

BgoFace User Manual

1.Introduction

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

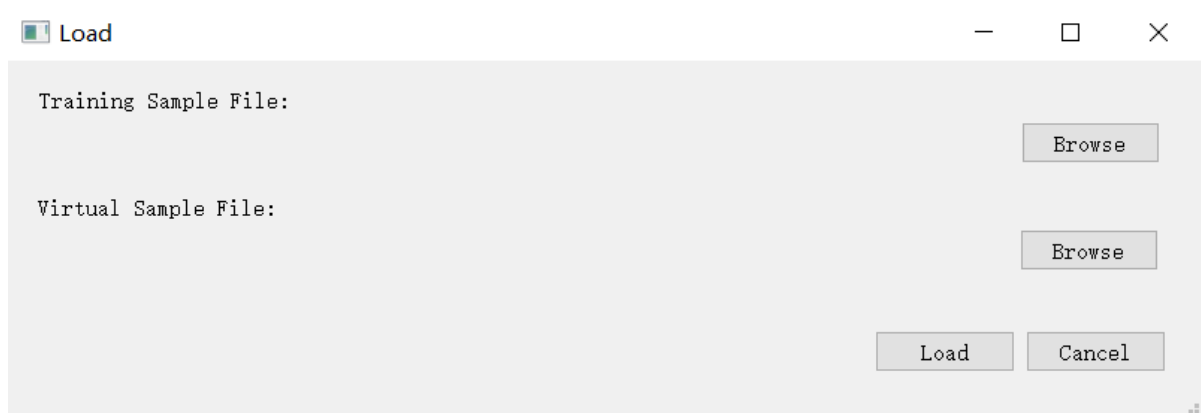
2.Upload sample file

2.1File format requirements

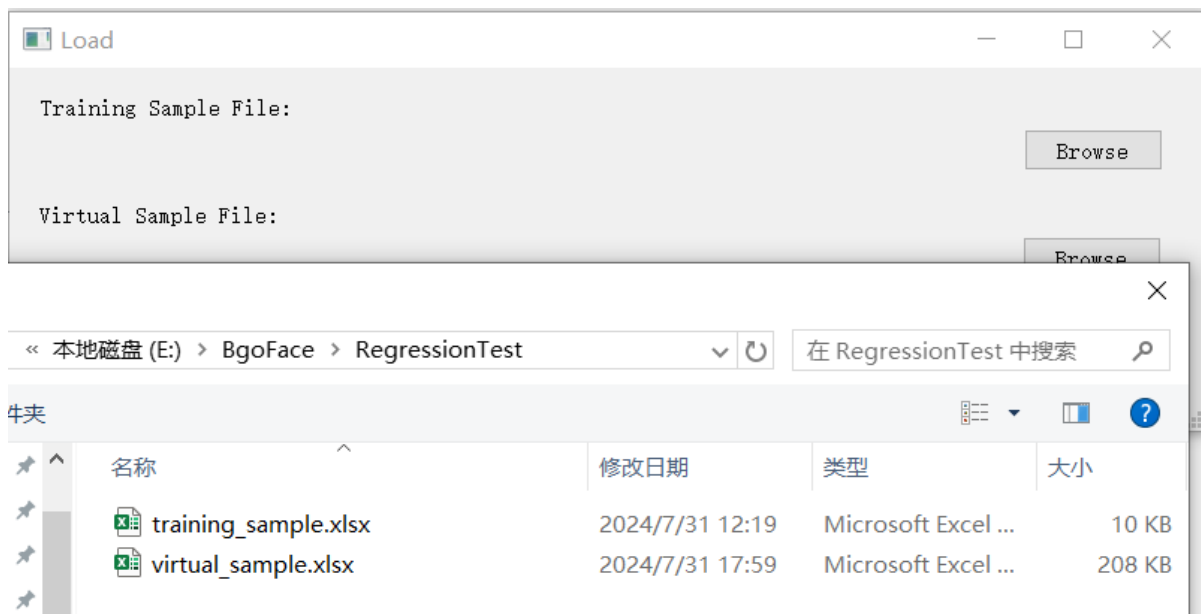
- The training sample files and virtual sample files are Excel files with the suffix 'xls' or 'xlsx'.
- The last column of the training sample file is used as a single target.

