spectral matrixes, this method can reduce the time for spectral transfer and modeling, which is called wavelet transform direct standardization (WTDS). Tan et al. ^[121] use wavelet packets to decompose the spectrum, and realize the transfer of spectrum between different instruments through wavelet packet coefficient transformation, which is called wavelet packet transform standardization (WPTS).

After Ni et al. ^[122] divide the spectrum by wavelet, use the PDS algorithm to transfer each sub-spectrum, and then use the consensus modeling strategy to establish a PLS model for each transferred sub-spectrum one by one, which is called stacked dual-domain piecewise direct standardization (SDDPDS). Poerio et al. ^[123] combined the dual-domain wavelet transform with orthogonal projection, and proposed the dual-domain transfer using orthogonal projection (DDTOP).

Based on the direct orthogonal signal correction (DOSC) algorithm, Lin et al. [124,125] used the regression of the virtual standard average spectrum to eliminate the background differences between sample batches, and proposed the Orthogonal Space Regression (OSR) calibration transfer method, which can correct the systematic errors between the spectra of multiple batches of preparations, and realize the calibration transfer of the chlorogenic acid quantitative model between batches during the water extraction process of the honeysuckle pilot-scale test. On this basis, Yang P. et al. [126,127] proposed a guided orthogonal projection technology combined with a calibration transfer method of SBC, which realized the transfer of the near-infrared

quantitative moisture model of the small-scale test to the pilot-scale test. Wang Q. et al. [128] used random forest to select the wavelength of the NIRS, and then used the DOSC algorithm to preprocess the spectrum to realize the sharing of calibration models between different instruments.

For the spectra collected at different temperature points, the transfer can be realized through the PDS algorithm. However, the traditional PDS algorithm cannot transfer the spectrum at any temperature between different temperature points ^[129]. Based on the PDS algorithm, Wulfert et al. ^[130,131] proposed a continuous piecewise direct standardization (CPDS) algorithm. The transfer matrix $F_{\Delta T}$ between two different temperatures and the temperature difference ΔT were subjected to polynomial regression to obtain two transfer matrix F_T at any temperature between two temperature points. In order to eliminate the influence of temperature on the online determination of electroplating bath composition content by AC voltammetry analyzer, Jaworski et al. ^[132] proposed continuous direct standardization (CDS), and used temperature as a variable to participate in the calibration model to eliminate the influence of temperature on the prediction results.

17.4 New algorithms

17.4.1 Canonical Correlation Analysis

Canonical correlation analysis (CCA) is a multivariate analytical method to study the correlation between two sets of variables, and which can reveal the linear dependence of them. CCA algorithm considers that the information of the measured object between two sets of spectra from the master and slave is consistent, and should be linearly related to each other, while the noise and interference information are random and independent. This method performs canonical correlation analysis on the master and slave spectral matrix, and then converts the obtained canonical correlation variables. Transfer of canonical correlation variables can extract spectral transfer information from the overall spectra, and can filter out noise and interference.

Specific calculation is as follows [133]:

(1) Execute CCA on the standard sample spectral matrix of the master and slave respectively.

$$L_m = X_m W_m \tag{17-2}$$

$$L_s = X_s W_s \tag{17-3}$$

 L_m and L_s are the score matrix of the master standard sample spectral matrix X_m and the slave standard sample spectral array X_s respectively, W_m and W_s are the loading matrix of X_m and X_s respectively.

(2) Calculate the transfer matrix F.

$$\boldsymbol{F}_1 = \boldsymbol{L}_s^+ \boldsymbol{L}_m \tag{17-4}$$

$$\boldsymbol{F}_2 = \boldsymbol{L}_m^+ \boldsymbol{X}_m \tag{17-5}$$

$$\mathbf{F} = \mathbf{W}_s \, \mathbf{F}_1 \mathbf{F}_2 \tag{17-6}$$

(3) Transfer of the slave spectrum \mathbf{x}_{un} to the master spectrum can be expressed as $\mathbf{x}_{un}^{P} = \mathbf{x}_{un} \mathbf{F}$.

CCA algorithm only considers extraction of the maximum correlation of typical variables, which may introduce redundant information that has nothing to do with the target, thereby complicating the calibration transfer function. On this basis, Zheng et al. ^[134] proposed to use PLS to extract the factors that are related to the target value with the largest variance, and then used CCA to perform spectral transfer, which improves the pertinence of spectral transfer to a certain extent.

Before CCA transfer, Bin et al. ^[135] used wavelet transform to preprocess the original spectra, and performed CCA by wavelet coefficients (WTCCA), which achieved a better transfer effect. Fan et al. ^[136] calculated the principal components of the master's standard sample spectral matrix X_m by the latent variables of master PLS model, and then performed spectral transfer (PC-CCA). The validation results were better than the single CCA method.

Similar with CCA, based on spectral regression (SR), Peng et al. ^[137] decomposed on X_m and X_s , and proposed the spectral regression transfer algorithm. It puts the issue of solving the characteristic function in the regression model, avoids the frequent eigenvalue decomposition process of dense matrix, and improves the calculation

efficiency. Zhang et al. ^[138] decomposed the spectra based on multi-level simultaneous component analysis (MSCA), and proposed a two-level strategy for spectral transfer algorithm.

17.4.2 Spectral Space Transformation

Spectral space transformation (SST) obtained the combined spectrum matrix $X_{comb} = [X_m, X_s]$ by combining the standard set spectra X_m and X_s measured by the master and slave respectively. The loading vectors of the combined spectrum matrix are obtained using PCA, and then the spectrum transfer matrix is calculated [139]. Caculation is as follows.

(1) Combine the standard set spectra X_m and X_s measured by the master and slave to obtain a combined spectrum matrix.

$$\boldsymbol{X}_{comb} = [\boldsymbol{X}_m, \ \boldsymbol{X}_S] \tag{17-7}$$

(2) PCA on the combined spectral matrix X_{comb} .

$$\boldsymbol{X}_{comb} = \boldsymbol{T} \left[\boldsymbol{P}_{m}^{t}, \ \boldsymbol{P}_{s}^{t} \right] + \boldsymbol{E} \tag{17-8}$$

Where, P_m^{t} and P_s^{t} are loading of the master and slave matrix.

(3) Calculate the transfer matrix F.

$$\mathbf{F} = \mathbf{I} + \left(\mathbf{P}_{s}^{t}\right)^{+} \left(\mathbf{P}_{m}^{t} - \mathbf{P}_{s}^{t}\right) \tag{17-9}$$

Where, *I* is the identity matrix.

(4) Transfer of the slave spectrum x_{un} to the master spectrum can be expressed as:

$$\boldsymbol{x}_{\mathrm{un}}^{\mathrm{P}} = \boldsymbol{x}_{\mathrm{un}} \boldsymbol{F} \tag{17-10}$$

The structure of the SST algorithm is relatively simple to be calibrated, and it can still maintain good prediction results under a low standard sample number. Similarly, Liu et al. ^[140] used ICA to decompose the combined spectral matrix obtained from multiple instruments, and the expression of the transfer matrix is consistent with the SST algorithm.

17.4.3 Alternating Trilinear Decomposition

Alternating trilinear decomposition (ATLD) is an algorithm commonly used to decompose three-dimensional data. For a group of standard samples with collected spectra from different instruments, a three-dimensional matrix \underline{X} can be obtained, the dimension of which is $I \times J \times K$, where I is the number of standard samples, J is the number of spectral points, K is the number of instruments. ATLD algorithm can decompose \underline{X} into three matrices as $A(I \times N)$, $B(J \times N)$, $C(K \times N)$, where N is the number of contributing factors, A represents the relative concentration matrix of the standard sample, B represents the relative spectral intensity matrix of the standard sample, and C represents the instrument information matrix. Algorithm is as follows [141].

