Support Information

Integrated hybrid modeling and SHAP (SHapley Additive exPlanations) to predict and explain the adsorption properties of thermoplastic polyurethane (TPU) porous materials.

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1. Experimental

Fig.1.TPU porous material

As shown in the Figure.1, we prepared the TPU porous material we tested its adsorption properties to obtain raw data for machine learning.

Table1. TPU Physical Parameters

	Soft segment	Hard segment	Density (g/ cm3)	Hardness (Shore A)
1185A	Polytetramethylene ether glycol	4,4′ -diphenylemethane diisocyanate +1,4-butanediol	1.12	85

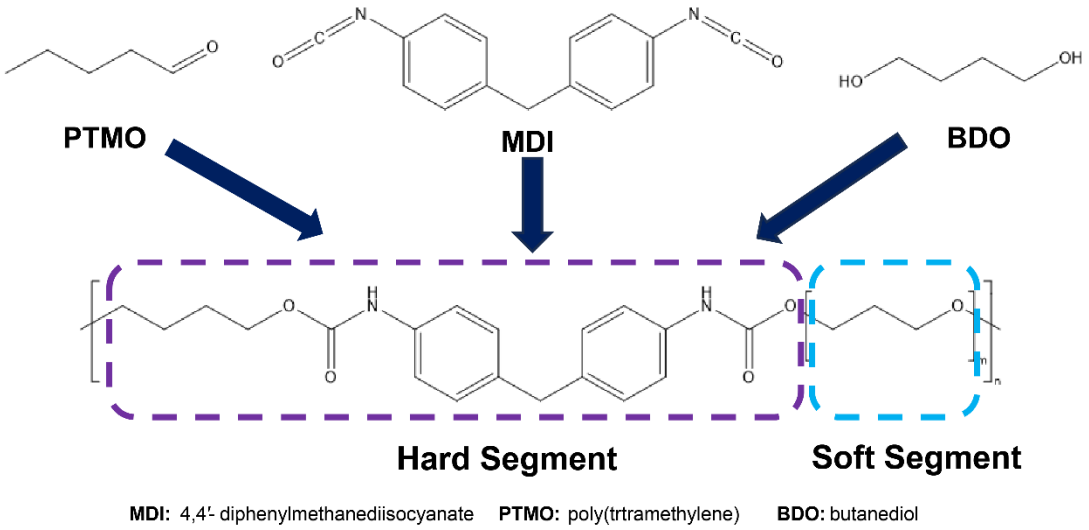

Fig.2. Thermoplastic Polyurethane Structures[1]

Table2. Experimental reagent table

Name of reagent	Manufacturer (of a product)	Purity
Deionized water	OSJ-II-100L Laboratory Water Purifier from Shandong BOKE Scientific Instrument Co.	-
1,4-Dioxane	Shanghai Xian Ding Biotechnology Co.	99%
Olive Oil	Jiangxi Gannan Natural Spice Oil Co.	99%
Olive Oil	Yihai Jiali Jinlongyu Cereals, Oils and Foodstuffs Co.	99%
Sweet almond oil	Guangzhou Xuan Yi Flavor & Fragrance Co	99%
Peanut oil	Shandong Luhua Group Co.	99%
Acetone	Shanghai Titan Technology Co.	AP
Cyclohexane	Shanghai Titan Technology Co.	AP
Toluene	Shanghai Titan Technology Co.	AP

