NWU Spectra Analysis (NWUSA) Toolbox
User manual

by

Dongliang Song, Shuang Wang*

Institute of Photonics and Photon-Technology, Northwest University,

Xi'an, Shaanxi, 710127, China

*Corresponding Author:

Dr. Shuang Wang

Associate Professor

State Key Laboratory of Photon-Technology in Western China Energy

Institute of Photonics and Photon-technology

Northwest University

#1 Xuefu Avenue, Guodu Education and Technology Industrial Zone

Chang'an District, Xi'an, 710127

Shaanxi, China

Email: swang@nwu.edu.cn

Tel: +86-29-8830-3281

Fax: +86-29-8830-3281

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1. Declaration

NWUSA toolbox is developed by Advanced Spectral Imaging Group, Institute of Photonics and Photonics Technology, Northwest University, Xi'an 710127, Shaanxi, China. If you need more detailed information about the software usage and operation or have certain suggestions for software improvement, please feel free to contact Dr. Shuang Wang, Institute of Photonics and Photonics Technology (Email: swang@nwu.edu.cn; wsnwuphy@163.com). The NWUSA toolbox can be downloaded at https://github.com/wsnwuphy/NWU-Spectra-Analysis-Toolbox.git.

This software is ONLY for academic research but NOT for commercial usage. The references where this software has been used are listed in the following.

1. Song D, Chen Y, Li J, et al. A graphical user interface (NWUSA) for Raman spectral processing, analysis and feature recognition. *J. Biophotonics*. 2021;e202000456. https://onlinelibrary.wiley.com/doi/10.1002/jbio.202000456

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6. Song D, Chen T, Wang S, et al. Study on the biochemical mechanisms of the micro-wave ablation treatment of lung cancer by ex vivo confocal Raman microspectral imaging. *Analyst*, 2020, 145:626-635. https://pubs.rsc.org/en/content/articlelanding/2020/an/c9an01524h

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2. Introduction

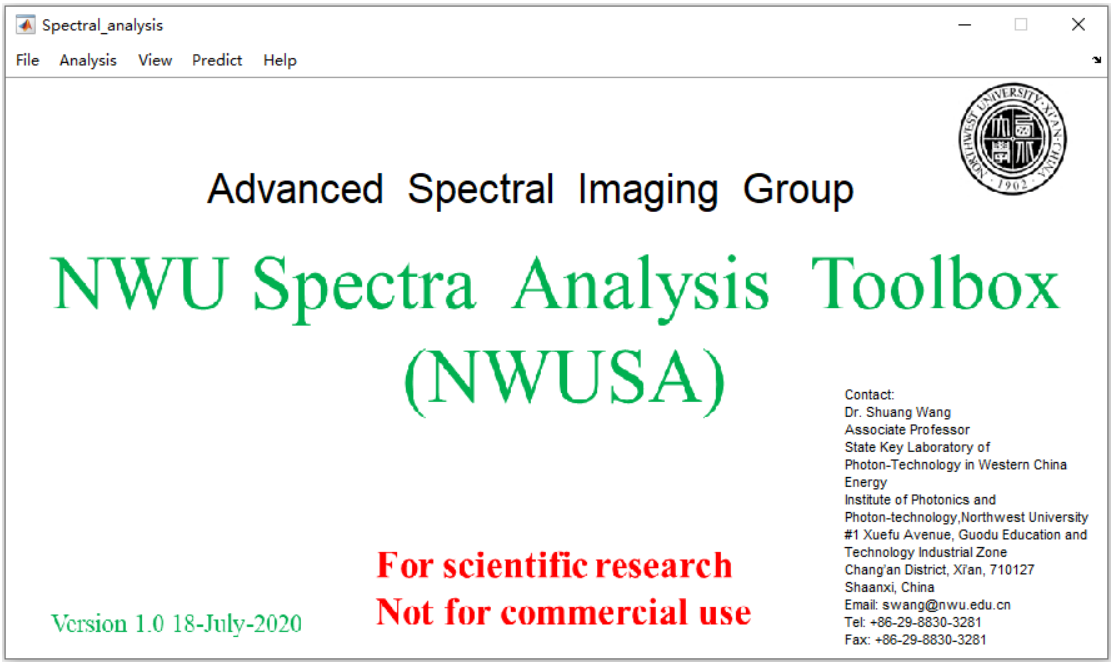


Figure 1. The main interface of the NWUSA toolbox.

NWUSA toolbox is designed for Raman spectral preprocessing and multivariate analysis. Its main functions include the spectra preprocessing techniques (wavenumber range selection, cosmic ray removal, background noise subtraction based on polynomial fitting and extended multiplicative signal correction (EMSC) algorithm, and Savitzky-Golay smoothing), additional spectral analysis functions (area normalization, mean-centered, vector normalization, the first and second derivatives, and spectral normalization under the specific peak), principal component analysis

(PCA), linear discriminant analysis (LDA), partial least squares-discriminant analysis (PLS-DA), support vector machine (SVM), and the PCA-SVM.

2.1 Principal Component Analysis

The PCA represents a multivariable analysis technique. It simplifies a complex dataset by reducing the data dimension and extracts significant features from the dataset. Therefore, the PCA can identify subtle differences between different types of samples. Usually, the first principal component (PC) can explain the largest variance in a dataset, and variances explained by subsequent PCs decrease gradually. In addition, the PC scores reflects a difference between different categories, and each PC loading is related to the characteristic spectrum through the PC scores.

2.2 Linear Discriminant Analysis

As a classical supervised classification algorithm, LDA aims to identify one or more optimal projection directions that maximize inter-group differences while minimizing intra-group differences. The number of discriminant functions generated by the LDA is equal to the number of sample categories decreased by one, and the projection data can be calculated by the discriminant functions. In this software, the PC scores obtained by the PCA dimensionality reduction process can be used as the input of the LDA algorithm to generate an effective discrimination model. In the LDA classification, it is feasible to calculate the probability of a sample belonging to a particular category using the Gaussian probability density function. In addition, in order to verify the performance of the classification model based on the PCA-LDA algorithm, it is necessary to perform the cross-validation.

2.3 Partial Least Squares–Discriminant Analysis

PLS-DA is a supervised technique that employs the fundamental principle of PCA, but further rotates the latent variables (LVs) by maximizing the covariance between spectral changes and group affinity, thus enabling the LVs to explain changes related to the diagnosis rather than the most significant variations in the spectral dataset. Before the PLS-DA modeling, it is necessary to select the number of LVs with the minimum sum square error as the optimal number of components using the leave-one-out

cross-validation (LOOCV) method. Since the predicted response value obtained by the PLS-DA model is not strictly equal to zero or one, it is necessary to calculate the posterior probabilities of samples belonging to each category using the probability density function and Bayesian formula, and the category with the highest probability is used as the prediction label.

2.4 Support Vector Machine

The SVM is also a supervised classification algorithm based on the VC dimension theory in the statistical learning theory and the principle of structural risk minimization. One of the basic ideas of the SVM is nonlinear mapping. When data are nonlinearly separable, the SVM maps a low-dimensional input space to the high-dimensional feature space by introducing kernel functions so that data samples may become linearly separable in the high-dimensional space. Another basic idea of the SVM is to construct an optimal hyperplane with the largest classification margin for separating different data types. The SVM was originally applied to solve the binary classification problems. As for multi-classification problems, it is feasible to construct multiple classifiers using the “one-versus-one” and “one-versus-all” strategies and then use these classifiers to conduct voting; next, the category with the largest number of votes should be selected as a prediction label. The SVM analysis process consists of model training and testing. First, the initial dataset is divided into training and test sets according to a certain proportion. Random selection and the Kennard-Stone algorithm are used to split the dataset. The training set is used for model construction and optimization of classification parameters. In the training process, the grid search and cross-validation are combined to obtain optimal parameters of each kernel, which are then used to build the final model. The performance of the final model is validated on the test set. The software uses three types of kernels: linear, polynomial, and radial basis function (RBF).

2.5 Principal Component Analysis–Support Vector Machine

In order to realize the visualization of the SVM classification and simplification of calculation without sacrificing the classification performance of the model, this

software uses the PCA to reduce the dimensions of the spectral dataset. Then, the first two most significant PC scores are used as the input variables of the SVM. The training and testing process of the PCA-SVM model are the same as those described in Section 2.4. PCA-SVM can not only extract the significant features of the spectral dataset and realize visual classification, but also reduce the computational complexity by reducing the input data characteristics, thus shortening the running time of the program.

3. Operation Guide

3.1 Data Loading

After openning the software, the operator can click “File > load data” button on the main interface to enter the data loading interface. At present, the NWUSA toolbox accepts spectra data in .mat and .txt file formats. If the spectral data are given in a .mat file format, it needs to include the spectra intensity matrix ($N \times M$), a wavenumber variable ($N \times 1$), and category label ($M \times 1$) to which each spectrum belongs, where N denotes the number of spectral features, and M represents the total number of spectra, that is, each column in the dataset represents an observed spectrum; it is recommended to use numerical vectors instead of category labels, such as [1. 1.... 2. 2.... 3. 3.…]. If the spectral data are given a .txt file format, it is allowed to load multiple .txt files in batches, and a operator only needs to create a .txt file containing the category labels. In addition, the software contains an editable tool that allows operators to edit the spectra category and intensity information in a table manually. In order to keep the data balanced, all categories should contain the same number of spectra.

Attention

The range and sparation of wavenumber in all spectra must be the same, otherwise, the data cannot be loaded.

In the process of loading data, the software will delete the duplicated spectral data and only retain one, so the number of processed spectra may not match the label.