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.

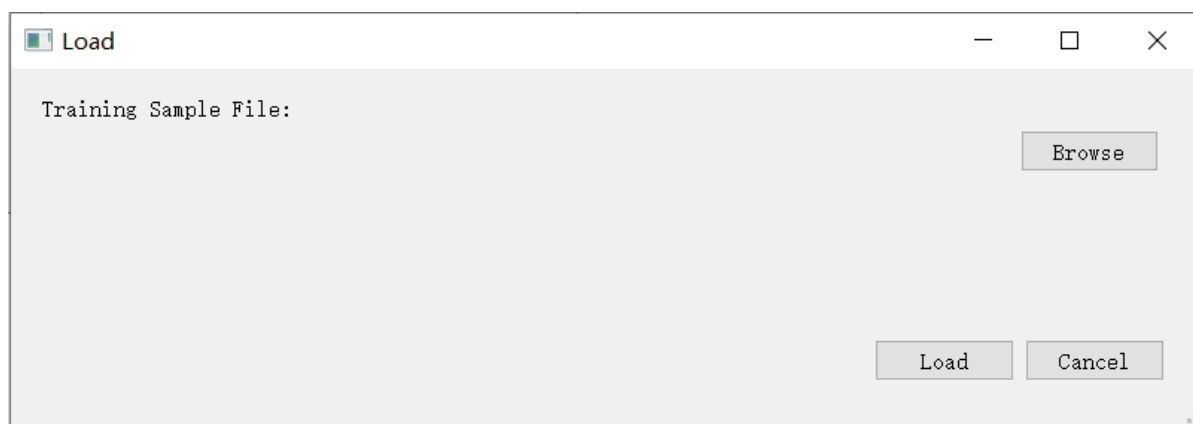


Click the "**Load**" button and the files will be loaded into the main window.



2.3 Upload 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.

BgoFace
Setting



香港科技大学(广州)
THE HONG KONG UNIVERSITY OF SCIENCE
AND TECHNOLOGY (GUANGZHOU)



材料信息学实验室
MATERIALS INFORMATICS



Bgolearn
贝叶斯优化材料设计

Virtual Sample

☐ Input

☒ Manual

Load Data

Fit

Result

Samples:

☒ Sn

☒ Bi

☒ In

☒ Ti

☒ T

Manual Virtual Sample:

Name: Sn

Minimum: 86.800

Maximum: 92.900

Step: 0.000

OK

Download

Training Sample:

	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

Citation:
Materials & Design : <https://doi.org/10.1016/j.matdes.2024.112921>
NPJ Computational Materials : <https://doi.org/10.1038/s41524-024-01243-4>

Virtual Sample:

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.

Samples:

☒ Sn

☒ Bi

☒ In

☒ Ti

☐ T

Manual Virtual Sample:

Name: Sn

Maximum: 92.900

Step: 0.000

OK

Download

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

Samples:

☒ Sn

☒ Bi

☒ In

☒ Ti

☐ T

Manual Virtual Sample:

Name: Sn

Minimum: 86.800

Maximum: 92.900

Step: 3.000

OK

Download

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.

Manual Virtual Sample:

Name:

