Supporting Information

Machine Learning Prediction of Physical Properties of Lignin Derived Porous Carbon via Catalytic Pyrolysis

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Code availability: The dataset and codes to perform machine learning and predict SSA, TPV, and MP of lignin-derived porous carbon are available at https://github.com//Zihao-Xie77/Machine-learning-for-physical-properties-of-LDPC.

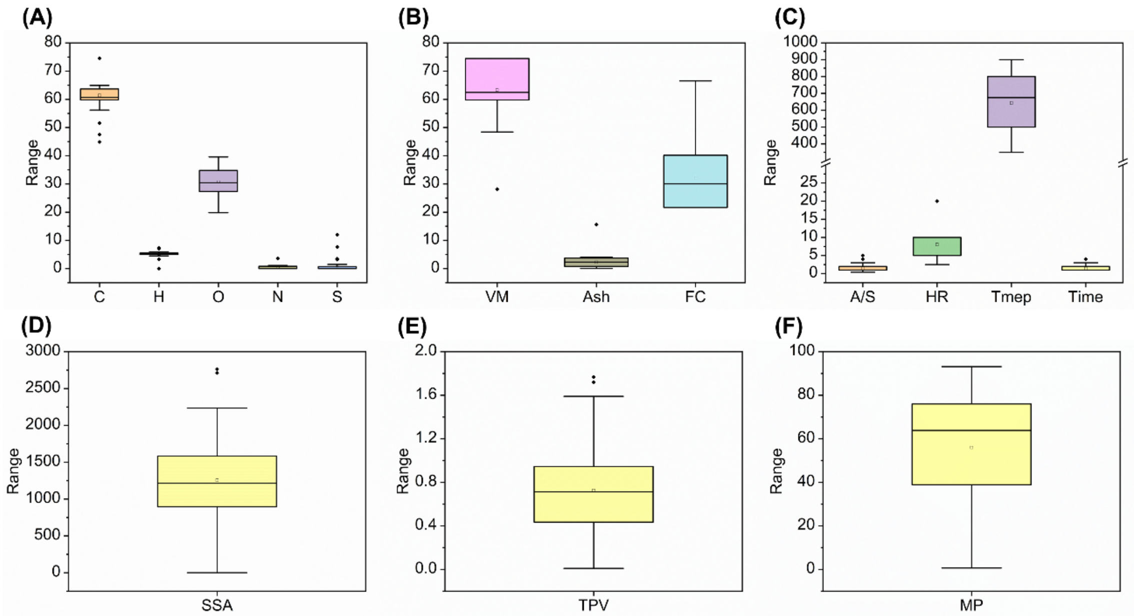

Fig. S1 The boxplot of input features and output targets of (A) elemental composition (C, H, O, N, S); (B) proximate composition (VM, Ash, FC); (C) pyrolysis condition (HR, Temp, Time) and chemical activators (A/S); (D) SSA; (E) TPV; (F) MP.

