Software Description

Active Learning Materials Optimization Software: BgoFace

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BgoFace

BgoFace is an easy-to-use active learning material optimization software that includes almost all functions of the Bgolearn library. BgoFace supports uploading training samples and generating virtual samples, using existing experimental data to search for optimal material composition designs to maximize or minimize required performance indicators. BgoFace supports a variety of utility functions, such as expectation lifting function, Gaussian supremum function and predictive entropy search function, etc., for Bayesian optimization material design problems of regression and classification.

Figure 1 : BgoFace Interface

Realize input sample processing, feature analysis, regression and classification task selection and optimal material composition recommendation. This manual analyzes and describes each function of the software.

Upload

The uploaded training sample files and virtual sample files support "xls", "xlsx" and "csv" formats. The last column of the default input training sample is the prediction target, and the first few columns are characteristics such as material composition or process parameters. Virtual samples can also be generated manually by uploading training sample files. The steps to upload and process training samples and virtual samples are as follows:

(Data upload mode 1, directly upload training samples and virtual samples)

When in "Input" mode, click the "Load Data" button to display the file upload interface.
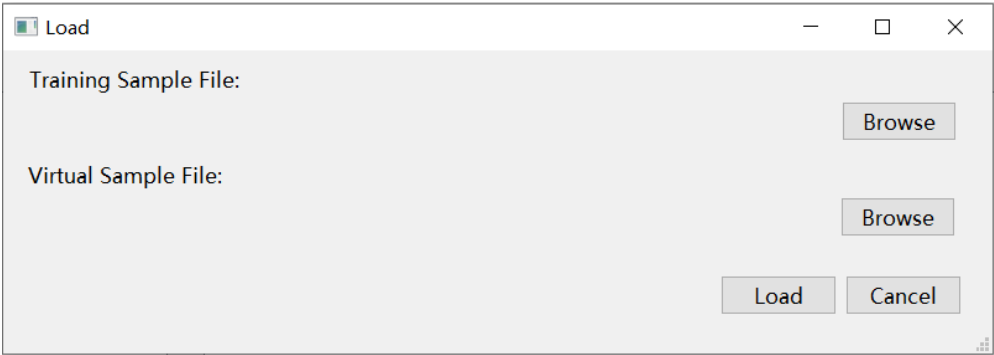
Figure 2 : Upload files

Click the "Browse" button to select the training sample and virtual sample files to upload.
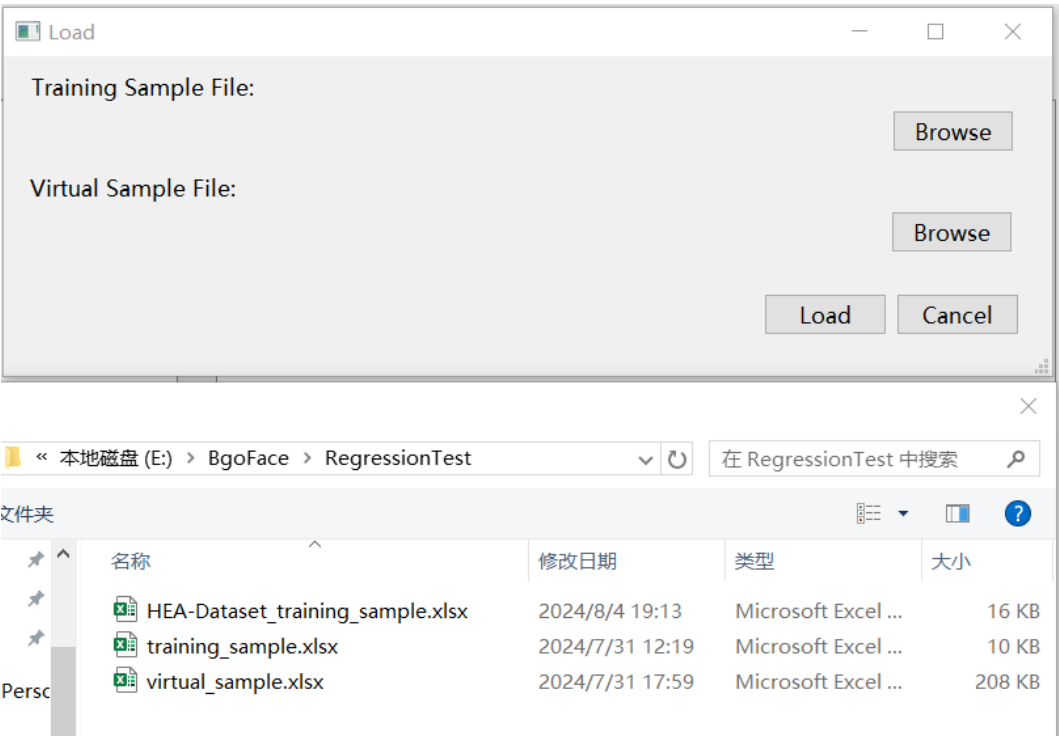