(1) Decompose \underline{X} by ATLD.

$$x_{ijk} = \sum_{n=1}^{N} a_{in} b_{jn} c_{kn} + e_{ijk}, (i=1,2,...,I, j=1,2,...,J, k=1,2,...,K)$$
 (17-11)

(2) calculate the transfer matrix F.

$$F_k = \operatorname{diag}(c_k)B^{t} \tag{17-12}$$

Where c_k is the k^{th} row of matrix C.

(3) For the new collected spectrum $x_{k1,new}$ from the k1 instrument, it can be transferred to the spectrum $x_{k2,trans}$ on the k2 instrument by the following formula.

$$\mathbf{x}_{\text{k2,trans}} = \mathbf{x}_{\text{k1,new}} \mathbf{F}$$
 (17-13)
Where, $\mathbf{F} = \mathbf{I} + \mathbf{F}_{kl}^{+} (\mathbf{F}_{k2} - \mathbf{F}_{kl})$

ATLD and SST algorithm have the same spectral transfer matrix formula, except that before the factor analysis, the SST algorithm expresses the standard sample spectral matrix collected from multiple instruments in an unfolded manner, while ATLD algorithm is a cube matrix. As for cube data decomposition, besides ATLD, there are also PARAFAC and Tucker3 that can also be used. Kompany-Zareh et al. [142] used Tucker3 algorithm to conduct the spectral transfer between different instruments as the missing data filling problem of the tensor array, and realized the calibration transfer from FT-Raman instrument to CCD-Raman spectrometer.

17.4.4 Multi-Task Learning

Multi-Task learning (MTL) calculating the transfer matrix can be summarized as solving a convex optimization problem with a regular trace norm. This regular optimization method can extend the linear transfer between the spectra of different instruments to the non-linear spectral transfer relationship. Compared with other transfer methods like neural networks, this method solves the final transfer matrix through a convex optimization problem. So it can efficiently and quickly obtain the global optimal solution, while requiring fewer preset parameters. Calculation is as follows [143].

(1) Calculate the Gram matrix of the spectral matrix X_s of the slave standard samples.

$$K = X_s X_s^{\mathsf{t}} \tag{17-14}$$

- (2) Perform eigenvalue decomposition on $n \times n$ order K matrix: K = UDU^t, where D is a diagonal matrix containing all eigenvalues, and each column of U is a corresponding eigenvector.
- (3) Solve a regular problem about the trace norm of matrix \mathbf{B} of order $n \times p$ (n is the number of standard samples, p is the number of wavelengths).

$$\frac{\min_{B} ||X_m - UD^{\frac{1}{2}}B||_F^2 + \rho||B||_{tr}}{(17-15)}$$

Where, $\|\cdot\|_F$ represents the Frobenius norm of the matrix, $\|\cdot\|_{tr}$ represents the trace norm of the matrix, and ρ is the regular term coefficient. Method of Accelerated Proximal Gradient can be used to solve the convex optimization problem of trace norm regularization.

(4) Calculate the transfer matrix F.

$$\boldsymbol{F} = \boldsymbol{X}_{S}^{t} \boldsymbol{U} \boldsymbol{D}^{-\frac{1}{2}} \boldsymbol{B} \tag{17-16}$$

(5) Transfer of the slave spectrum x_{un} to the master spectrum can be expressed as:

$$\boldsymbol{x}_{\mathrm{un}}^{\mathrm{P}} = \boldsymbol{F}^{\mathrm{t}} \boldsymbol{x}_{\mathrm{un}} \tag{17-17}$$

Boucher et al. [144] also proposed the Proximal Methods for spectral transfer between different instruments based on the regularization framework, which used

alternating direction method of multipliers (ADMM) to solve convex optimization problems. It has a good result on the transfer from a narrow band range spectrum to a wide band range spectrum.

As for the transfer of multiple qualitative models, Hu et al. [145] proposed an optimization framework using the maximum margin criterion (MMC) criterion.

$$\operatorname{argmin}||X_{m} - X_{s}F||_{F}^{2} + \rho||F^{t}(S_{w} - S_{b})F||_{tr}$$
 (17-18)

Where, S_{w} is the intra-class scatter matrix, S_{b} is the inter-class scatter matrix, S_{b} is the spectral transfer matrix. MMC algorithm has certain advantages in transfering spectra for qualitative analysis.

17.4.5 Generalized Least Squares

Generalized least squares (GLS) takes the difference matrix of the master and slave standard samples as a reference to establish a weighted filtering model to eliminate the influence of the difference between the instruments on the spectra. Main steps of algorithm are as follows [146, 147].

(1) Calculate the mean-centered difference matrix of the master and slave standard sample spectra.

$$\boldsymbol{X}_{d} = (\boldsymbol{X}_{m} - \overline{\boldsymbol{X}_{m}}) - (\boldsymbol{X}_{s} - \overline{\boldsymbol{X}_{s}})$$
 (17-19)

(2) Calculate the covariance matrix of X_d .

$$\boldsymbol{C}_d = \frac{\boldsymbol{X}_d \, {}^{\mathrm{t}} \boldsymbol{X}_d}{n-1} + \alpha \boldsymbol{I} \tag{17-20}$$

Where, n is the number of standard samples, α is the coefficient (usually $1 \times e^{-6}$), and I is the identity matrix.

(3) Perform singular value decomposition on the covariance matrix C_d .

$$C_d = USV^t \tag{17-21}$$

(4) Calculate the weighted filter matrix W.

$$W = V S_{adi}^+ V^t \tag{17-22}$$

Where, $S_{adj} = \mathbf{sqrt}(\frac{S \times m}{\mathbf{trace}(S)})$, m is the number of wavelength variables.

(5) Transform the spectral matrix of the master calibration set and that of the

slave prediction set separately.

$$X_{\text{trans}} = (X - \overline{X})W \tag{17-23}$$

17.4.6 Other algorithms

Based on the principle of orthogonal projection, Andrew et al. [148] obtained the average spectrum of a set of standard samples on multiple instruments, and performed PCA on the average spectra. The first few representive projection space formed by the different spectral loadings between the instruments can perform transfer by orthogonal projection (TOP) on the spectra on multiple instruments. From the concept of TOP, Zhu et al. [149] replaced the average spectral matrix with a change matrix of a set of sample repetitive spectra, performed PCA to obtain the projection space, and proposed an error removalby orthogonal subtraction (EROS). Subsequently, in view of EROS, Zeaiter et al. [150] calculated the virtual spectrum of the slave through the kernel function. According to the difference matrix between the measured and virtual spectrum, the PCA was performed to obtain the projection space, and the dynamic orthogonal projection (DOP) was proposed. Dabros et al. [151] used the DOP algorithm for the maintenance of the online infrared calibration model, and achieved good application results. Igne et al. [152] reviewed and compared the effects of the above-mentioned orthogonal projection algorithms for the transfer of NIRS models. Siska et al. [153] used wiener filter (Wiener Filter) method to process the spectra for the transfer of fixed filter-type NIRS instruments, and proposed a method of optimizing the master instrument.

Chen et al. ^[154] proposed a loading space standardization (LSS) algorithm for the influence of temperature on the spectrum. PCA was performed on the spectra collected from the standard set samples at different temperatures, and then the quadratic function relationship between the spectral loading and the temperature at each temperature was established. Spectrum measured at a certain temperature can be standardized in the loading space to obtain corresponding spectrum at standard temperature. Afterward, Chen et al. ^[155] combined the LSS algorithm with the optical

path length estimation and correction (OPLEC) and proposed the extended loading space standardization (ELSS), which was used to correct the effects of temperature and composition changes on the spectra. Similarly, Shi X. et al. [156] effectively eliminated the influence of temperature changes on the NIRS during the production of sugar and flavoring based on LSS algorithm.