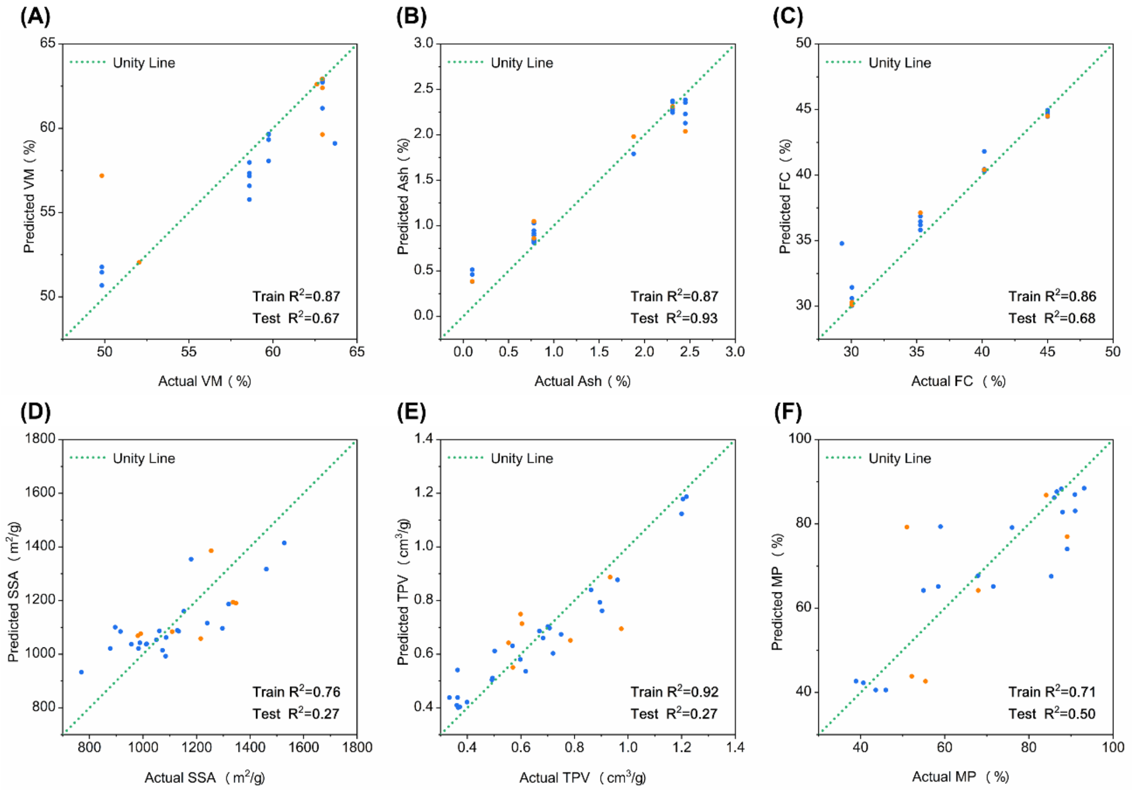

Fig. S2 Comparison of predicted and actual values using pre-trained interpolation model for (A, B, C) VM, Ash and FC; (D, E, F) SSA, TPV and MP.