Figure 3 : Select files to upload

After selecting the training sample and virtual sample, the file path is displayed in the Load window.
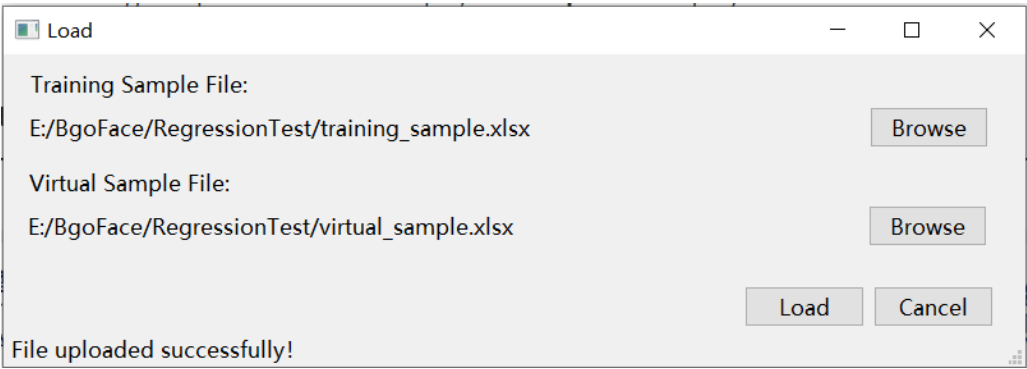

Figure 4 : Display file path

Click the "Load" button and the files will be loaded into the main window.

Figure 5 : Show sample file

(Data upload mode 2, directly upload training samples and synthesize virtual samples through BgoFace)

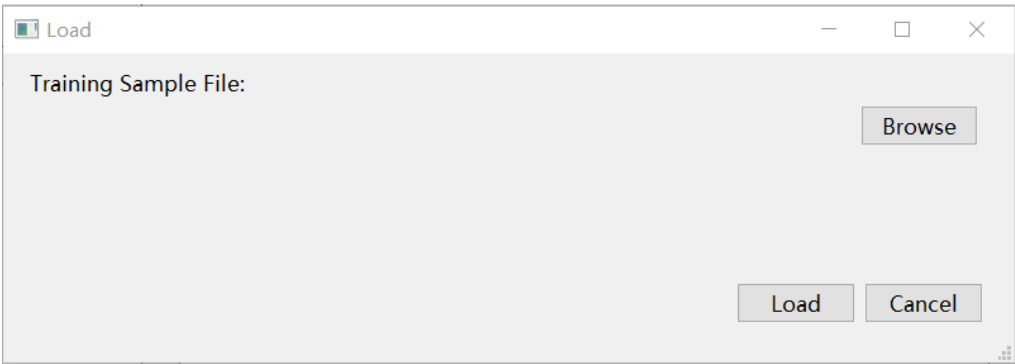When in "Manual" mode, click the "Load Data" button to display the file upload interface.

Figure 6 : Upload training sample

Similar to the above steps, upload and load the training sample file into the main window.
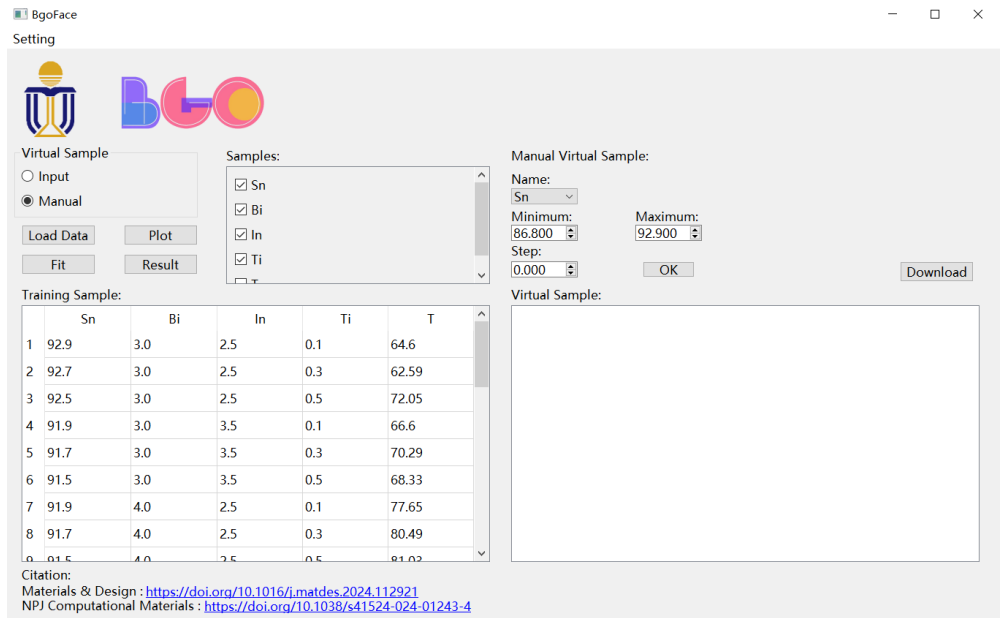
Figure 7 : Display training sample

In the Samples area, you can see the selected samples. **Use the selected samples to generate virtual samples.**

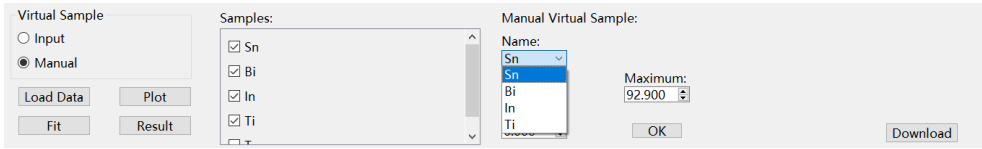For example, use "Sn", "Bi", "In" and "Ti" to generate the virtual sample.

