https://github.com/Bgolearn

https://bgolearn.netlify.app

BgoFace User Manual

1.Introduction

The BgoFace is the user interface of the Bgolearn Platform. This user manual describes how to use BgoFace.

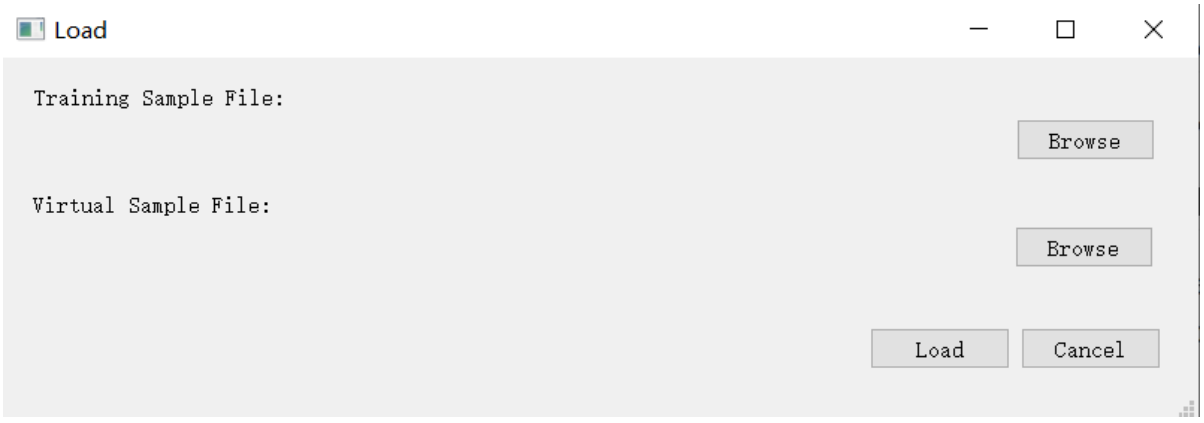
2.Upload sample file

2.1File format requirements

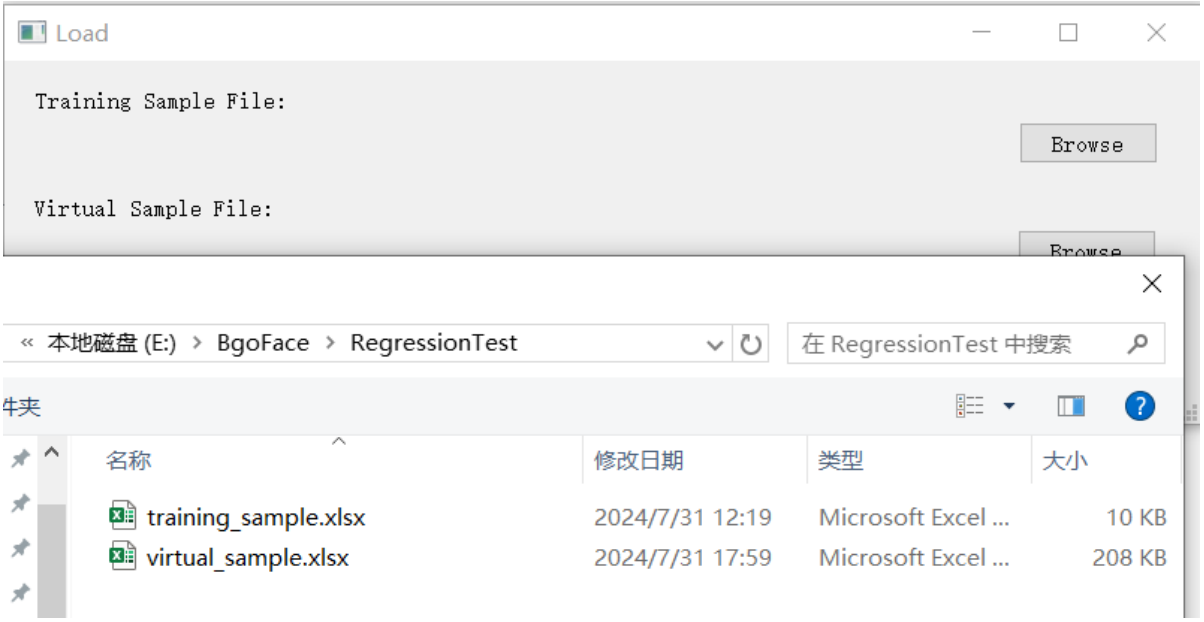
- **The training sample files and virtual sample files are Excel files with the suffix 'xls' or 'xlsx'.**
- **The last column of the training sample file is used as a single target.**