Zhang et al. ^[157] regarded calibration transfer as a global affine transformation problem:

$$\hat{x}_{i,n} = a_i x_{i,n} + b_i, i = 1, ..., k, n = 1, ..., N$$

Where, $\mathbf{x}_{i,n}$ represents the spectrum of the n^{th} standard sample on the i^{th} slave instrument, k represents the number of slave instruments, and N represents the number of standard samples, $\hat{\mathbf{x}}_{i,n}$ represents the spectrum of the n^{th} standard sample sample on the i^{th} slave instrument transferred to the master. The transfer coefficients \mathbf{a}_i and \mathbf{b}_i are calculated by the robust weighted least square algorithm (RWLSA). Deshmukh [158] also used a robust regression method to achieve inter-station signal transfer among the electronic nose systems for emission detection in paper mills.

Zhao et al. ^[159] proposed an algorithm of calibration transfer based on affine invariance (CTAI) for calibration transfer based on affine invariance. This method first establishes PLS model to obtain the score matrix and prediction vector of the master spectra, as well as, the pseudo score matrix and pseudo prediction vector of the slave spectra. Secondly, the regression coefficients of master and slave are obtained by least squares respectively, and then the angle and deviation between master and slave are calculated by the regression coefficients. Finally, the prediction result of the slave spectra is obtained based on the affine transformation.

Folch-Fortuny et al. [160, 161] proposed a new spectral transfer method using Joint-Y partial least squares regression (JYPLS).

$$Y_{J} = \begin{bmatrix} Y_{m} \\ Y_{s} \end{bmatrix} = \begin{bmatrix} T_{m} \\ T_{s} \end{bmatrix} Q_{J}^{t} + E$$

$$X_{m} = T_{m} P_{m}^{t} + E$$

$$X_{s} = T_{s} P_{s}^{t} + E$$

$$T_{m} = X_{m} W_{m}$$

$$T_{S} = X_{S}W_{S}$$

Where, Y_m and Y_s are the concentration matrixes of the calibration set and standard set samples of the master. T_m and T_s are score matrixes of X_m and X_s , respectively. P_m and P_s are loading matrixes of X_m and X_s , respectively. W_m and W_s are weighting matrixes of X_m and X_s , respectively. Q_J is the loading matrix of the combined Y concentration matrix.

Spectrum $x_{i,m}$ in the master calibration set can be transferred into the spectrum $\widehat{x}_{i,s}$ of the slave by the following formula:

$$\widehat{\boldsymbol{x}}_{i,s} = \left(\boldsymbol{Q}_{I} \; \boldsymbol{Q}_{I}^{t}\right)^{-1} \boldsymbol{Q}_{I} \; \boldsymbol{x}_{i,m} \tag{17-24}$$

Shan et al. ^[162] proposed a joint spectral subspace spectral transfer method (JPCA) based on principal component analysis and kernel principal component analysis. The method combines the spectral matrixes of the master and slave standard sample sets for PCA or kernel PCA, so as to obtain the transfer matrix through least squares in the low-dimensional feature space.

Khaydukova et al. ^[163] proposed a standardization method with regularization coefficients (SRC) based on Tikhonov regularization (TR), which uses the following formula to obtain the transfer matrix:

$$\boldsymbol{F} = \left(\boldsymbol{X}_{s}^{\mathsf{t}} \boldsymbol{X}_{s} + a\right)^{-1} \left(\boldsymbol{X}_{s}^{\mathsf{t}} \boldsymbol{X}_{m}\right) \tag{17-25}$$

In the formula, a is the regularization coefficient, usually from 1 to 30000.

Spectrum $x_{i,m}$ in the master calibration set can be transferred into the spectrum $\hat{x}_{i,s}$ of the slave by the following formula:

$$\widehat{\boldsymbol{x}}_{i,m} = \boldsymbol{x}_{i,s} \boldsymbol{F} \tag{17-26}$$

Zhao et al. ^[164] used the PLS model of the master to project the spectra of master and slave standard sample sets respectively, and then established the transfer between two instruments in the PLS projection space. For the spectrum collected from the slave, the projection vector on the master was obtained by transfer relationship in the projection space, and then the PLS model of the master produced the final prediction result. Zhang et al. ^[165] used *X* weight matrix of PLS model built by the master to

project the master standard sample spectrum to further obtain the matrix L, and then to obtain the transfer matrix F between L and the slave standard sample spectral matrix. It was a PLS-based weight matrix transfer method. Chen et al. ^[166] used the master model to predict the deviation of the concentration value of the slave standard sample set from the actual concentration, and established a deviation prediction model for systematic prediction error correction (SPEC).

Mou et al. ^[167] aimed the minimization of the robust Cauchy Estimator function of subspace learning, and proposed a robust spectral transfer method. It calculated the shared base matrix of the master and slave spectra and its corresponding expression coefficients in an iterative manner, and then established a transfer matrix based on the expression coefficients, which can reduce the impact of outlier samples and spectral noise on the spectral transfer. Seichte et al. ^[168] proposed a Bayesian calibration transfer method based on Lagrangian multiplier method and hierarchical model, which used the Markov chain Monte Carlo method to estimate the error bounds. It was successfully performed in calibration transfer of oxygen sensors. Subsequently, they used similar methods to eliminate the influence of oxygen on the determination of carbon dioxide content by mid-infrared spectroscopy ^[169]. Based on the multiple block orthogonal projections to latent structures (OnPLS), Skotare et al. ^[170] proposed a joint and unique multiblock analysis (JUMBA) for spectral transfer of multiple instruments.

Andries used the penalty matrix decomposition algorithmof domain adaptation in transfer learning method, such as transfer component analysis (TCA) and scatter component analysis (SCA) for spectral matrix transfer and model maintenance ^[171]. Similarly, Liu C. et al. ^[172] used the TCA to realize the NIRS transfer of edible oil on different instruments. In terms of soil researches, TCA was successfully applied to transfering the NIRS among arsenic and available phosphorus models ^[173, 174]. Specically, TCA addresses the problem of different data distribution in the source domain and the target domain, and maps the data from two domains to a high-dimensional regenerative kernel Hilbert space, where, the data distance between the source and target are minimized, while their respective internal attributes to the

greatest extent retains.

Shi G.et al. ^[175] transferred the NIRS of the two types of wood by adaptive component analysis (ACA) and established a deep transfer learning model of oak wood defect classification with the color wood data as the source domain and oak wood data as the target domain. Shan et al. ^[176] proposed a joint spectral subspace method for calibration transfer based on PCA and KPCA. Based on the principle of domain adaptation, Nikzad-Langerodi et al. ^[177, 178] proposed a domain-invariant PLS (di-PLS) method, which can be used for unsupervised, semi-supervised and supervised spectral model maintenance and calibration transfer. Huang et al. ^[179] also proposed a partial least squares method for domain adaptation. A transfer sample based coupled task learning (TCTL) method was proposed based on transfer learning and multi-task learning, which could be used for transfer between electronic nose instruments and compensation for drift over time ^[180]. Based on the active learning algorithm from machine learning, Hu et al. ^[181] solved the problem of multivariate quantitative correction for hyperspectral imaging of different types of blueberries through iterative screening of standard samples.

Li et al. ^[182] proposed a double digital projection slit algorithm for Raman spectrometers with different resolutions to solve the problem of spectral consistency. Gradient descent method was adopted to obtain the optimal solution of the transfer matrix, and a better transfer result was achieved. In the study of Liu et al., the deep autoencoder (DAE) method was employed to establish a nonlinear mapping between spectra of different NIR instruments. An error function penalty term based on conditional probability and parameter maximum likelihood method was designed, and the network parameters of deep auto-encoding was optimized by combining with gradient back propagation algorithm ^[183].