Figure 8 : Generate virtual sample

Select a sample and generate the corresponding virtual sample by adjusting the minimum, maximum and step size.

Figure 9 : Adjust values to generate

Click the "OK" button to select the next sample. **When all selected samples are processed, the virtual sample is generated and displayed in the main window.**

Figure 10 : Display virtual sample

After the virtual sample is generated, you can choose to click the "**Download**" button to select the download folder to download the virtual sample. **There is no need to re-generate the software next time and upload the data through method 1.**
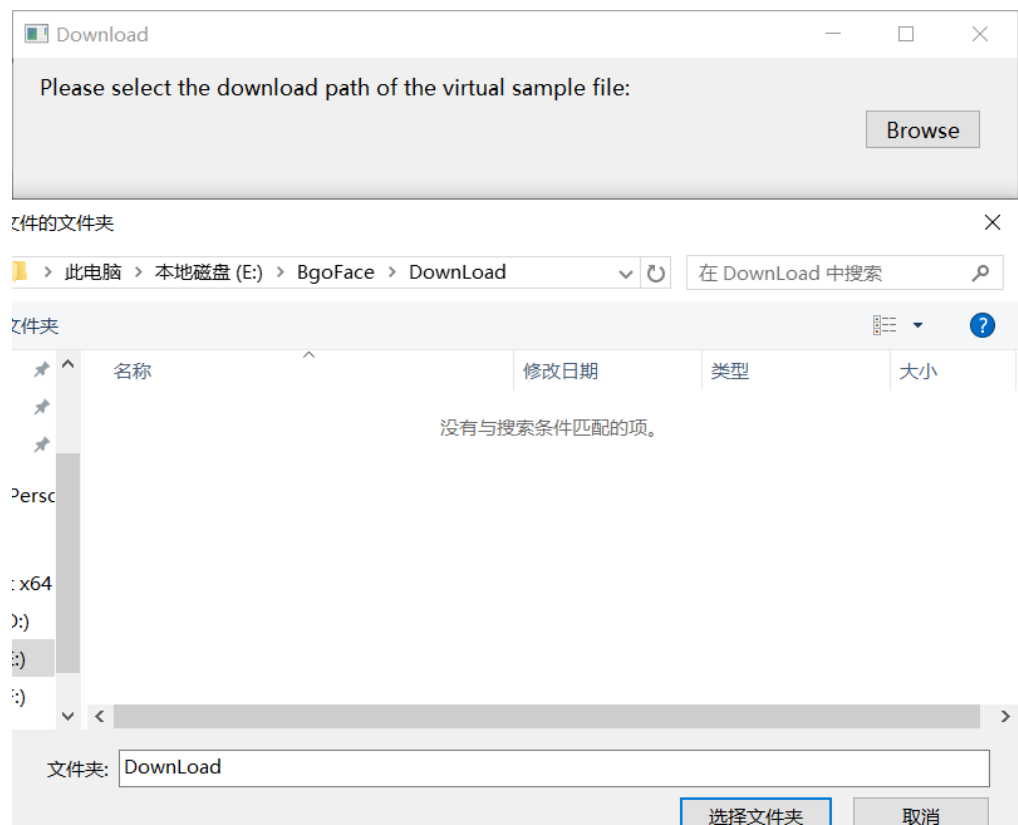
Figure 11 ：Download virtual sample

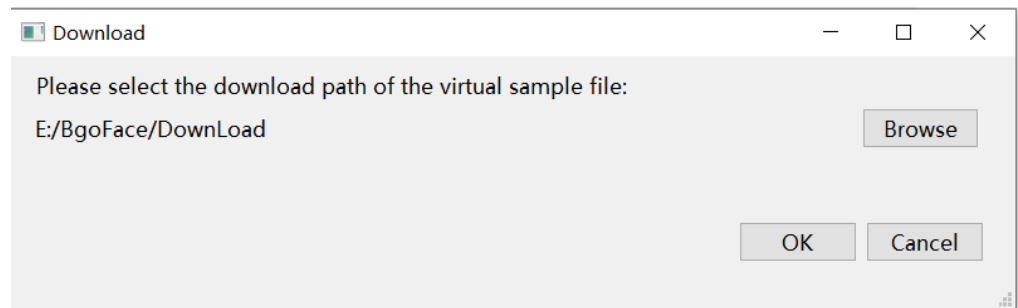Click the "OK" button to download the virtual sample to the specified folder.
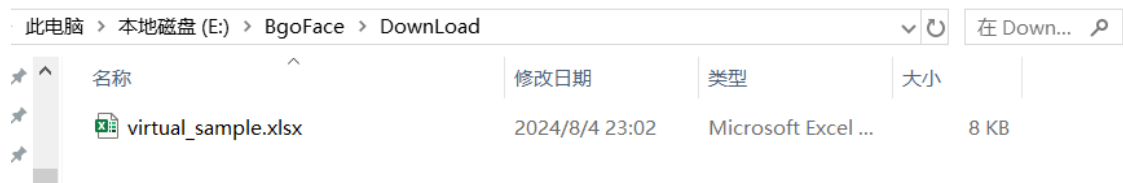

