https://github.com/Bgolearn

https://bgolearn.netlify.app

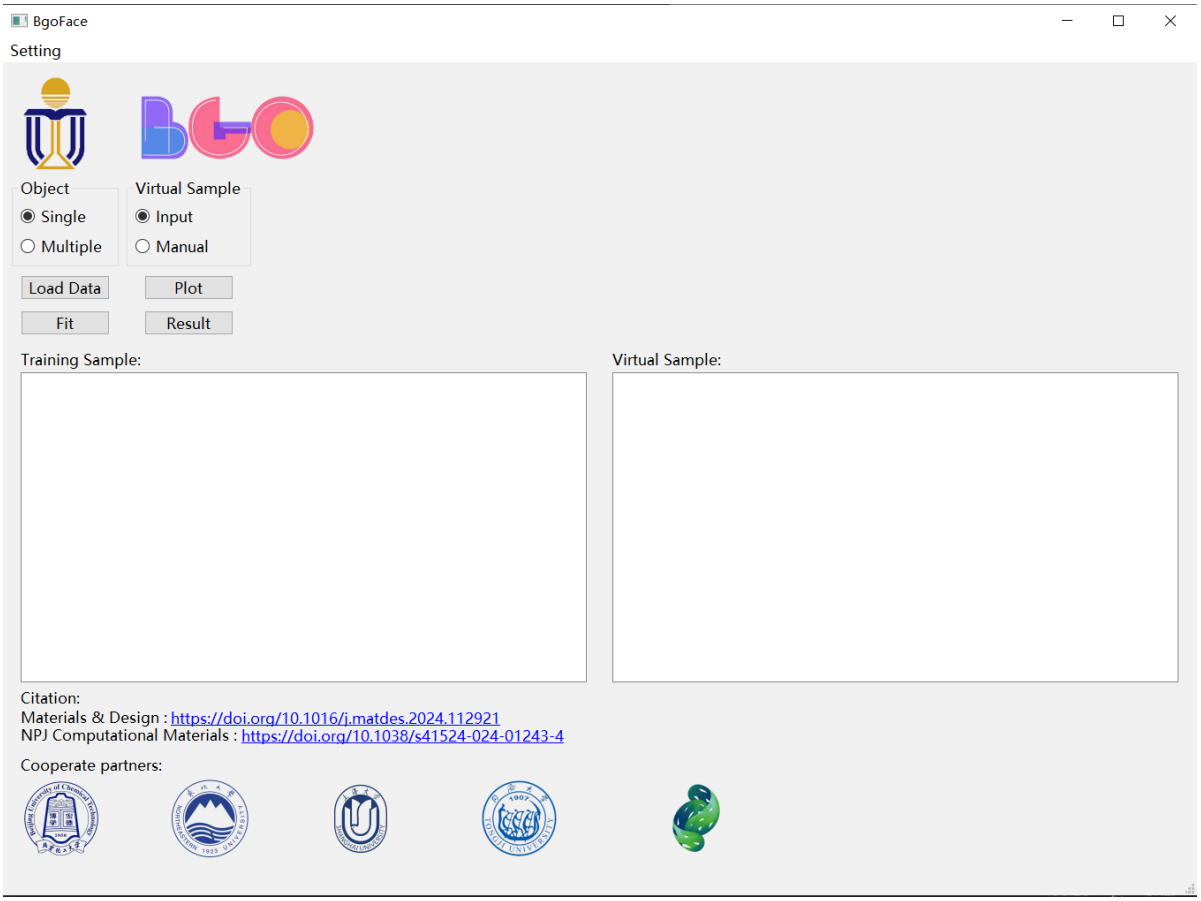
BgoFace User Manual

1.Introduction

The BgoFace is the user interface of the Bgolearn Platform. 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 classifications.

BgoFace also add the MultiBgolearn module. MultiBgolearn is a Python package designed for multi-objective Bayesian global optimization (MOBO), sepcifically tailored for materials design. It extends the functionalities of the Bgolearn package, which focuses on single-objective optimization, by enabling the simultaneous optimization of multiple material properties.

This user manual describes how to use BgoFace.



2.Single-Object

Choose the "**Single-Object**" method to perform regression tasks and classification tasks.

2.1Upload sample file

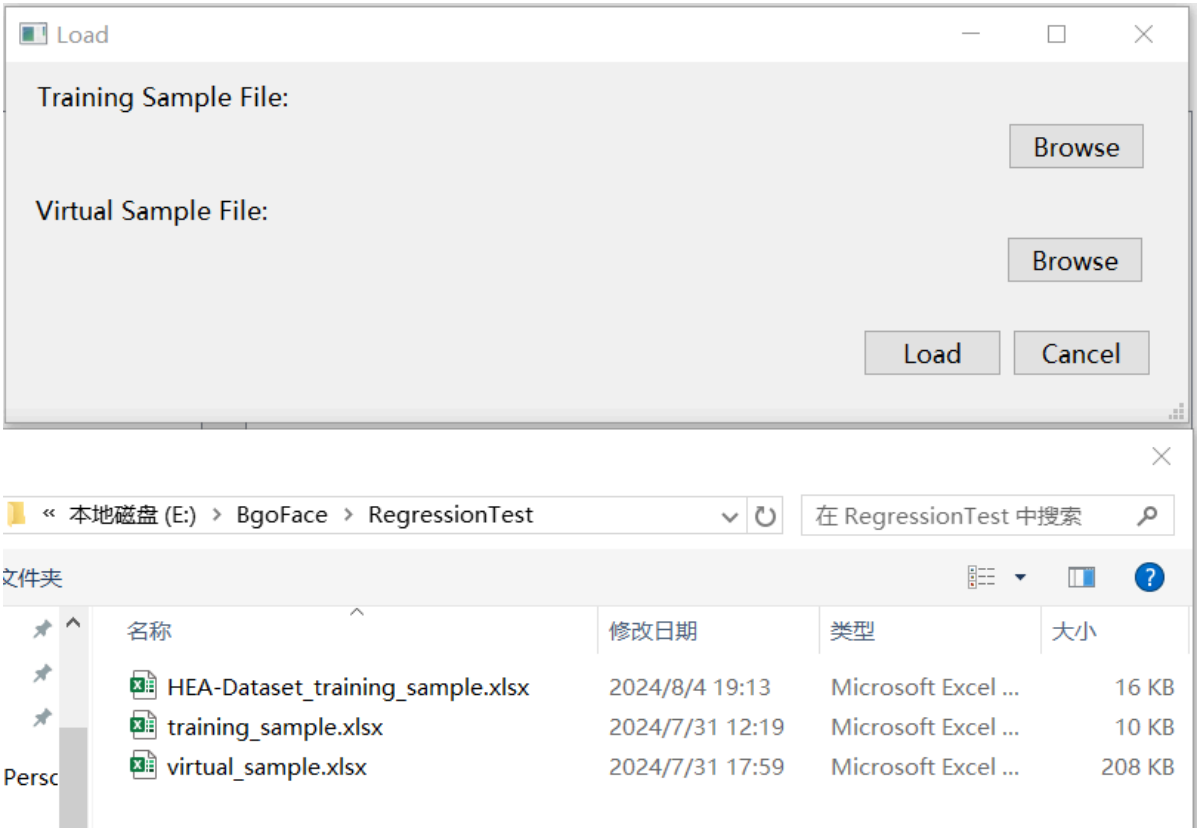
2.1.1File format requirements

- **The training sample file and virtual sample file support 'xlsx', 'xls' and 'csv' formats.**
- **The last column of the training sample file is used as a single target.**

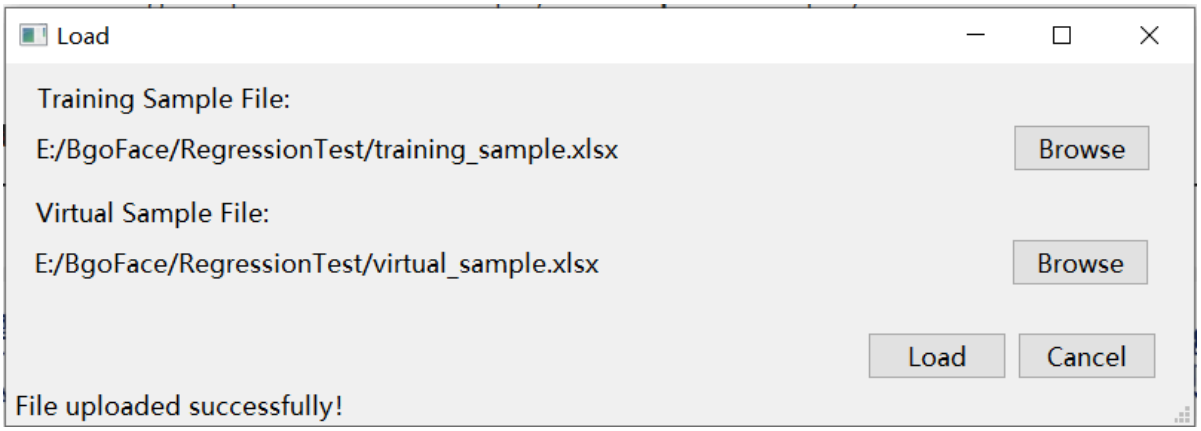
2.1.2Upload training sample and virtual sample