In addition to the transfer of the calibration spectra matrix, some new methods have also been applied in order to realize the transfer of the master calibration model. Liu et al. ^[184] proposed a linear model correction (LMC) which can realize the transfer of PLS model regression coefficients. Subsequently, the method was further improved to obtain the globally optimized regression coefficients ^[185]. Kauppinen et al. ^[186]

realized the transfer of the online NIR model of the moisture content of drug freeze-drying process by converting the PLS regression coefficients. With regard to the evaluation issue of the transferred model, Eskildsen et al. ^[187] proposed to use the prediction results of the model instead of original reference data to evaluate the effect of the calibration transfer.

17.5 Global calibration, robust calibration and model update

Three keywords of global calibration, robust calibration and model update (or model maintenance) are often refered confusingly in spectral multivariate calibration analysis, and actually they have a lot in common. The global model calibartion, also known as the augmented hybrid calibration, hybrid calibration, spiking method in the literature, usually refers to the expansion of the calibration set of the master by adding spectra under different test conditions, spectra measured from different instruments, etc. to build a model, so as to achieve model sharing under different instruments, different measurement environments or different sample types. Robust calibration often refers to the establishment of a model that is not sensitive to external influence factors through spectral preprocessing algorithms, wavelength variable screening algorithms, etc [188, 189]. Therefore, it can be considered that the establishment of a global calibration is a means to achieve the robust model, and both two methods can also be combined to establish a robust global model. However, the model updating or calibration maintenance covers a broader range. In the traditional concept, when encountering samples outside of the model (chemical composition or physical state of the sample changes) or the instrument is aging over time, what we need is model update or model maintenance. In general concept, the process of establishing a global model or a robust calibration actually also belongs to the category of model update or model maintenance [190, 191]. Thus, global calibration, robust calibration and model updates (or model maintenance) are usually employed to solve calibration transfer problems [192].

Koehler et al. [193, 194] introduced a self-designed FIR matrix to filter the MIR

interference data, combined with model update, accurately classifying the data obtained by two MIR remote sensing spectrometers based on piecewise linear discriminant analysis (PLDA). FIR algorithm was used by Song et al. to eliminate the changes in the spectra from the same instrument at different times and under different environmental conditions, and a more robust NIRS model for predicting soil organic matter content was established [195, 196]. By means of spectral error analysis, Wang Y. et al. [197] proved that the combination of the first derivative and SNV can significantly improve the calibration transfer results between FT-NIR spectrometers with integrating sphere diffuse reflectance measurement.

Milanez et al. [198] involved successive projections algorithm (SPA) to select characteristic wavelength variables for establishing NIRS and UV-vis models. The discriminant models can be used among different instruments, and their recognition accuracy was equivalent to DS and PDS methods. Similar study was reported that, SPA and competitive adaptive reweighted sampling (CARS) were combined to select special wavelengths, and together with SBC algorithm, the established NIRS model predicted the soluble solid content of apple spicked for consecutive years [199]. A double CARS strategy was proposed by Zheng et al. [200] for NIRS global modeling. Based on the concept of standard deviation, Ni et al. [201-203] proposed a stable and consistent wavelength variable selection method between spectrometers, which can establish a robust calibration model and realize the sharing of models on multiple instruments. Hong S. et al. [204] used the scale invariant features transform (SIFT) algorithm to screen the stable characteristic wavelengths for establishing NIRS model of the total alkaloids of tobacco leaves, which can realize the standard-free transfer of the model. Xu et al. [205] proposed a correlation-analysis-based wavelength selection (CAWS) based on the correlation coefficient between the master and slave spectra, which was used to establish a robust calibration model and obtained good results. Based on the multi-model consensus strategy, Zhang et al. [206, 207] proposed the Guided Model Reoptimization (GMR) method to solve the problem of model update and calibration transfer, which selected wavelength variables to filter and weight by PLS regression coefficients, and screened calibration set samples through a method

similar to stepwise multiple linear regression to select variables.

When establishing the global model between master and slave, it is necessary to collect the spectra of a certain number of representative samples from the slave, and the corresponding concentration value is granted to get better results ^[208]. To address this problem, Kalivas et al. ^[209,210] proposed a strategy of models update and transfer based on the weighting method of slave samples and the Tikhonov regularization framework.

The common weighting modeling can be expressed as:

$$\begin{pmatrix} \mathbf{y} \\ \lambda \mathbf{y}_{\mathrm{L}} \end{pmatrix} = \begin{pmatrix} \mathbf{X} \\ \lambda \mathbf{L} \end{pmatrix} \mathbf{b} \tag{17-27}$$

Where, y is the concentration vector of the master calibration set, X is the spectra matrix of the master calibration set, y_L is the concentration vector of the slave calibration, L is the spectra matrix of the slave calibration, λ is the weighted value, and b is the regression coefficient.

Under Tikhonov regularization (L2 regularization), the optimization framework is:

$$\min(||Xb - y||_2^2 + \lambda^2 ||Lb - y_L||_2^2)$$
 (17-28)

The solution of this equation is:

$$\widehat{\boldsymbol{b}} = (\boldsymbol{X}^{\mathsf{t}}\boldsymbol{X} + \lambda^2 \boldsymbol{L}^{\mathsf{t}}\boldsymbol{L})^{-1} (\boldsymbol{X}^{\mathsf{t}}\boldsymbol{y} + \lambda^2 \boldsymbol{L}^{\mathsf{t}}\boldsymbol{y}_{\mathsf{L}})$$
 (17-29)

If *L* represents the difference spectramatrix of a set of standard sample sets measured on the master and slave respectively, or a set of spectral baseline background matrix under different test conditions, or a set of spectramatrix of blank samples, etc., its corresponding *y*_Lbecomes a zero concentration vector. Then the optimization framework can be simplified as:

$$\min(\left||X\boldsymbol{b} - \boldsymbol{y}|\right|_{2}^{2} + \lambda^{2}|\left|\boldsymbol{L}\boldsymbol{b}\right|\right|_{2}^{2})$$
 (17-30)

The solution of this equation is:

$$\widehat{\boldsymbol{b}} = (\boldsymbol{X}^{\mathsf{t}}\boldsymbol{X} + \lambda^2 \boldsymbol{L}^{\mathsf{t}}\boldsymbol{L})^{-1}\boldsymbol{X}^{\mathsf{t}}\boldsymbol{y}$$
 (17-31)

In order to obtain more stable regression coefficients, based on the idea of ridge regression, the weighting method modeling can be improved as:

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{0} \\ \lambda \mathbf{y}_{\mathbf{I}} \end{pmatrix} = \begin{pmatrix} \mathbf{X} \\ \tau \mathbf{I} \\ \lambda \mathbf{L} \end{pmatrix} \mathbf{b}$$
 (17-32)

Among which, τ is the penalty coefficient, I is the identity matrix.

The optimization framework is:

$$\min(||X\boldsymbol{b} - \boldsymbol{y}||_2^2 + \tau ||\boldsymbol{b}||_2^2 + ||L\boldsymbol{b} - \boldsymbol{y}_L||_2^2)$$
(17-33)

The solution of this equation is:

$$\widehat{\boldsymbol{b}} = (\boldsymbol{X}^{\mathsf{t}}\boldsymbol{X} + \tau^{2}\boldsymbol{I} + \lambda^{2}\boldsymbol{L}^{\mathsf{t}}\boldsymbol{L})^{-1}(\boldsymbol{X}^{\mathsf{t}}\boldsymbol{y} + \lambda^{2}\boldsymbol{L}^{\mathsf{t}}\boldsymbol{y}_{\mathsf{L}})$$
(17-34)

Regarding to the model update and transfer strategy of Tikhonov's regularization, Kunz et al. ^[211,212] discussed the influence of standard design selection. Shahbazikhah et al. ^[213] proposed a consensus modeling strategy to optimize the selection of regularization parameters. While, Tencate et al. ^[214] brought forward a method for selecting model update parameters based on the fusion strategy. Farrell et al. ^[215] used Tikhonov's regularization strategy to update the drug NIRS model under different conditions, and obtained satisfactory results. Similar study was done for sharing the model on different NIRS instruments based on Tikhonov's regularization strategy ^[216].