Figure 12 ：Download path

Figure 13 ：Download successfully

Statistics

After uploading the training sample, **click the "Plot" button to see some feature statistics.**

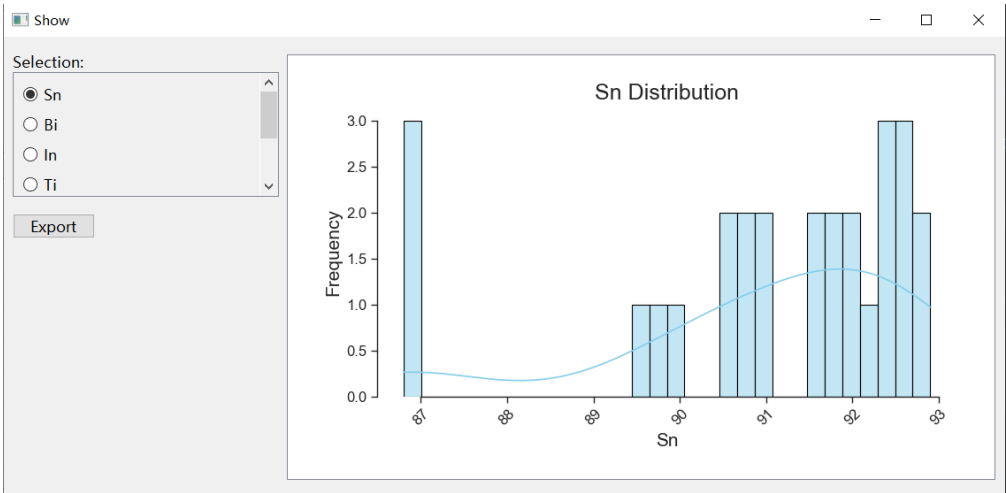For example, this is the distribution chart of "Sn".

Figure 14 : Sample distribution

This is the distribution chart of single target labels (mainly for categorical variable label statistics).
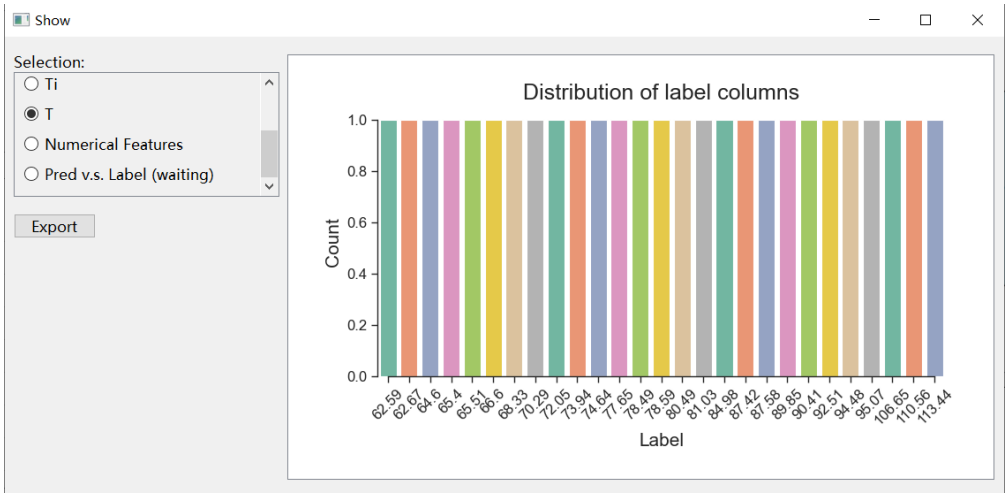

Figure 15 : Label distribution

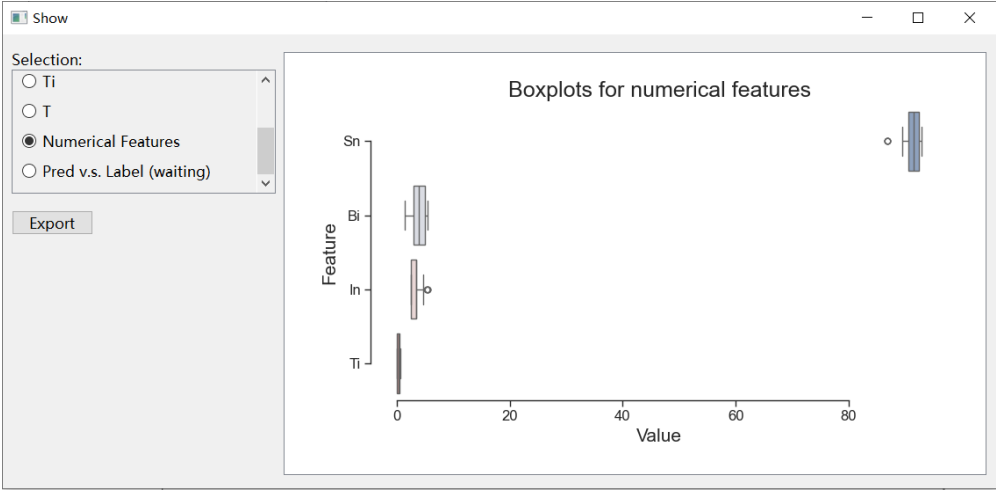This is the boxplots for numerical features.