2.2Upload training sample and virtual sample

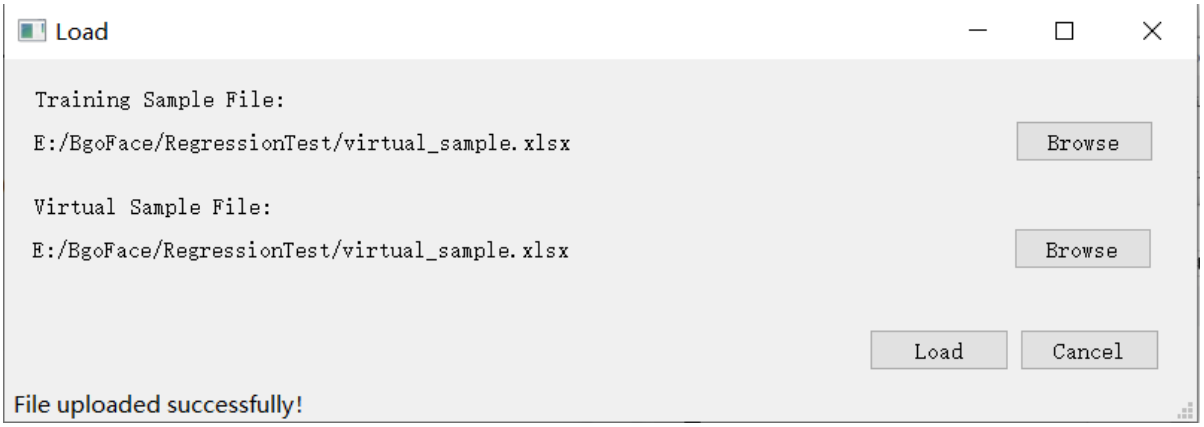
When in **"Input" mode**, click the **"Load Data"** button to display the file upload interface.



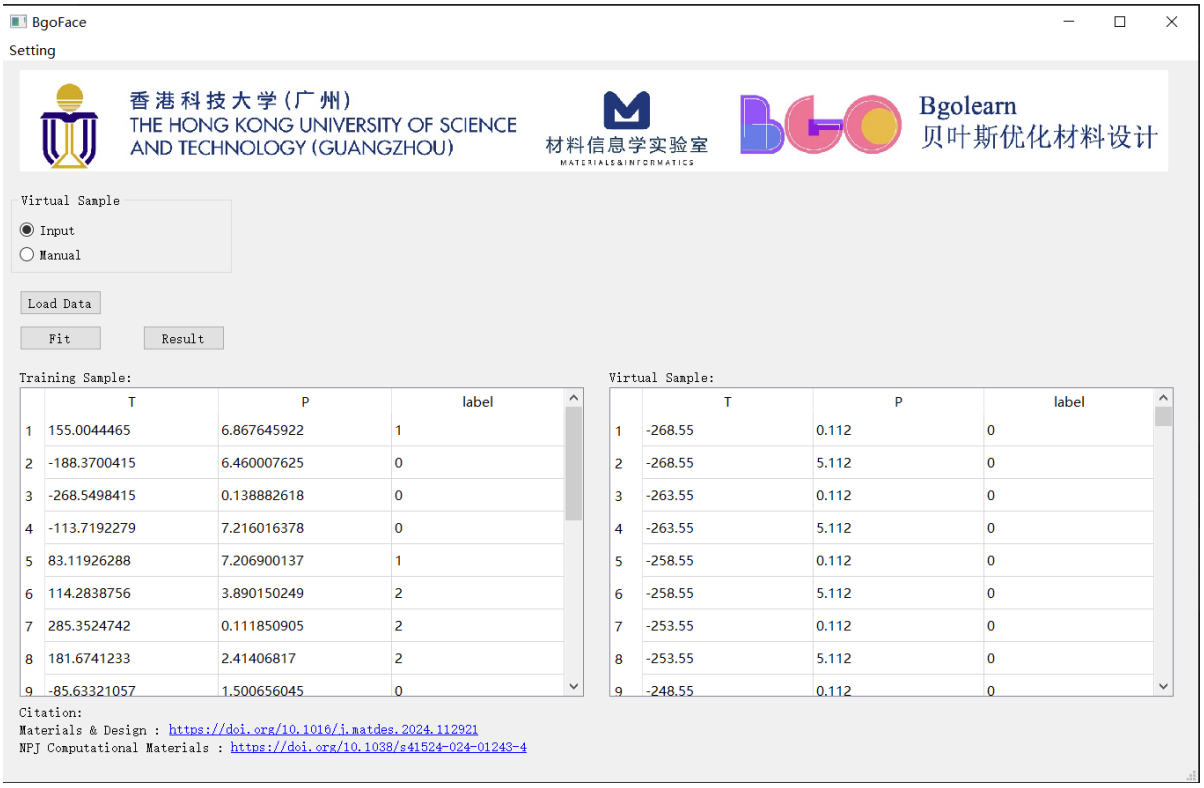
Click the **"Browse"** button to select the training sample and virtual sample files to upload.



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.