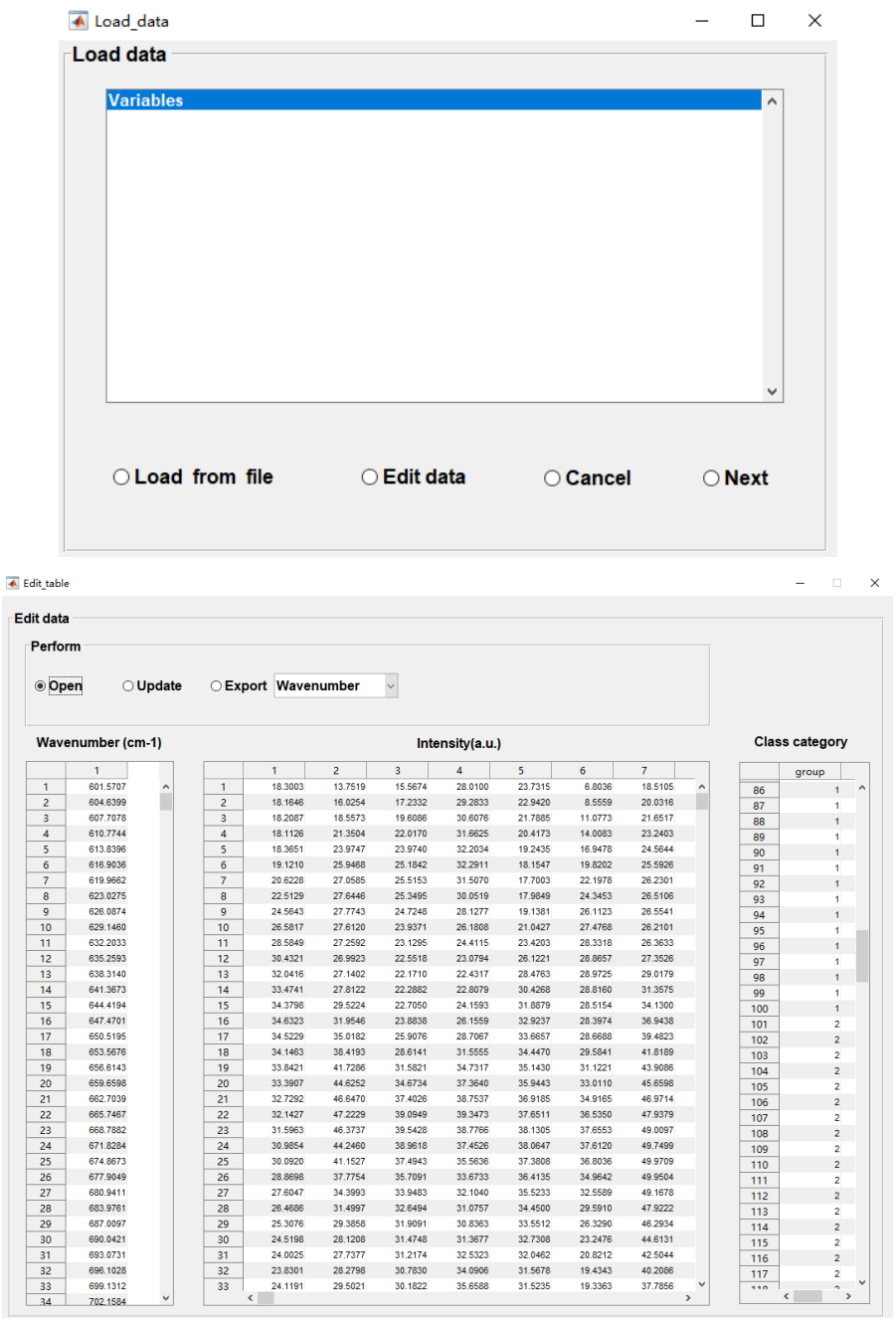


Figure 2. Data loading and editing interface.

3.2 Spectra Preprocessing

When performing the Raman spectra preprocessing process, a operator first needs to choose the following options to enter the spectral preprocessing interface: “Analysis > Preprocessing > Spectral Preprocessing,” and then to click on the button “Load” on the right side of the preprocessing interface to load the spectral data in the form of a .mat file or multiple .txt files. The spectral data in .txt format are selected to be processed in the list box, and then the spectral selection is completed by clicking on the “Select”

button. The operator can view the processing results in the drawing window in real time by clicking different buttons and parameters in the “Methods” panel on the left of the preprocessing interface. For the spectral data in the format of a .mat file, the operator only needs to enter the spectra serial number to be viewed in the “Spectrum sequence number” on the right side, and the rest of the operation is the same as in the previous case. After that, the operator can query peak information by clicking on the “Find peaks” button and save the preprocessed spectral data by clicking on the “Output data” button.

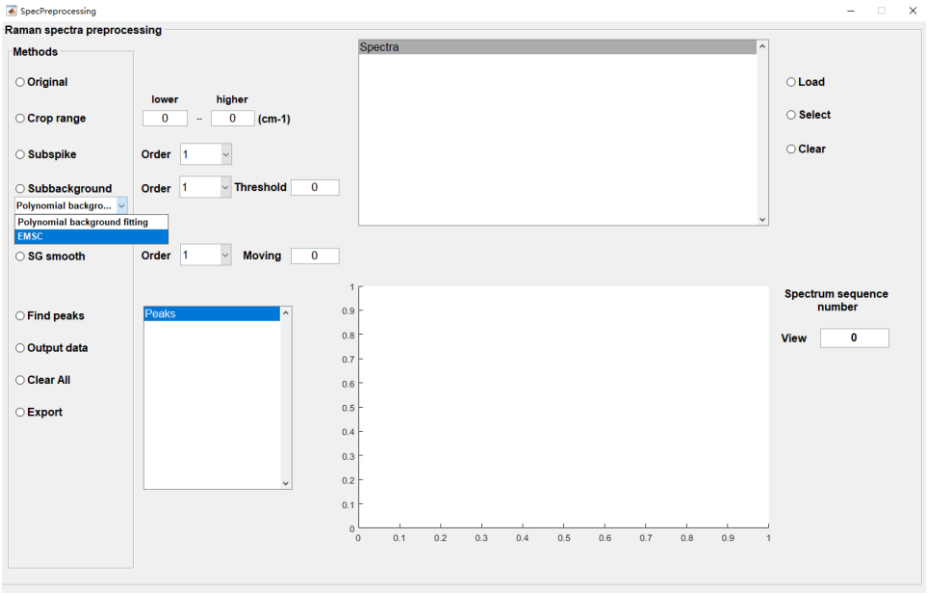


Figure 3. The preprocessing interface in the NWUSA toolbox.

3.2.1 Selecting Spectral Range (Crop Range)

The operator needs to input the spectral range of interest in the box and clicks the “Crop range” button.

3.2.2 Removing Cosmic Rays (Subspike)

The operator can select appropriate parameter (order) for removing cosmic rays. As shown in the figure below, the red lines represent the spectrum after the spectral range is cut, and the blue lines represent the spectrum after the cosmic rays are removed.

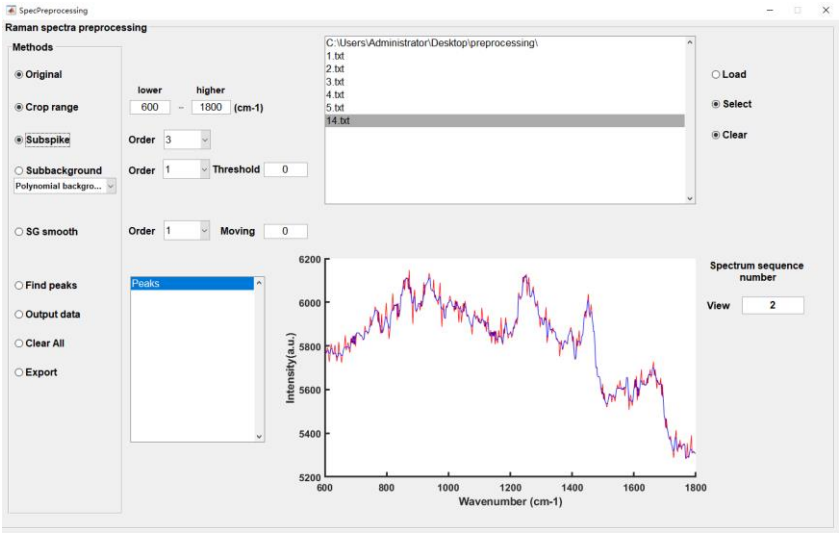


Figure 4. Spectrum with cosmic rays removed.

3.2.3 Background Noise Subtraction (Subbackground)

Before using the background subtraction function, the operator needs to select the method for background subtraction from the pop-up menu, such as “Polynomial background fitting” or “EMSC”. In this example, the red lines represent the spectrum after removing cosmic rays, and the blue lines represent the baseline of the polynomial fitting. Subtracting these two will yield the spectral data after background noise subtraction. “Order” stands for polynomial order, and “Threshold” can be used to adjust the position of the baseline. In addition, the open-source EMSC toolbox developed by Kristian *et al*. is included in the software, and when the EMSC is used as the light scattering correction method, the baseline correction is not required. The EMSC toolbox has been approved for use in the NWUSA toolbox by Prof. Kristian Hovde Liland in Norwegian University of Life Sciences. If the operator chooses to use “EMSC” for baseline correction, he/she needs to click “Subbackground” to enter the EMSC menu, click “Select data” button, select “rawdata” variable in the list box of the subinterface, and click “OK” button to complete data selection. After that, the operator clicks the “EMSC” button to enter the EMSC processing interface, in which the operator is free to set parameters and reference spectrum, and clicks the “Apply EMSC” button to complete the baseline correction.