Figure 16 : Boxplot

This graph uses leave-one-out and cross-validation to evaluate the predictive performance of a Gaussian process regression model, and plot a scatter plot of the model's predicted values versus the true values.

When selecting the "Pred vs. Label" picture, a large amount of calculations will be performed and it may take a long time to load (please wait patiently).
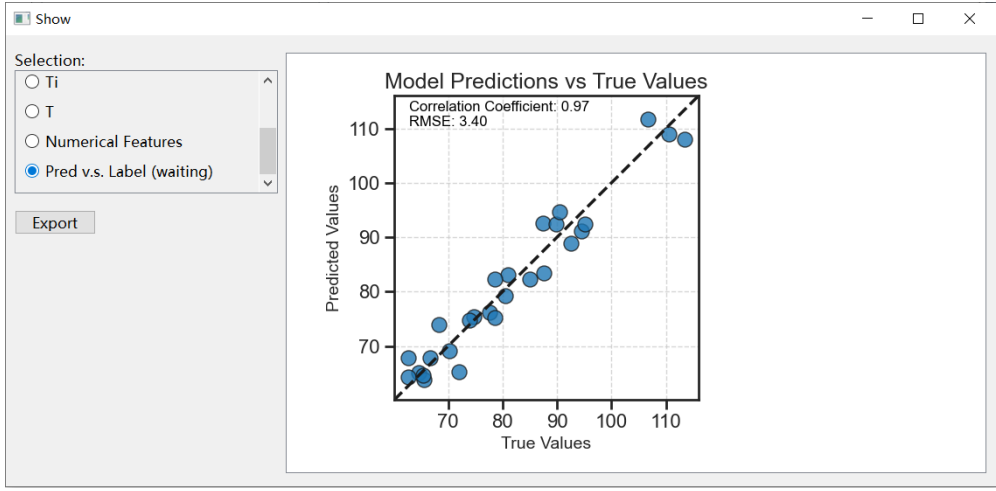

Figure 17 : Pred v.s. Label

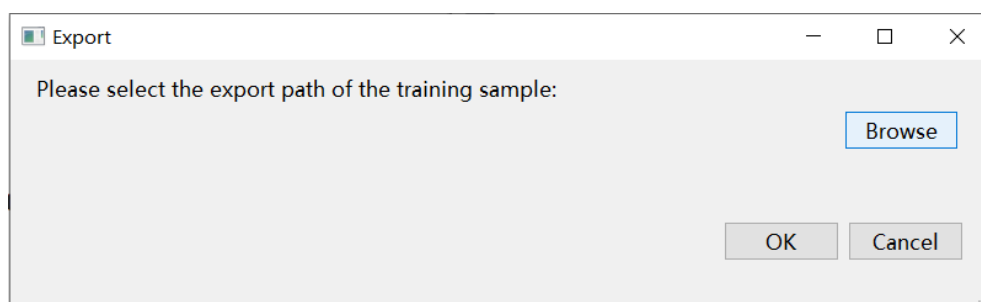Similar to the previous operation, click the "Export" button to download these images to the specified folder.

Figure 18 : Export

Parameters Setting

After obtaining the training sample and virtual sample, set the operating parameters.
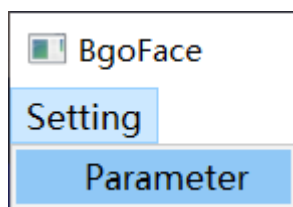

Figure 19 : Set parameters

Click "Parameter" button in the menu bar and set the parameters in the Parameter window.
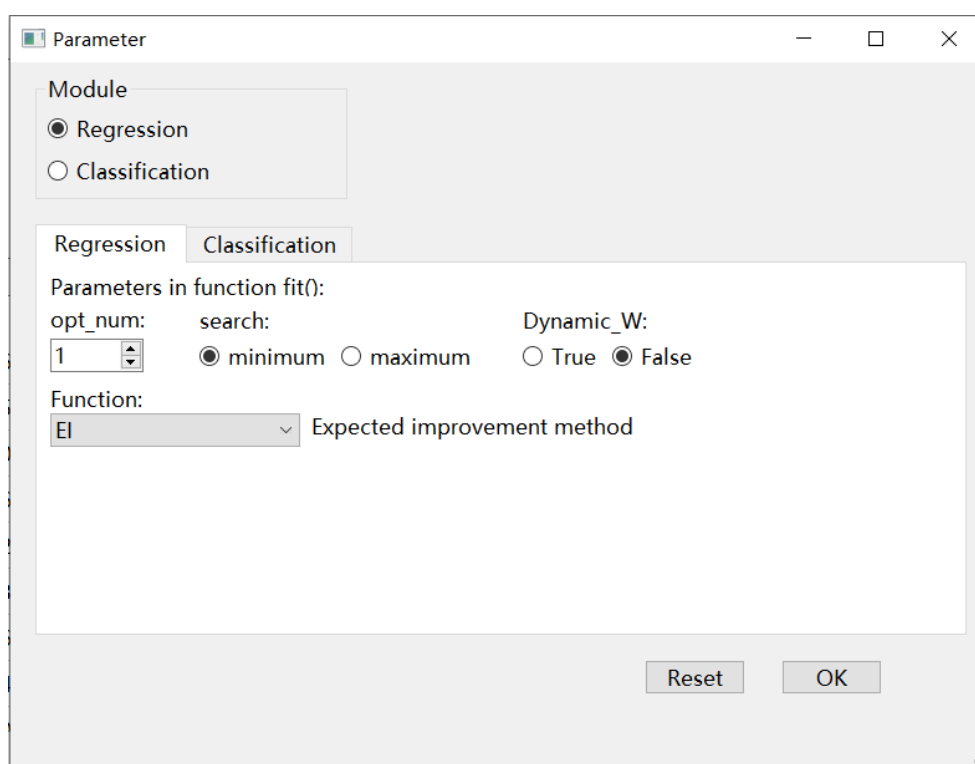