Except for sample augmentation, model update can also take samples and features to augment at the same time, which can be expressed as [217]:

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{0} \\ \lambda \mathbf{y}_{L} \end{pmatrix} = \begin{pmatrix} \mathbf{X} & \mathbf{0} \\ \mathbf{0} \mathbf{X} \\ \lambda \mathbf{L} & \lambda \mathbf{L} \end{pmatrix} \begin{pmatrix} \mathbf{b}_{m} \\ \mathbf{b}_{s} \end{pmatrix}$$
(17-35)

Rudnitskaya et al. ^[218] compared the results of DS algorithm, Tikhonov regularization and Joint-Y PLS on calibration transfer and update for the potential sensor array instrument, proving that Tikhonov regularization and Joint-Y PLS can get better results. On the basis of the least absolute shrinkage and selection operator (LASSO), Kunz et al. ^[219] proposed a robust fused LASSO algorithm (RFL) for the maintenance and transfer of the calibration model. Genetic algorithm was performed by Guo et al. ^[220] to correct the wavelength variables from multiple Raman spectra, and the updated model by Tikhonov regularization obtained satisfactory results. Based on the ridge regression updating, Zhang et al. ^[221] combined the prediction optimization and the 2-norm constraint of model coefficients, realized the update of

model coefficients, and solved the problem of deterioration of model prediction ability and reliability caused by instrument drift or sample changes.

Based on the Lambert Beer's law, Sulub et al. [222] proposed a spectral simulation calculation method. Spectra of the mixture can be generated by the absorption signal of the pure substance and the background signal of the instrument. In this way, whether for master or slave instrument, the calibration set can be quickly established by measuring the spectra of the pure substance in the mixture. Haaland et al. [223] synthesized spectra by adding the temperature-affected background signal to the calibration spectraas to solve the problem of the model's adaptability to temperature. The temperature-affected background signal was obtained by the least square expansion of the temperature spectra. By PDS, Sulub et al. [224] realized the spectral transfer of multiple NIRS instruments (including grating scan and FT instruments) to determine the content of active ingredients in medicines, and updated the slave model by preparing a placebo. This method can analyze 30 medicines in 12 minutes, instead of 5 hours by HPLC method. Saiz-Abajo et al. [225] established a robust calibration model by adding different types of noise and interference to the calibration spectra, as well as the ensemble modeling strategy. Pierna et al. [226] added the spectral changes of different instruments and samples with different states (water content and particle size, etc.) to the spectra of 10 calibration samples, generating hundreds of virtual modeling spectra, and obtaining a robust prediction model.

Cooper et al. ^[227] took the spectra of several calibration samples from the master as the target, and obtained the same number of virtual spectra through mathematical mixing calculation to form a virtual spectral matrix. The master model predicted the virtual spectral matrix of master and slave, and established the SBC calibration curve based on the predicted value of master and slave. In the further study, they also used the spectra of 13 pure compounds to transfer the NIRS of jet fuel by the above method, which can accurately predict the properties and composition of aromatics, hydrogen content, density, viscosity, etc ^[228]. Rauscher et al. ^[229] also refered this method to transfer the spectra of the non-dispersive infrared spectrometer to monitor the quality of oil. Similarly, Abdelkader et al. ^[230] used the spectra of 15 pure compounds and

calculated the virtual spectra in segments, improving the transfer results of the method. Silva et al. ^[231] established the spectral transfer coefficient on the virtual spectral matrix using DS algorithm, and realized the transfer of oil from the desktop NIR spectrometer to the handheld instrument.

Ni et al. ^[232] combined the stacked PLS method with model update to establish a robust calibration model for the sharing of multiple NIRS instruments. Honorato et al. ^[233] selected wavelength variables by the continuous projection algorithm (SPA) to establish a robust MLR model shared by multiple instruments, and the results were slightly better than PDS-PLS. With establishment of a local calibration model, Igne et al. ^[234] realized the model sharing of four NIRS instruments from two brands. Liu et al. ^[235] first constructed the 3D spectral cube collected from multiple instruments, and employed Tchebichef discrete orthogonal moments to extract chemical features. Finally, a stepwise regression method was conducted to establish a universal model on multiple instruments.

Moving window MSC was employed by Kramer et al. ^[236] for the preprocessing of jet fuel spectra on two NIRS instruments, and a better result was obtained by optimizing the size of the moving window. Also, Liu et al. ^[237] mainly used the MSC algorithm to standardize the line-scan NIR imaging system. Sahni et al. ^[238] compared the effects of MSC, OSC, FIR, PDS and global models on the correction of optical path changes of optical fiber probes, and results revealed that PDS and global models proved to be the better solutions. Extended multiplicative signal correction (EMSC) was used for the preprocessing of bacterial Raman spectra on multiple instruments. The PLS-DA algorithm can successfully establish a discriminant model for different bacterial species ^[239]. Preys et al. ^[240] combined orthogonal signal correction (OSC) with external parameter orthogonalisation (EPO) to establish a robust calibration model, which solved the problem that OSC can not consider the influence of external interference and the predictive performance degradation of EPO when the influence of external factors on the target value is too high.

Wijewardane et al. [241, 242] modelled the air-dried ground soil to predict the organic and inorganic carbon content at different moisture levels by EPO, DS and a

global model. Ackerson et al. and Roudieret al. ^[243, 244] also solved similar problems through EPO and DS algorithms. Amat-Tosello et al. ^[245] used the EPO algorithm to simultaneously realize the sharing of gasoline short-wave NIRS on four instruments. EPO was employed by Hans et al. ^[246] to reduce the influence of temperature and humidity on the NIRS to predict the calorific value of biomass, and to establish a model that was not sensitive to temperature and humidity. Similarly, the temperature mixing model strategy can eliminate the influence of temperature on NIRS prediction of reducing sugar and moisture content in longan honey. Thygesen et al. and Thamasopinkulet al. ^[247, 248] successfully built a temperature mixing model for predicting moisture content in wood using NIRS, which was more effective than single PDS algorithm.

Luoma et al. ^[249] attempted to use additive partial least squares modeling strategy for model maintenance. According to different measurement conditions, the residual PLS model was established to solve the problem of model inapplicability by addition. Elizalde et al. ^[250] also adopted a similar strategy to solve the problem of model inapplicability caused by changes in the online Raman spectrometer. Nouri et al. ^[251] established a hybrid model of soil NIRS from lab and airborne hyperspectral images, and updated the model with the difference spectra and zero concentration of the standard spectra. This model can be used for prediction of airborne hyperspectral imaging.

Local model that is based on the local kernel function is often established in the SVR method, which may not work when the new spectrum from the new instrument is added to the calibration set. Based on the transfer learning idea, Yu et al. ^[252] used regularized multi-task learning (RMTL) to estimate the relationship between the SVR model in the new condition and the original model, and successfully improved SVM regression. Highlight of this method is that the most important support vectors of SVR model can be selected as the sample for model update.