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

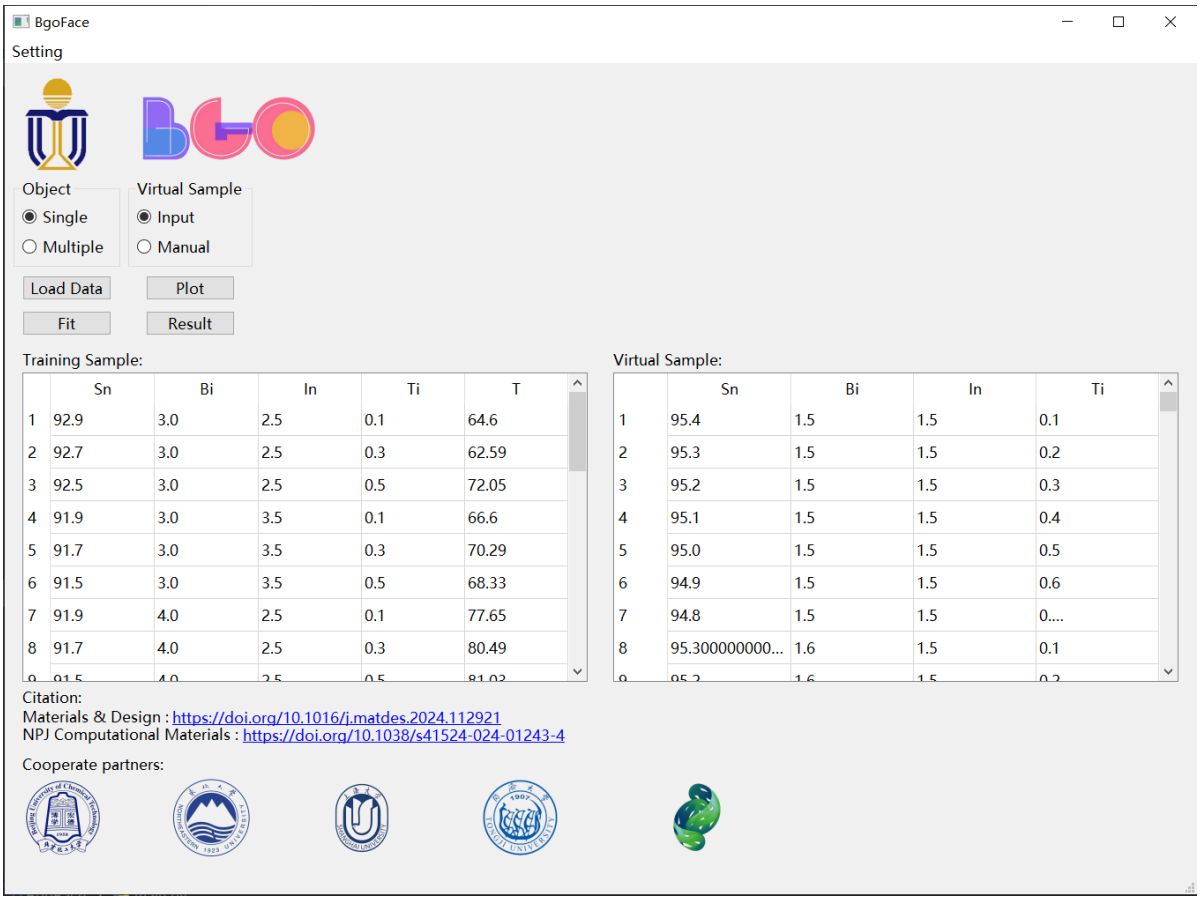
Click the **"Browse"** button to select the training sample and virtual sample files to upload.



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



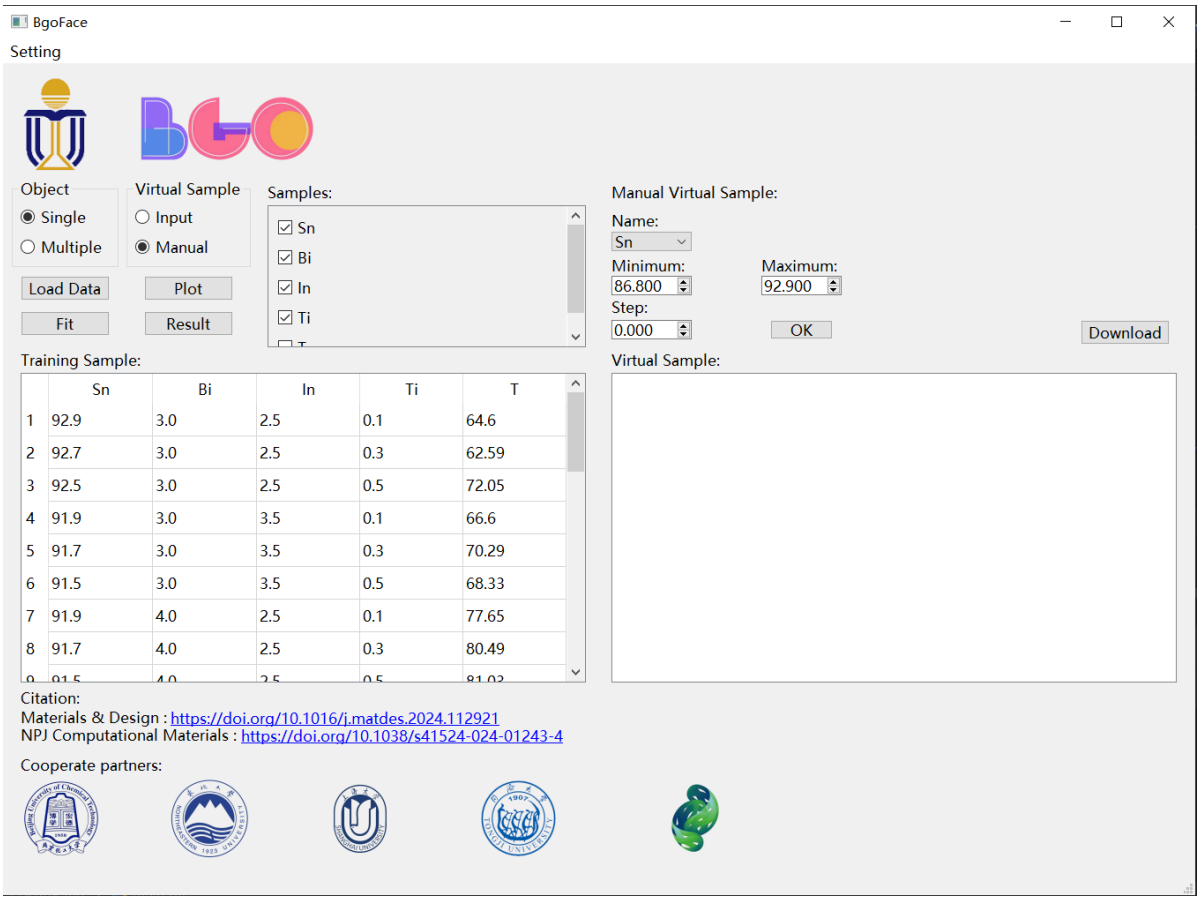
Click the **"Load"** button and the files will be loaded into the main window.



2.1.3Upload training sample and generate virtual sample

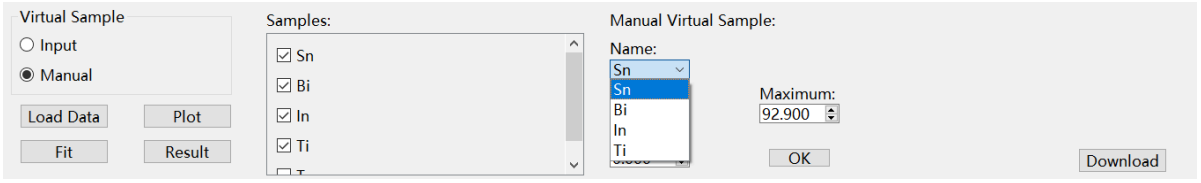
When in **"Manual" mode**, click the **"Load Data"** button to display the file upload interface.