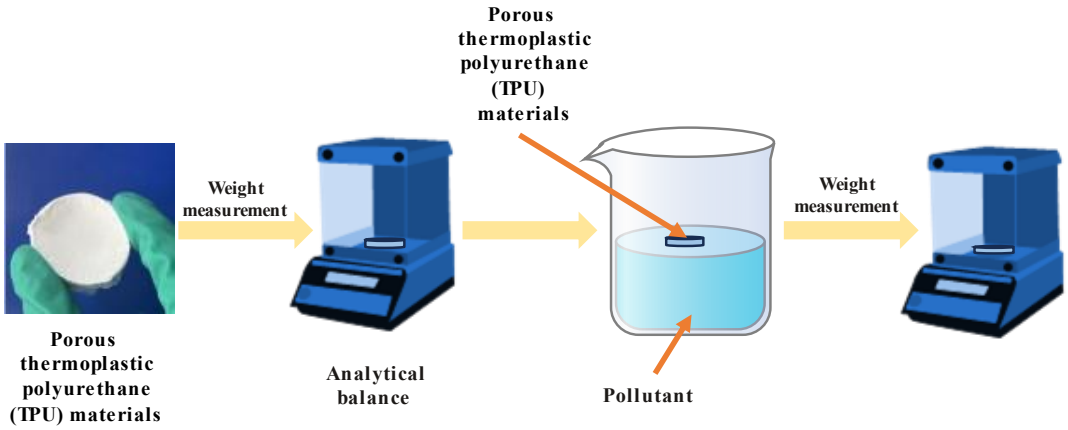

Fig.3. Adsorption capacity test procedure

2.Machine Learning

2.1 Machine learning data part

Table.3. Machine learning data

adsorption	Concentration （g/ml）	temperature （℃）	time （min）	mixture ratio	acetone	olive	peanut	Cyclohexane	toluene	Sweet almonds	Anhydrous alcohol	coconut oil
14.39	0.04	0	15	9.00	1	0	0	0	0	0	0	0
5.79	0.04	0	15	9.00	0	1	0	0	0	0	0	0
5.17	0.04	0	15	9.00	0	0	1	0	0	0	0	0
4.348	0.04	0	15	9.00	0	0	0	1	0	0	0	0
5.91	0.04	0	15	9.00	0	0	0	0	1	0	0	0
6.16	0.04	0	15	9.00	0	0	0	0	0	1	0	0
5.65	0.04	0	15	9.00	0	0	0	0	0	0	1	0
6.21	0.04	0	15	9.00	0	0	0	0	0	0	0	1
10.41	0.04	0	30	5.67	1	0	0	0	0	0	0	0
3.55	0.04	0	30	5.67	0	1	0	0	0	0	0	0
2.41	0.04	0	30	5.67	0	0	1	0	0	0	0	0
2.59	0.04	0	30	5.67	0	0	0	1	0	0	0	0
5.46	0.04	0	30	5.67	0	0	0	0	1	0	0	0
5.41	0.04	0	30	5.67	0	0	0	0	0	1	0	0
4.60	0.04	0	30	5.67	0	0	0	0	0	0	1	0
4.030	0.04	0	30	5.67	0	0	0	0	0	0	0	1
11.33	0.04	0	30	19.00	1	0	0	0	0	0	0	0
3.85	0.04	0	30	19.00	0	1	0	0	0	0	0	0
3.47	0.04	0	30	19.00	0	0	1	0	0	0	0	0
2.68	0.04	0	30	19.00	0	0	0	1	0	0	0	0
9.34	0.04	0	30	19.00	0	0	0	0	1	0	0	0
3.31	0.04	0	30	19.00	0	0	0	0	0	1	0	0
2.028	0.04	0	30	19.00	0	0	0	0	0	0	1	0
4.98	0.04	0	30	19.00	0	0	0	0	0	0	0	1
13.40	0.04	0	30	9.00	1	0	0	0	0	0	0	0
6.36	0.04	0	30	9.00	0	1	0	0	0	0	0	0
6.62	0.04	0	30	9.00	0	0	1	0	0	0	0	0
6.16	0.04	0	30	9.00	0	0	0	0	0	1	0	0
8.36	0.04	0	30	9.00	0	0	0	0	0	0	1	0
5.23	0.04	0	30	9.00	0	0	0	0	0	0	0	1
9.49	0.06	0	15	9.00	1	0	0	0	0	0	0	0
4.21	0.06	0	15	9.00	0	1	0	0	0	0	0	0
3.79	0.06	0	15	9.00	0	0	1	0	0	0	0	0
4.86	0.06	0	15	9.00	0	0	0	0	0	1	0	0
4.19	0.06	0	15	9.00	0	0	0	0	0	0	1	0
3.77	0.06	0	15	9.00	0	0	0	0	0	0	0	1
8.69	0.06	0	30	9.00	1	0	0	0	0	0	0	0
2.079	0.06	0	30	9.00	0	1	0	0	0	0	0	0
2.12	0.06	0	30	9.00	0	0	1	0	0	0	0	0