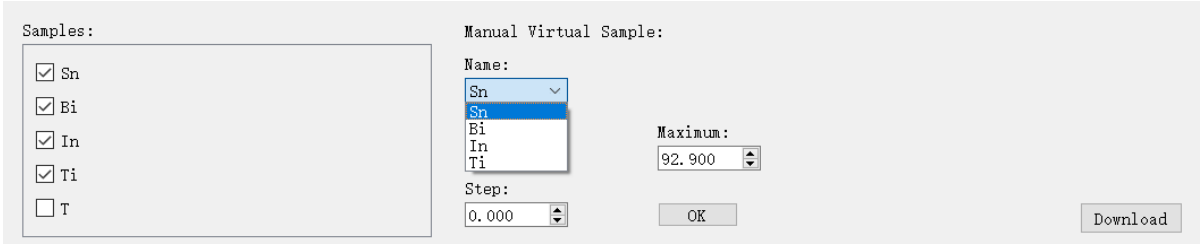
2.3Upload training sample and generate virtual sample

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

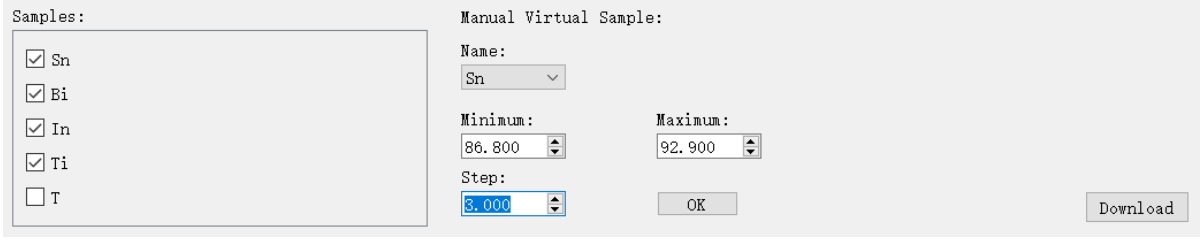
Similar to the above steps, upload and load the training sample file into the main window.

In the Samples area, you can see that all samples are selected. **Select the samples you need to create virtual samples.**

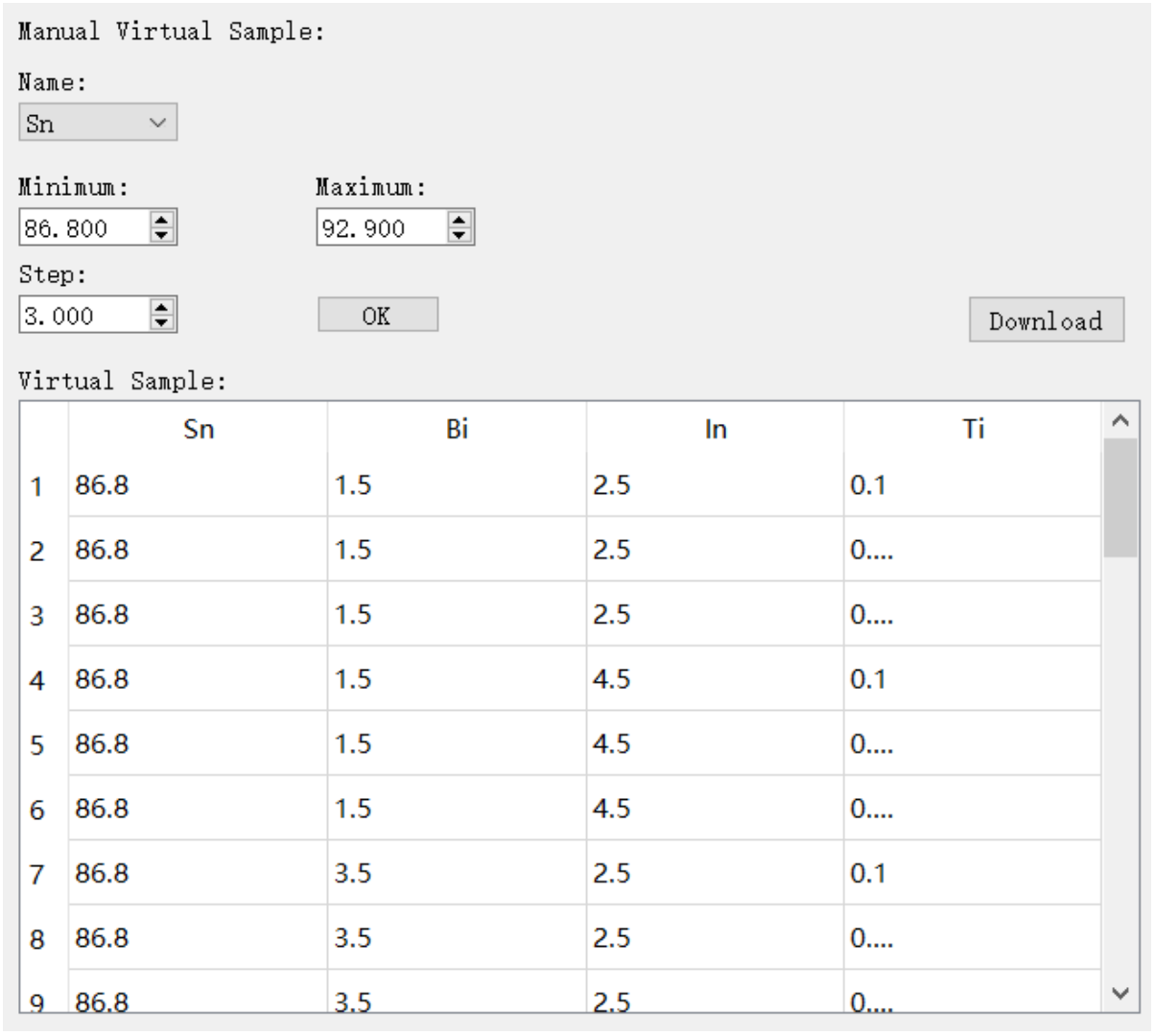
For example, "Sn", "Bi", "In" and "Ti" to generate the virtual sample.