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

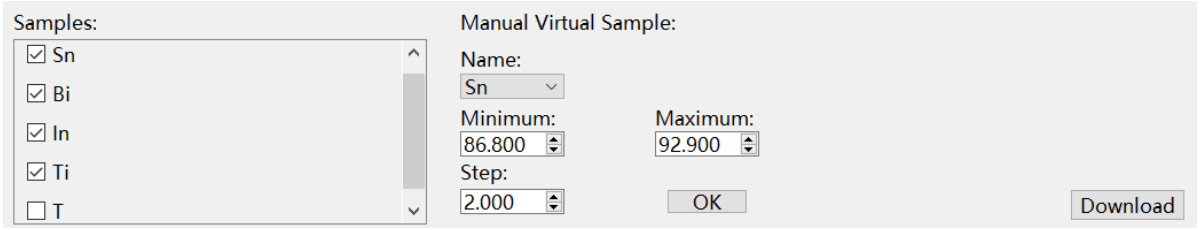


In the Samples area, you can see the selected samples. **Use the selected samples to generate virtual samples.**

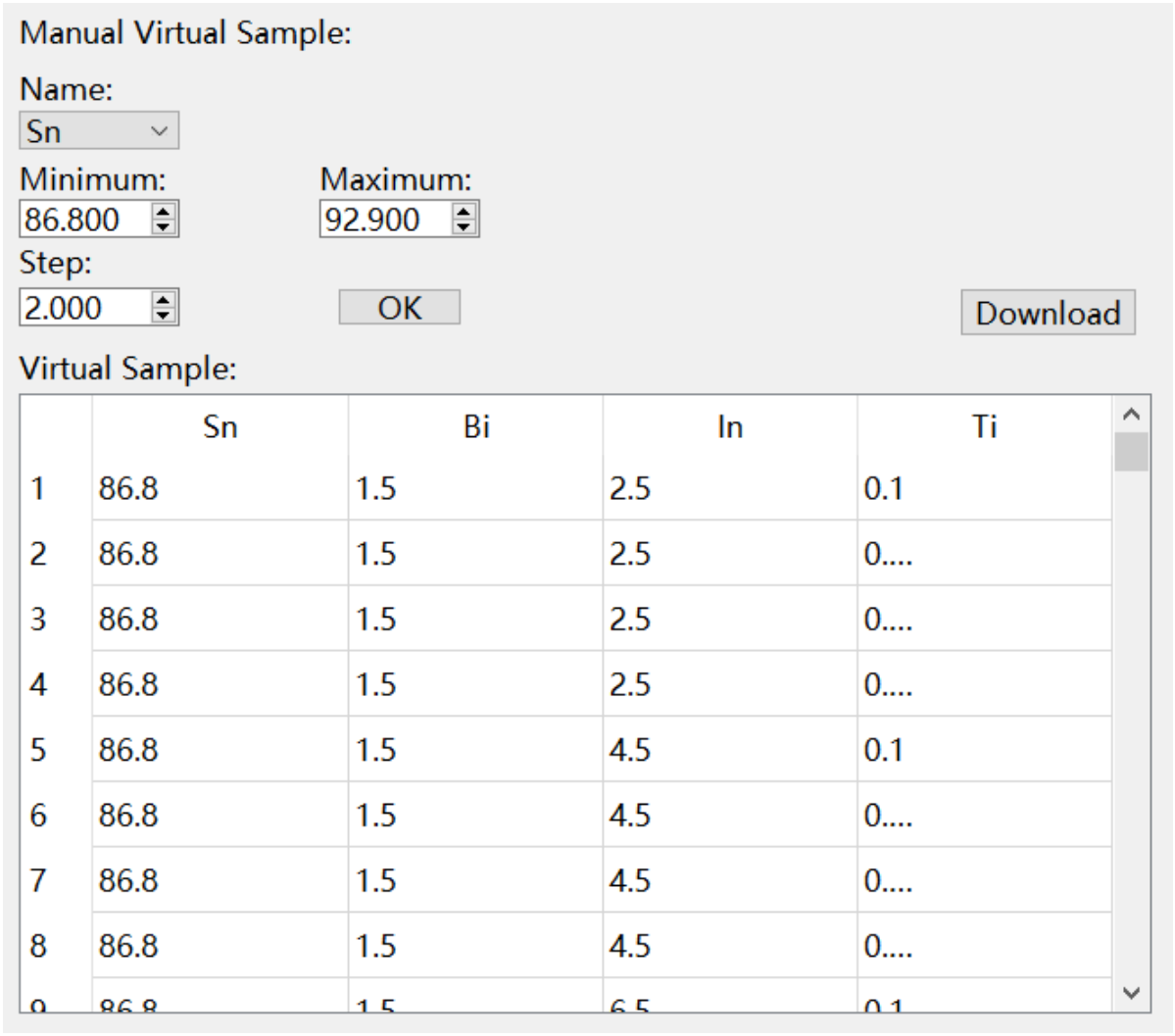
For example, use "Sn", "Bi", "In" and "Ti" to generate the virtual sample.



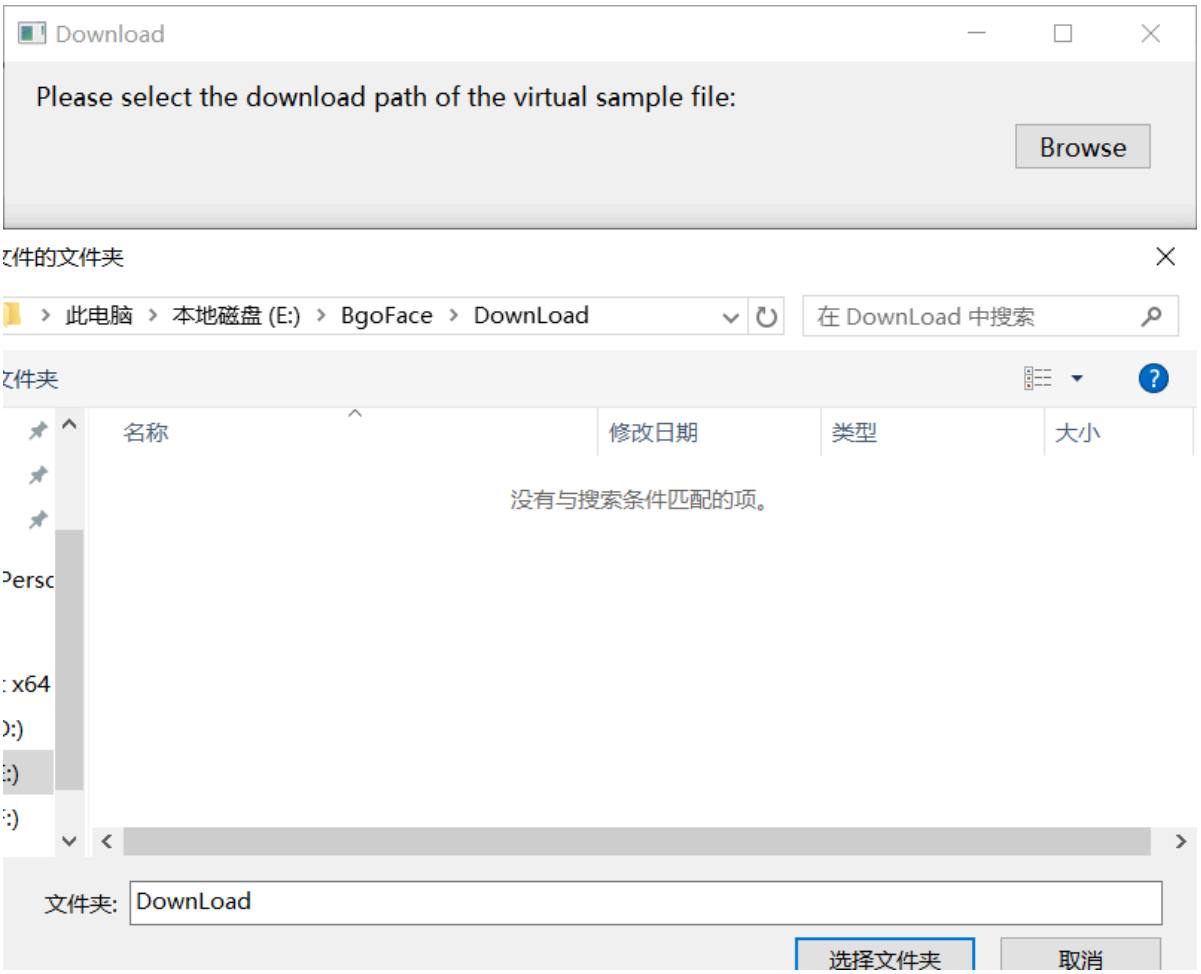
Select a sample and generate the corresponding virtual sample by adjusting the minimum, maximum and step size.



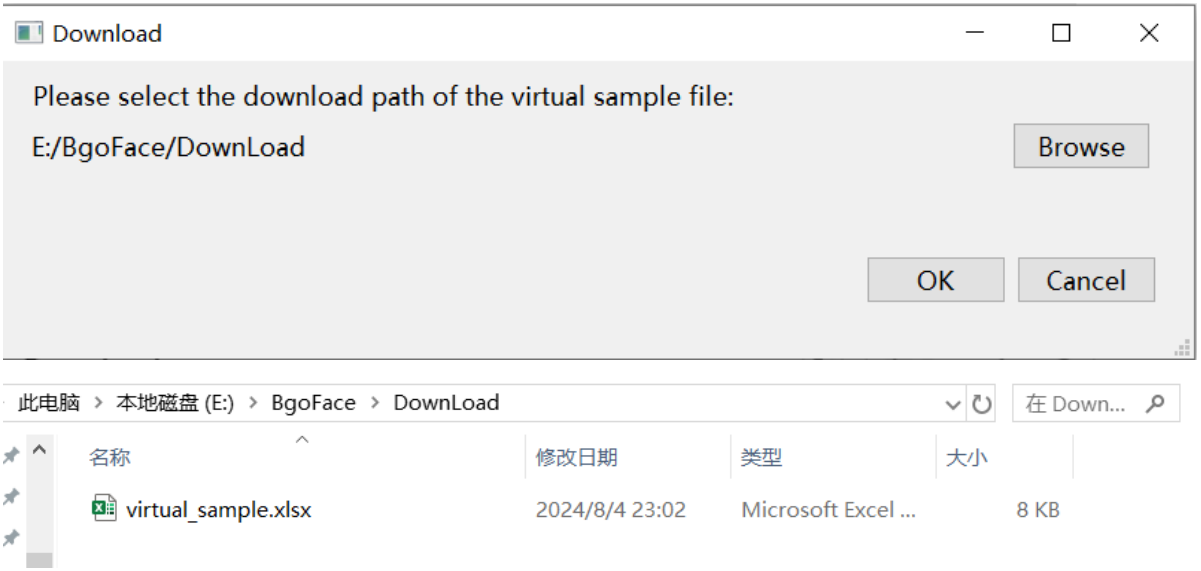
Click the "OK" button to select the next sample. When all selected samples are processed, the virtual sample is generated and displayed in the main window.