17.6 Progress of applications

17.6.1 SBC method

Brito et al. ^[253] used the SBC algorithm to correct the model prediction values of the total suspended solids (TSS) and chemical oxygen demand (COD) of waste water by UV spectroscopy, and the result was better than the SSC algorithm and the SLRDS algorithm. Brouckaert et al. ^[254] also used the SBC algorithm to correct the predicted values of the Raman spectroscopy established in the laboratory for the determination of the content of the two components of the liquid detergent, and used it for industrial-level online analysis, and obtained satisfactory results. Dambergs et al. ^[255] used the SBC algorithm to quickly analyze the predicted value of the tannin content in red wine by ultraviolet spectroscopy and corrected it on multiple instruments, and obtained relatively consistent prediction results.

According to the PCA classification model of different types of coffee beans in the NIR spectroscopy, Myles et al. ^[256] used the SBC algorithm to transfer the PCA scores on the two instruments, and obtained a better result. Wang J. et al. ^[257] conducted a similar study on the hyperspectral prediction models of lamb protein from different origins, and the result is that the SBC algorithm has a better effect. Li T. et al. ^[258] used SBC algorithm to correct the acid value and peroxide value of edible oil predicted on two NIRS instruments.

17.6.2 SSC method

Pierna et al. ^[259] used the spectral difference correction algorithm (SSC) to transfer the spectrum of more than 9000 feed samples on the dispersive desktop NIR spectrometer to the MEMS handheld spectrometer using 25 transfer standard samples to establish the determination of feed fat, fiber, and protein, and starch PLS model. Zamora-Rojas et al. ^[260] used the SSC algorithm to transfer the pork spectrum collection on the desktop NIR spectrometer to the handheld instrument to realize the

routine quality analysis beside the pork processing line. Daikos et al. ^[261] used a method similar to the SSC algorithm to subtract the background of the substrate, and transferred the near-infrared imaging spectrum of the coating on one substrate material to another substrate material, realizing the sharing of PLS models. Smith et al. ^[262,263] used the SSC algorithm to realize the spectral transfer of different near-infrared spectroscopy instruments to predict the content of active ingredients in the whole paracetamol tablets. This article also tried to use six standard materials to establish a spectral response correction model through the SLRDS algorithm, which was slightly inferior to the SSC algorithm.

Hayes et al. [264] calibrated the wavelength of the array detector type short-wave near-infrared spectrometer, and then used the SSC algorithm to update the model. In predicting the soluble solid content of apples, the results are equivalent to PDS, but the implementation process is simple and easy. Xu H. et al. [265] aimed at the lack of universality in the multi-channel grading detection model for fruit quality, and adopted the DS algorithm (MSSC-DS) for correction of the average spectral difference to transfer the online detection spectrum of the crown pear sugar content between the two spectrometers, the prediction accuracy of the model can meet the actual requirements of production (less than 0.5 Brix). Roggo et al. [266] used the SSC algorithm to transfer the near-infrared reflectance spectrum of sugar beet, and good results can be obtained no matter whether the actual sample or the general sample is used as the transfer standard sample. Saranwong et al. [267] used the SSC algorithm for the NIRS transfer of the online fruit screening machine, which greatly improved the MLR and PLS correction models, and the compensation of the average spectral difference of the standard sample set was better than the result of linear fitting or polynomial fitting.

Soldado et al. ^[268] combined the SSC algorithm with the transfer by orthogonal projection (TOP) method to transfer the silage spectrum from the desktop NIR spectrometer to a portable instrument, the built model can accurately predict the content of dry matter, neutral detergent fiber and crude protein. Sun H. et al. ^[269] first screened the characteristic variables through regression coefficients, and then

compensated the absorbance through the SSC algorithm, and established a universal NIR analysis model for the quality of fresh jujubes between different instruments.

17.6.3 Shenk's method

Qin et al. ^[270] compared the transfer results of PDS, DWPDS and Shenk's algorithms on the NIRS of tobacco leaf and smoke powder. Shenk's algorithm is superior to other methods. It is also a feasible way to establish a NIRS mixed model of tobacco leaf and powder. Based on Shenk's algorithm, Garcia-Olmo et al. ^[271] investigated the transfer results of four standard sample components on fatty acid liquid near-infrared spectroscopy, and the results showed that the closer the composition of the sample to the test sample, the better the transfer result. Roza-Delgado et al. ^[272] used Shenk's algorithm to transfer the milk spectrum between desktop and portable near-infrared spectrometers, and established a model that can quickly detect milk composition on site. Masahiro et al. ^[273] used a similar Shenk's algorithm to calibrate the wavelength and absorbance of the NIRS respectively, to solve the problem of spectrum changes before and after the online instrument maintenance, and to achieve the correction and maintenance of the vinyl content prediction model in molten polypropylene. Perezmarin et al. ^[274] used Shenk's algorithm to successfully transfer the NIRS of feed on different scanning instruments.

17.6.4 DS method

Milanez et al. ^[275] used the DS algorithm to transfer the NIRS of the adulterated ethanol gasoline on two instruments, and a 100% recognition success rate can be obtained for PLS-DA discriminant analysis. Sil et al. ^[276] used the DS algorithm to transfer the FT-NIRS of drugs to multiple handheld spectrometers, and established an analysis model for predicting the content of different crystal forms. Brito et al. ^[277] used the DS algorithm to transfer the NIRS of the flour from the desktop instrument to the handheld instrument, and then re-established the PLS model on the handheld instrument, which can obtain better results. Jinayu et al. ^[278] used the UVE-SPA

wavelength screening method combined with the DS algorithm to realize the transfer of the NIRS of the apple on the same model and different models of fruit portable instruments. Hu R. et al. ^[279] realized calibration transfer of navel orange total sugar prediction by near-infrared spectroscopy using DS algorithm.

Chen Y. et al. [280] used the DS algorithm to transfer the NIR hyperspectral spectra of soil under different humidity, and realized that the model based on the air-dried soil spectrum could be used for soil samples with different moisture content. Wang S. et al. [281] used the DS algorithm to convert the NIRS of soil under different humidity to eliminate the interference of moisture on the prediction of soil organic matter content. Ji et al. [282] used the DS algorithm to transfer the NIRS of the water-bearing untreated soil, and made predictions through a quantitative calibration model established by dry and ground soils. Silva et al. [283] used the DS algorithm to transfer the gasoline spectra measured by three mid-infrared spectrometers, and based on the global modeling strategy, the PLS-DA or SIMCA method can be used to distinguish gasoline from different origins. Liu C. et al. [284] used the DS algorithm to transfer two edible oil spectra above the NIRS, and established an analysis model for predicting acid value and peroxide value. Lopez-Moreno et al. [285] used the DS algorithm to transfer the LIBS spectrum at room temperature to the spectrum at high temperature, and established a model for predicting the metal content in a high-temperature environment.

Khaydukova et al. ^[286] used the DS algorithm to transfer the volt-ampere signal and the potential signal in the electronic tongue sensor, so that the regression model based on the potential data can be used for the prediction of the volt-ampere signal. Weng H. et al. ^[287] used the DS algorithm to transfer citrus spectra between different models of hyperspectral imaging, and the extreme learning machine discriminant model of citrus canker has an accuracy of 86.2% on the slave spectra. Fonollosa et al. ^[288,289] used DS, PDS and other algorithms to transfer the signal of the metal oxide gas sensor matrix on multiple sensors and obtained satisfactory results. Panchuk ^[290] used the DS algorithm to convert different types of spectra, such as the transfer between energy-dispersive XFS and vis-UV, and the transfer between different NIRS

wavelength ranges. Vaughan et al. ^[291] used the DS combined with PLS algorithm to convert the spectra of two LC-MS, and initially solved the problem of metabolomics data fusion. Morais et al. ^[292] realized the transfer of digital imaging on two devices using DS algorithm for predictive analysis of serum creatinine content. Khoshkam et al. ^[293,294] embedded the DS algorithm in the multivariate resolution analysis of the extended matrix for the study of reaction kinetics and obtained good results. Surkova et al. ^[295] successfully transferred the spectrum from the UV-Vis spectrometer to the optical multi-sensor system composed of four LEDS by using DS algorithm, and realized the transfer between optical multi-sensor systems.