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



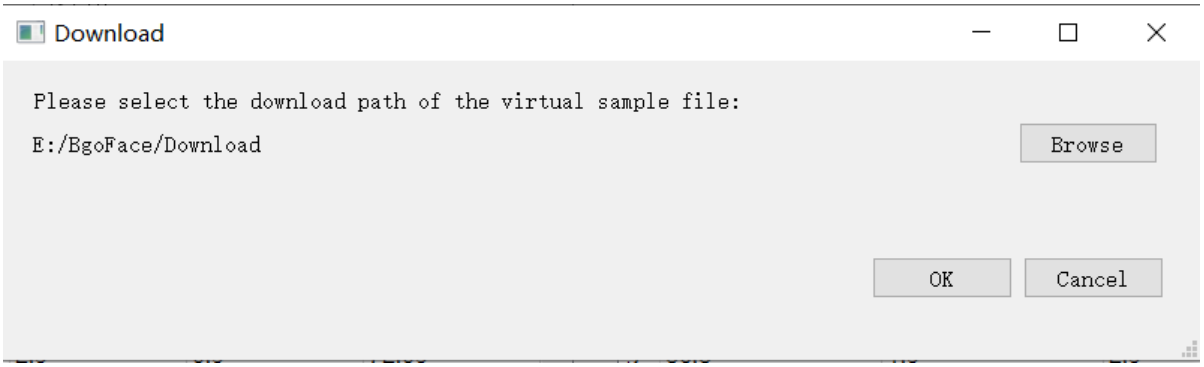
Click the "OK" button to select the next sample. When all selected samples are processed, the virtual sample is generated and displayed in the main window.



	Sn	Bi	In	Ti
1	86.8	1.5	2.5	0.1
2	86.8	1.5	2.5	0....
3	86.8	1.5	2.5	0....
4	86.8	1.5	4.5	0.1
5	86.8	1.5	4.5	0....
6	86.8	1.5	4.5	0....
7	86.8	3.5	2.5	0.1
8	86.8	3.5	2.5	0....
9	86.8	3.5	2.5	0....

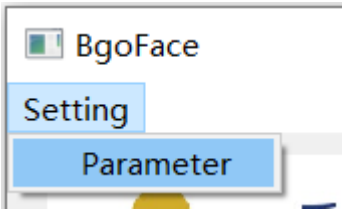
After the virtual sample is generated, click the **"Download"** button and **select the downloaded folder to download the virtual sample.**