After the virtual sample is generated, click the **"Download"** button and **select the downloaded folder to download the virtual sample.**



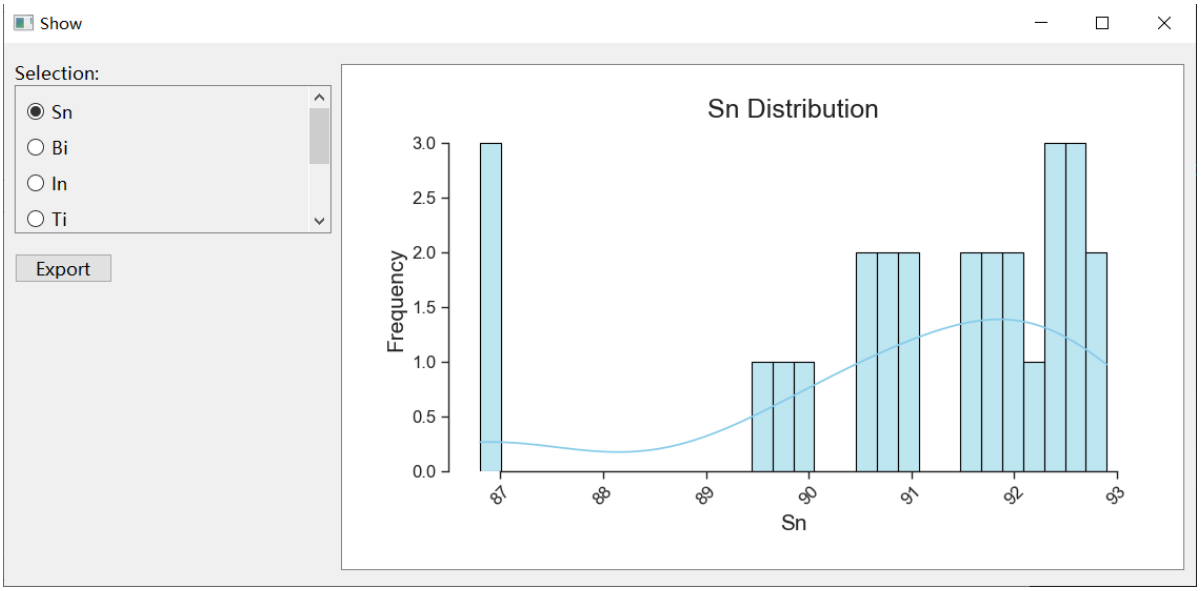
Click the **"OK"** button to **download the virtual sample to the specified folder**.



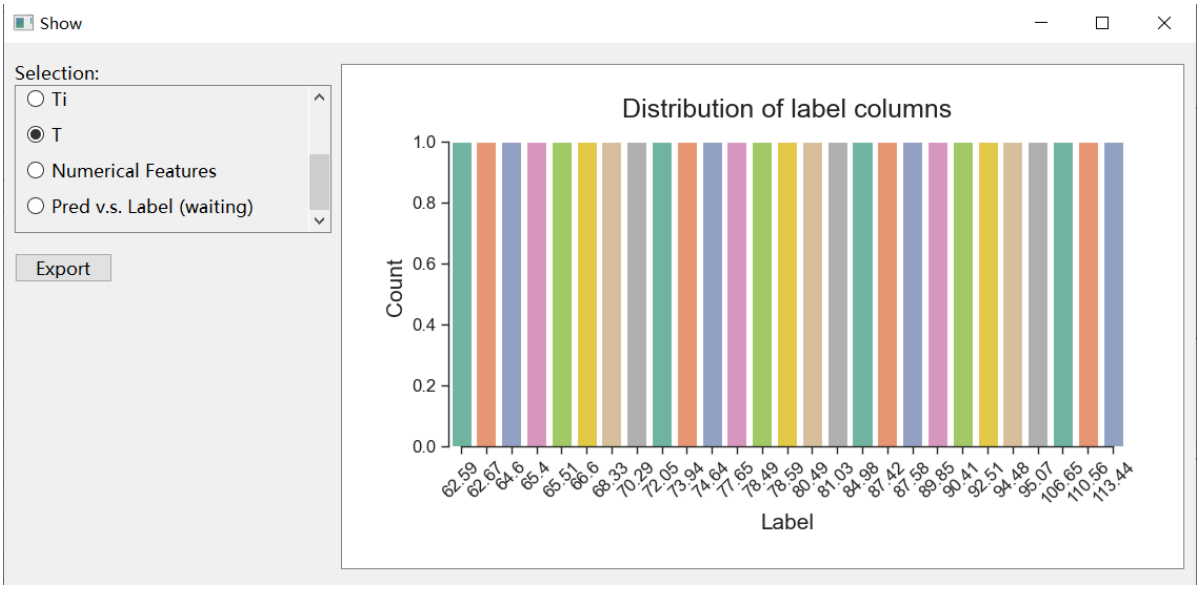
2.2Plot

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

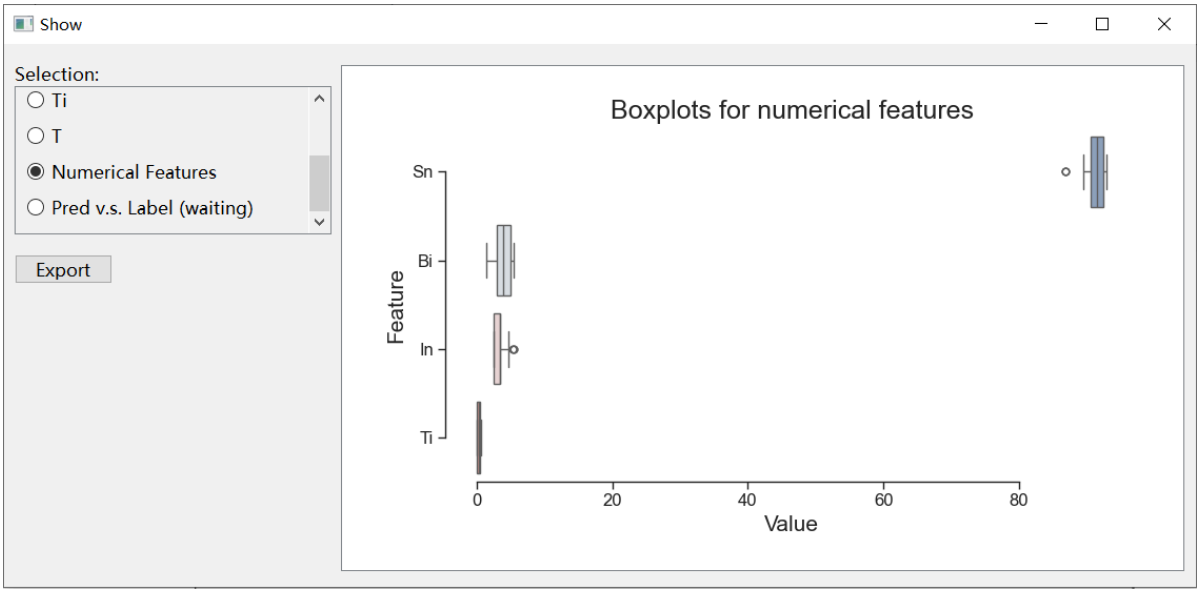
For example, this is the distribution chart of "Sn".



This is the **distribution chart of single target label**.

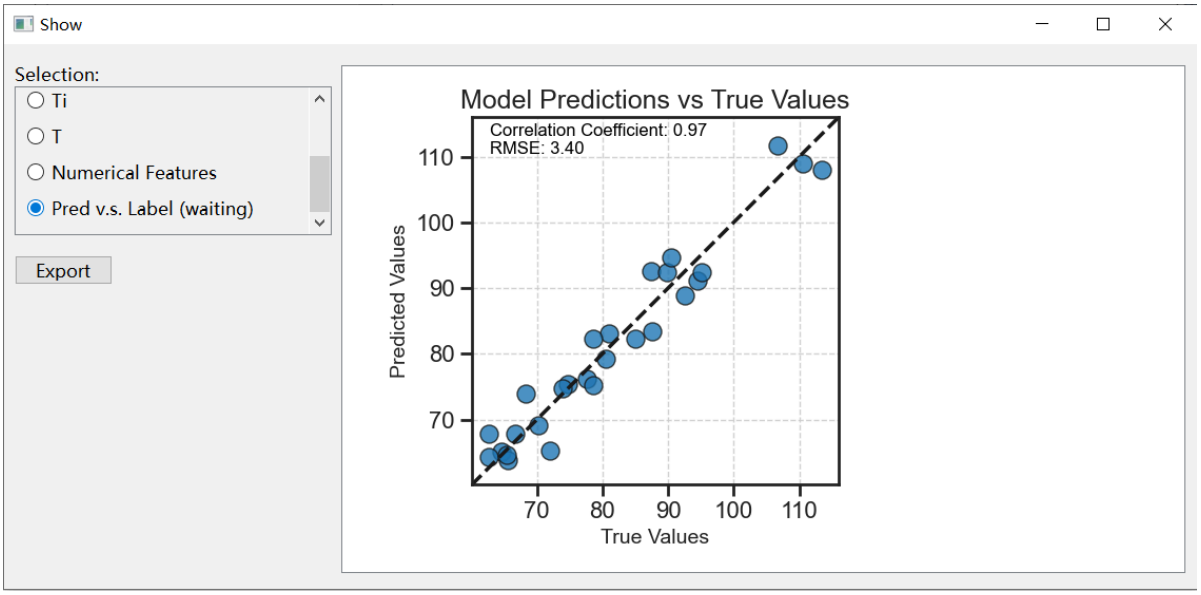


This is the **boxplots for numerical features**.