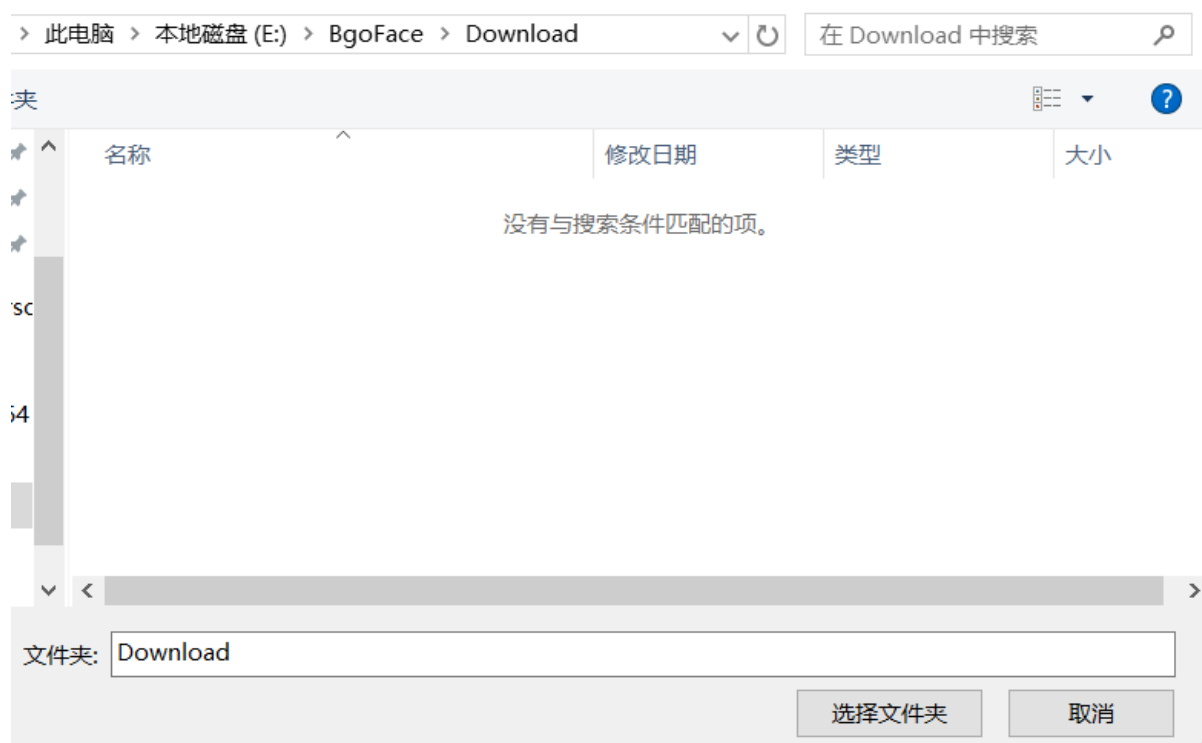
Minimum: Maximum:

Step:

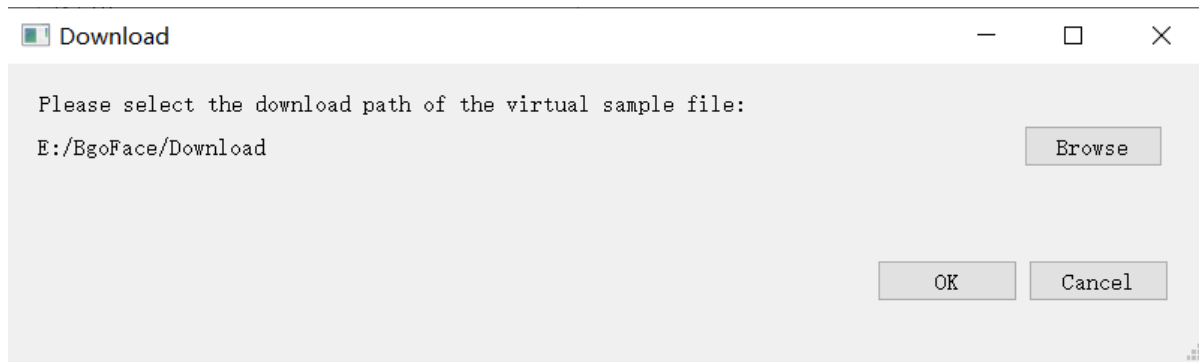
Virtual Sample:

	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.**

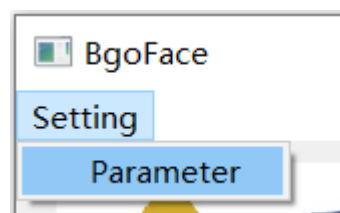


Click the **"OK"** button to **download the virtual sample to the specified folder.**