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

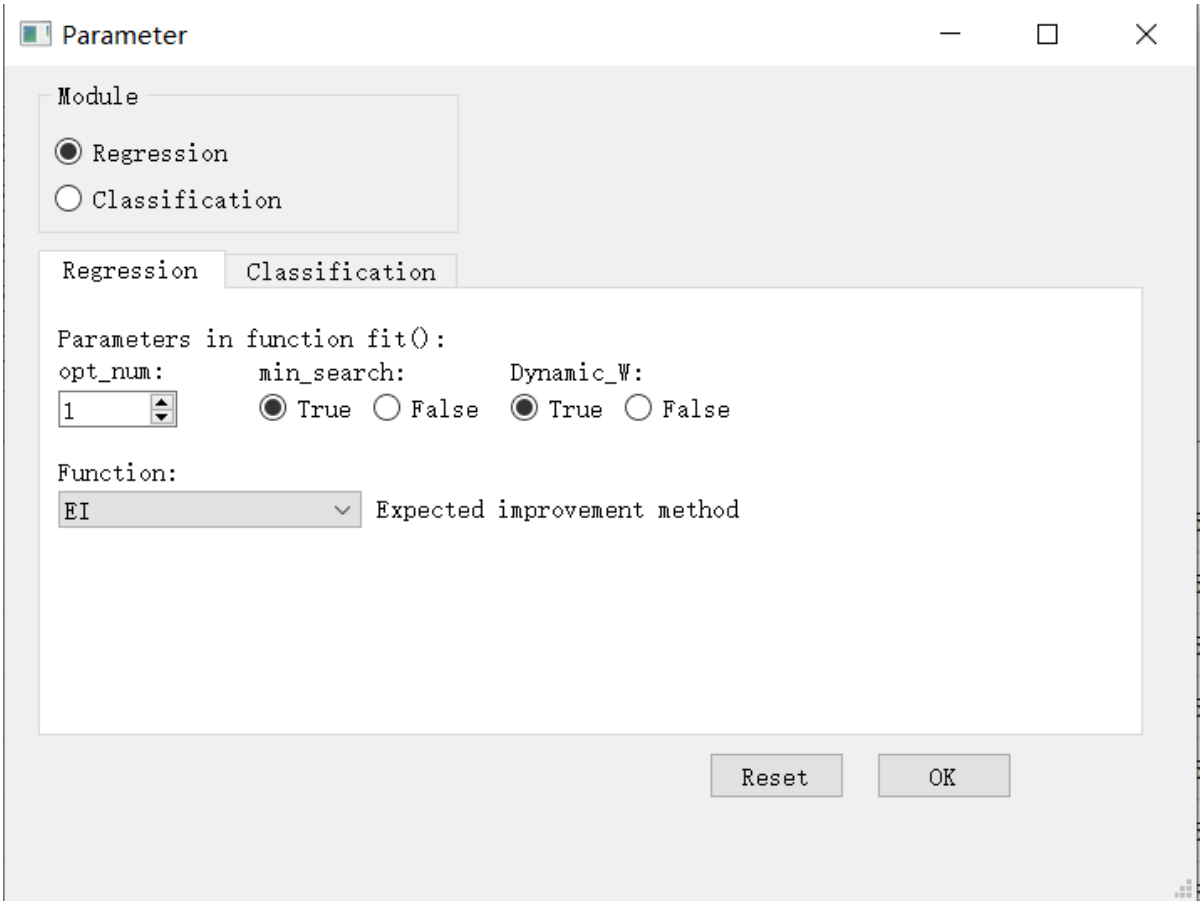


3.Parameter setting

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

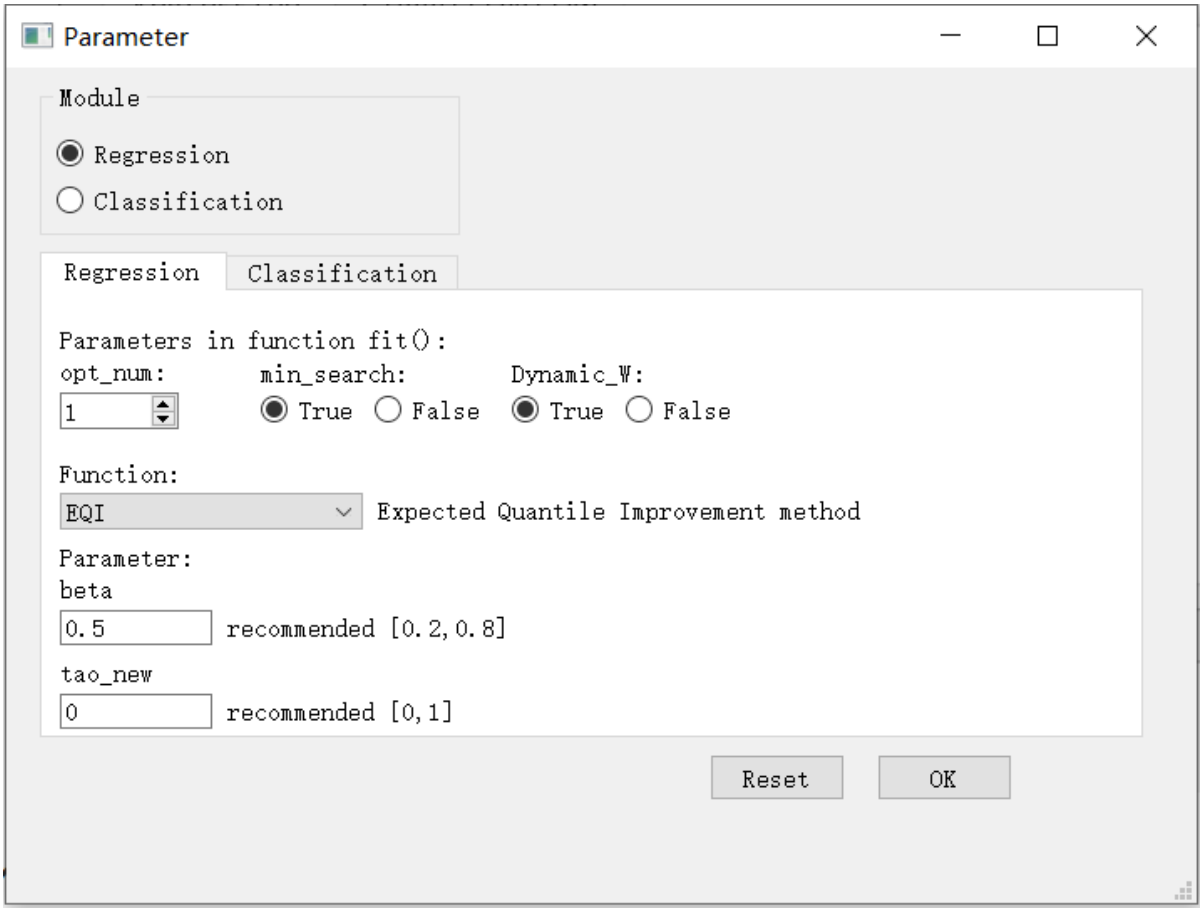


Click **"Parameter"** in the menu bar and **set the parameters in the Parameter window**.