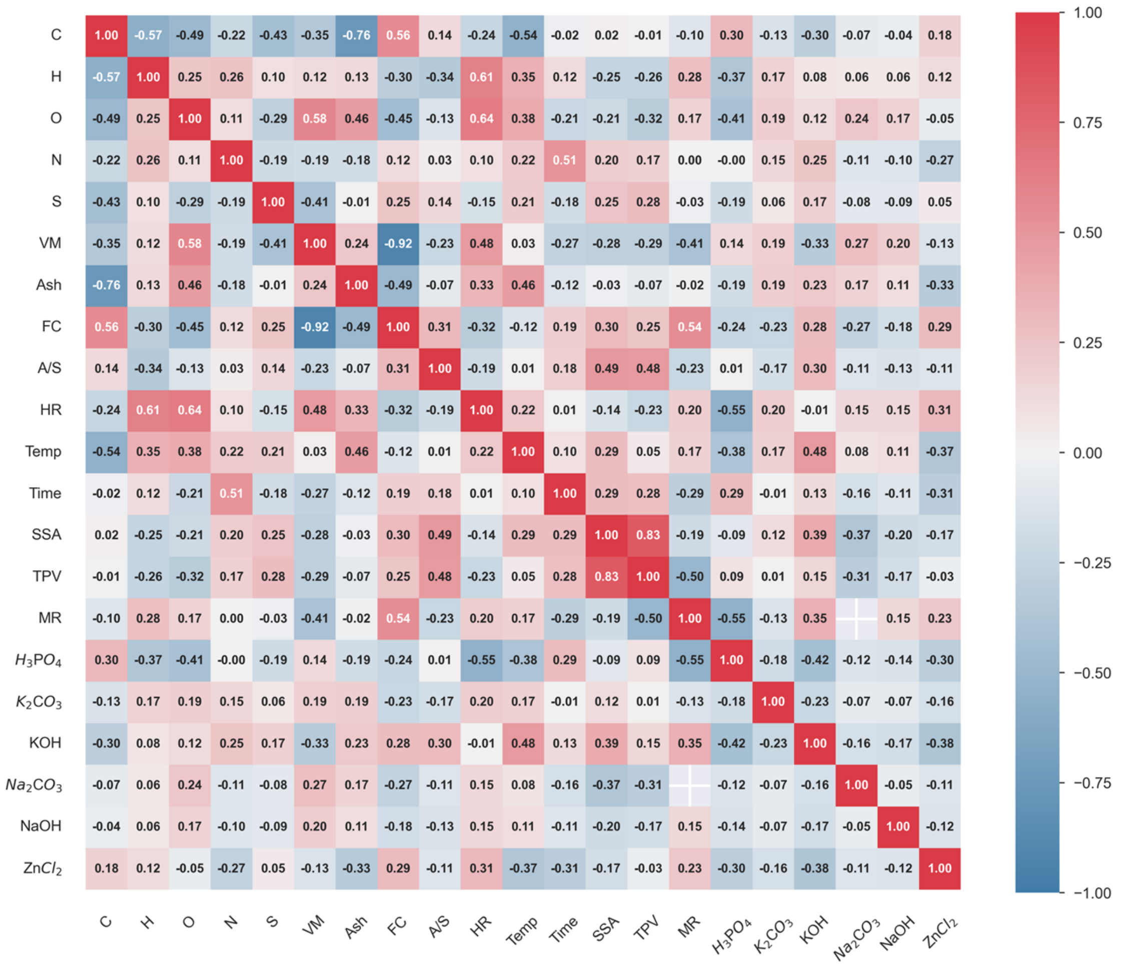

Fig. S3 Pearson correlation matrix between any two features in the original dataset.

Table S1 Information of references for the original used for the hybrid machine learning framework

No.	Lignin Type	Chemical Agent	Ref.
1	Black liquor lignin	$KOH/ZnCl_2$	1
2	Kraft softwood lignin	KOH	2
3	Sodium lignosulfonate	H_3PO_4	3
4	lignosulfonate	K_2CO_3	4
5	Kraft lignin	KOH	5
6	Kraft lignin	KOH/ H_3PO_4/ K_2CO_3	6
7	Alkali lignin	KOH	7
8	Sodium lignosulfonate	KOH	8
9	Sodium lignosulfonate	KOH	9
10	Alkali lignin	KOH/NaOH	10
11	Alkali lignin	KOH	11
12	Alkali lignin	H_3PO_4	12
13	sodium lignosulfonate	$ZnCl_2$	13
14	Alkali lignin	KOH	14
15	Enzymatic hydrolysis lignin	$ZnCl_2$/ K_2CO_3	15
16	Alkaline lignin	KOH	16
17	Enzymatic hydrolysis lignin	KOH/ H_3PO_4/ K_2CO_3	17
18	Sodium lignosulfonate	KOH	18
19	Lignin	$ZnCl_2$/ K_2CO_3/ H_3PO_4	19
20	Lignin	K_2CO_3	20
21	Bioethanol lignin	KOH/NaOH	21
22	Sodium lignosulphonate	KOH	22
23	Sodium lignosulfonate	KOH	23
24	Enzymatic hydrolysis lignin	KOH	24
25	Kraft lignin	KOH	25
26	Lignin	KOH	26
27	Akali lignin	KOH	27

28	Lignin	$ZnCl_2$	28
29	Lignin	H_3PO_4	29
30	Lignin	$ZnCl_2$/ K_2CO_3/KOH	30
31	Lignin	KOH	31
32	Lignin	KOH	32

Table S2 Description of dataset features.