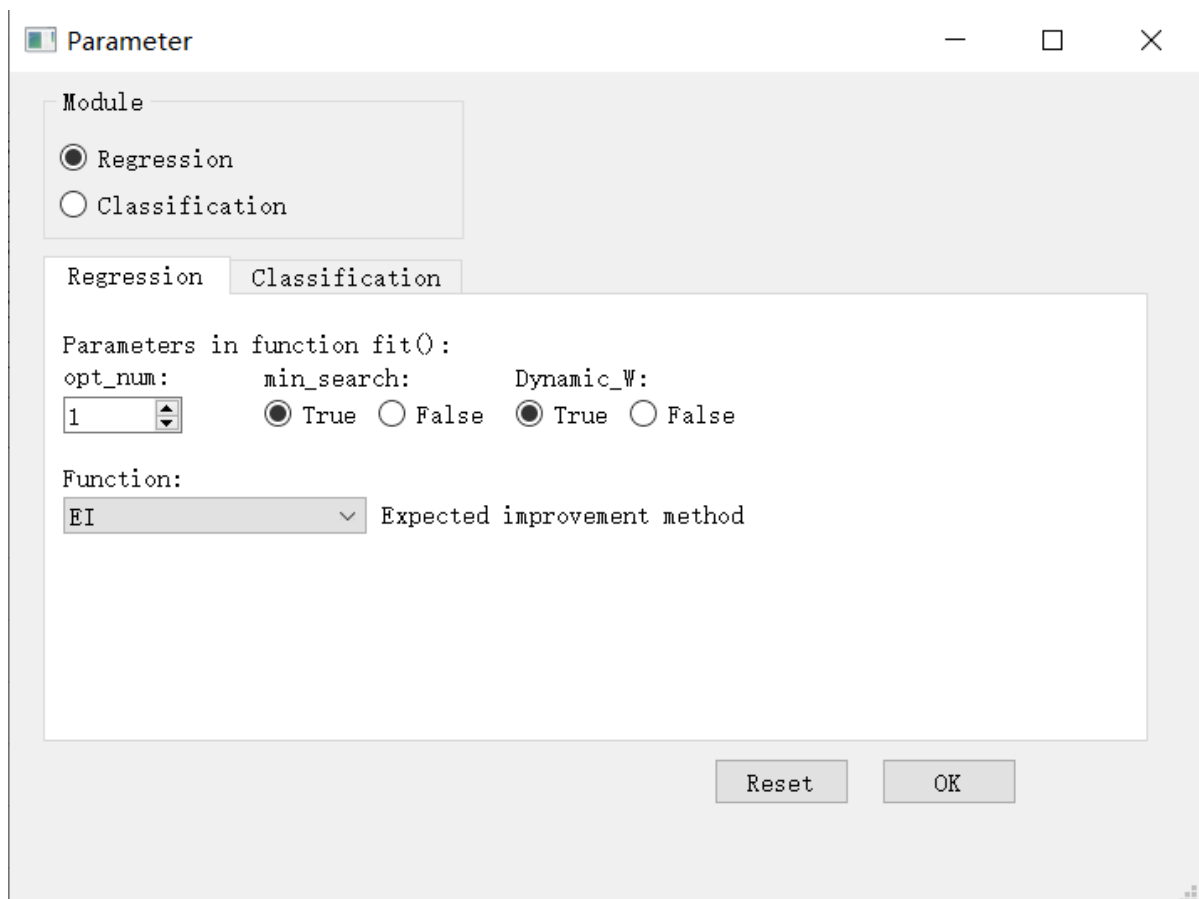


3.Parameter setting

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

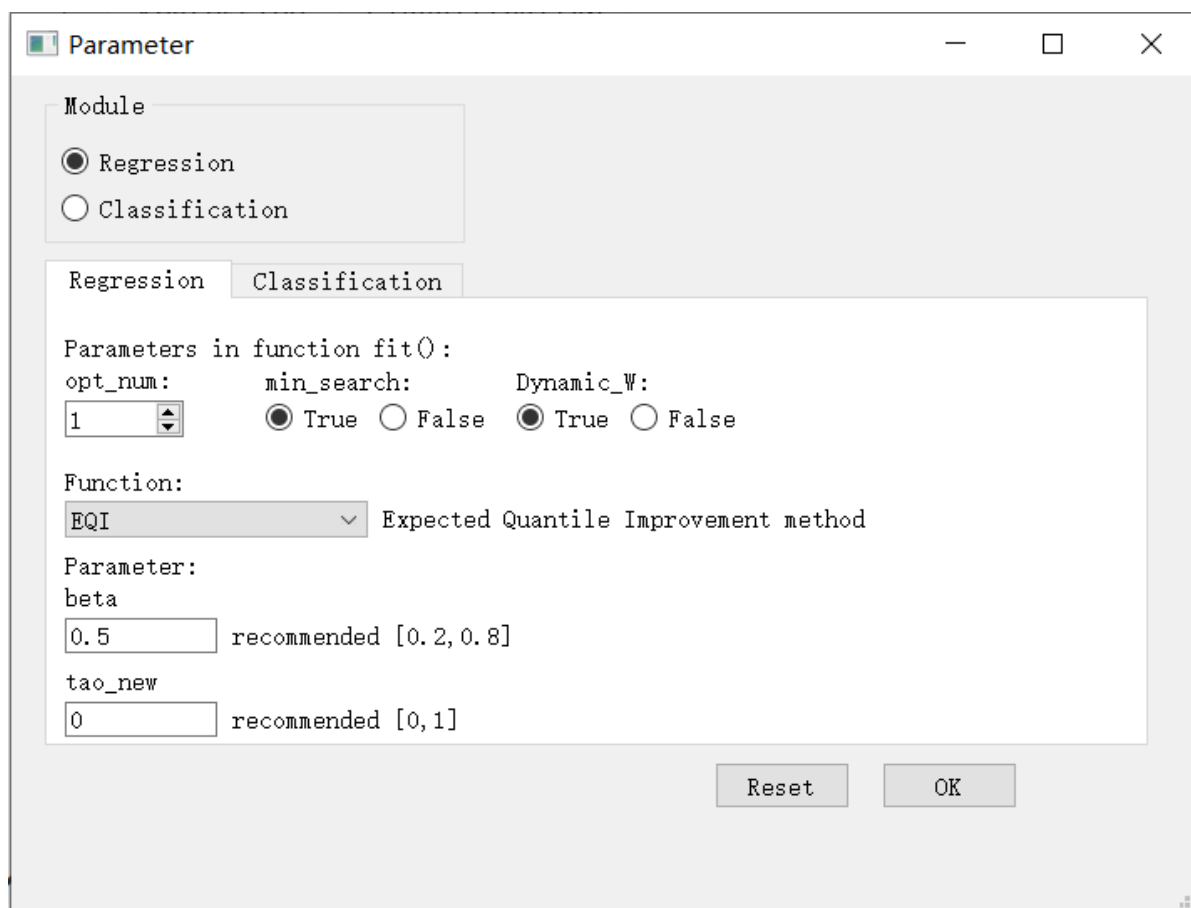


Click "**Parameter**" in the menu bar and **set the parameters in the Parameter window**.



3.1Regression

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



The dialog box is titled "Parameter" and has standard window controls (minimize, maximize, close). It contains a "Module" section with two radio buttons: "Regression" (selected) and "Classification". Below this are two tabs: "Regression" (active) and "Classification". The "Parameters in function fit():" section contains three settings: "opt_num" is a spinner box set to "1"; "min_search" has two radio buttons, "True" (selected) and "False"; "Dynamic_W" has two radio buttons, "True" (selected) and "False". The "Function:" section has a dropdown menu set to "EQI" with the text "Expected Quantile Improvement method" to its right. The "Parameter:" section has two entries: "beta" with a text box set to "0.5" and the text "recommended [0.2, 0.8]" to its right; and "tao_new" with a text box set to "0" and the text "recommended [0,1]" to its right. At the bottom right are "Reset" and "OK" buttons.