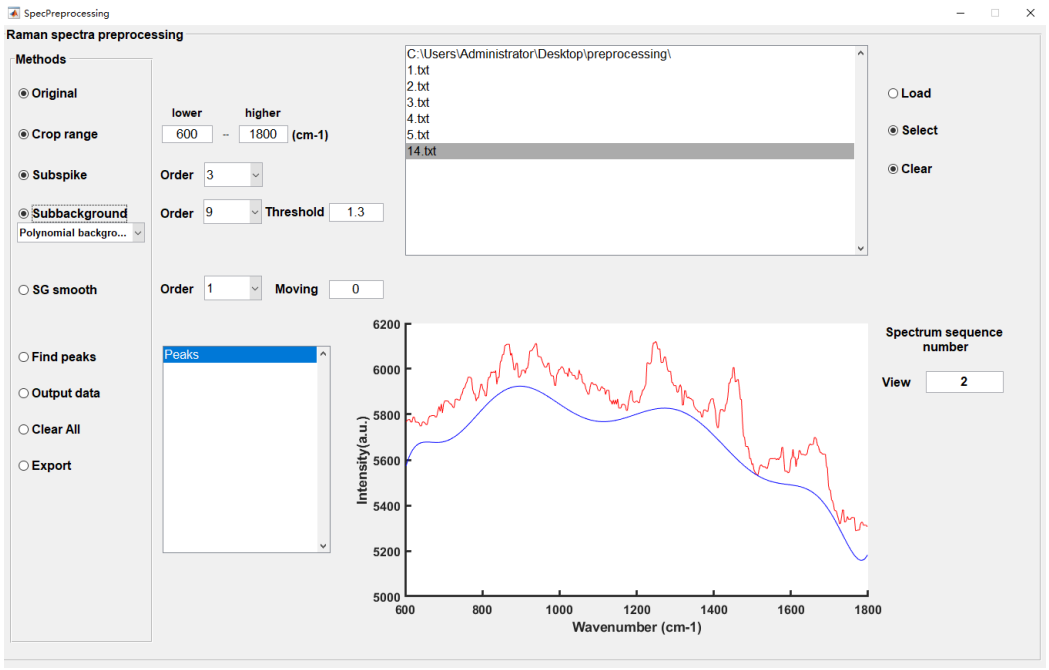


Figure 5. The baseline of the polynomial fitting.

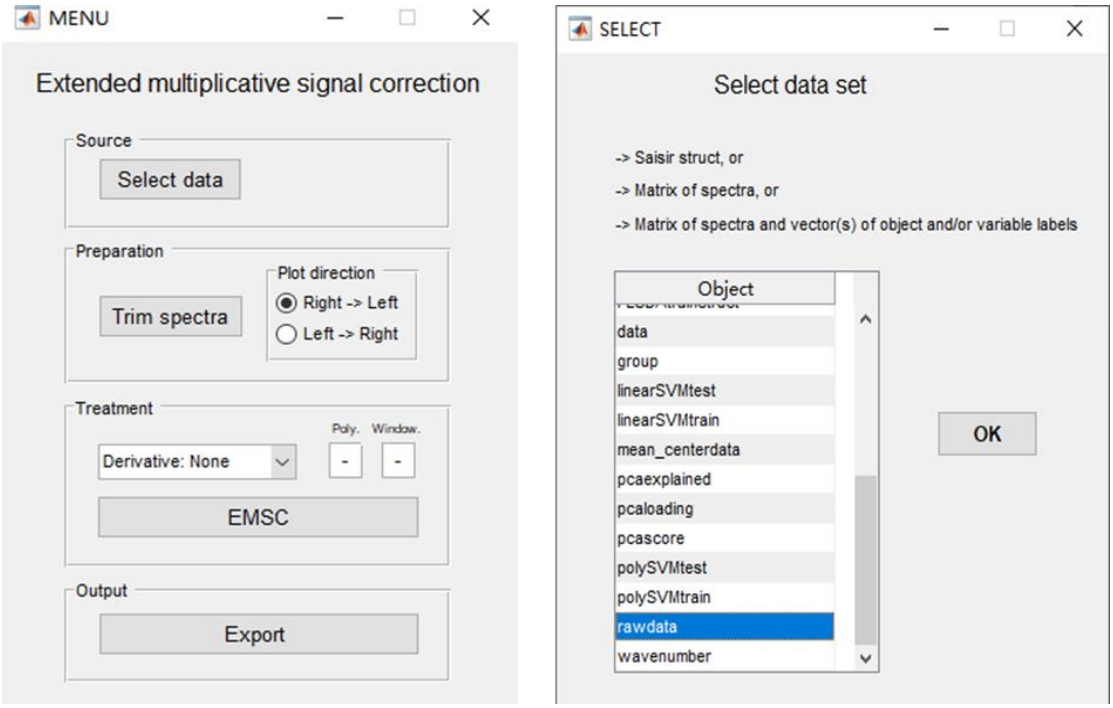


Figure 6. EMSC menu and data selection interface.

3.2.4 Savitzky-Golay Smoothing (SG Smoothing)

Finally, a smoother spectrum can be obtained by performing Savitzky-Golay smoothing based on the least square principle, as shown in the figure below.

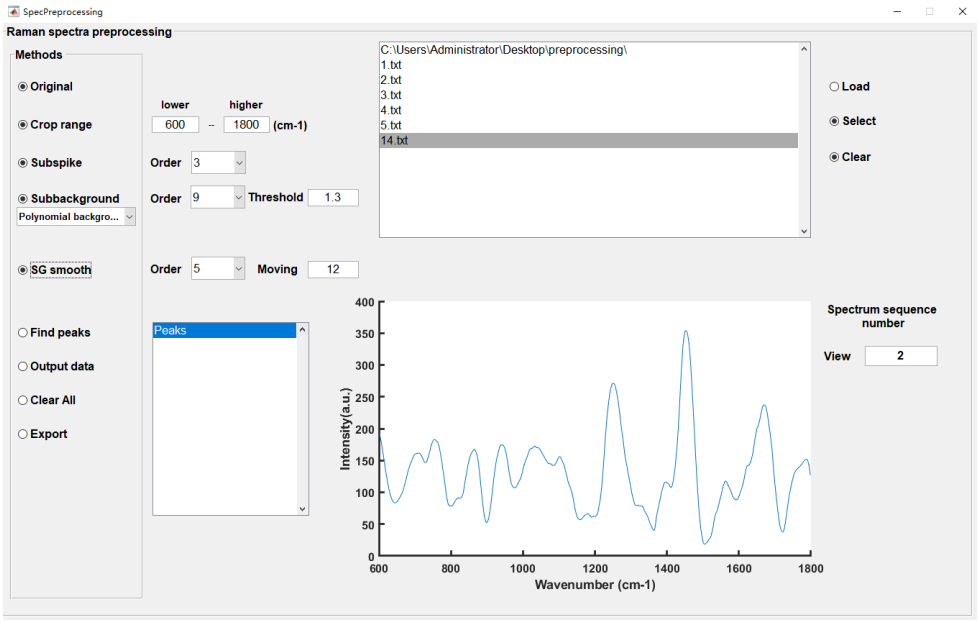


Figure 7. The smoothed spectral by Savitzky-Golay algorithm.

3.3 Additional Spectral Analysis Functions

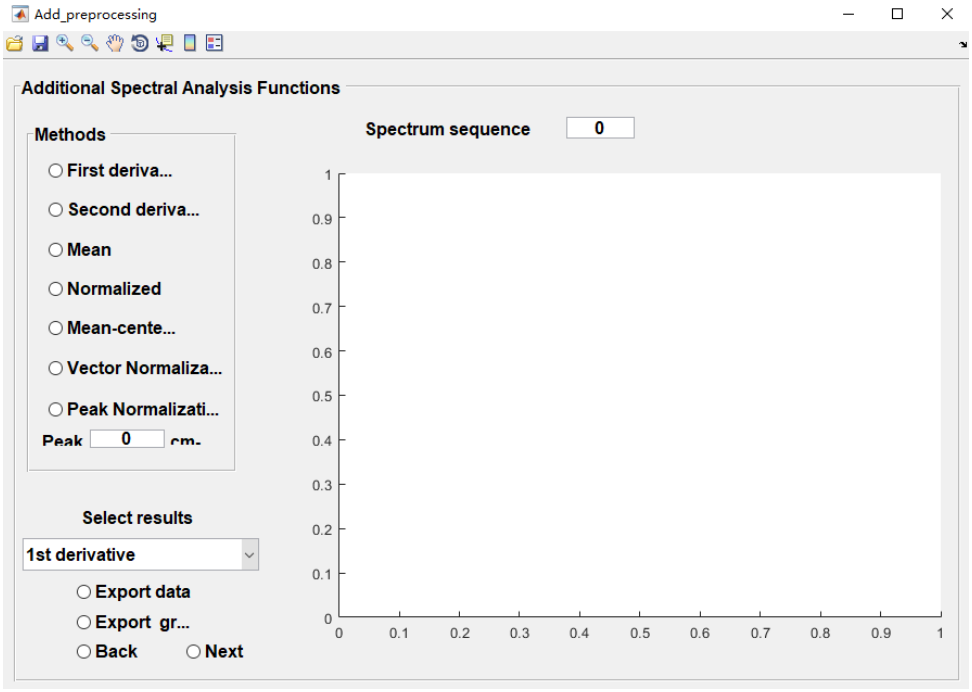


Figure 8. Additional spectral analysis functions in the NWUSA toolbox.

"Back" button at the bottom of the interface is used to return the previous step, and "Next" button is used to perform the next step. By clicking the "Next" button, the operator can find a option terface in which the multivariate analysis method can be freely selected by entering the corresponding interface.

3.3.1 First and Second Derivatives

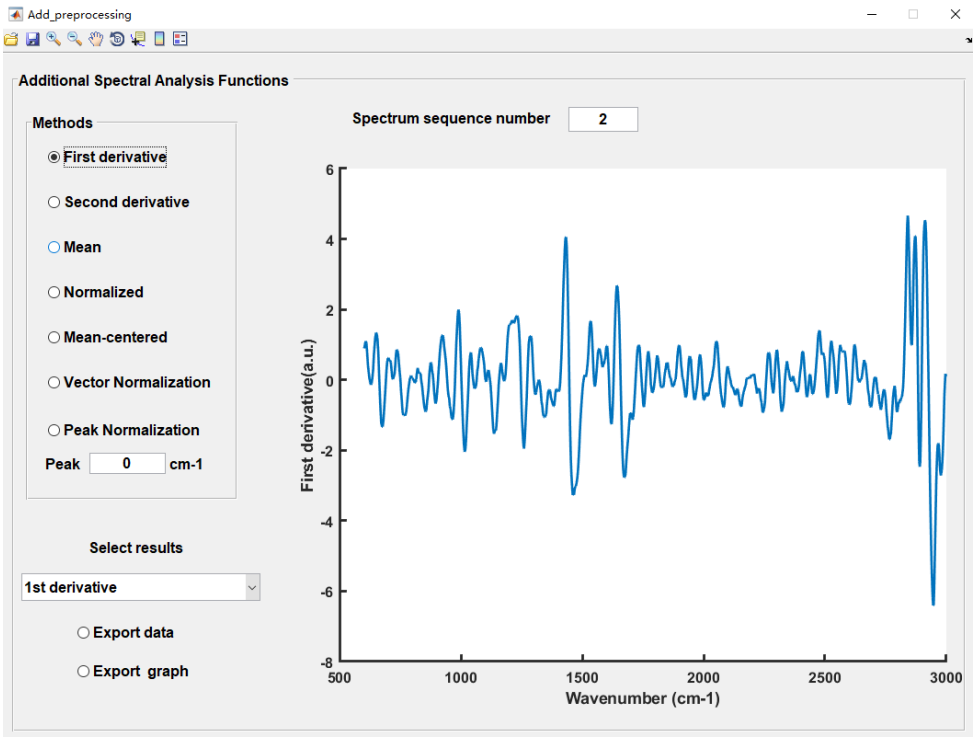


Figure 9. The first derivative of an example spectrum.