17.6.5 PDS method

Barreiro et al. [296] used the PDS algorithm to transfer the spectrum from the desktop NIR spectrometer to the portable spectrometer, and established an analytical model that can detect the olive breeding process in the field. Alamar et al. [297] used the PDS algorithm to transfer the FT-NIRS of 447 Jonagold apples to the array spectrometer, and before the spectrum transfer, the wavelength of the FT-spectrum was normalized by the segmented cubic Hermite interpolation, and then the analytical model of the soluble solid content was established. Sulub et al. [298] used the PDS algorithm and the wavelet hybrid direct correction algorithm (WHDS) to achieve spectral transfer on five NIR spectrometers for rapid analysis of the uniformity of the active ingredient content of the tablet. Luo et al. [299,300] combined wavelength selection and PDS algorithm for the transfer of bovine blood near-infrared spectroscopy, which can achieve rapid diagnosis of bovine anemia on multiple instruments. Cen H. et al. [301] used PDS to transfer the hyperspectral spectrum of citrus canker, and then established a least squares support vector machine discriminant model. The recognition rate of the model for the prediction set increased from 26% before transfer to 97%.

Pereira et al. ^[302] used the dual-window PDS algorithm (DWPDS) to transfer the NIRS of the drug powder to the spectrum of the tablet, which provides a feasible way

to quickly obtain a sample of the drug spectrum calibration set. Sohn et al. ^[303] also used the DWPDS algorithm to transfer the NIRS for analyzing the cellulose content of flax between different instruments, and achieved good results. Galvan et al. ^[304] used the DWPDS algorithm to transfer the low-field nuclear magnetic resonance spectrum of gasoline between different instruments, among which the resolution of low-field nuclear magnetic instruments is different.

Yang Y. et al. ^[305] used DS and PDS algorithms to effectively transfer the surface-enhanced Raman prediction model of potassium sorbate in sweet-scented osmanthus wine to bayberry wine to realize the transfer of the same analyte prediction model among different species. Similar examples of transferring models between different sample types include the application of quality analysis of chilled pork and eggs ^[306-308]. Boiret et al. ^[309] used the PDS algorithm to transfer the transmission NIRS of the coated tablets between two Fourier transform spectrometers of the same model, and the predicted standard deviations of the active ingredient content before and after the transfer were 4.0% and 2.4%, respectively. Sales et al. ^[310] used the PDS algorithm to transfer the signal of the potential sensor under the two test conditions, and selected the transfer standard sample based on the K-S algorithm, and obtained satisfactory results. Marchesini et al. ^[311] used the PDS algorithm to transfer the NIRS from the desktop instrument of the undried whole maize plant to two portable instruments.

Ge et al. ^[312] used the PDS algorithm to convert the diffuse reflectance spectra of the soil measured on multiple NIRS instruments of different types, and established a model to predict the organic carbon content in the soil. Rodrigues et al. ^[313] used the PDS algorithm to transfer the MIRS of crude oil on two instruments, and then used the orthogonal projections to latent structures (OPLS) to establish a crude oil density prediction model, and got better results. Li et al. ^[314] used the PDS algorithm to transfer the spectrum of propylene glycol-water solution measured on multiple handheld NIR spectrometers, and realized the rapid identification of ethylene glycol adulteration. Gryniewicz-Ruzicka et al. ^[315] used the PDS algorithm to transfer the spectra of multiple Raman spectrometers measuring the content of propylene glycol in

glycerol. Thygesen et al. ^[316] used algorithms such as DS and PDS to transfer excitation-emission three-dimensional fluorescence spectra, and then took advantage of PARAFAC to obtain satisfactory results. Sanllorente ^[317] also used a similar method to transfer the three-dimensional fluorescence spectrum between the portable fluorescence spectrometer of the LED light source and the fluorescence spectrometer of the xenon light source. Sun et al. ^[318] used the PDS algorithm to transfer the three-dimensional fluorescence spectra on the two instruments, and then used the self-weighted alternating normalized residual fitting algorithm (SWANRF) to establish a three-linear decomposition multidimensional quantitative model. The results show that PDS can maintain the "second-order advantage" of the second-order tensor calibration methods.

Wang et al. ^[319] used PDS to realize the transfer of NIRS of leaves picked from different tree species and different periods, and solved the problem of standard spectra based on chlorophyll content through linear interpolation. Watari et al. ^[320] also used a similar method to transfer the NIRS of random polypropylene and block polypropylene in the molten state, so that the model of ethylene content in one type of polypropylene can predict another type of polypropylene. Li Y. et al. ^[321] discussed the influence of the number of PLS latent variables on the transfer performance of the model when the PLS model is established by the NIRS after PDS. The results show that too high number of latent variables can easily cause over-fitting, affect the robustness of the model, and make the error of calibration transfer larger.

Sun et al. ^[322] used the PDS algorithm to transfer the NIRS of the plasma alcohol precipitation process between two different types of instruments, and established an analytical model for predicting the content of total protein, albumin and globulin. Xiao et al. ^[323] combined linear interpolation with the PDS algorithm to transfer the FT-NIRS of a single grape to a portable grating spectroscopic spectrum, and established a model for predicting the content of soluble solids. Fernandez ^[324] compared DS, PDS, OSC, GLSW and other methods to transfer the signal of the gas sensor matrix at different temperatures, and the results of the PDS algorithm are better. Hoffmann et al. ^[325] used the PDS algorithm to transfer the FT-NIRS to the linear

variable filter handheld instrument, and the quantitative and qualitative models obtained good results. Di Anibal et al. ^[326] used the PDS algorithm to transfer the UV spectrum used to determine whether illegal substances are added to the fragrance, and combined with the PLS-DA method to obtain satisfactory results. Zheng Y. et al. ^[327] used the PDS method to transfer the NIRS of fish meal on the grating-type instrument to the Fourier-type instrument, and there was no significant difference in predicting the content of crude protein, crude fat, methionine, lysine and other components.

Pu et al. ^[328] used the PDS algorithm to successfully transfer the banana spectrum from the handheld NIR spectrometer to the hyperspectral imaging instrument, and established a model for predicting the soluble solid content. Xi C. et al. ^[329] used the PDS algorithm to transfer the NIRS of amoxicillin capsules and the NIRS of its contents, so that the amoxicillin capsule quantitative model can accurately predict and analyze the powder spectrum of the content, and proposed an index to judge whether the spectrum is successfully transferred. Gislason et al. ^[330] used the PDS algorithm to realize the transfer of process nuclear magnetic resonance spectrum on different instruments, and compared the result of DS combined with SSC algorithm. Monakhova et al. ^[331] used the PDS algorithm to transfer the spectrum of the sunflower lecithin and soybean lecithin mixture obtained by three high-resolution NMR instruments, and the result was better than the DS algorithm and the establishment of a hybrid model.

Chen et al. ^[332] used the PDS algorithm to transfer the UV-visible spectrum of the cuvette with a 10mm optical path to a fiber optic probe with a 2mm optical path. Before using the PDS algorithm for transfer, the spectrum was subjected to Fourier transform processing. Lin et al. ^[333] used the PDS algorithm to transfer the spectrum from the scanning NIRS instrument (cuvette) to the Fourier transform (fiber probe) instrument. Shi et al. ^[334] used the PDS algorithm to better solve the transfer of the NIRS of the mixture of fish meal and soybean meal on two different spectroscopic types of instruments. Tortajada-Genaro et al. ^[335] used the PDS algorithm for the transfer of chemiluminescence signals on two instruments, and established a model for the rapid determination of Cr(III), Cr(VI) and total Cr content in water through the

PLS method. Griffiths et al. ^[336] used the PDS algorithm combined with the variable selection method to solve the problem of the failure of the multivariate calibration model caused by the drift of the ICP-AES instrument over time.

