Neural Network Model for Forecasting the Cetane Number in the Diesel Fuels

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ABSTRACT

The cetane number is important for the process of production of the diesel fuels. This article offers a model for forecasting the cetane number by neural networks. The proposed model is compared with a standardized by the organization ASTM method for forecasting, used in the factories of LUKOIL. For this purpose the laboratories of LUKOIL have tested 140 samples of diesel fuel, and the data, provided by them include the cetane number and the density, plus three more indicators expressed in a scale defined by the organization ASTM, also established empirically. As a result, estimation made by the neural network has less error than the method used in the enterprise.

Keywords
Neural network, forecasting, diesel fuels.

1. INTRODUCTION

The process of the distillation of petroleum products is complex and continuous, and during its progress, it is needed to monitor and modify multiple parameters. An important indicator of the quality of diesel fuels is their cetane number. An article from British Petroleum defining cetane number states that: The cetane number is a measure of the combustion roughness. [1]. This is equivalent to octane rating of gasoline. This is an important indicator for the process of production because when it changes, it is required to respond as quickly as possible, by modifying the parameters of the process. Usually determination of its value is done by burning a sample of the fuel in an engine, and cetane number is determined as a function of engine power under certain conditions. To determine the cetane number in this way the standard D613A was developed [2]. In practice, determination of the cetane number in this way is associated with several drawbacks, since on the one hand it is not always possible (e.g., a sample of the fuel is very small for such tests) and on the other hand the technical time that is needed for conducting the tests, evaluation and analysis of results appears to be a problem. For this reason a number of methods for theoretical determination of cetane number based on indicators which values are known have been developed. Chevron Research Co developed a standard that includes a methodology for determining cetane number based on four indicators [3]. The authors claim that the resulting error amounts to ±2 cetane numbers for the estimated distillate fuels. Interest of scientific and practical point of view represents the construction of a neural network model which is able to predict the cetane number with similar, and perhaps even less error level.

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2. ANALYSIS

In the source [4] the authors consider the possibility of predicting the cetane number of diesel fuels on the basis of their chemical composition. They assume that the cetane number and the density of the diesel fuels may be determined on the base of indicators derived from the chemical analysis such as liquid chromatography, gas chromatography and mass spectrometry. The extract of data available to them consisted of 69 samples. They find correlation between the cetane number and the data for 12 hydrocarbon groups (derived from chemical analysis). In order to obtain a more accurate model they developed GRNN (general regression neural network) neural network. After a comparison of the resulting error with error produced by prediction of the cetane number with the help of linear regression, they found out that the neural network model is doing better.

The authors [5] considered the problem of predicting the cetane number of biodiesel fuels as important to the production process. Authors note that empirical determination of cetane number is a difficult process and built a forecasting model based on fatty acid composition of the raw material for biodiesel production. They built different models for forecasting, examined multi-layer feed forward, radial base, generalized regression and recurrent neural network models. The developed models successfully cope with the task of predicting the cetane number.

In source [6], the authors consider the possibility of building a neural network to predict the cetane number on the base of data obtained from nuclear magnetic resonance. The authors had difficulties constructing the model, as their input parameters are numerous - 18, and the extract with sample data contain very few examples - 60 in number. To solve this problem, they use intermediate neural network, which reduced the input parameters to 8 in number. Based on the transformed extract they trained a neural network, which performed with satisfactory results in predicting the cetane number. The model is calibrated with the help of a test engine unit that empirically established the cetane number.

The authors [7] obtained Neural network models for estimation of cetane number of biodiesel. They evaluated twenty four neural networks by using two topologies. The best accuracy neural network for predict the cetane number was selected. It was backpropagation network with the Levenberg–Marquardt algorithm for the second step of the network training. They also developed model using multiple regression which compared to two other models from literature, was able to predict cetane number with 89% of accuracy. Their Neural network model had even better accuracy with 92%.

3. STANDARDS USED IN THE ENTERPRISE

In the studied enterprise LUKOIL [8] data is measured, stored and converted in the standard ASTM D86. The organization ASTM (American Society for Testing and Materials) offers standards and methods to standardize the properties of over 12,000 products, including diesel fuels. While less popular in Europe than the standard ISO (International Organization for Standardization), which publishes standards, ASTM plays a major role overseas. As it is well known traditionally oil prices are in U.S. dollars, and from there follows that the measures used in the production of oil should also be in U.S. units and standardized according to the U.S. standards. Therefore it is not surprising that the production in a European plant uses U.S. scales to assess different indicators.

