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Shuzo Ohe

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A Neural Network Prediction System for Critical Temperature of Paraffin

Shuzo Ohe

Faculty of Engineering, Science University of Tokyo
1-3, Kagurazaka, Shinjukuku, Tokyo, JAPAN,162

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This paper presents a neural network-based methodology for providing a potential solution to the problems encountered in the area of prediction of critical temperatures of hydrocarbons from their fundamental properties. The neural network-based system successfully determined the property.

There have been various kinds of prediction methods of physical properties based on the theory of physical chemistry and statistics. Most of them are composed of correlation equations with empirically determined parameters. In this study, the critical temperature of substances are determined directly by the association ability of neural network learned by the back propagation method.

There is a correlation between critical temperature and carbon numbers in hydrocarbons, molecular weight, boiling point, and acentric factor. Giving network carbon numbers, molecular weight, boiling point, and acentric factor as input and critical pressure as output for teaching, learning was executed until the sum of error squared between output and ideal output becomes with sufficient small values.

NEURAL NETWORK METHODOLOGY

Neural network applications to various industries have been used extensively since the learning method called back propagation method was presented by Rumelhart et al.,[1]. The neural network consists of a set of artificial neurons connected with each other in the form of a multi-layered network. In most cases,three layers are used as input, hidden, and output layers, respectively. The weights of all interconnections are dynamically modified to generate the desired output pattern for each presented input pattern. In this way, learning is accomplished. Each node receives the bias and weighted sum of all the inputs to it. The output is normalized between zero and one by the sigmoid transfer function; therefore, all the values of the input and output nodes should be normalized in this way.

NETWORK LEARNING: The neural network contains 4 input nodes and 1 output node which represent the fundamental properties of the substance and its critical temperature, respectively. Table 1 lists the learning data for the 35 substances involved. The learning data presented total of 100,000 iterations or time steps.

BACK PROPAGATION LEARNING PARAMETERS: In all computations, the learning rate parameter was set at 0.7, the momentum term was set at 0.8, and the gain term was set at 1.0. The initial weights of the network were assigned random values to prevent the hidden units from acquiring identical weights during learning.

Table 1 Learning Data for Network to Predict Critical Temperature

No.	Substance Name	Carbon Number	Molecular Weight[-]	Boiling Point[C]	Acentric Factor[-]	Critical Temperature[K]
1	METHANE	1	16.0	-161.5	0.008	190.6
2	ETHANE	2	30.1	-88.5	0.097	305.5
3	PROPANE	3	44.1	-42.0	0.152	369.8
4	BUTANE	4	58.1	-0.5	0.198	425.2
5	PENTANE	5	72.2	36.1	0.251	469.6
6	HEXANE	6	86.2	68.7	0.300	507.7
7	HEPTANE	7	100.2	98.4	0.349	540.2
8	OCTANE	8	114.2	125.7	0.401	568.6
9	NONANE	9	128.3	150.9	0.445	594.6
10	DECANE	10	142.3	174.1	0.488	617.6
11	UNDECANE	11	156.3	195.9	0.537	638.8
12	DODECANE	12	170.3	216.3	0.568	659.0
13	TRIDECANE	13	184.4	235.5	0.622	675.8
14	TETRADECANE	14	198.4	253.6	0.643	694.6
15	PENTADECANE	15	212.4	270.7	0.705	707.0
16	HEXADECANE	16	226.4	286.8	0.775	717.0
17	HEPTADECANE	17	240.5	302.1	0.774	733.0
18	OCTADECANE	18	254.5	316.4	0.801	745.0
19	NONADECANE	19	268.5	330.0	0.827	756.0
20	ETHYLENE	2	28.1	-103.6	0.084	282.7
21	PROPYLENE	3	42.1	-47.0	0.139	365.0
22	1-BUTENE	4	56.1	-6.3	0.208	419.6
23	1-PENTENE	5	70.1	30.0	0.293	464.7
24	1-HEXENE	6	84.2	63.5	0.296	504.0
25	1-HEPTENE	7	98.2	93.6	0.347	537.2
26	1-OCTENE	8	112.2	121.3	0.403	566.6
27	1-NONENE	9	126.2	147.0	0.383	601.0
28	1-DECENE	10	140.3	170.6	0.491	617.6
29	1-UNDECENE	11	154.3	192.7	0.519	637.0
30	1-DODECENE	12	168.3	213.4	0.558	657.0
31	1-TRIDECENE	13	182.4	232.8	0.599	674.0
32	1-TETRADECENE	14	196.4	251.2	0.645	689.0
33	1-PENTADECENE	15	210.4	268.4	0.686	704.0
34	1-HEXADECENE	16	224.4	285.0	0.725	717.0
35	1-OCTADECENE	18	252.5	316.4	0.801	745.0

ACCURACY CALCULATIONS: As shown in Table 1, the learning data are real values, varying from minus to plus values and most of their absolute values are greater than unit [2]. The outputs are also real values which have greater values than unit. Therefore, the learning data were normalized to the values between zero and unit. The outputs from the network were then gained as normalized values, which were converted to the original digits number. The network error in prediction for learning is computed as the sum of the output node errors for 34 of 35 substances. The remaining substance was taken out of the learning data to examine the network accuracy for prediction using the learned connection weights.