Figure 20 : Parameters Setting Interface

Choose the "Regression" mode, select different functions and their corresponding parameter settings.
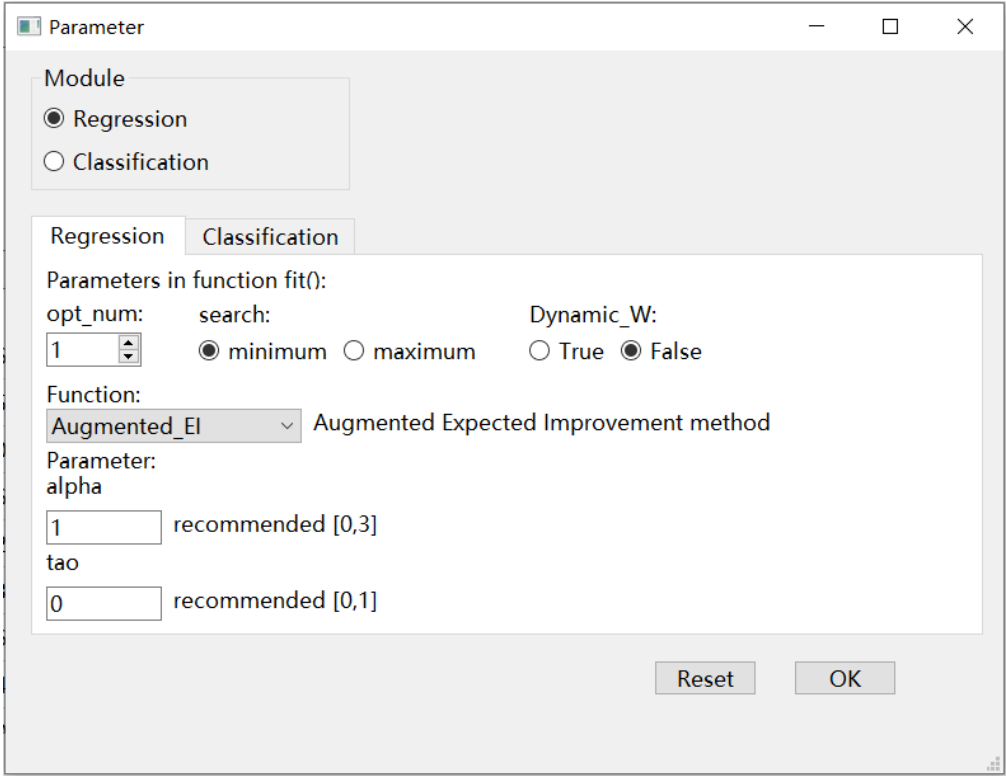
Figure 21 : Regression Task

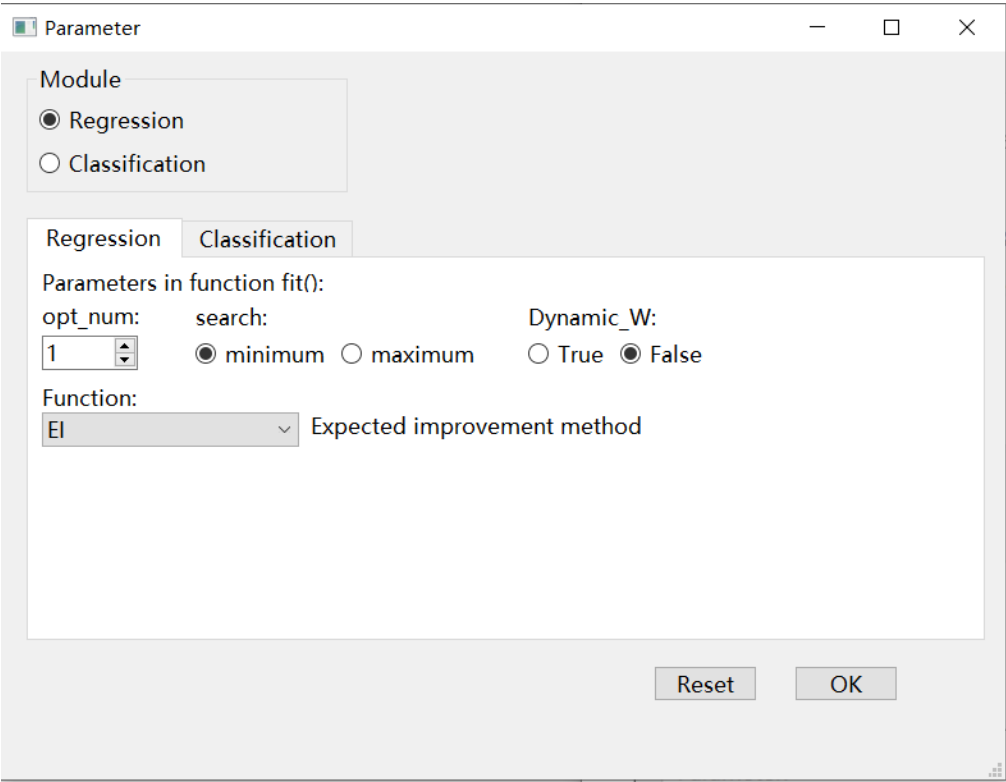Click the "Reset" button and the parameters are set to default setting.