The provided data include analysis of 140 samples of diesel fuel in the laboratories of LUKOIL, and consist of the values of 5 indicators, which are given in normalized form in order to preserve the privacy of the dynamics of the process. The formula used for normalization of the data is: new value = (old value - min) / (max - min), where max and min are the maximum and minimum values of a given indicator. This formula puts all indicators in a uniform scale [0; 1]. This scale is very convenient and in assessing the error, for example, at error rate of 0.15 (or deviation of 0.15 in predicting an indicator of the target value) directly reflects 15% error of the model.

Data courtesy of LUKOIL include the following indicators:

- Physical property Density (ρ) of the produced diesel distillate measured at 15* C in grams per cubic centimeter; this indicator is an input for the forecasting model;

Data for three indicators that take into account the process of distillation in degrees C, standardized by ASTM standard D86:

- degrees, at which are evaporated 10% of the volume of distillate;
- degrees, at which are evaporated 50% of the volume of distillate;
- degrees, at which are evaporated 90% of the volume of distillate.

The three indicators above will also be used as an input for the forecasting model.

- The indicator cetane number, measured by standard ASTM D613, is empirically measured in the laboratory of the enterprise. This indicator is an output for the forecasting model (its value is the subject of the forecast). Its value is the result of burning fuel in a test engine. In this report, this value is used as a target for training and testing neural network models. Subsequently it will be used in assessing the error of the neural network model and the error resulting from the prediction by the method ASTM D4737 (which is the value of the next available for research purposes indicator):
- The last indicator is the estimated value of cetane number. This value is estimated by the method ASTM D4737. The object of this article is the evaluation of the error of this estimation on the scale [0; 1], thereby achieving an accurate basis for comparison with the error obtained in forecasting by the neural network model.

Four of these indicators are measured and stored in scales, standardized by the organization ASTM.

4. EXTRACT OF DATA

The extract of data consists of 140 samples of diesel fuel. The first step of the analysis was to normalize the data by the above described formula. As a second step, on the indicators is applied bivariate correlation analysis with the SPSS statistical software [9], and the results are shown in Table 1.

Measure unit of data in the columns is Pearson correlation. Since the correlation between the indicators do not exceed 0.9, it is not necessary to exclude any of the variables. This is due to the fact that in the statistics similar issue is considered, as two measures of a single indicator. It is generally seen that the different indicators have little correlation with the indicator of interest (D613). This complicates the construction of linear regression models for predicting this indicator.

5. NEURAL NETWORK - RESULTS

Neural Network simulation was conducted in two phases - training and forecasting. For the training stage, from the extract were allocated 119 training examples, and the remaining 21 examples were allocated for the stage of forecasting. The separation of the two parts of the extract was performed on a mechanical principle: the first 119 examples were separated from the last 21. At this stage it is important to note that the more examples are put in the training extract, the better neural network model will be trained and the more accurate it will be. On the other hand this will lead to less data remaining in the extract, which serve to evaluate the error. The neural network was constructed with four inputs, which corresponds to the input parameters of the model:

Physical property Density (ρ) of the produced diesel distillate measured at 15 * C in grams per cubic centimeter;

- degrees, at which are evaporated 10% of the volume of distillate;
- degrees, at which are evaporated 50% of the volume of distillate;
- degrees, at which are evaporated 90% of the volume of distillate;

The output of the neural network corresponds to the indicator Cetane Number. In the learning process, the inputs of the neural network are fed with training examples, which consist of the values of the four input parameters for a given sample of diesel fuel. The output of the neural network is fed with the values of the resulting parameter, in this case a cetane number assessed by an empirical test according to the standard ASTM-D86 (sample combustion engine).

The values of the synaptic weights are reset by the learning algorithm in such a way that in the following stage of forecasting when the same values (or close to them) are passed to the input of the neural network, at its output is the same (or close to it) predicted value, submitted to its output during the training. The above algorithm is applied sequentially over all training examples of the training extract.

The neural network was built on the architecture Multi-layer Perceptron, with one hidden layer with sigmoid activation function of neurons, and an output layer with linear activation function.

Table 1. Results obtained from bivariate correlation analysis of data

Indicator	ASTM_D613	Density_15	ASTM_D_86_10	ASTM_D_86_50	ASTM_D_86_90
ASTM_D613	1,0000	-0,6323	0,2205	0,1712	0,1767
Density_15	-0,6323	1,0000	0,4820	0,6157	0,4534
ASTM_D_86_10	0,2205	0,4820	1,0000	0,8023	0,3717
ASTM_D_86_50	0,1712	0,6157	0,8023	1,0000	0,8187
ASTM_D_86_90	0,1767	0,4534	0,3717	0,8187	1,0000

Scheme of the neural network is shown in Table 2.