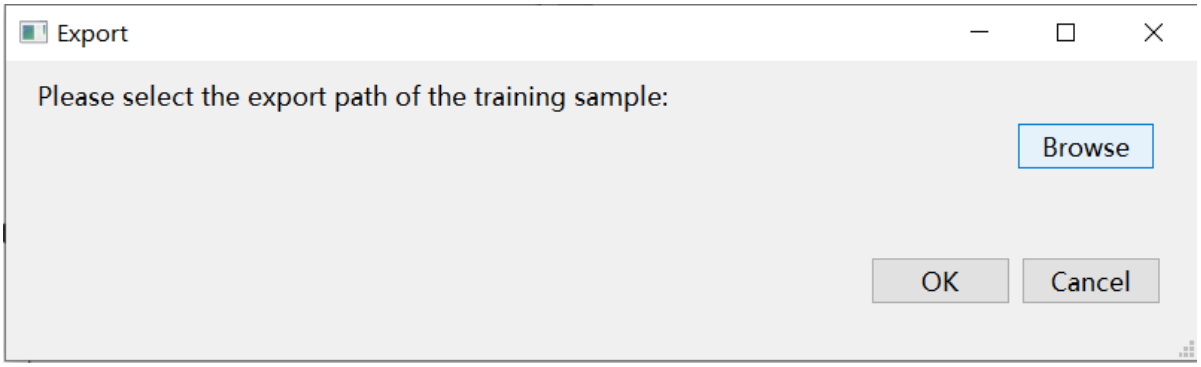


This graph uses **leave-one-out and cross-validation** to evaluate the predictive performance of a **Gaussian process regression model**, and plot a scatter plot of the model's predicted values versus the true values.

A lot of calculations will be done when you select this image, and it may **take a long time to load**.

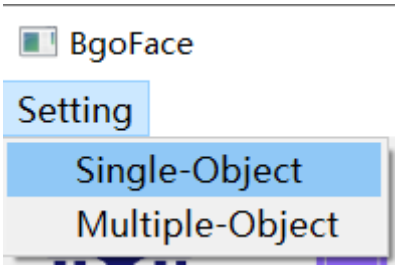


Similar to the previous operation, click the **"Export"** button to download these images to the specified folder.

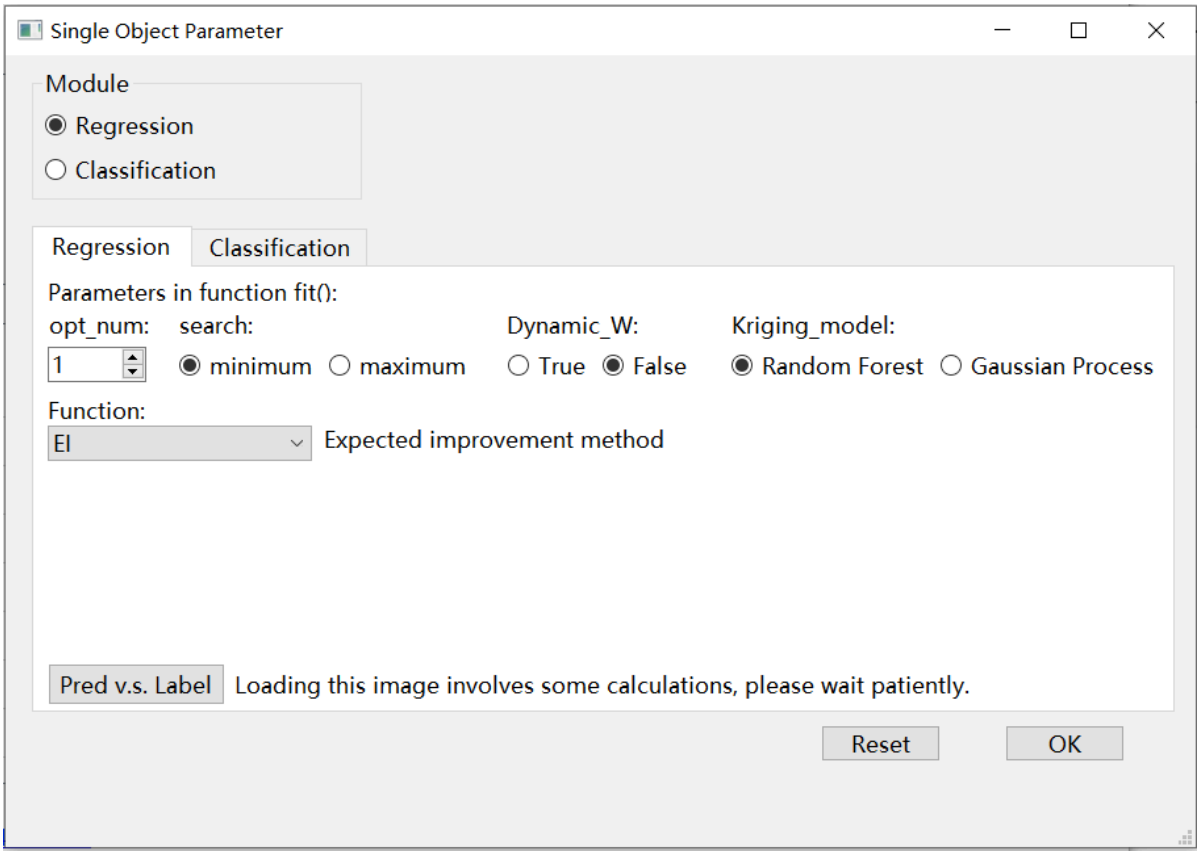


2.3Parameter setting

After obtaining the training sample and virtual sample, set the operating parameters of **single-object task**.

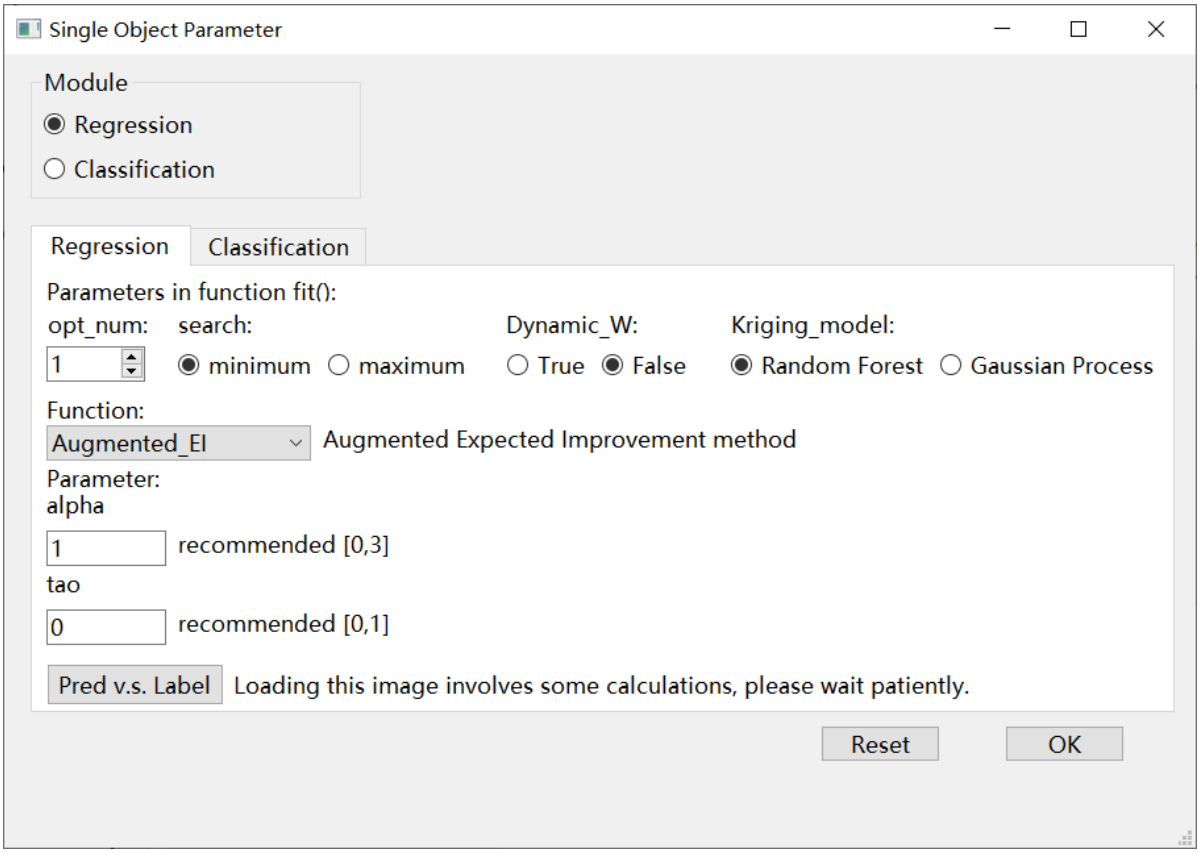


Click **"Single-Object"** in the menu bar and **set the parameters in the Single Object Parameter window**.

