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Steps:

**Training the surrogate forward model**

1. First, open the data generation folder, forward\_NN\_periodic\_BC\_training\_data

2. Run the Module1\_R3\_GSO\_R.m file (line 21 sets the training data size, line 22 sets the test data size)

3. Then run the Module\_2\_1\_actual\_model\_R3\_target.m file

4. Put the training data previously generated in the forward\_NN\_periodic\_BC\_training\_data folder into the current GA\_forward\_NN folder.

The required files are:

phi\_final\_testing.txt

phi\_final\_training.txt

phi\_final\_training\_test.txt

phi\_target\_3\_3\_testing.txt

phi\_target\_3\_3\_training.txt

phi\_target\_3\_3\_training\_test.txt

Th\_large\_testing.txt

Th\_large\_training.txt

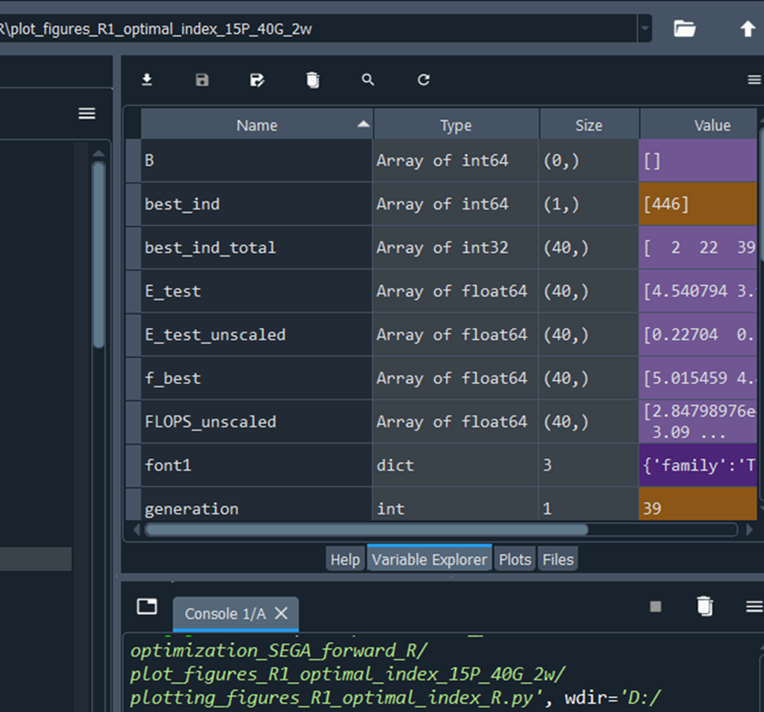
Th\_large\_training\_test.txt

5. Open the GA\_forward\_NN folder, open main.py, and click "run" to run.

6. Place f\_best.txt and progress\_forwardnn.txt generated in the GA\_forward\_NN folder into the plot\_and\_optimized\_nn folder, then open plotting\_figures\_R1\_optimal\_index.py and click "run" to run.

7. After the operation is completed, the screen will appear, forward nn optimal value index: X (any possible number)

8. Then click on the variable explorer in the figures below. All variables will appear. Open the variable nn\_parameter\_data, find row X-1, and record the values ​​in column 0, column 1, and column 2. They correspond to the number of hidden layers, the number of nodes, and the number of iterations respectively. Write them down and save them in the optimized\_nn.docx file that exists in the plot\_and\_optimized\_nn folder.





9. After that, open the GA\_forward\_NN folder and find the file named net\_paramsX.pkl. This file is the optimized network. Put this file into the plot\_and\_optimized\_nn folder and change its file name to net\_params1.pkl.

**Testing the trained surrogate forward model**

10. Open the forward\_NN\_periodic\_BC\_new\_testing\_data folder,

Run the Module1\_R3\_GSO\_R.m file (line 21 sets the training data size, line 22 sets the test data size, the size does not need to be changed.)

11. Run the Module\_2\_1\_actual\_model\_R3\_target.m file

12. Place the following files generated in the forward\_NN\_periodic\_BC\_new\_testing\_data folder into the test\_output\_trained\_surrogate\_forward\_model folder.

Th\_large\_testing.txt，

phi\_target\_3\_3\_testing.txt，

phi\_final\_testing.txt

Then put net\_params1.pkl in the plot\_and\_optimized\_nn folder into the test\_output\_trained\_surrogate\_forward\_model folder

Run output\_trained\_surrogate\_forward\_model\_R.py.

**Training the controller**

13. Open the controller\_data\_generation folder,

First run the Module1\_R3\_GSO\_R.m file (line 21 sets the training data size and line 22 sets the test data size).

Then run the Module\_2\_1\_actual\_model\_R3\_target\_inverse.m file.

Place the following files into the controller\_train folder.

phi\_final\_training\_inverse.txt

phi\_final\_training\_test\_inverse.txt

phi\_target\_3\_3\_training.txt

phi\_target\_3\_3\_training\_test.txt

14. Open the testing\_data\_genration\_R\_inverse folder and run the testing\_data\_for\_inverse\_nn.m file. Place phi\_final\_testing\_inverse.txt and phi\_target\_3\_3\_testing.txt into the controller\_train folder.

15. Then put net\_params1.pkl in the plot\_and\_optimized\_nn folder into the controller\_train folder.

16. Open the optimized\_nn.docx file in the plot\_and\_optimized\_nn folder. Set the hyperparameters to the corresponding locations in the nn\_adam\_inverse\_R\_1305\_16\_R2\_PFM\_1.py file in the controller\_train folder.

Line 24 EPOCHS\_2 is the number of iterations

Line 27 HIDDEN\_DIM\_2 is the number of nodes,

Line 28 NUM\_LAYERS\_2 is the total number of layers, which equals to the number of hidden layers + 2.

Line 32, set EPOCHS\_1 equal to EPOCHS\_2

Line 35, set HIDDEN\_DIM\_1 equal to HIDDEN\_DIM\_2

Line 36, set NUM\_LAYERS\_1 equal to NUM\_LAYERS\_2

After that, run the nn\_adam\_inverse\_R\_1305\_16\_R2\_PFM\_1.py file.

17. Place the Th\_out\_phi\_target\_testing.txt file generated in the controller\_train folder into the Th\_to\_PFM folder. And run the Th\_inputting\_into\_PFM\_R2.m file.

18. Put the phi\_final\_testing\_PFM.txt generated in the Th\_to\_PFM folder into the microstructure\_comparison folder, put the phi\_final\_testing\_inverse.txt in the controller\_train folder into the microstructure\_comparison folder, and put the phi\_final\_net\_out\_1\_testing.txt in the controller\_train folder into microstructure\_comparison. folder.

Run final\_microstructure\_comparison.m to get the comparison figures.