2.37	0.06	0	30	9.00	0	0	0	1	0	0	0	0
5.86	0.06	0	30	9.00	0	0	0	0	1	0	0	0
2.56	0.06	0	30	9.00	0	0	0	0	0	1	0	0
3.77	0.06	0	30	9.00	0	0	0	0	0	0	1	0
3.62	0.06	0	30	9.00	0	0	0	0	0	0	0	1
7.10	0.08	0	15	9.00	1	0	0	0	0	0	0	0
2.53	0.08	0	15	9.00	0	1	0	0	0	0	0	0
1.51	0.08	0	15	9.00	0	0	1	0	0	0	0	0
1.92	0.08	0	15	9.00	0	0	0	1	0	0	0	0
5.27	0.08	0	15	9.00	0	0	0	0	1	0	0	0
2.11	0.08	0	15	9.00	0	0	0	0	0	1	0	0
2.090	0.08	0	15	9.00	0	0	0	0	0	0	1	0
2.83	0.08	0	15	9.00	0	0	0	0	0	0	0	1
6.98	0.08	0	30	19.00	1	0	0	0	0	0	0	0
4.041	0.08	0	30	19.00	0	1	0	0	0	0	0	0
2.41	0.08	0	30	19.00	0	0	1	0	0	0	0	0
2.22	0.08	0	30	19.00	0	0	0	1	0	0	0	0
6.45	0.08	0	30	19.00	0	0	0	0	1	0	0	0
3.75	0.08	0	30	19.00	0	0	0	0	0	1	0	0
4.073	0.08	0	30	19.00	0	0	0	0	0	0	1	0
3.99	0.08	0	30	19.00	0	0	0	0	0	0	0	1
6.094	0.08	0	30	9.00	1	0	0	0	0	0	0	0
3.13	0.10	4	30	9.00	0	0	1	0	0	0	0	0
1.35	0.08	0	30	9.00	0	1	0	0	0	0	0	0
1.062	0.08	0	30	9.00	0	0	1	0	0	0	0	0
1.46	0.08	0	30	9.00	0	0	0	1	0	0	0	0
1.10	0.10	4	30	9.00	0	0	0	0	0	0	0	1
5.75	0.08	0	30	9.00	0	0	0	0	1	0	0	0
2.72	0.08	0	30	9.00	0	0	0	0	0	1	0	0
2.54	0.08	0	30	9.00	0	0	0	0	0	0	1	0
2.76	0.08	0	30	9.00	0	0	0	0	0	0	0	1
4.91	0.10	0	30	9.00	1	0	0	0	0	0	0	0
3.22	0.10	0	30	9.00	0	1	0	0	0	0	0	0
3.36	0.10	0	30	9.00	0	0	1	0	0	0	0	0
1.46	0.10	0	30	9.00	0	0	0	1	0	0	0	0
5.13	0.10	0	30	9.00	0	0	0	0	1	0	0	0
3.54	0.10	0	30	9.00	0	0	0	0	0	1	0	0
3.35	0.10	0	30	9.00	0	0	0	0	0	0	1	0
4.057	0.10	4	30	9.00	1	0	0	0	0	0	0	0
3.23	0.10	4	30	9.00	0	1	0	0	0	0	0	0
1.63	0.10	4	30	9.00	0	0	0	1	0	0	0	0
5.25	0.04	0	30	9.00	0	0	0	1	0	0	0	0
10.32	0.04	0	30	9.00	0	0	0	0	1	0	0	0
2.47	0.10	4	30	9.00	0	0	0	0	1	0	0	0
3.20	0.06	0	15	9.00	0	0	0	1	0	0	0	0
7.61	0.06	0	15	9.00	0	0	0	0	1	0	0	0
1.81	0.10	0	30	9.00	0	0	0	0	0	0	0	1
5.75	0.08	0	30	9.00	0	0	0	0	1	0	0	0
2.72	0.08	0	30	9.00	0	0	0	0	0	1	0	0