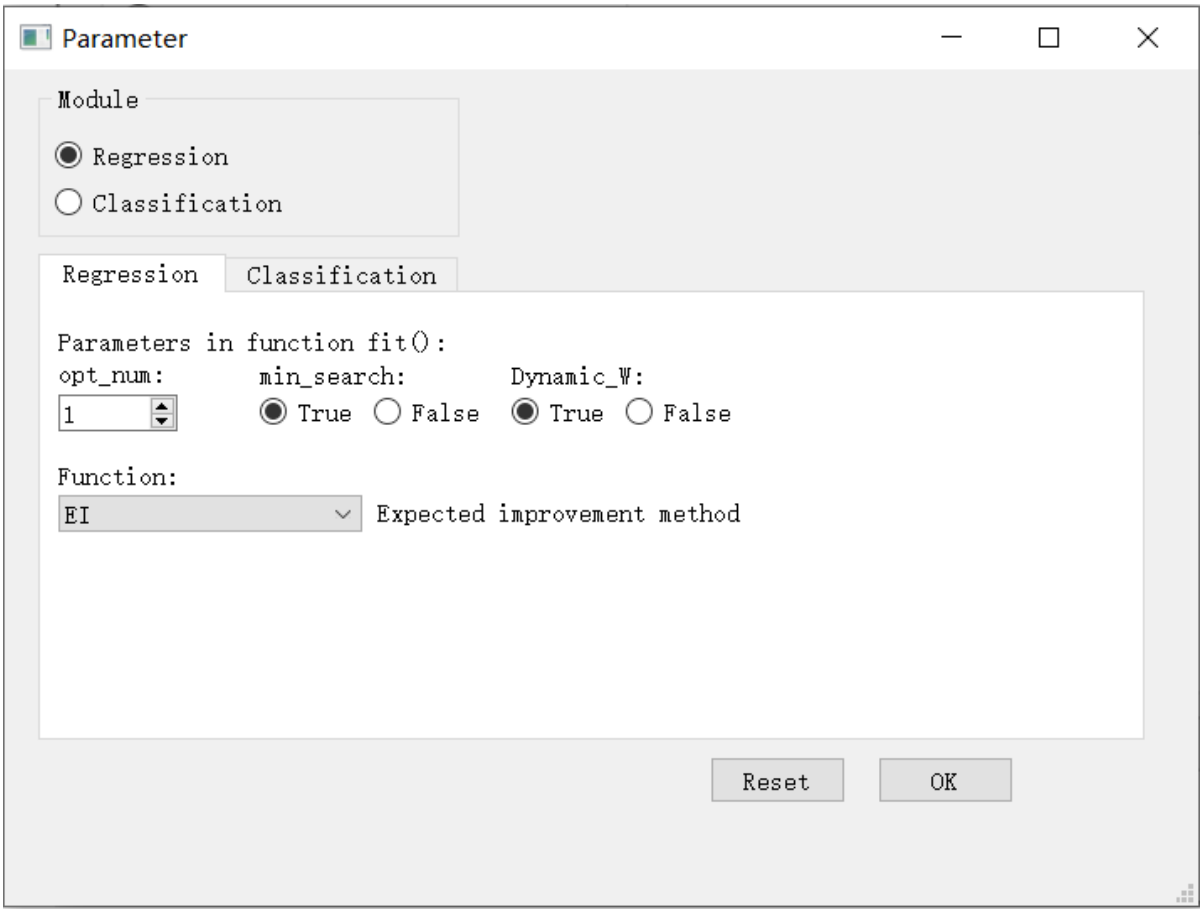


3.1Regression

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



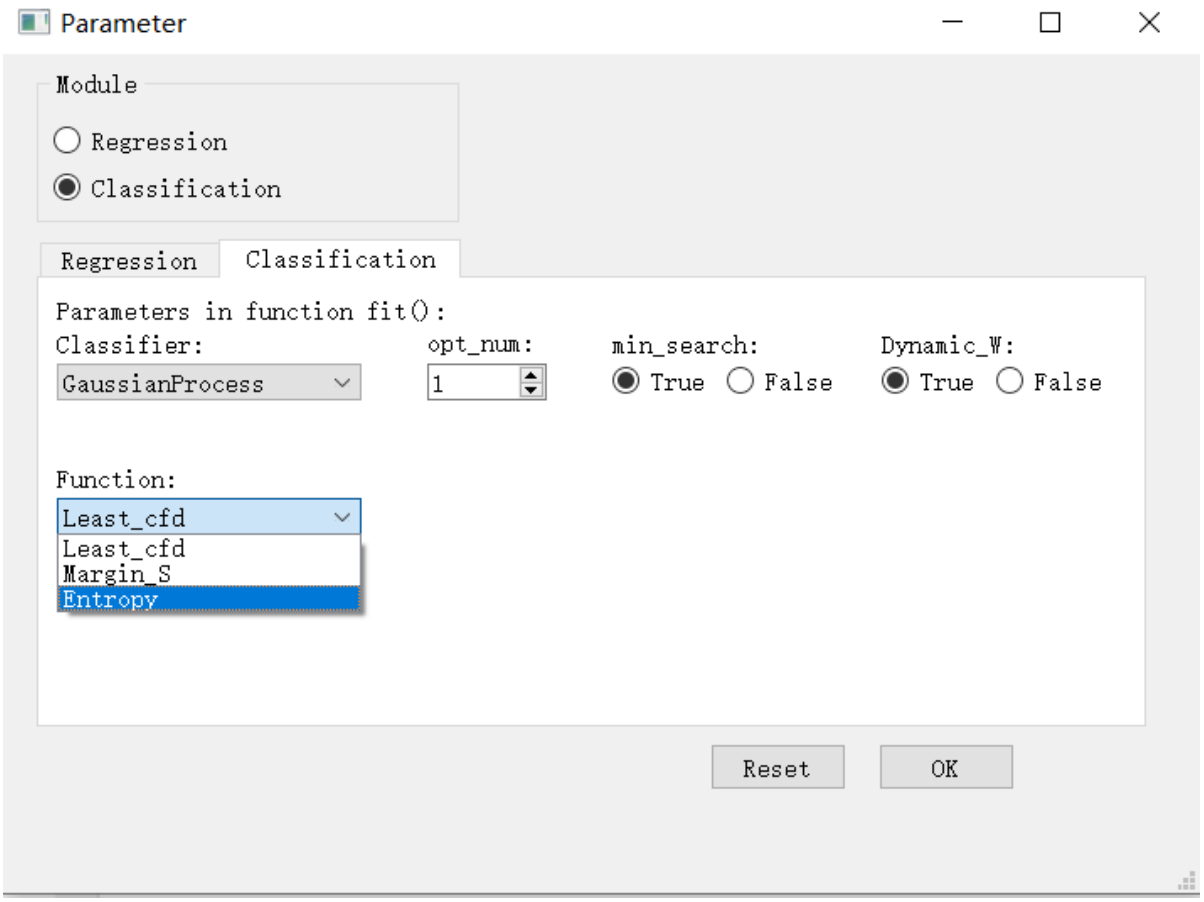
Click the **"Reset"** button and the parameters are set to default setting.