Figure 22 : Reset Parameters

Click the "OK" button to complete the parameter setting.

Choose the "Classification" mode, set the parameters and choose the function.
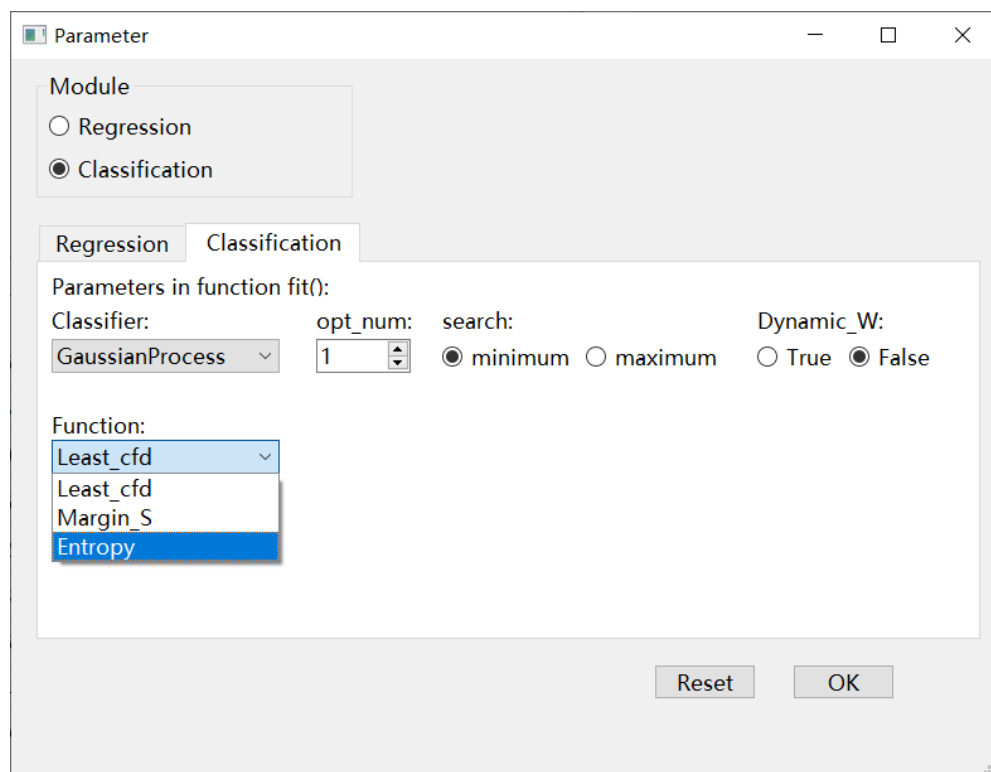

Figure 23 : Classification Task

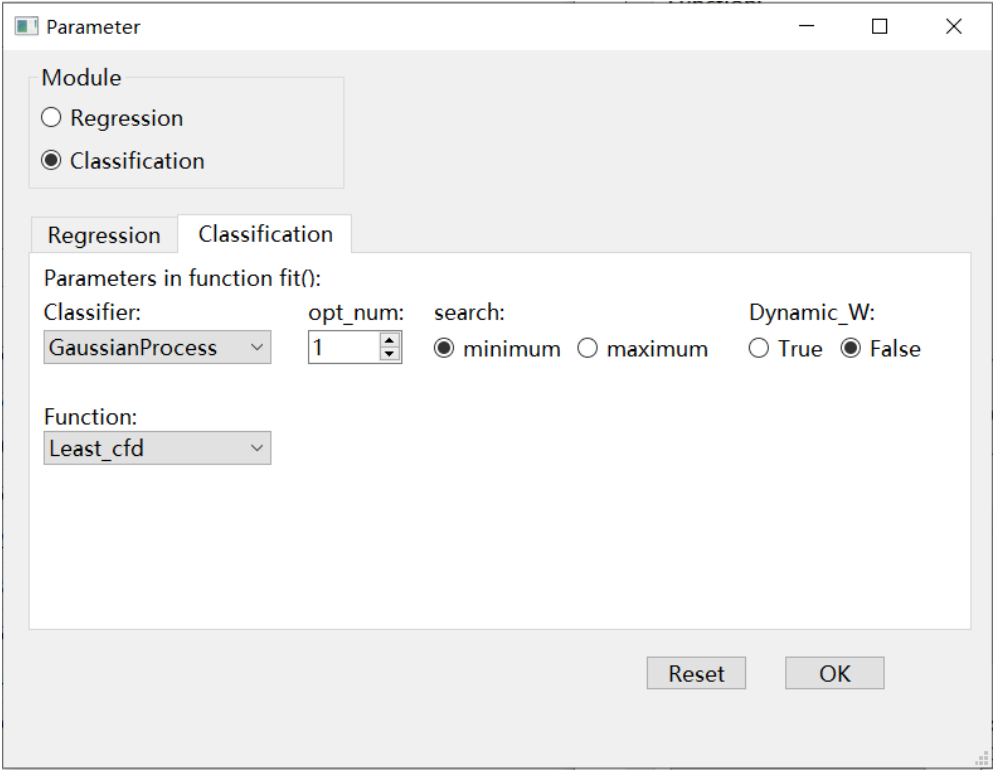Click the "Reset" button and the parameters are set to default setting.