3.3.2 Mean spectral intensity (Mean)

This function can be used in two modes. One is to obtain the mean intensity of the preprocessed spectral data, and another is to obtain the mean intensity of the spectral data after area normalization. Operators can choose the mode according to their needs.

3.3.3 Area Normalization

Spectrum normalization through the integration of the area under the spectral curve can reduce the influence of certain factors, such as laser power disturbance. This function can also be used in two modes. One is to normalize the area under the preprocessed spectral curve, and the other is to perform normalization for the mean spectral. Operators can choose the mode according to their needs.

3.3.4 Mean-centering

The software subtracts the mean value from the spectral intensity matrix after area normalization to obtain the mean-centered matrix, and used for subsequent multivariate

analysis. The mean-centered approach can eliminate the influence of intra-subject and/or inter-subject spectral variability on multivariate analysis.

3.3.5 Vector normalization

During vector normalization, the software first calculates the norm of the spectrum, which is defined as the square root of the sum of squares of spectrum intensities. Then, the intensity corresponding to each Raman shift is divided by the norm to obtain the normalized spectrum.

3.3.6 Spectral Normalization Under Specific Peak (Peak Normalization)

During the normalization under specific peak, the intensity value corresponding to the center frequency of a specific Raman shift is used as a reference and defined as I_P. Next, the Raman intensity of the whole spectrum is divided by I_P to obtain the normalized spectrum. The operator can set the position of the reference peak freely.

Operators have an option to save results using the pop-up menu on the "Add preprocessing" interface, and the data and graph can be saved in a specified file by clicking on the "Export data" and "Export graph" buttons. The software supports exporting data in several formats, including .txt, .mat, and .xls formats.

3.4 Multivariate Analysis

3.4.1 Principal Component Analysis

The operator can also enter the PCA analysis interface by clicking "Analysis > PCA," where he can update the variable name in the list box by clicking on the "Update" button and select the variable used for the PCA analysis by clicking on the "Select" button; it is recommended to select "mean_centerdata" in the list box. Then, the operator can customize the dataset splitting method and training set ratio to divide the dataset into training and test sets. The range of 0.6–0.8 is recommended for determing the proportion of the training set, that is, the training set accounts for 60%–80% of the overall number of data samples.

Attention

In this step, all training proportions can be set by moving slider. When the left and right arrows of the slider are clicked, the moving step of the slider is 0.01; when the gray area is clicked, the moving step is 0.1. The following operation process of PLS-DA, SVM and PCA-SVM is in the same procedure.

Click the "Run" button to calculate and select the number of components with the minimum error rate as the optimal number of components. After that, the operator can select the optimal number of PCs to be retained and click "PCA Score / Loading / Explained" in the calculation panel to complete the PCA analysis. Finally, the operator selects the result to be exported from the pop-up menu at the bottom of the interface and completes the exporting process by clicking on the "Export data" button.

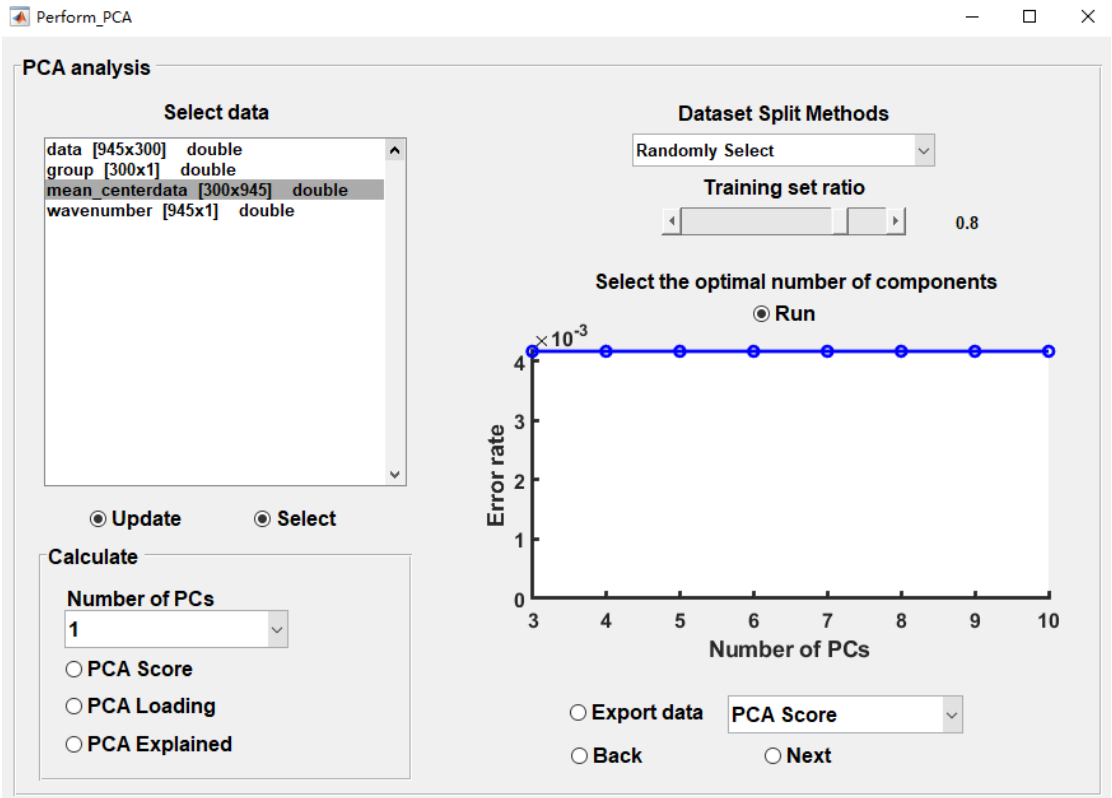
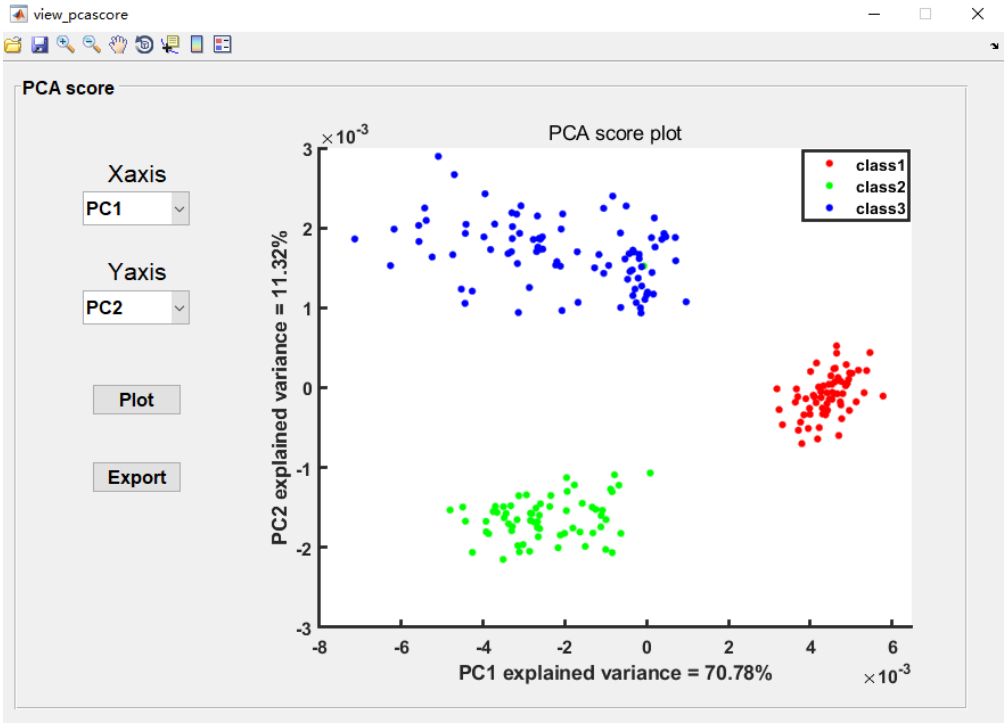
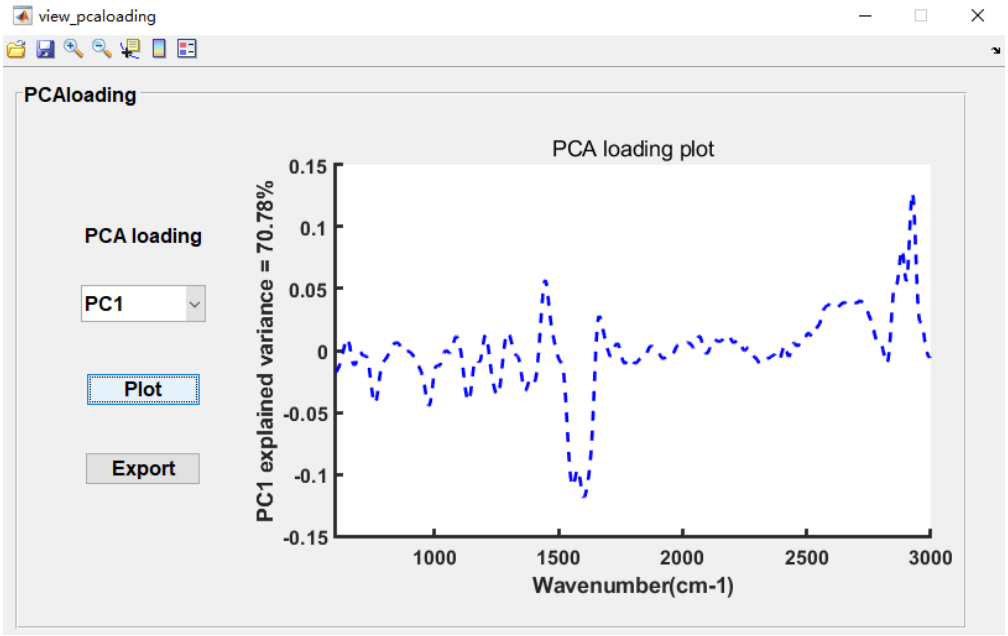


Figure 10. PCA analysis interface in the NWUSA toolbox.