Feature	Abbreviation	Unit
Carbon content of lignin	C	%
Hydrogen content of lignin	H	%
Oxygen content of lignin	O	%
Nitrogen content of lignin	N	%
Ash proportion of lignin	S	%
Volatile matter proportion of lignin	VM	%
Ash proportion of lignin	Ash	%
Fixed carbon proportion of lignin	FC	%
Hate rate during the pyrolysis	HR	(^{o}C/min)
Highest temperature during the pyrolysis	Temp	^{o}C
Mass ratio of lignin to chemical activator	A/S	-
Using chemical activator	Agent	-
Specific surface area of the porous carbon	SSA	m^2/g
Total pore volume of the porous carbon	TPV	cm^3/g
Microporosity of the porous carbon	MP	%

Table S3 Statistical summary of input features and output targets of the original dataset

I/O	Type of features	feature	Min	Max	Mean	SD	No. of samples (% of total samples)
Input	Elemental composition	C (%)	44.90	74.56	61.41	5.38	112 (100%)
		H (%)	0	7.34	4.87	1.50	112 (100%)
		O (%)	19.82	39.57	30.66	3.81	112 (100%)
		N (%)	0	3.60	0.48	0.77	112 (100%)
		S (%)	0	12	0.95	2.53	112 (100%)
	Proximate composition	VM (%)	28.14	74.46	63.30	9.93	90 (80.36%)
		Ash (%)	0.04	15.62	2.29	2.05	90 (80.36%)
		FC (%)	21.65	66.52	32.26	9.75	90 (80.36%)
	Pyrolysis condition	HR (^{o}C/min)	2.5	20	8.05	2.98	112 (100%)
		Temp (^{o}C)	350	900	643.30	157.47	112 (100%)
		Time (h)	1	4	1.42	0.56	112 (100%)
	Chemical activators	A/S	0.4	5	1.45	0.85	112 (100%)
		Agent	-	-	-	-	112 (100%)
Output		SSA (m^2/g)	1.4	2762.5	1256.15	552.04	101 (90.18%)
		TPV (cm^3/g)	0.01	0.45	0.73	0.38	112 (100%)
		MP (%)	0.66	93.14	56.01	26.75	73 (65.18%)

Table S4 Performance of the pre-trained interpolation model.

Target	R^2		RMSE		
	Train	Test	Train	Test	Unit
VM	0.87	0.67	3.78	6.81	%
Ash	0.87	0.93	0.44	0.22	%
FC	0.86	0.68	4.03	6.84	%
SSA	0.76	0.27	275.25	120.98	m^2/g
TPV	0.92	0.27	0.19	0.14	cm^3/g
MP	0.71	0.50	15.48	14.59	%

$$y = B1x + B2x^2 + B3x^3 + Intercept$$

Note: The fitting lines are all fitted using polynomials, which are completed within a cubic polynomial. The formula for cubic polynomial fitting is shown in the above equation

Table S5 The formula of all fitted lines of top four important input features on each target

Target	Feature	B1	B2	B3	Intercept	R^2
SSA	A/S	167.26	-32.65	-	68.59	0.87
	Temp	157.98	-101.93	-	64.22	0.78
	C	-47.5	81.03	27.53	-23.91	0.96
	Time	44.77	-6.37	-	-9.39	0.99
TPV	C	-0.05	0.09	0.03	-0.04	0.94
	Temp	0.10	-0.03	0.018	-0.047	0.79
	A/S	0.20	-0.03	-	0.01	0.84
	VM	-0.07	-0.01	-	0.02	0.81
MP	A/S	-6.09	4.39	-	-3.25	0.73
	Temp	5.86	-0.57	-3.89	1.47	0.61
	Ash	16.93	12.47	-	-6.20	0.99
	Time	-1.99	0.42	-	-0.13	0.98

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