Figure 24 : Reset Parameters

Click the "OK" button to complete the parameter setting.

Fit

After completing the parameter settings, click the "Fit" button to view the results in the Result window.
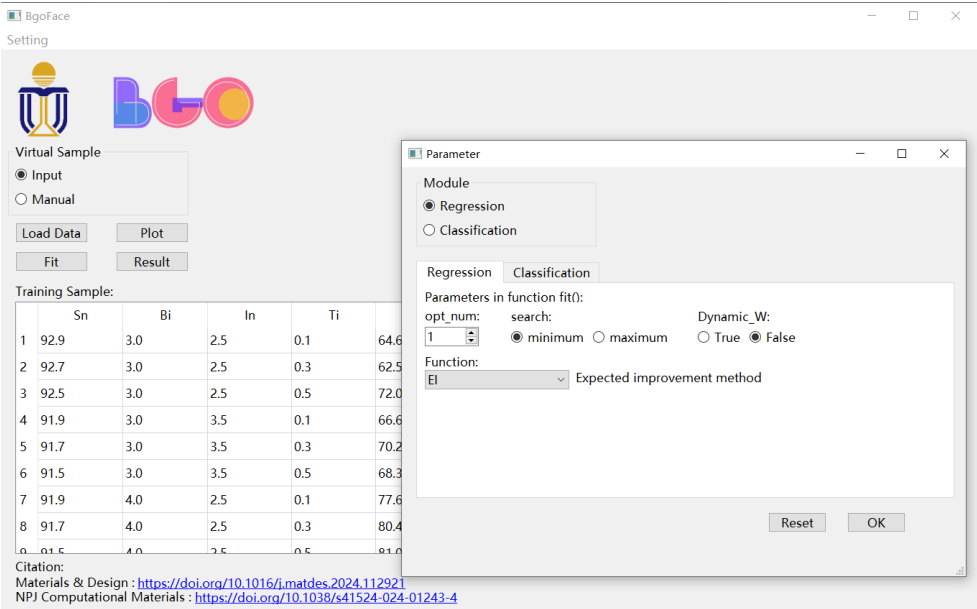

Figure 25 : Sample files loading
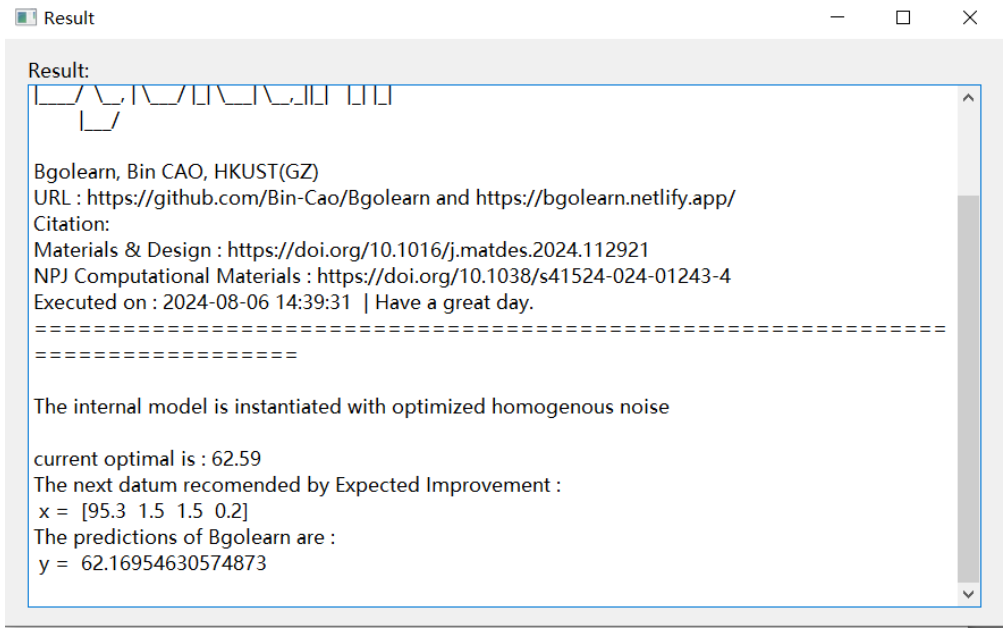

Figure 26 : Set parameters

Figure 27 : Show results