Module

☒ Regression
☐ Classification

Regression Classification

Parameters in function fit():

opt_num: min_search: Dynamic_W:

1 ☒ True ☐ False ☒ True ☐ False

Function:

EQI Expected Quantile Improvement method

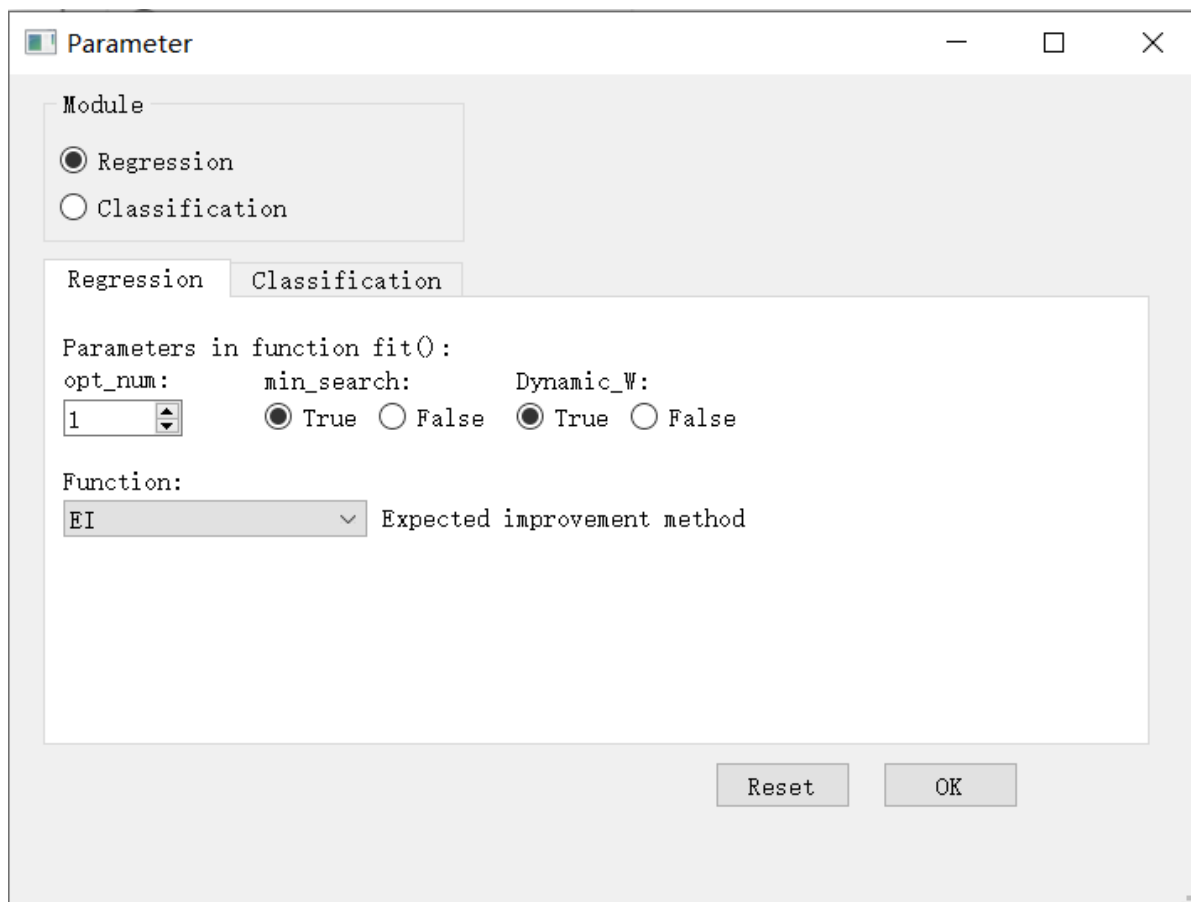
Parameter:

beta
0.5 recommended [0.2, 0.8]

tao_new
0 recommended [0,1]

Reset OK

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



The dialog box is titled "Parameter" and has standard window controls (minimize, maximize, close). It contains a "Module" section with two radio buttons: "Regression" (selected) and "Classification". Below this are two tabs: "Regression" (active) and "Classification". The "Parameters in function fit():" section contains three settings: "opt_num" is a spinner box set to "1"; "min_search" has two radio buttons, "True" (selected) and "False"; "Dynamic_W" has two radio buttons, "True" (selected) and "False". The "Function:" section has a dropdown menu set to "EI" with the text "Expected improvement method" to its right. The "Parameter:" section is empty. At the bottom right are "Reset" and "OK" buttons.