Wang et al. [337] used the PDS to transfer the NIRS of Poriacocos samples measured on two different brands of NIR spectrometers, and established a model to predict alkali-soluble polysaccharides in Poriacocos. Morais et al. [338] used the DS and the PDS to standardize the MIR spectrochemical database of complex biological tissues and established a complete spectrum standardization process. Grelet et al. [339,340] used the PDS algorithm to standardize the instruments in the European dairy MIR spectroscopy network, which can convert spectra on spectrometers of different brands into spectra on the master computer to realize the sharing of quantitative calibration models. Ji et al. [341] used the PDS algorithm to eliminate the influence of moisture and environment on the NIRS of the field soil, and the transferred spectrum can be accurately predicted by the model established in the laboratory. Pierna et al. [342] designed and produced a standard sample pool for the transfer of NIRS microscopic imaging instruments. Different parts of the standard sample pool are equipped with meat and bone meal of different animals, and the spectral transfer of multiple imaging instruments is realized through the PDS algorithm.

17.6.6 CCA method

Zheng et al. ^[343] used the CCA algorithm to convert the NIRS between different times and different brands of milk, and the content of dimethyl fumarate in milk can be predicted by the sample enrichment-NIRS measurement method. Liu Y. et al. ^[344,345] used the DS algorithm and the CCA algorithm to realize the transfer of the near-infrared spectroscopy analysis model of wood lignin content between different types of portable spectrometers. Yang et al. ^[346] compared the transfer effects of algorithms such as CCA, SST, CTWM, ICA, and PDS on the transfer of tobacco NIRS on desktop, portable and handheld instruments, and the results showed that the CCA algorithm is superior to other methods. Luo J. et al. ^[347] used the CCA algorithm

to transfer the NIRS that predicts the content of polyester in textiles, and the results are better than the PDS method. Fan P. et al. [348] used CCA or PDS algorithm combined with linear interpolation method for the transfer of soil near-infrared spectroscopy. A soil nutrient content model can be used to accurately predict soil nutrient content in different regions.

17.6.7 Establishment of global model

Eliaerts et al. ^[349] used the S/B algorithm, the PDS algorithm and the method of establishing a hybrid global model to transfer the cocaine classification and quantitative SVM models on desktop and portable infrared spectrometers. The results showed that the method of establishing the hybrid model has better results. Yang Z. et al. ^[350] transferred the model established in the laboratory to feed production enterprises for online application by using the method of hybrid modeling of near-infrared spectroscopy and online spectroscopy, and the predicted values of moisture content and crude protein content were in good agreement with the actual measured values, which can meet the requirements of online analysis. Chen et al. ^[351] used TrAdaBoost algorithm based on principal component analysis and weighted extreme learning machine to establish a global model to realize the sharing of models on multiple instruments. Ni et al. ^[352] used the establishment of a global hybrid model of multiple instruments to realize the sharing of tobacco models on different near-infrared spectroscopy instruments.

Pereira et al. ^[353] compared the transfer effects of DS, PDS, OSC and model update methods based on the NIRS of gasoline on different instruments. The results show that DS combined with model update strategy can get better results. Fernandez-Ahumada et al. ^[354] used Shenk's algorithm and PDS algorithm to transfer the feed spectrum measured on the laboratory grating near-infrared spectrometer to the online array instrument, and then through the model update, the transfer of the model can be better realized. Debus et al. ^[355] used the method of establishing a hybrid model to solve the problem of sharing the multi-element calibration model of

mid-infrared spectroscopy evaluation environment carbon-containing particulate matter among multiple instruments of the same type.

Krapf et al. ^[356] used the PDS algorithm to transfer the laboratory NIRS of the samples during the anaerobic digestion process of energy crops to the online analysis instrument, and the problem of online analysis model establishment was better solved through model update. Li X. et al. ^[357] used the combination of Shenk's, PDS and CCA algorithms and hybrid modeling technology to establish a hybrid model based on a homogeneous tobacco powder model, which was successfully applied to the prediction of nicotine content in heterogeneous cut tobacco samples and tobacco flake samples. Clavaud et al. ^[358] constructed a global calibration set of more than 3000 spectra of various types of freeze-dried drugs and their moisture content on two NIRS of the same model, and established a global model by PLS, SVR, Bayesian Ridge regression, KNN and other methods. The results show that the predictive ability of SVR was better. Ozdemir et al. ^[359] used a hybrid global model combined with genetic regression to establish a model of four vis-UV spectrometers, one of which is a array spectrometer, and the other three are dual-beam scanning instruments.

Kupyna et al. ^[360] used a global model to solve the problem of the application of acoustic multivariate quantitative correction models under different test conditions (temperature, flow rate, etc.). Igne et al. ^[361] compared the effects of multiple transfer methods on the same type and different types of NIRS instruments, and the results proved that establishing a stable and sound local model is a better strategy. On the basis of Shenk's algorithm, Fontaine et al. ^[362] can accurately predict and analyze the model of amino acid content in feed ingredients on dozens of instruments in the NIR network through the model update strategy. Steinbach et al. ^[363] established a hybrid calibration model for the drug transmission Raman spectra measured on the two instruments, and the model built can be accurately applied to the spectra obtained on the two instruments.

17.6.8 Other Methods

Xu et al. ^[364] realized the transfer between NIR spectra of rice single grains and rice flours of different varieties by spectral space transformation. Online monitoring of tobacco nicotine and total sugar was realized through the SST from offline model ^[365]. In addition, calibration transfer by SST algorithm has also been applied to edible oil acid value and peroxide value ^[366], rice ^[367], hyperspectral image on plant phenotype ^[368] and Terahertz spectral instruments ^[369].

Yang H. et al ^[370] successfully transferred the apple spectra on two portable NIR spectrometers using simple linear regression direct standardization (SLRDS) algorithm. Salguero-Chaparro et al. ^[371] used Transfer by Orthogonal Projection (TOP) algorithm to transfer the olive spectra from the grating NIR spectrometer to the array portable spectrometer, established an analytical model to predict fat, free acid and moisture content. Liu et al. ^[372] compared the transfer results of SBC, OSC, DS, PDS, and local centralization to the silage NIR spectra on the same and different types of spectrometers. They further studied the influence of different temperatures and measuring accessories on the NIRS of rice straw and found local centralization method can eliminate the influences on the spectra to a certain extent ^[373]. Similar study on pharmerceutical samples was done by Bergman et al. and result revealed local centralization can be realized with less standard samples ^[374].

Li et al. ^[375] combined the wavelet multiscale piecewise direct standardization (WMPDS) with SBC algorithm to realize the transfer of NIR spectra of different types of soils and the correction of prediction for total nitrogen and total carbon content. Greensill et al. ^[376, 377] compared the effects of DS, PDS, DWPDS, OSC, FIR, and WT on the transfer of citrus spectra between micro-array detector NIR spectrometers, and the results showed WT and model update is better than others.

Martins et al. ^[378] combined SPA wavelength selection algorithm with the multi-model consensus strategy to establish calibration model by MLR, which was proved to be more effective than PDS-PLS model. Youn et al. ^[379] performed first-order derivative and OSC preprocessing on NIRS of gasoline, and then

transferred the spectra on the two instruments through PDS algorithm, eventually established the model for predicting the benzene content in gasoline. Yahaya et al. [380] established an analytical method for rapid prediction of mango acidity by the variable screening coupled with MLR, realizing the application to multiple instruments by optimization of variable selection.

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