The mixture ratio in Table 3 of the Machine Learning data refers to the proportion

of 1,4-dioxane to deionized water. For the definition of adsorption please see the text section. Detailed information on adsorption data for TPU porous materials can be found at https://osf.io/jnu9d/

2.2. Models Development

2.2.1. XGBoost Developmet

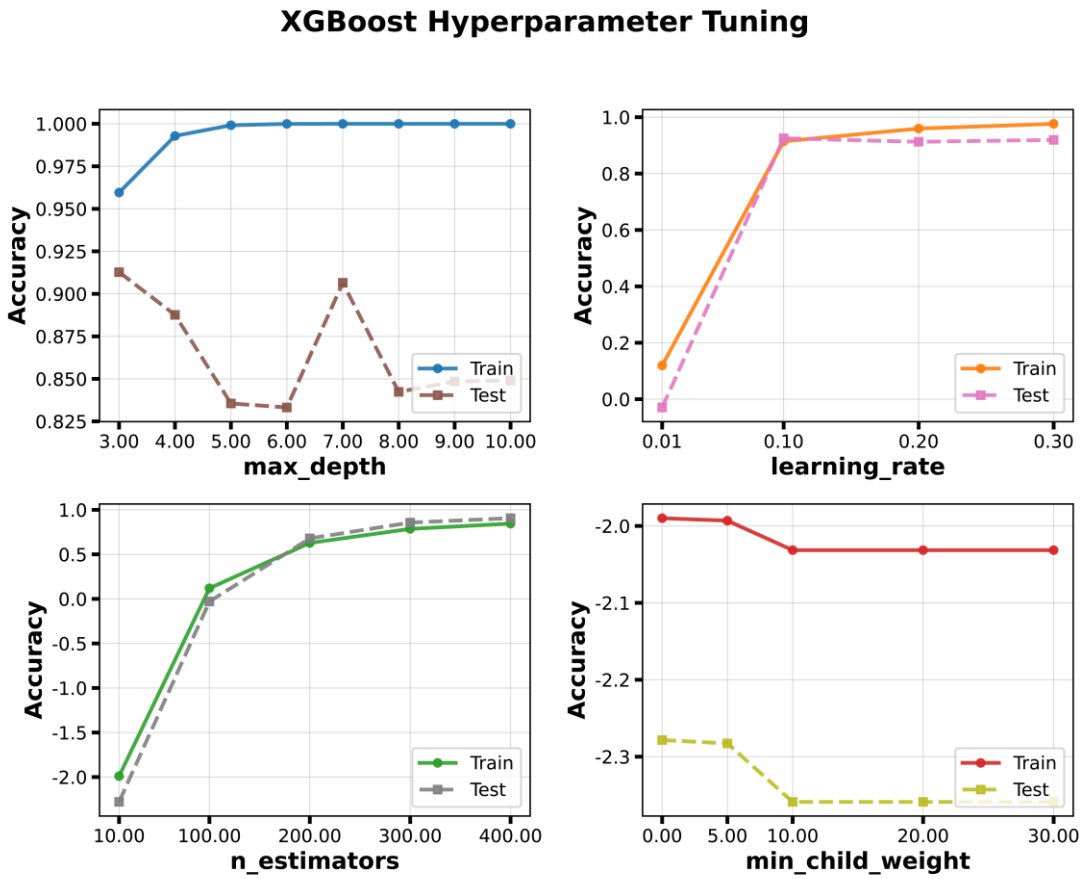

Fig.4.Relationship between XGBoost parameters and accuracy

2.2.2. Decision Tree Regressor Developmet

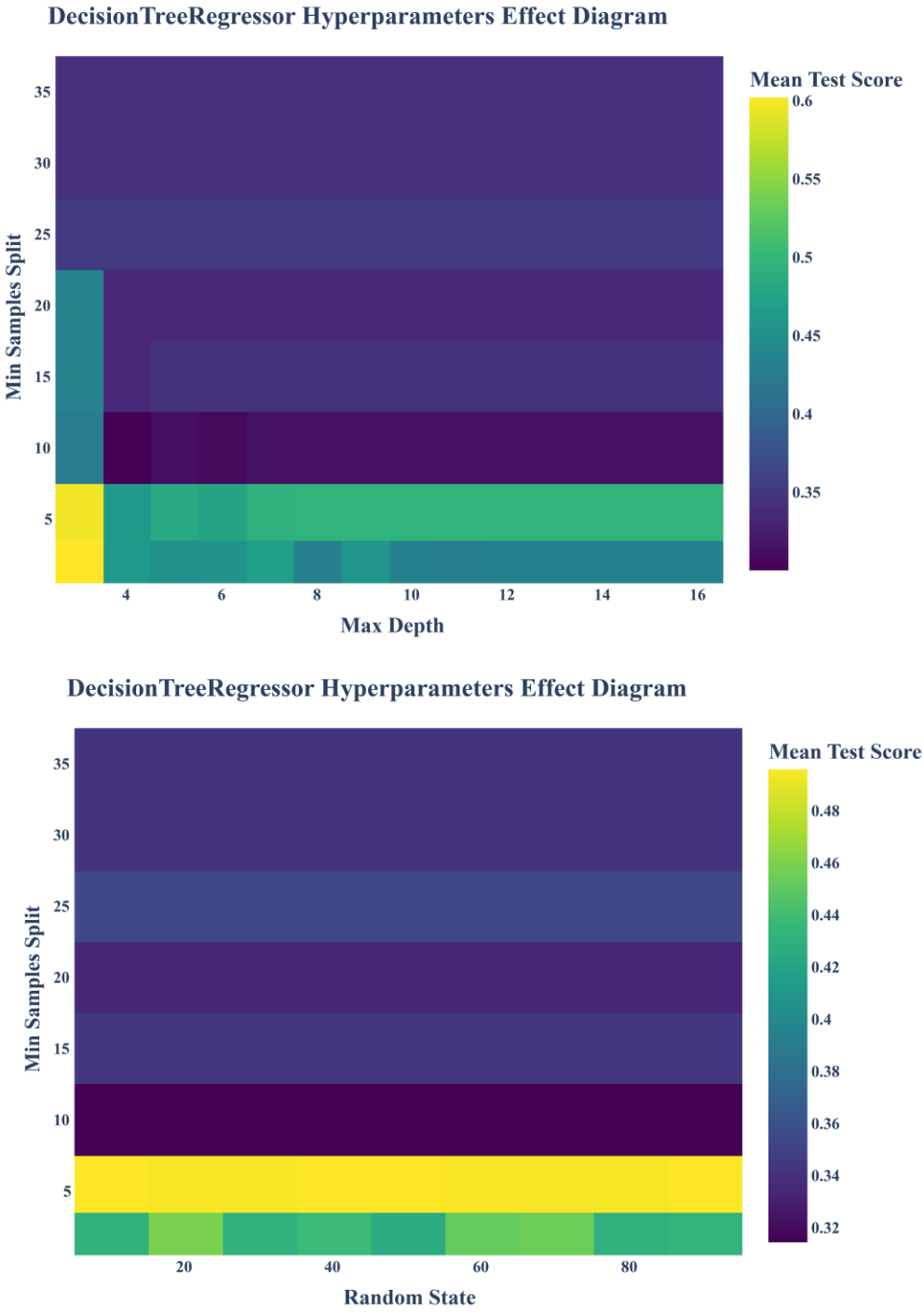

Fig.5.Relationship between DTR parameters and accuracy

2.2.3. KNeighbors Regressor Development