The operator can view the PCA results, including the projection data (score), loading, and variance percentage, by clicking "View > viewPCA > view PCAscore / loading / explained" to open the corresponding drawing interface and then click the "Plot" button and select the variables to plot through the pop-up menu. By clicking "Export" in each

drawing window, the graph is output. The “Back” button at the bottom of the interface is used to return the previous step, and “Next” button is clicked to perform the next step.





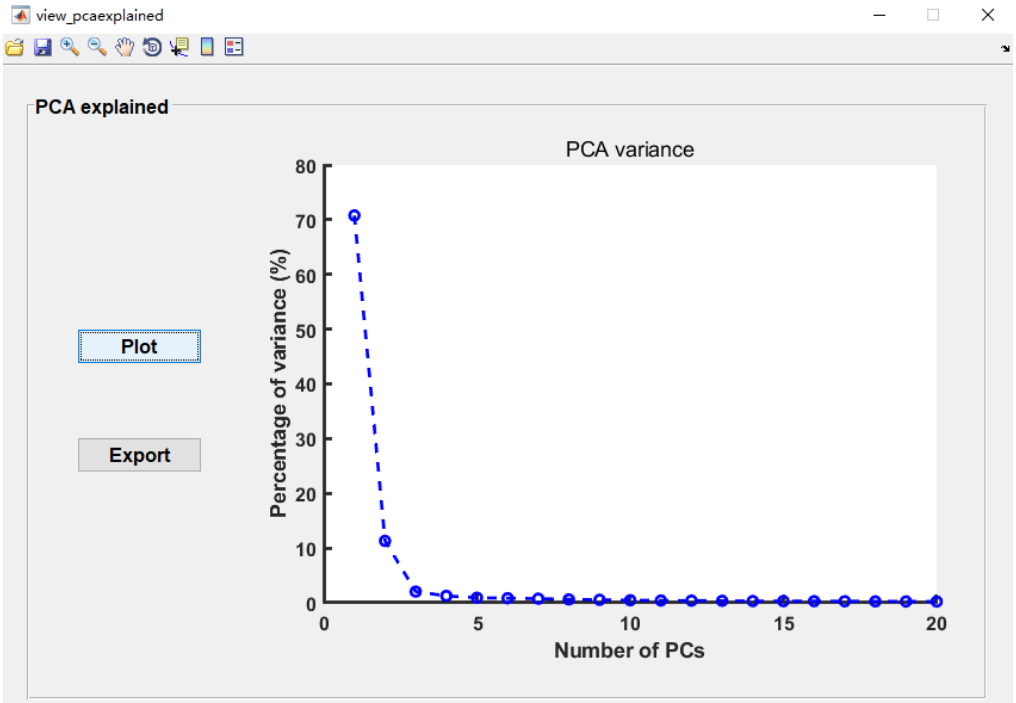


Figure 11. PCA scores scatter plot, loading of PC1, and variance percentage of the first 20 PCs.

3.4.2 Linear Discriminant Analysis

To execute the LDA, the operator can also to click "Analysis > LDA > ProjData." After entering the interface, the operator has to select the number of components (the number of selected components should be at least equal to the number of sample categories) and then to click on the "Calculate" button to obtain the data after the LDA projection and the posterior probability of samples belonging to each category. Similarly, the operator can select the result to be exported from the pop-up menu and click on the "Export data" button to complete the export. Then, the operator can click "View > view LDA > view LDAprojData" to view the scatter plot of linear discriminant scores. Also, the operator can click "View > view LDA > view LDAprobability" to view the posterior probability of samples. By clicking on "Analysis > LDA > LDA classification" view the classification results and performance evaluation indicators of the PCA-LDA model on the training set, including sensitivity, specificity, accuracy, F1-score, G-score, Macro-F1 score, overall accuracy and the confusion matrices.

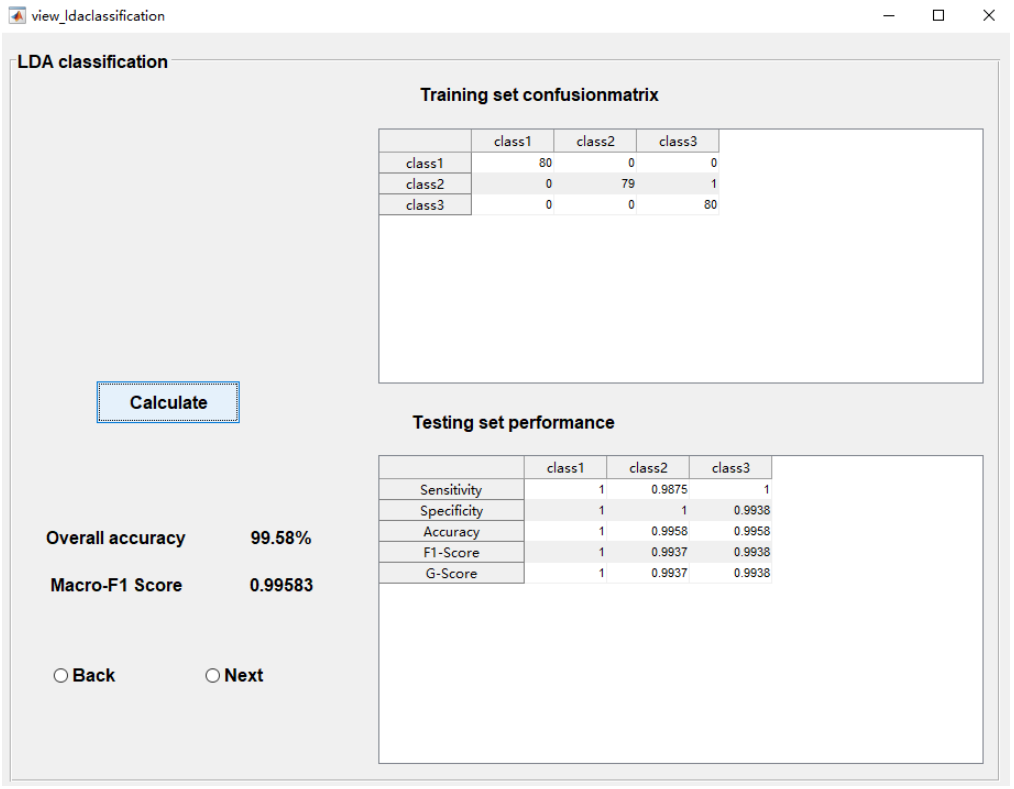


Figure 12. The classification results and performance evaluation of the PCA-LDA model on the training set.

The next step is to assess the classification performance of the model by performing cross-validation. This is done by clicking the "Next" button as shown in Figure 12 or clicking "Analysis > LDA > Cross validation" to enter the cross-validation interface, and then selecting the number of PCs and groups for cross-validation. The number of PCs is the same as the number of components selected previously. The type of cross-validation can be set to five-fold, ten-fold, or leave-one-out cross-validation. The operator can click on the "Calculate" button to view the classification results of the model for different categories of samples represented by the confusion matrices, as well as the corresponding performance evaluation indicators, including sensitivity, specificity, accuracy, F1-score, G-score, Macro-F1 score, and the overall accuracy. In the "LDA Testing" panel, the operator can view the classification result and performance evaluation indicators of the PCA-LDA model on the test set by clicking the "Calculate" button. In addition, the operator can obtain the ROC curve of each category by clicking "Analysis > LDA > ROC."