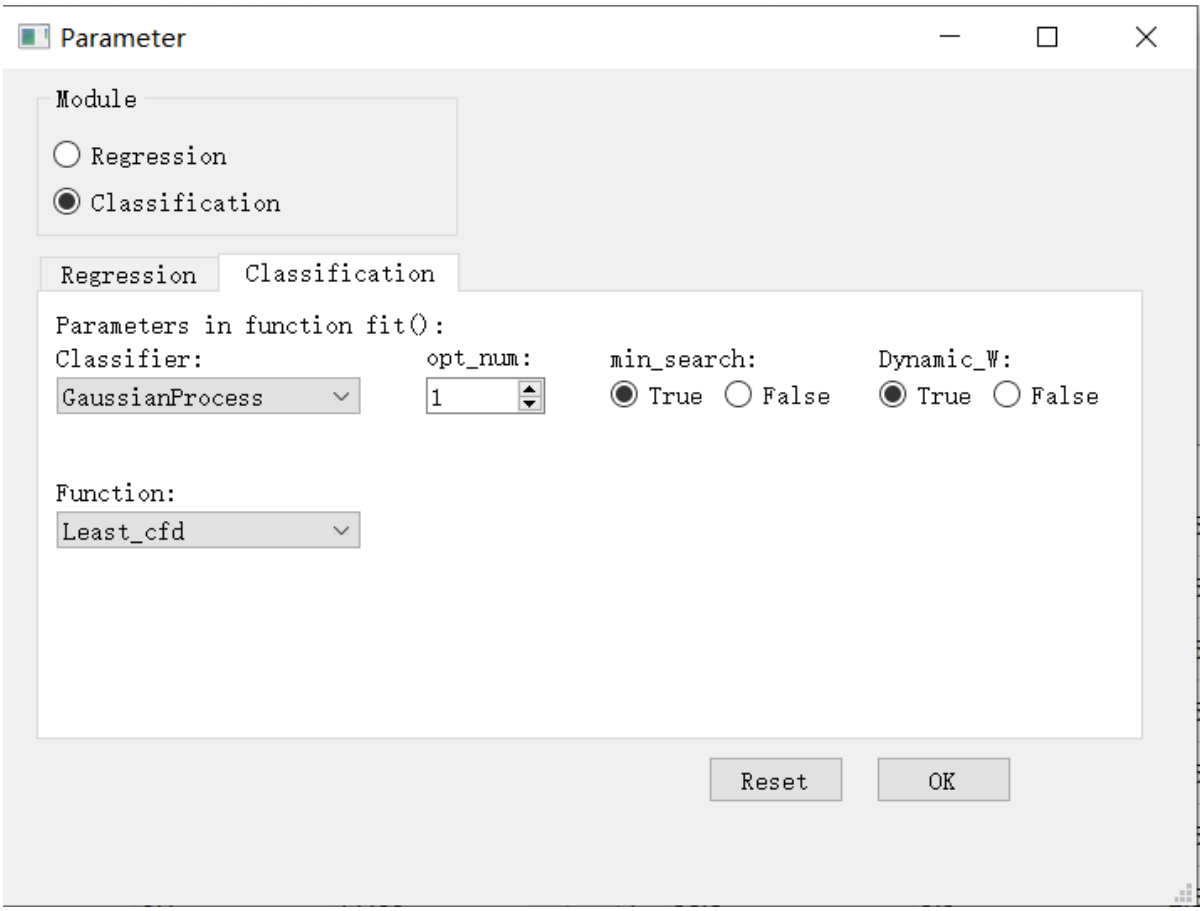
Click the "OK" button to complete the parameter setting.