NUMBER OF HIDDEN LAYERS AND HIDDEN UNITS : Neural networks associate the non-learned data from the learned data. The association capability is a function of both the number of hidden layers

Table 2 Result Learned by Network after 100,000 Time Steps

No.	Substance Name	Tc[K] learned	Tc[K] observed	Error (%)
1	METHANE	190.72	190.60	0.061
2	ETHANE	302.87	305.50	-0.861
3	PROPANE	370.40	369.80	0.162
4	BUTANE	425.25	425.20	0.012
5	PENTANE	470.46	469.60	0.184
6	HEXANE	508.28	507.70	0.115
7	HEPTANE	540.82	540.20	0.115
8	OCTANE	569.01	568.60	0.073
9	NONANE	594.85	594.60	0.042
10	DECANE	617.91	617.60	0.050
11	UNDECANE	638.19	638.80	-0.095
12	DODECANE	658.29	659.00	-0.107
13	TRIDECANE	674.54	675.80	-0.186
14	TETRADECANE	692.23	694.60	-0.341
15	PENTADECANE	704.89	707.00	-0.298
16	HEXADECANE	715.74	717.00	-0.176
17	HEPTADECANE	731.42	733.00	-0.215
18	OCTADECANE	743.51	745.00	-0.200
19	NONADECANE	754.69	756.00	-0.173
20	ETHYLENE	283.19	282.70	0.172
21	PROPYLENE	362.47	365.00	-0.694
22	1-BUTENE	418.48	419.60	-0.268
23	1-PENTENE	461.81	464.70	-0.623
24	1-HEXENE	502.60	504.00	-0.277
25	1-HEPTENE	535.66	537.23	-0.292
26	1-OCTENE	564.03	566.60	-0.453
27	1-NONENE	596.49	601.00	-0.751
28	1-DECENE	613.79	617.60	-0.617
29	1-UNDECENE	636.56	637.00	-0.070
30	1-DODECENE	656.19	657.00	-0.123
31	1-TRIDECENE	673.88	674.00	-0.017
32	1-TETRADECENE	689.56	689.00	0.081
33	1-PENTADECENE	704.20	704.00	0.028
34	1-HEXADECENE	717.92	717.00	0.129
35	1-OCTADECENE	742.54	745.00	-0.331

Note : Number of hidden units ; 4

and hidden units. In this work, neural networks with one hidden layer were used in computations. The number of hidden units required to perform accurate prediction was determined empirically. All series of computations were repeated using networks from one to twelve hidden units.

PERFORMANCE EVALUATION OF NEURAL NETWORK

To test the learning proficiency and thus the network convergence, the critical temperatures resulting from the 35 substances were presented to all of the learned networks. During this stage, all output values were quickly and accurately determined to the correct value.

The networks were able to learn the correct association between the fundamental physical properties and critical temperature. The best average performance was achieved by a network with 9 hidden units which attained 0.090 sum of learned error

squared for 35 substances in 100,000 time steps. There was an insignificant increase in performance with the number of hidden units between four and nine.

Comparison between learned values by the network and observed values are shown in Table 2. Hidden units numbered four and time steps 100,000. From Table 2, the average absolute error of learning was 0.240% for the thirty five hydrocarbons(No.1 - 35, in Table 2), 0.182% for the nineteen paraffins (No.1 - 19), and 0.308% for the sixteen olefins (No.20 - 35) whereas maximum error for learning was -0.861% of ethane. Minimum error was 0.012 % for butane (No.4, in Table 2). The characteristic of the learning can be confirmed on Table 2. The network ability to learn such numeric data is almost perfect.

The comparison between the values predicted by the network and observed values were performed. The predictions were performed for the thirty five hydrocarbons listed in Table 1 after learning 100,000 time steps with four hidden units.

During learning the predicted substance was taken from example data, thus the prediction by the network was performed from the other thirty four hydrocarbons. The maximum, minimum, and average absolute error for the thirty five hydrocarbons were 3.722, -0.011, and 0.389%, respectively. On the other hand, the conventional Lydersen's method gave the maximum, minimum, and average absolute error -1.814, -0.055, and 0.589%, respectively. The maximum, minimum, and average absolute error for the nineteen paraffins were 3.722, -0.039, and 0.399%, respectively. The maximum, minimum, and average absolute error for the sixteen olefins were 0.833, -0.011, and 0.377%, respectively. The errors show that the neural network based method is equivalent and/or superior to the conventional method.

CONCLUSIONS

In this work, a neural network based methodology for developing prediction systems for critical temperature from fundamental physical properties is presented. As demonstrated, neural networks are able to acquire numeric knowledge of physical properties from examples of series of substances. This knowledge acquisition is an automatic process driven by a learning algorithm called the back propagation algorithm. The neural network's recall of learned data is nearly perfect with an average absolute error 0.389%. Thus, the network has the useful characteristic of being able to deal with incomplete numeric information. The ability to learn from example and extract correlation from data makes neural networks ideal for the prediction of physical properties. It is believed that an integration of neural networks together with traditional correlation methods is effective in developing prediction systems using numeric data.

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Keywords

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