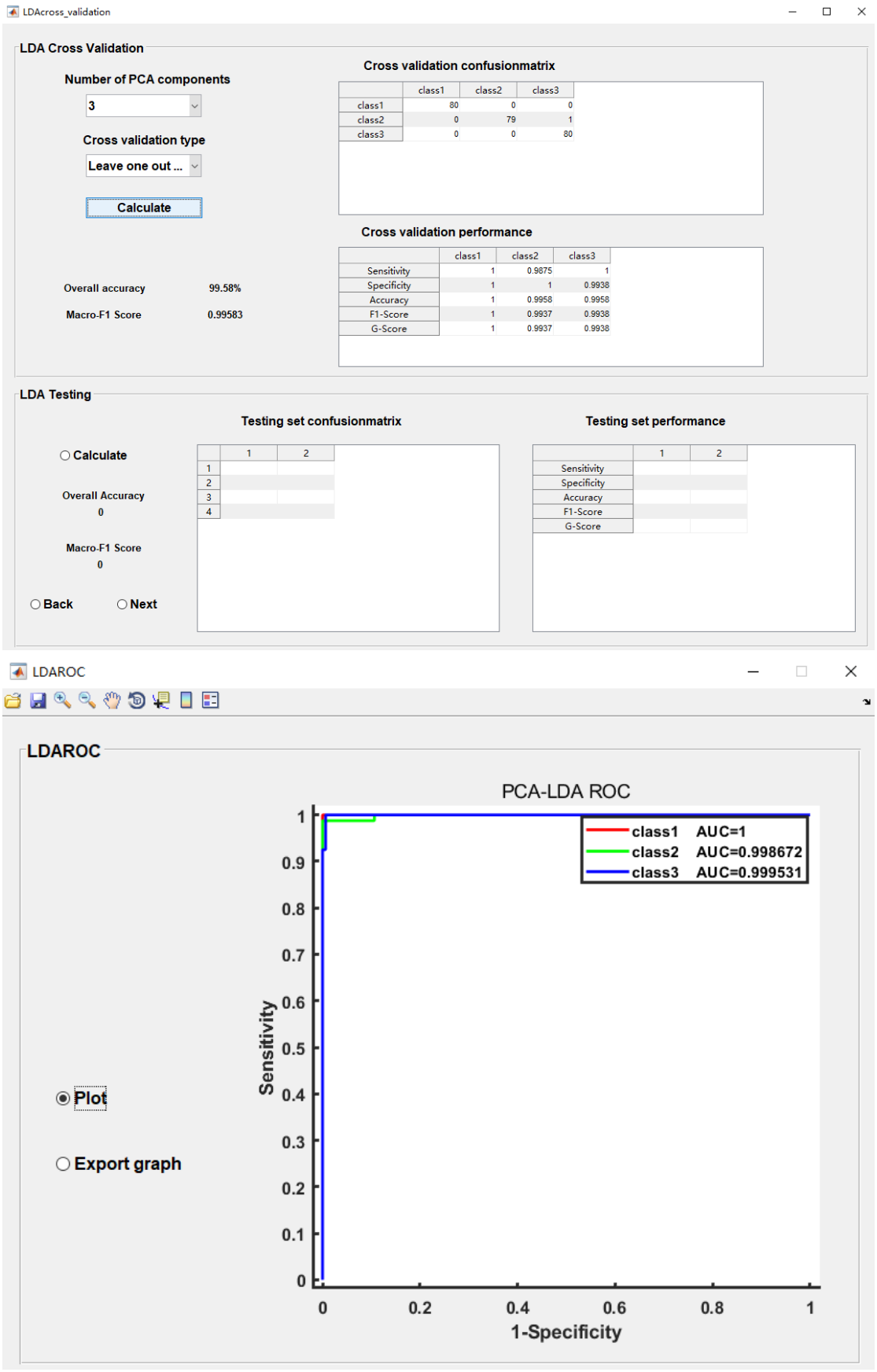


Figure 13. The cross validation results, classification results and performance evaluation of the model on the test set, and the ROC curve of each class.

3.4.3 Partial Least Squares-Discriminant Analysis

The operator can enter the PLS-DA analysis interface by clicking "Analysis > PLSDA > Perform PLSDA," and then the "Update" button should be clicked to update the variable name in the list box; then, the variable for the PLS-DA analysis should be selected, and lastly, the "Select" button should be clicked to complete data selection; it is recommended to select "mean_centerdata" in the list box. The operator can customize the dataset splitting method and training set ratio (like 60%–80% of the overall number of data samples) to divide the dataset into training and test sets. By clicking the "PLSDA SSE" button in the calculation panel, the sum of squared errors (SSE) of the first 20 latent variables (LVs) is calculated for drawing SSE curve by clicking "Plot"; the number of LVs with the minimum SSE is chosen as the optimal number of components required for modeling. Next, the corresponding PLSDA execution results can be obtained by selecting the number of LVs and clicking "PLSDA Score / Loading / Explained / probability". The drawing interface of PLSDA analysis results can be opened by clicking "View > viewPLSDA > view PLSDAscore / loading," and different LVs can be chosen for drawing. To output the graph in each drawing interface, it is needed to click on the "Export" button.

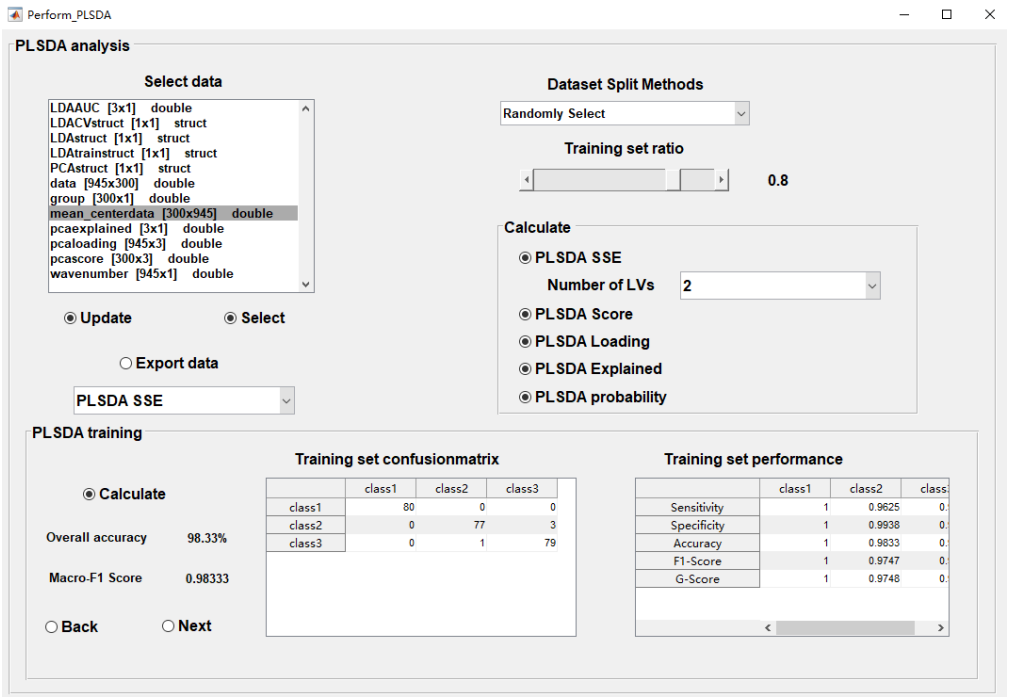


Figure 14. PLSDA analysis interface in the NWUSA toolbox.

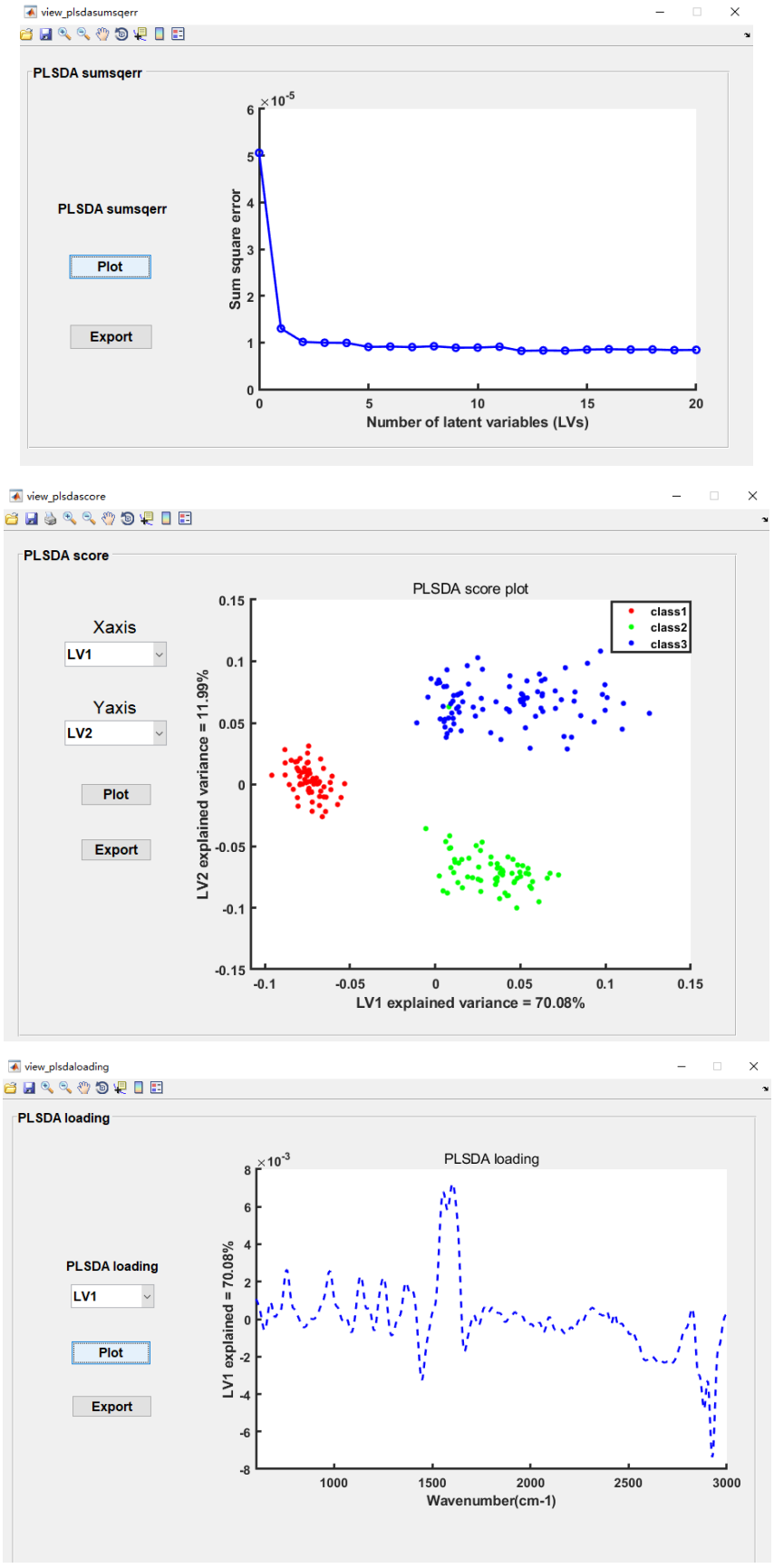
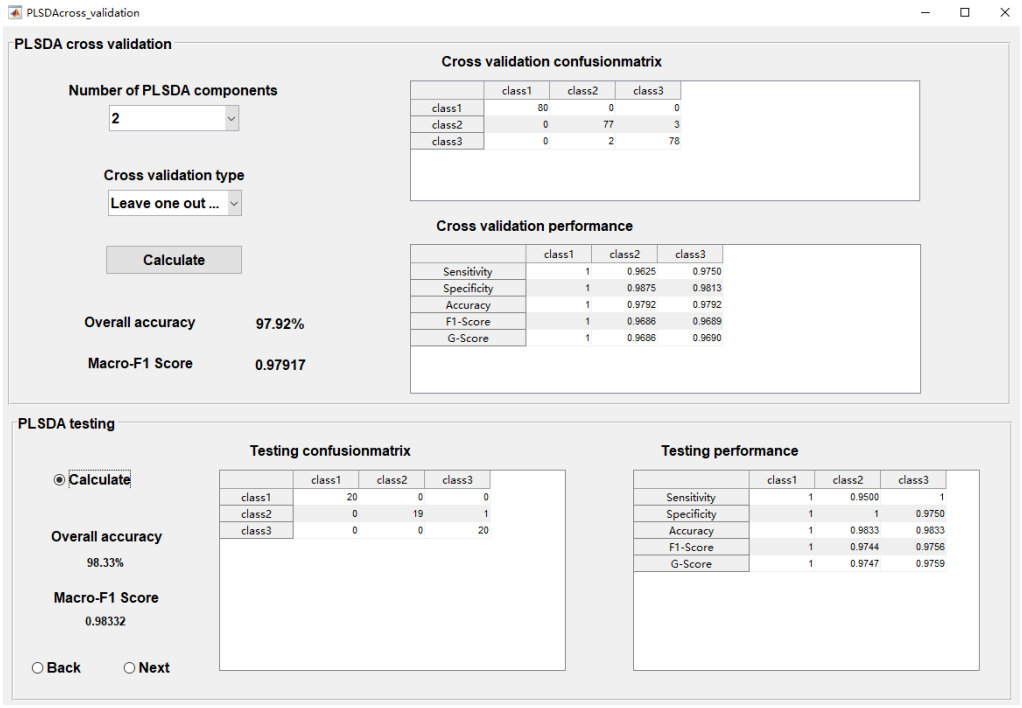