3.2Classification

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



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



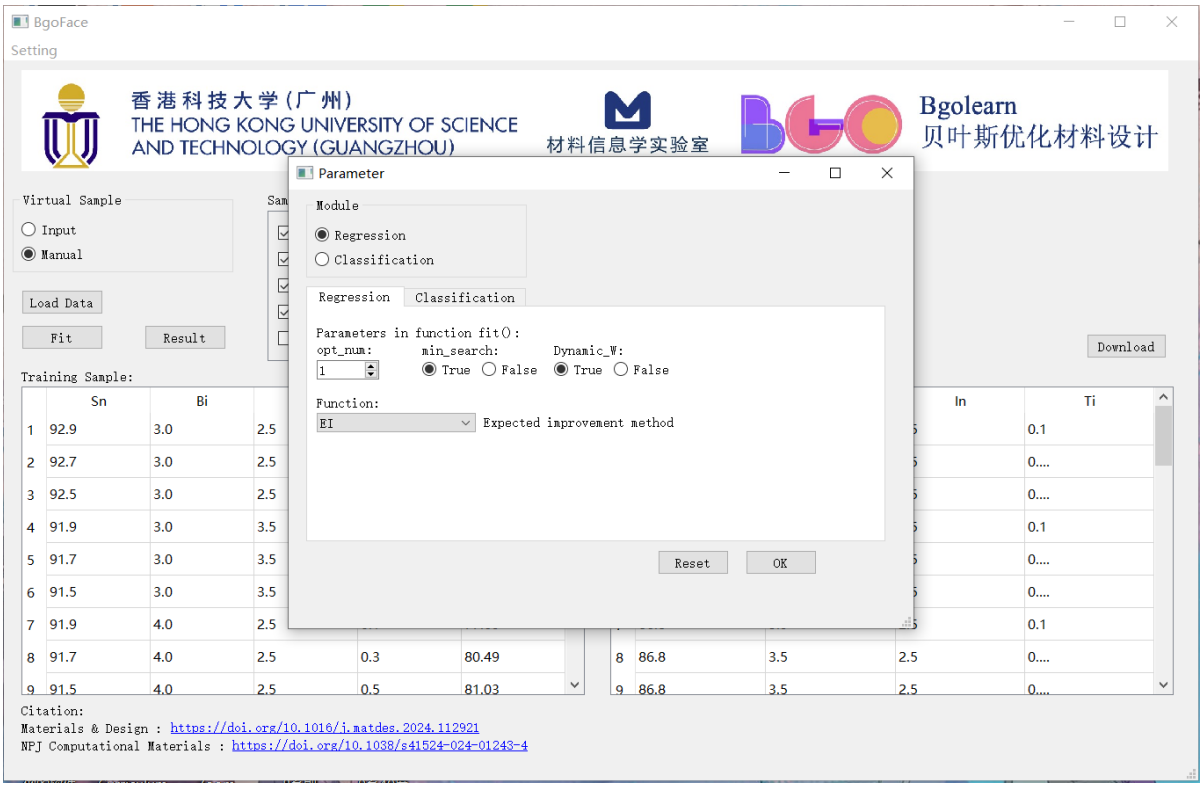
Click the "OK" button to complete the parameter setting.

4.Fit

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

	Sn	Bi	In	Ti	T
1	92.9	3.0	2.5	0.1	64.6
2	92.7	3.0	2.5	0.3	62.59
3	92.5	3.0	2.5	0.5	72.05
4	91.9	3.0	3.5	0.1	66.6
5	91.7	3.0	3.5	0.3	70.29
6	91.5	3.0	3.5	0.5	68.33
7	91.9	4.0	2.5	0.1	77.65
8	91.7	4.0	2.5	0.3	80.49
9	91.5	4.0	2.5	0.5	81.03

	Sn	Bi	In	Ti
1	86.8	1.5	2.5	0.1
2	86.8	1.5	2.5	0....
3	86.8	1.5	2.5	0....
4	86.8	1.5	4.5	0.1
5	86.8	1.5	4.5	0....
6	86.8	1.5	4.5	0....
7	86.8	3.5	2.5	0.1
8	86.8	3.5	2.5	0....
9	86.8	3.5	2.5	0....


BgoFace
Setting
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材料信息学实验室
Bgolearn
贝叶斯优化材料设计
Parameter
Module
Regression
Classification
Regression
Classification
Parameters in function fit():
opt_num:
min_search:
Dynamic_W:
True
False
True
False
Function:
EI
Expected improvement method
Reset
OK
Virtual Sample
Input
Manual
Load Data
Fit
Result
Download
Training Sample:
Sn
Bi
In
Ti
Citation:
Materials & Design : https://doi.org/10.1016/j.matdes.2024.112921
NPJ Computational Materials : https://doi.org/10.1038/s41524-024-01243-4


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材料信息学实验室
Bgolearn
贝叶斯优化材料设计
Result
Result:
current optimal is : 62.59
The next datum recomended by Expected Improvement :
x = [89.8 1.5 2.5 0.3]
The predictions of Bgolearn are :
y = 65.5175300927587
Virtual Sample
Input
Manual
Load Data
Fit
Result
Download
Training Sample:
Sn
Bi
Ti
Citation:
Materials & Design : https://doi.org/10.1016/j.matdes.2024.112921
NPJ Computational Materials : https://doi.org/10.1038/s41524-024-01243-4