Module

☒ Regression
☐ Classification

Regression Classification

Parameters in function fit():

opt_num: min_search: Dynamic_W:

1 ☒ True ☐ False ☒ True ☐ False

Function:

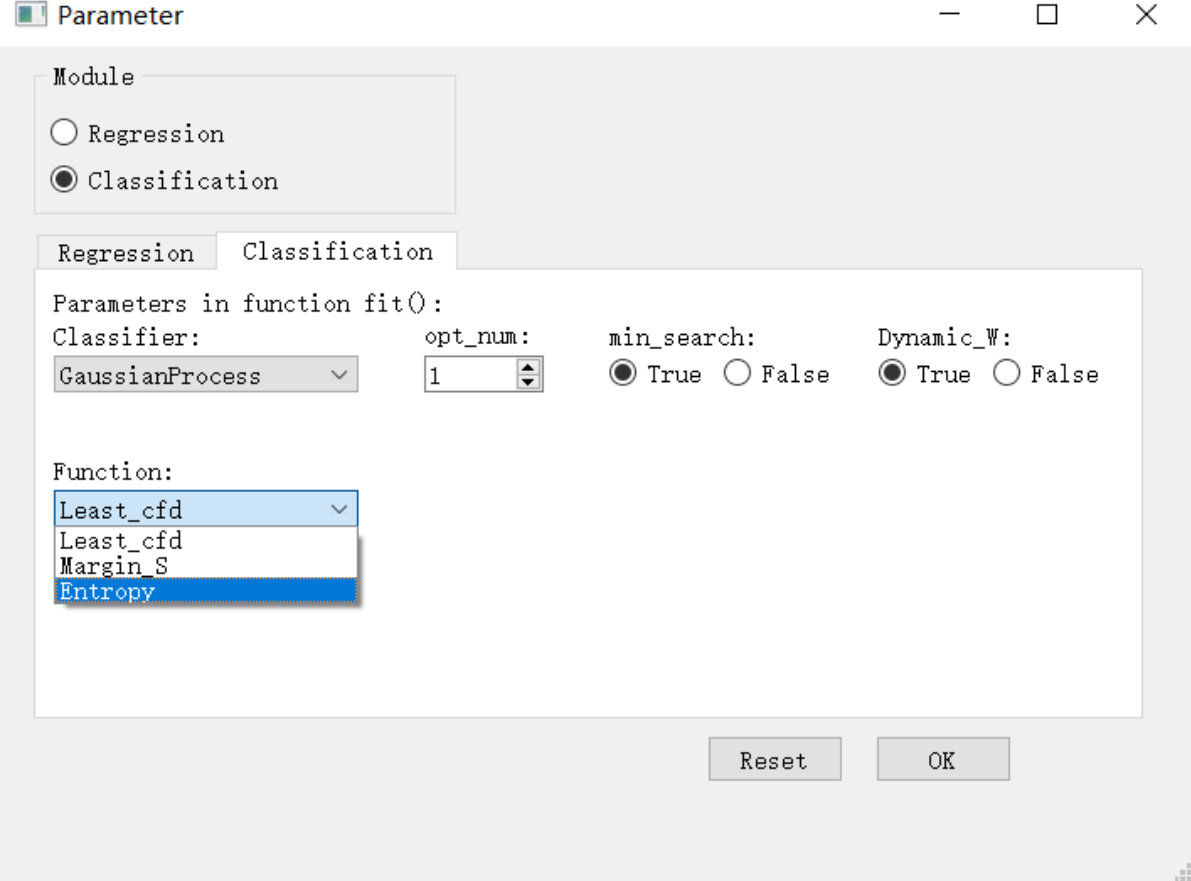
EI Expected improvement method

Reset OK

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

3.2 Classification

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



The image shows a software window titled "Parameter" with standard window controls (minimize, maximize, close). Inside, there's a "Module" section with two radio buttons: "Regression" and "Classification", with "Classification" selected. Below this are two tabs: "Regression" and "Classification", with "Classification" active. The main area is titled "Parameters in function fit():" and contains four settings: "Classifier:" with a dropdown menu showing "GaussianProcess"; "opt_num:" with a numeric spinner set to "1"; "min_search:" with two radio buttons "True" (selected) and "False"; and "Dynamic_W:" with two radio buttons "True" (selected) and "False". At the bottom left, there's a "Function:" label above a dropdown menu that is open, showing a list with "Least_cfd" at the top, followed by "Least_cfd", "Margin_S", and "Entropy" (which is highlighted in blue). At the bottom right, there are two buttons: "Reset" and "OK".