Figure 15. The variance percentage of the first 20 LVs, scores scatter plot, and loading of LV1.

In the “PLSDA training” panel, the operator can click on the “Calculate” button to view the classification results and performance evaluation indicators of the PLSDA model on the training set, including sensitivity, specificity, accuracy, F1-score, G-score, Macro-F1 score, overall accuracy and the confusion matrices. After that, the operator can click the “Next” button or “Analysis > PLSDA > PLSDA Cross validation” to enter the cross-validation and testing interface. The number of PLSDA components is the optimal number of LVs selected in the first step, and the cross-validation types can be set to five-fold, ten-fold, or leave-one-out cross-validation. The operator can click on the “Calculate” button to view the cross-validation results of the PLSDA model for training set samples represented by the confusion matrices, as well as the corresponding performance evaluation indicators, including sensitivity, specificity, accuracy, F1-score, G-score, Macro-F1 score, and the overall accuracy. In the “PLSDA testing” panel, the operator can obtain the classification results and performance evaluation indicators of the PLS-DA model on the test set by clicking the “Calculate” button. In addition, the operator can obtain the ROC curve by clicking “Analysis > PLSDA > PLSDA ROC.”



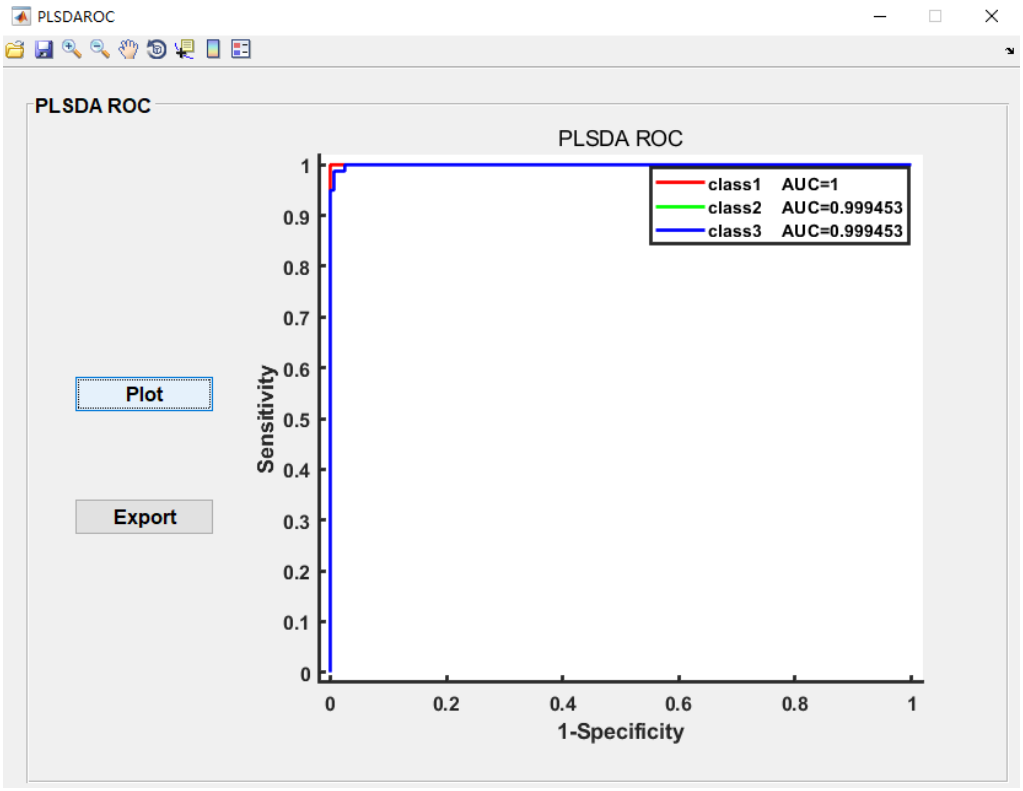


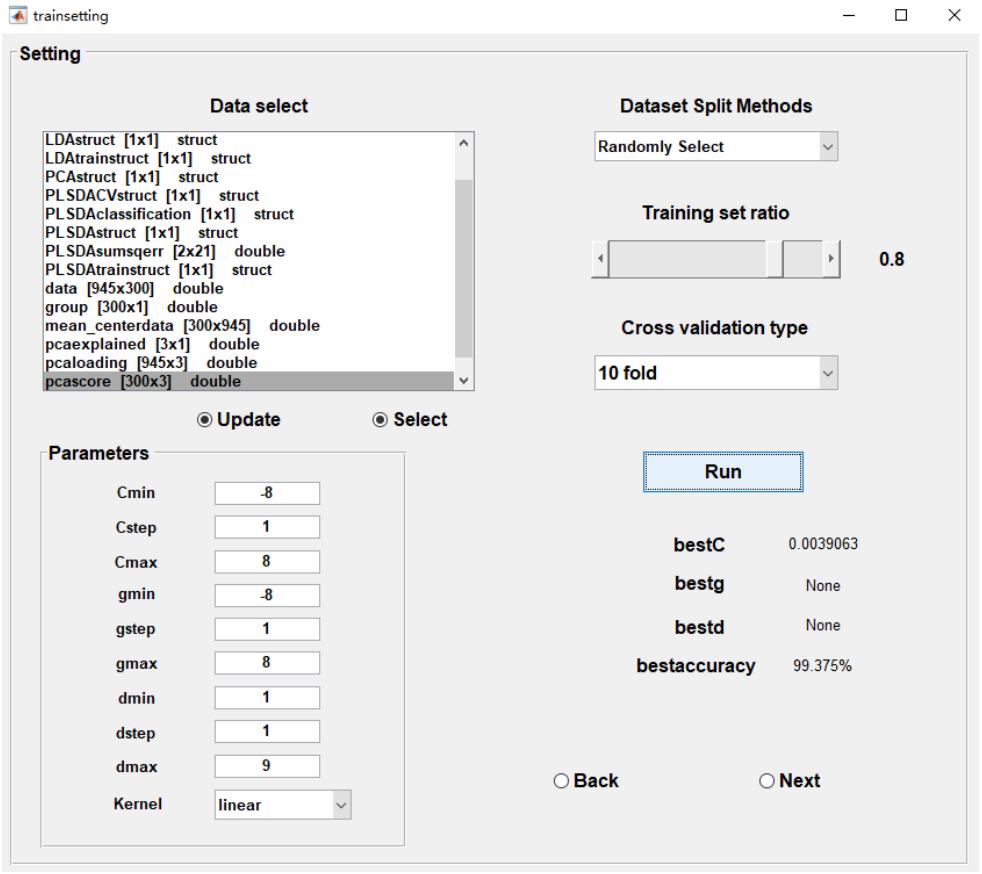
Figure 16. The cross validation results, classification results and performance evaluation of the model on the test set, and the ROC curve of each class.

3.4.4 Support Vector Machine

In the execution process of the SVM, the selection of kernel type and parameters is crucial. Operator can enter the interface for setting the SVM training parameters by clicking "Analysis > SVM > TrainSVM," and then click on the "Update" button to update the variable name in the list box, select the variable used for the SVM training, and click on the "Select" button to complete data selection; it is recommended to select "mean_centerdata" in the list box. Then, the operator can customize the dataset splitting method, the proportion of the training set, the cross-validation types, kernel type, and the corresponding parameter ranges. It is recommended to use the range of 0.6–0.8 for the proportion of the training set, that is, the training set accounts for 60%–80% of the overall number of data samples.

For a linear kernel, it is only necessary to set the range of parameter C (C_{min}, C_{step}, and C_{max} represent the minimum value, step size, and maximum value, respectively). For a polynomial kernel, it is necessary to specify the ranges of parameter C and polynomial order d (d_{min}, d_{step}, and d_{max} represent the minimum value, step size, and

maximum value of polynomial order, respectively, and they are all positive integers). For an RBF kernel, the ranges of parameters *C* and *gamma* (g_{min}, g_{step}, and g_{max} represent the minimum value, step size, and maximum value of *gamma*, respectively) should be specified. It is worth noting that for the convenience of use, the parameters *C* and *g* (*gamma*) in the setting interface can be expressed in the form of rational numbers (e.g., C_{min} = -10, and g_{min} = 10), but they are expressed by default in the form of logarithm with the base number of two (e.g., $C_{min} = 2^{-10}$, $g_{min} = 2^{10}$) in the process of program execution, so the parameter ranges should be properly selected. Finally, the operator can click on the "Run" button to view the combination of optimal parameters (*bestC* / *bestg* / *bestd*) and the corresponding best accuracy. To verify the SVM performance on the test set, it is necessary to click "Analysis > SVM > TestSVM," select the kernel type, and then click the "View confusionmat" button to view the classification results of each kernel on the test set, as well as performance evaluation indicators, including sensitivity, specificity, accuracy, F1-score, G-score, Macro-F1 score, and the overall accuracy.