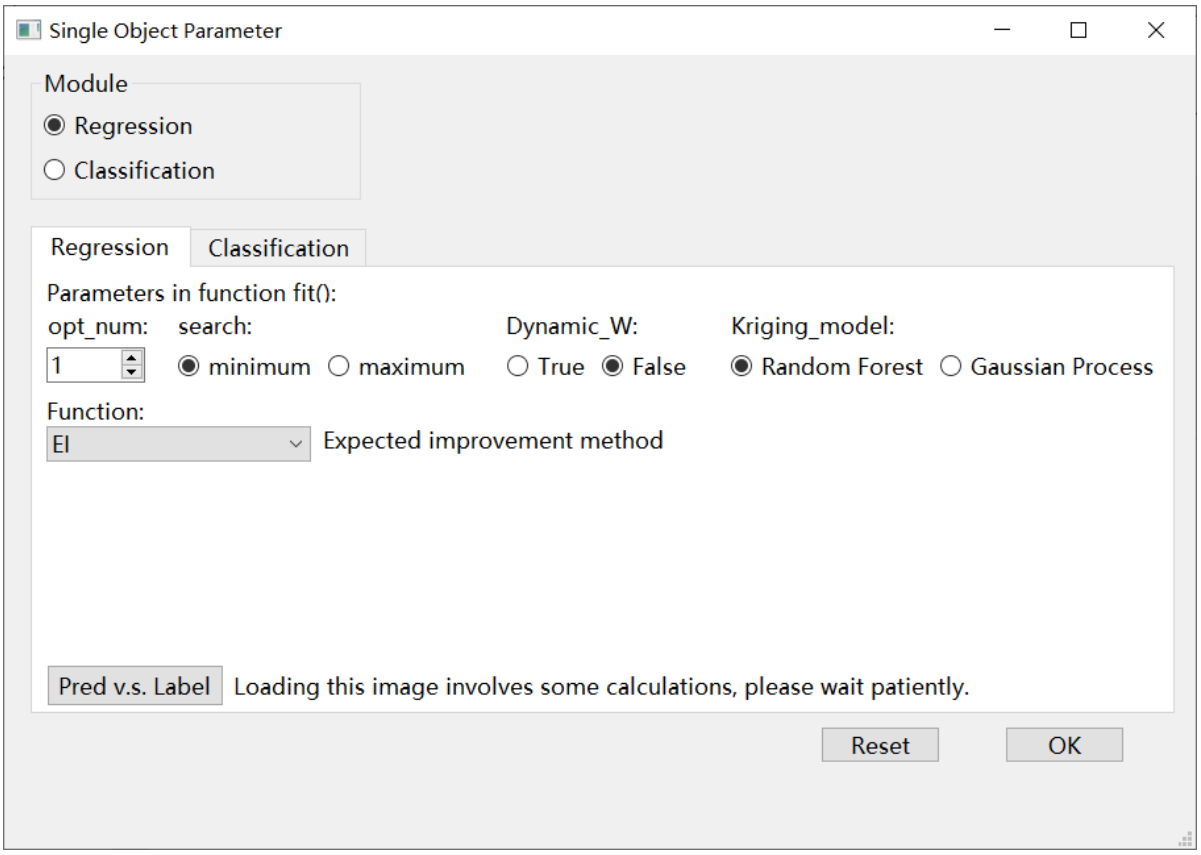


2.4Regression

Choose the **"Regression"** mode, select different functions and their corresponding parameter settings.



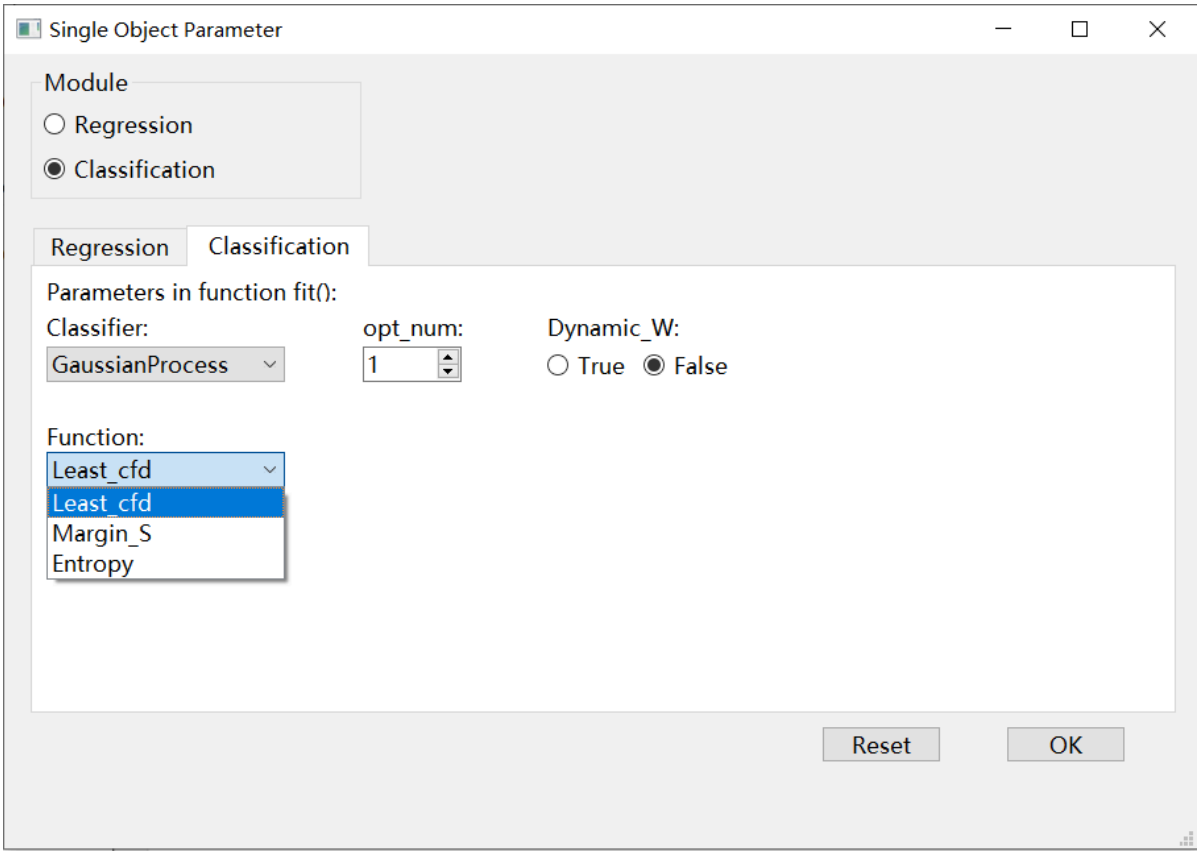
Click the **"Reset"** button and the parameters are set to default setting.



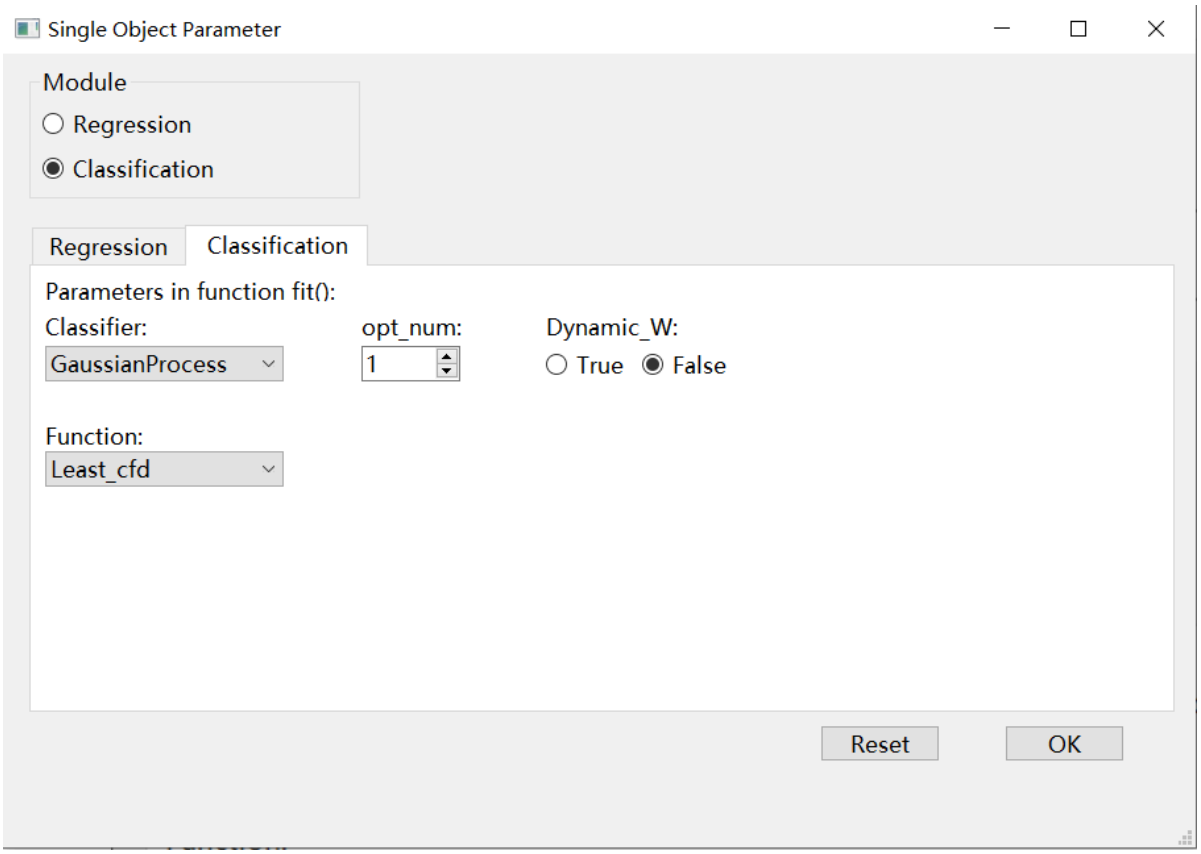
Click the "OK" button to complete the parameter setting.