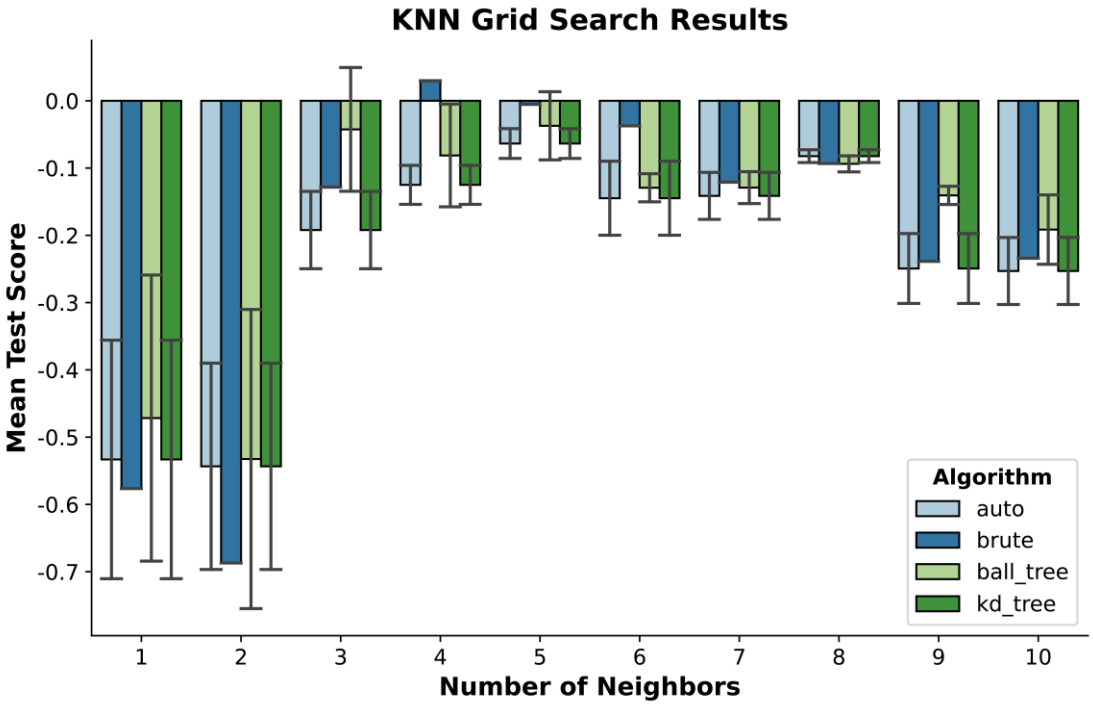

Fig.6.Relationship between KNN parameters and accuracy

2.2.4. Bagging Regression Development

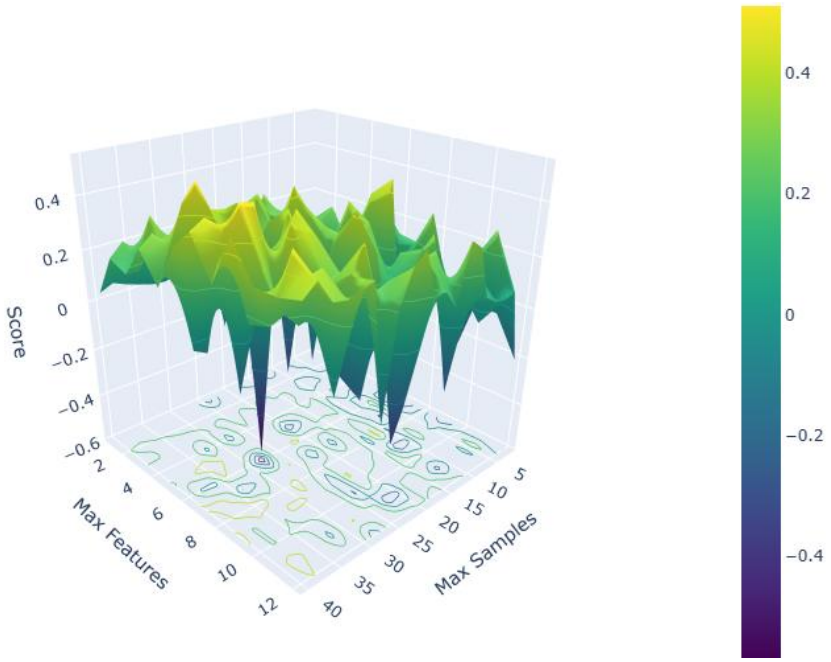

Fig.7. Relationship between BGR parameters and accuracy

2.2.5. Extra Trees Regression Development