Parameter

Module

☐ Regression

☒ Classification

Regression Classification

Parameters in function fit():

Classifier: GaussianProcess

opt_num: 1

min_search: ☒ True ☐ False

Dynamic_W: ☒ True ☐ False

Function:

Least_cfd

Least_cfd

Margin_S

Entropy

Reset OK

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

Parameter

Module

☐ Regression
☒ Classification

Regression

Classification

Parameters in function fit():

Classifier:

GaussianProcess

opt_num:

1

min_search:

☒ True
☐ False

Dynamic_W:

☒ True
☐ False

Function:

Least_cfd

Reset

OK

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.

BgoFace

Setting



香港科技大学(广州)
THE HONG KONG UNIVERSITY OF SCIENCE
AND TECHNOLOGY (GUANGZHOU)



材料信息学实验室
MATERIALS INFORMATICS



Bgolearn
贝叶斯优化材料设计

Virtual Sample

☐ Input
☒ Manual

Load Data

Fit

Result

Samples:

☒ Sn
☒ Bi
☒ In
☒ Ti
☐ T

Manual Virtual Sample:

Name:

Sn

Minimum:

86.800

Maximum:

92.900

Step:

3.000

OK

Download

Training Sample:

	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

Virtual Sample:

	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....

Citation:

Materials & Design : <https://doi.org/10.1016/j.matdes.2024.112921>
NPJ Computational Materials : <https://doi.org/10.1038/s41524-024-01243-4>

BgoFace
Setting

香港科技大学 (广州)
THE HONG KONG UNIVERSITY OF SCIENCE
AND TECHNOLOGY (GUANGZHOU)

材料信息学实验室

Bgolearn
贝叶斯优化材料设计

Virtual Sample
☐ Input
☒ Manual

Load Data

Fit

Result

Training Sample:

	Sn	Bi	
1	92.9	3.0	2.5
2	92.7	3.0	2.5
3	92.5	3.0	2.5
4	91.9	3.0	3.5
5	91.7	3.0	3.5
6	91.5	3.0	3.5
7	91.9	4.0	2.5
8	91.7	4.0	2.5
9	91.5	4.0	2.5

Citation:
Materials & Design : <https://doi.org/10.1016/j.matdes.2024.112921>
NPJ Computational Materials : <https://doi.org/10.1038/s41524-024-01243-4>

Parameter

Module
☒ Regression
☐ Classification

Regression Classification

Parameters in function fit():
opt_num: 1 min_search: ☒ True ☐ False Dynamic_W: ☒ True ☐ False

Function:
EI Expected improvement method

Reset OK

	In	Ti
		0.1
		0....
		0....
		0.1
		0....
		0....
		0.1
		0....
		0....
		0....

Download

BgoFace
Setting

香港科技大学 (广州)
THE HONG KONG UNIVERSITY OF SCIENCE
AND TECHNOLOGY (GUANGZHOU)

材料信息学实验室

Bgolearn
贝叶斯优化材料设计

Virtual Sample
☐ Input
☒ Manual

Load Data

Fit

Result

Training Sample:

	Sn	Bi	
1	92.9	3.0	
2	92.7	3.0	
3	92.5	3.0	
4	91.9	3.0	
5	91.7	3.0	
6	91.5	3.0	
7	91.9	4.0	
8	91.7	4.0	2.5
9	91.5	4.0	2.5

Citation:
Materials & Design : <https://doi.org/10.1016/j.matdes.2024.112921>
NPJ Computational Materials : <https://doi.org/10.1038/s41524-024-01243-4>

Result

Result:
current optimal is : 62.59
The next datum recommended by Expected Improvement :
x = [89.8 1.5 2.5 0.3]
The predictions of Bgolearn are :
y = 65.5175300927587

	Ti
	0.1
	0....
	0....
	0.1
	0....
	0....
	0.1
	0....
	0....
	0....

Download