2.5Classification

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



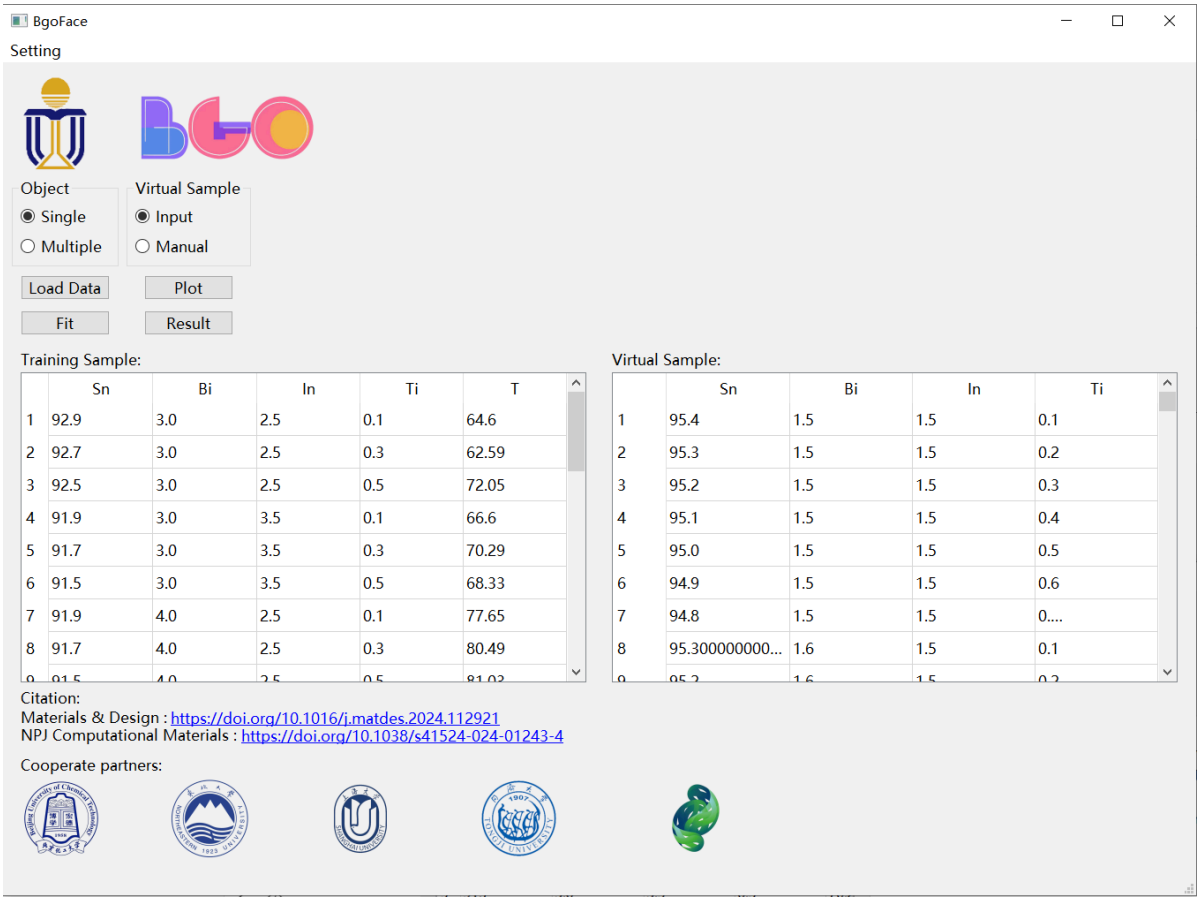
Click the **"Reset"** button and the parameters are set to default setting.