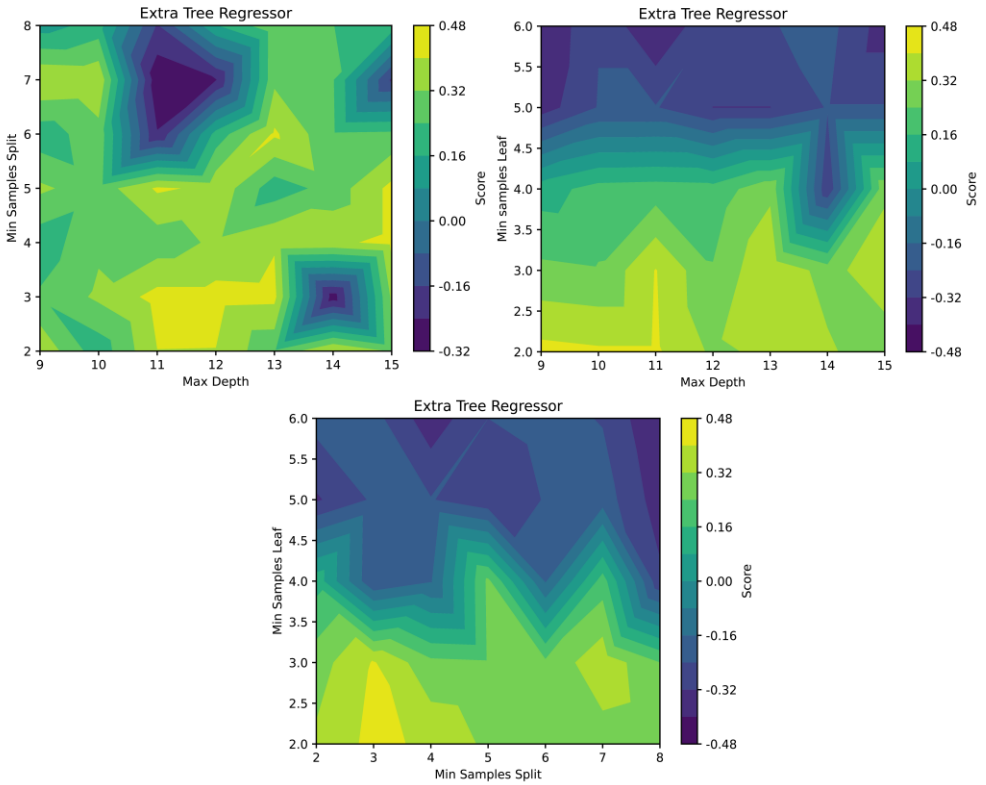

Fig.8. Relationship between ETR parameters and accuracy

2.2.6. Ensemble Hybrid Model Development

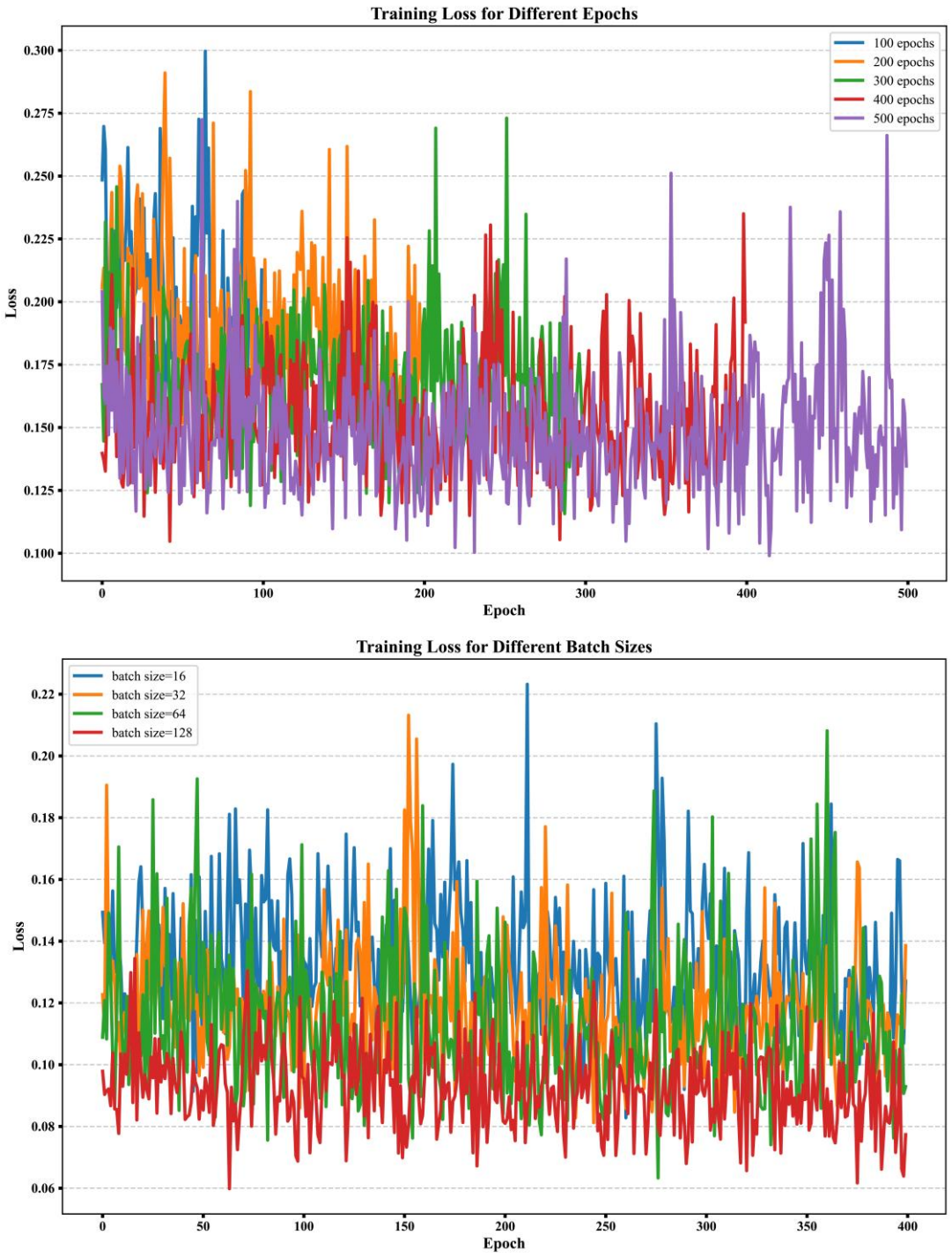

Fig.9. Training Loss for Different Batch sizes and Epoch

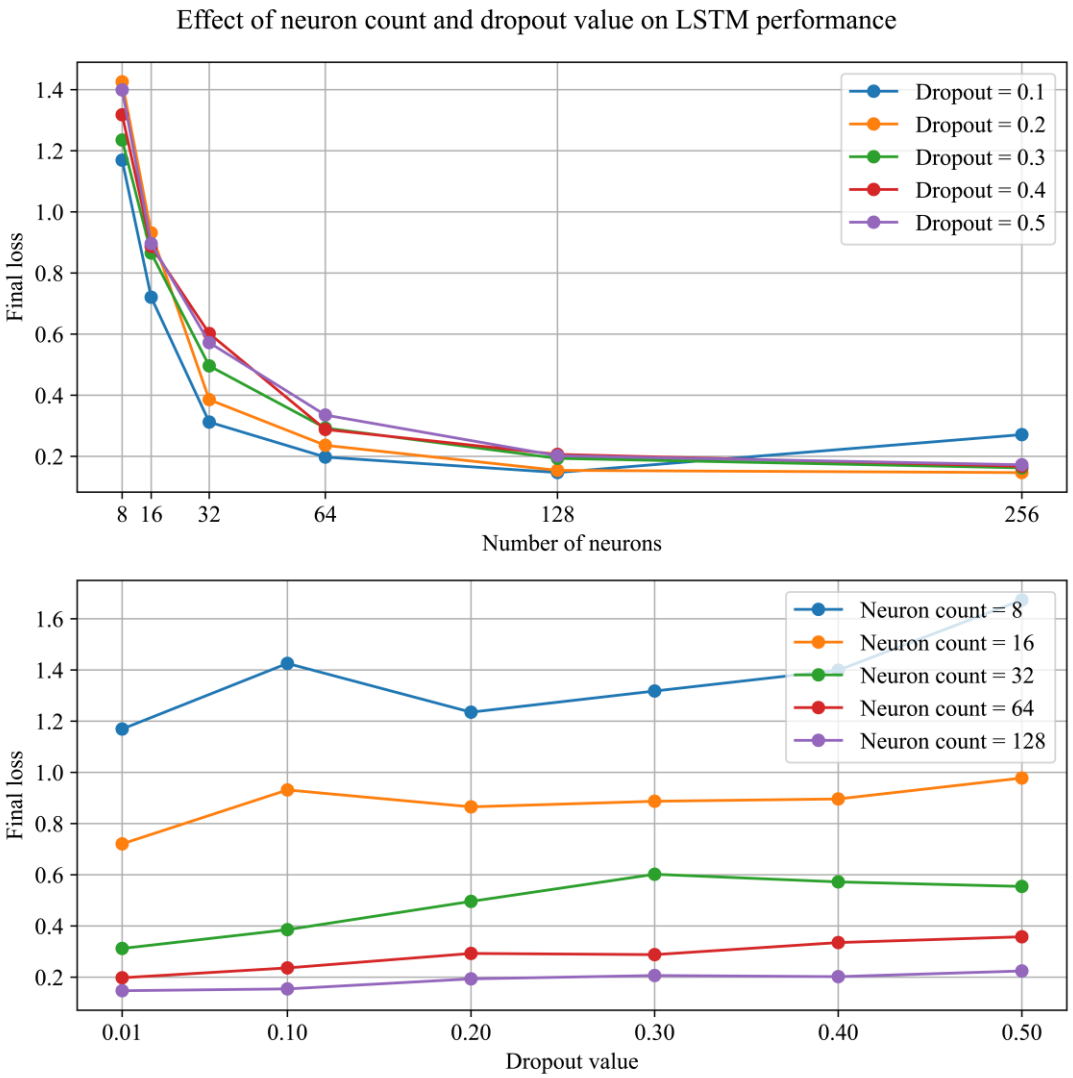

Fig.10. Effect of neuron count and dropout value on LSTM performance

References

[1] Wang Y, Zou G, Shang L. Effects of temperature and hard segment content on the interfacial mechanical properties of graphene/thermoplastic polyurethane composites: a molecular dynamics study[J]. Computational Materials Science, 2022, 213: 111635.