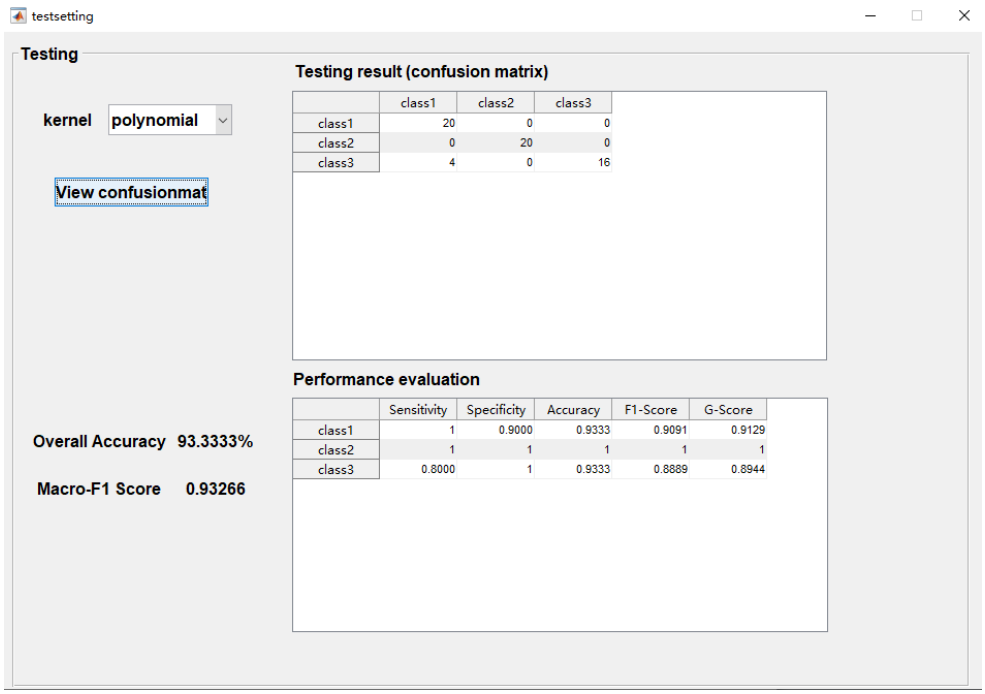


Figure 17. Training and testing interfaces of SVM and PCA-SVM models.

The influence of each parameter on the accuracy of the SVM model when a combination of optimal grid search parameters is used can be depicted by a 2D graph or a 3D surface. To perform this function, it is needed to click "View > viewSVM > SVMgridsearch," select the kernel type, click on the "Plot" button to draw the diagram, and then click on the "Export" button to export the graph. To make the 3D surface more uniform, parameters C and g are expressed in the exponential form, i.e., $\log_2 C$ and $\log_2 g$, respectively.

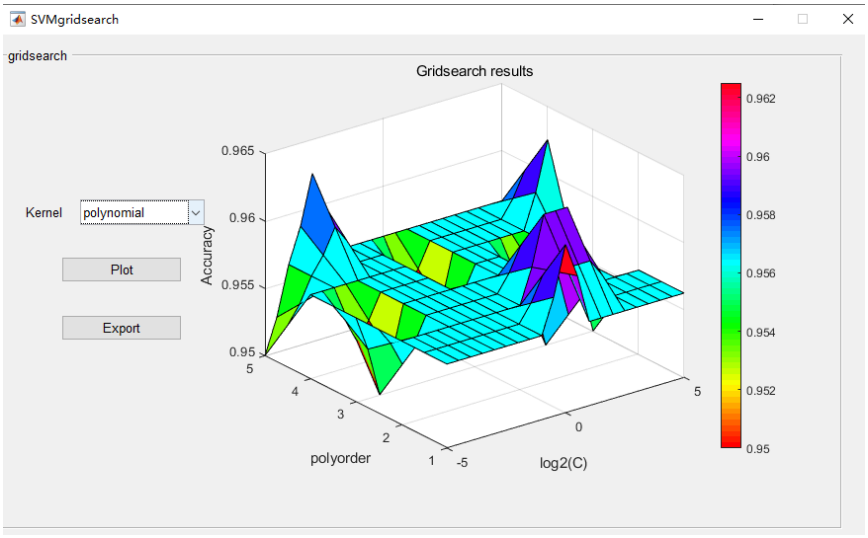


Figure 18. The 3D surface plot of classification accuracy as the function of the parameter C and polynomial order d in the polynomial kernel.

3.4.5 PCA-SVM

The implementation process of the PCA-SVM is basically the same as that of the SVM, with the exception of the form of input data. In the PCA-SVM, the data to be selected in the list box is “pcascore,” and only the first two significant PCs are used for the PCA-SVM model. To view the visualized classification result, the operator can click “View > viewPCASVM > PCASVMplot,” select the dataset and kernel type, and then click on the “Plot” button to draw a diagram. Finally, by clicking on the “Export” button, the graph is exported.

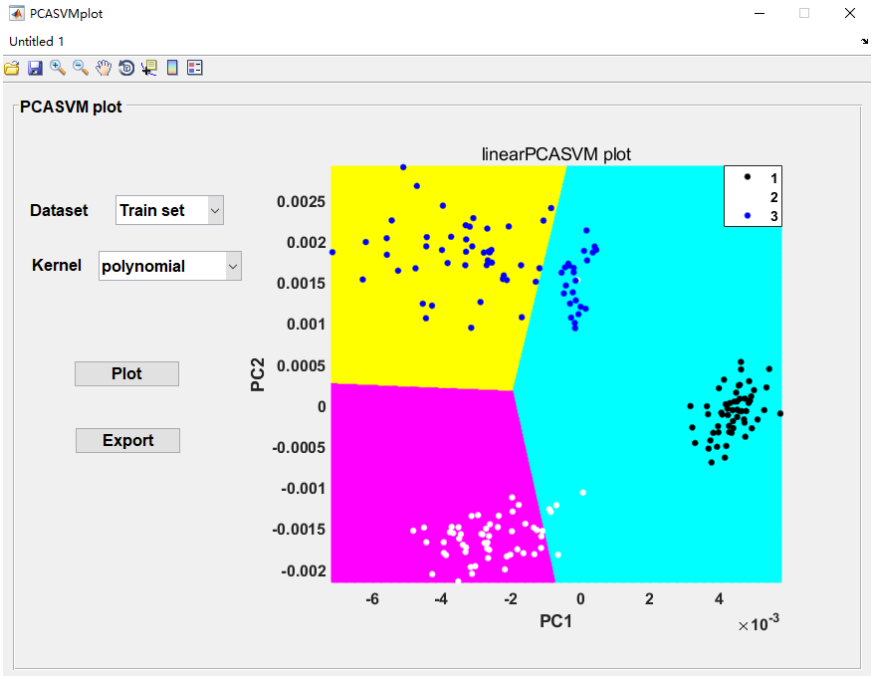


Figure 19. The polynomial kernel PCA-SVM classification scatter plots.

4. Model saving and loading

After each model training, the operator can save all the information (e.g., training parameters, training methods, and other parameters) on the trained model by clicking “Save model” in the “File” in the main menu. The operator selects the name of the model to be saved in the pop-up menu of the “Save Model” interface, and clicking on the “Save” button to save the model to the specified location. After the information on the trained model is saved, there is no need to perform data preprocessing and establish classifiers again when the model is used to predict a new dataset. When the operator wants to predict an unknown spectral dataset, he should click “Predict” in the main

menu, select the required model, and then click “Load model” and “Load data” in the subinterface to load the model and new dataset, respectively. By clicking on the “Predict label” button in the subinterface, the new dataset is predicted, and prediction results are displayed in the table.

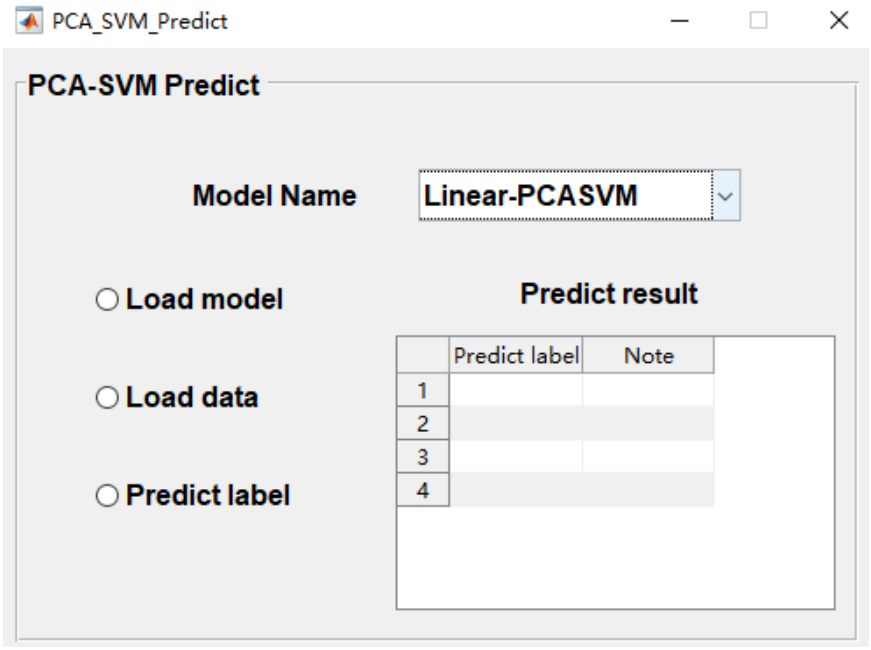


Figure 20. The saved model's prediction interface for unknown data. The example is the PCA-SVM model.

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