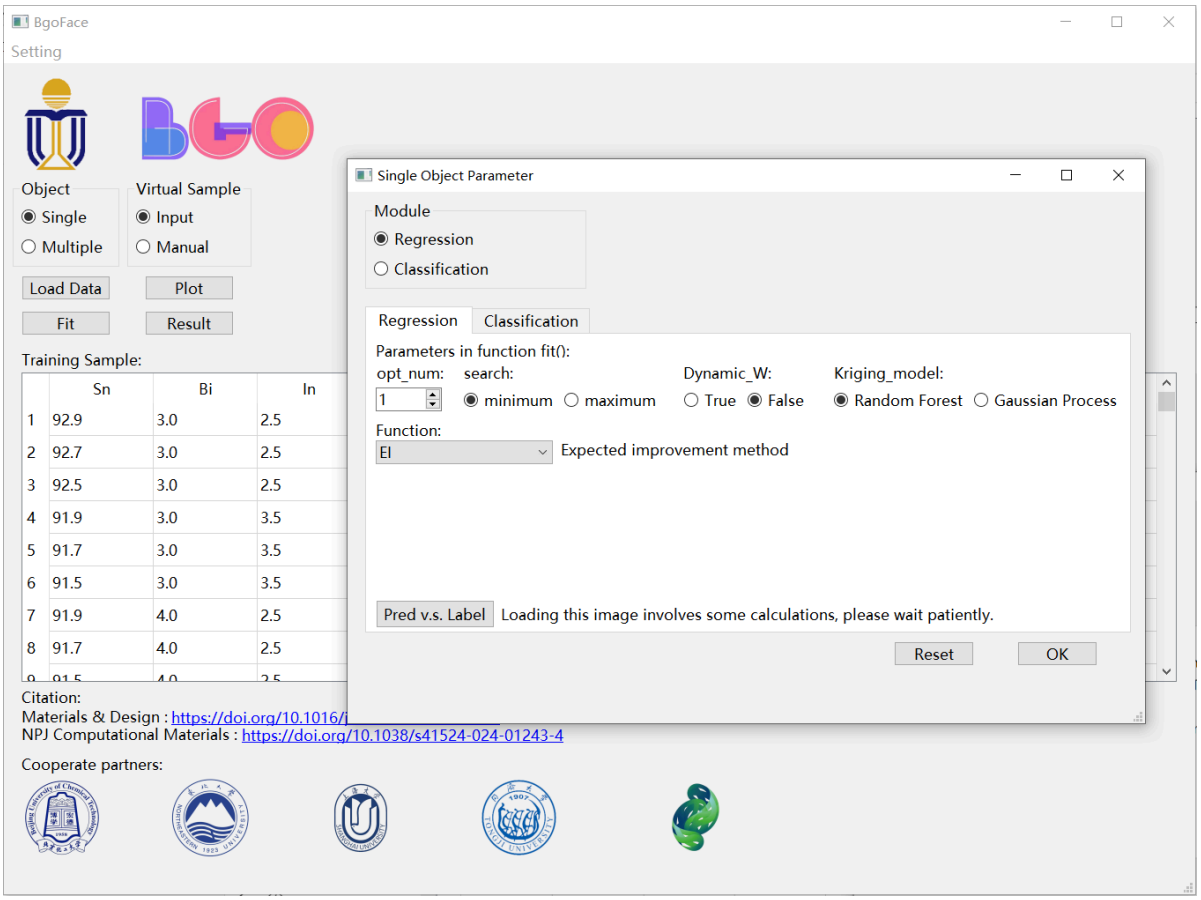


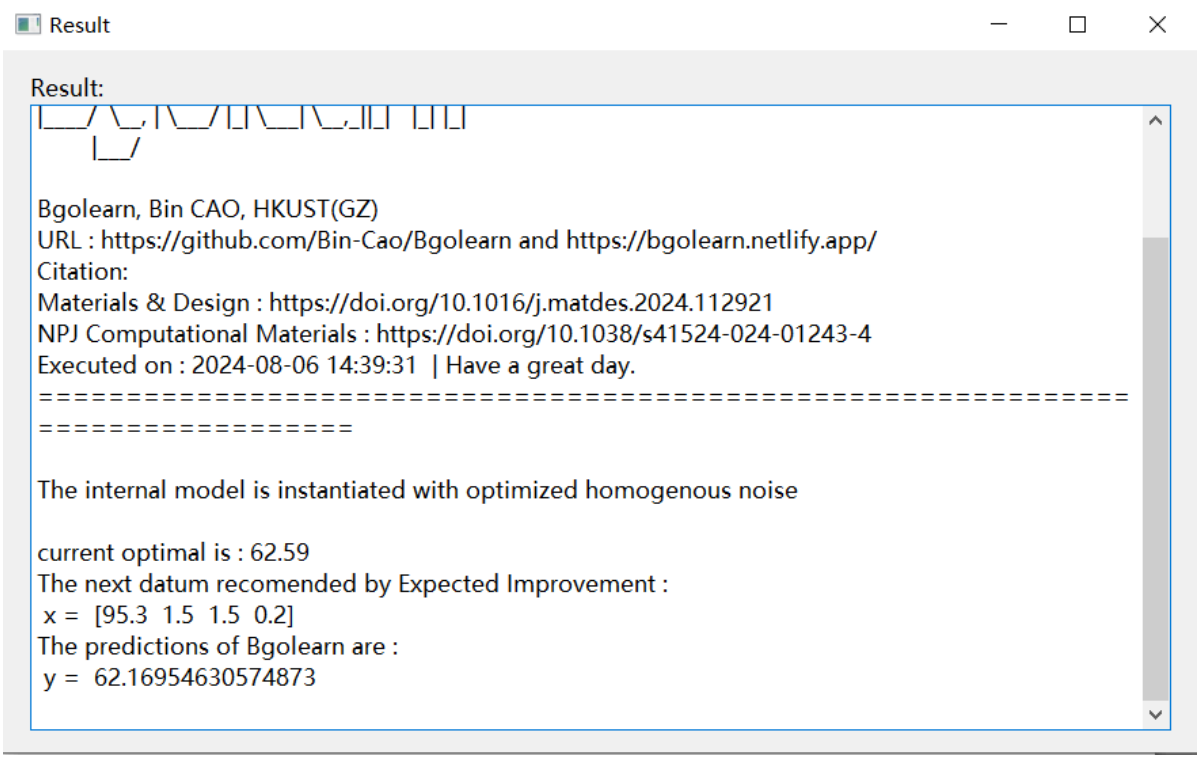
Click the "OK" button to complete the parameter setting.

2.6Fit

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





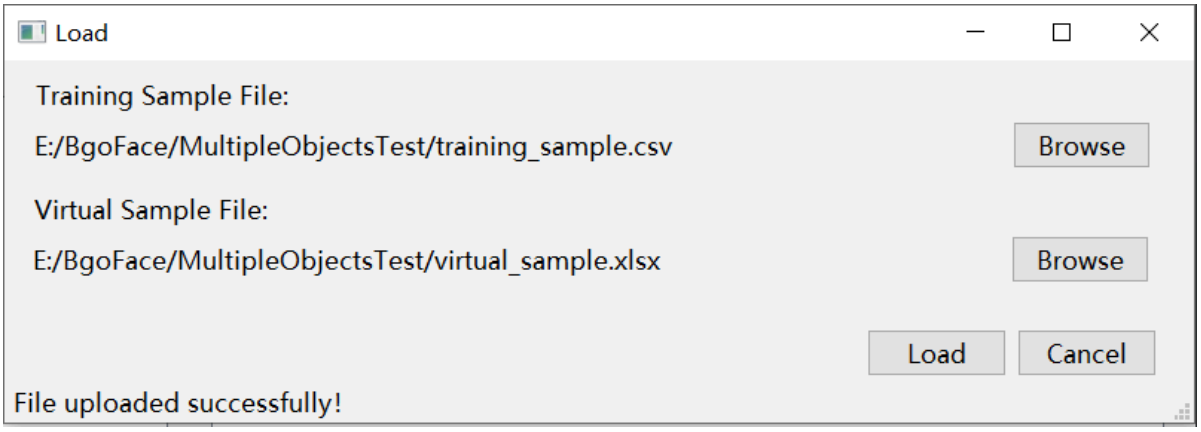


3.Multiple-object

Choose the "**Multiple-Object**" method to perform multiple-objective Bayesian global optimization.

3.1Upload training sample file and virtual sample file

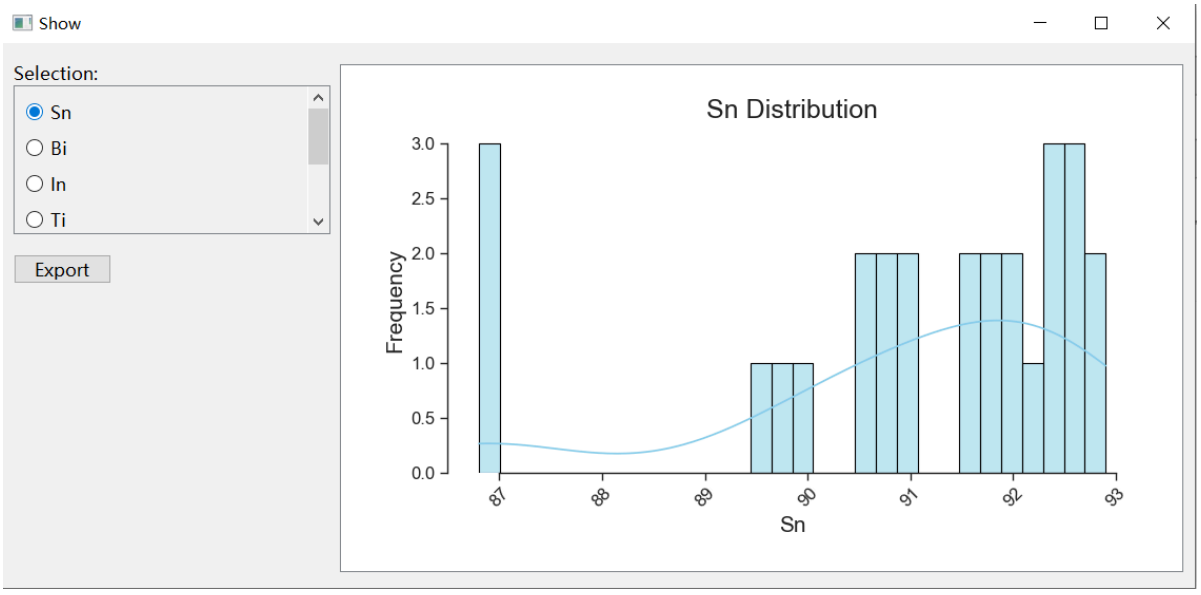
When in **"Input" mode**, click the **"Load Data"** button to display the file upload interface. Then upload training sample file and virtual sample file.



3.2Plot

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

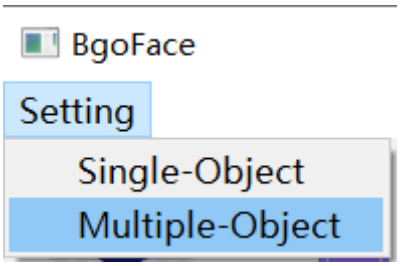
For example, this is the distribution chart of "Sn".



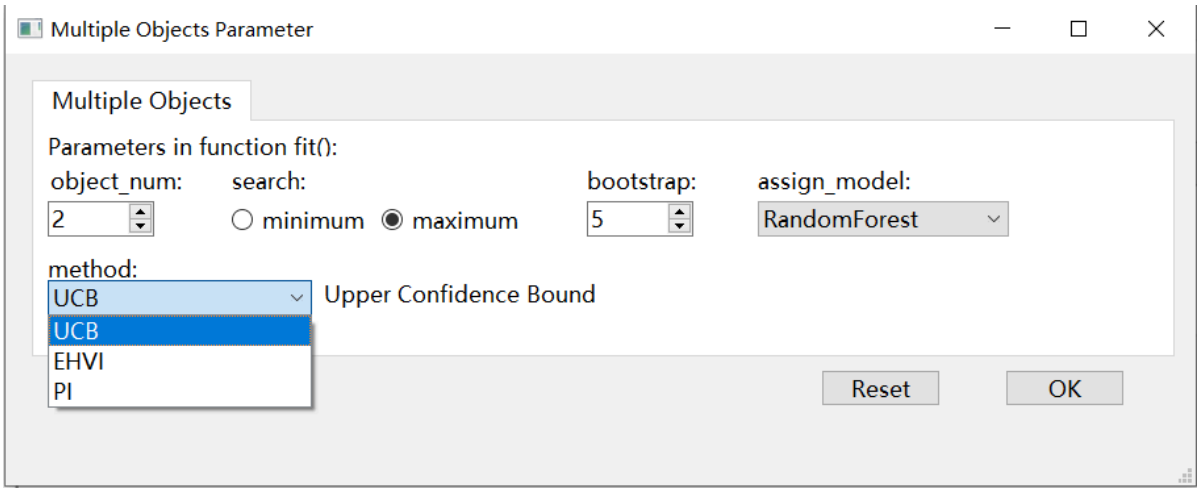
Some of the statistical characteristics here are the same as above.

3.3Parameter setting

After obtaining the training sample and virtual sample, set the operating parameters of **multiple-object task**.



Click **"Multiple-Object"** in the menu bar and **set the parameters in the Multiple Object Parameter window**.



Choose different method to perform regression tasks. And the variable object_num needs to be appropriately selected according to the target number of training sample file.

3.4Fit

Click the "Fit" button, we can see the results of multi-object regression task.