Table 2. Scheme of the neural network

Layer	Activation function	Number of Neurons	Variable
Input	N/A	4	•density (ρ) of the produced diesel distillate measured at 15 * C; •degrees, at which are evaporated 10% of the volume of distillate; •degrees, at which are evaporated 50% of the volume of distillate; •degrees, at which are evaporated 90% of the volume of distillate;
Hidden	Sigmoid	10	N/A
Output	Linear	1	Cetane index

Results and graph of the resulting error relative to the target value of the estimated parameter can be seen in Table 3 with the 21 examples used for the prediction.

At this point it may be noted that it is possible to calculate the averages of the different measures of the error: dispersion, average for further analysis.

In Table 3 are displayed:

- The first column Cetane index is the value of the cetane number predicted by the mathematical method described in the ASTM D4737 standard and applied to data from the manufacturer; According to the mentioned standard, the error that results amounts to +/-2 cetane number (in this case, this error can be interpreted as 2 * 100/30 = +/ -6.77 %, as the cetane number of the fuel oil is between 30 and 60).
- The second column Cetane number is a cetane number of the fuel sample as measured by the method described in the standard ASTM D613. In short, the cetane number is determined empirically by burning a sample of the fuel in a test engine;
- column Physical property density (ρ) reflects the density of the sample at 15 * C in a g/cm3; Data from this column must be submitted as an input parameter in the forecasting process
- The next three columns Distillation, % evaporates (v / v) 10%, 50 %, 90% contain the information on the volatility of the fuel samples. Also used as input for the Neural Network in the forecasting process;
- ASTM D4737 error column contains the difference between the estimated by the forecasting methodology D4737, now used in the laboratory and the empirical evaluation of the laboratory sample (second column Cetane Number of the table).
- The column Neural network forecast (output) contains data with the predicted values obtained from the Neural Network model. The estimates in this column were obtained by passing to the input of Neural Network the data from the input for the model parameters.
- Neural Network error column contains the difference between the second column Cetane Number of the table and the column described above (NN Forecast).

The last row of the table contains the average error of forecasting methodology ASTM D4737 used in the enterprise, and the average error obtained from the Neural network model in predicting the same indicator.

The data in this table are not used in the training process of Neural network, so it can be concluded that the ability of NN to predict new data was assessed. In establishing, training and simulation of NM solution was used the scientific research software Matlab [10].

Table 3. Examples used for prediction

Cetane index ASTM D4737 (estimated)	Cetane number ASTM D613-target (measured)	Density at 15 oC g/cm3 (input1)	Distillation, % evaporates (v/v) 10% at (input2)	50% at (input3)	90% at (input4)	ASTM D4737 error	Neural network forecast (output)	Neural Network error
0,7215	0,7800	0,1384	0,3925	0,5565	0,8779	0,0585	0,7914	0,0114
0,6829	0,7900	0,1743	0,3972	0,5785	0,8895	0,1071	0,7521	0,0379
0,6510	0,7100	0,1653	0,3832	0,5069	0,8430	0,0590	0,7095	0,0005
0,5654	0,6167	0,2281	0,3832	0,4959	0,8605	0,0513	0,5812	0,0355
0,7620	0,8500	0,1070	0,3972	0,5289	0,7558	0,0880	0,8453	0,0047
0,7433	0,8350	0,1204	0,3972	0,5344	0,7674	0,0917	0,8260	0,0090
0,7239	0,8117	0,1070	0,3738	0,4848	0,7326	0,0878	0,8075	0,0042
0,6674	0,7667	0,1249	0,3645	0,4463	0,7035	0,0993	0,7391	0,0276
0,7609	0,7733	0,1608	0,4673	0,6281	0,7267	0,0124	0,8492	0,0759
0,7406	0,7733	0,1608	0,4673	0,5950	0,7326	0,0327	0,8198	0,0465
0,7390	0,7750	0,1608	0,4626	0,5950	0,7384	0,0360	0,8189	0,0439
0,7728	0,7733	0,1608	0,4720	0,6446	0,7442	0,0005	0,8616	0,0883
0,7339	0,7683	0,1608	0,4673	0,5840	0,7442	0,0344	0,8084	0,0401
0,6392	0,6667	0,2102	0,4252	0,5785	0,7442	0,0275	0,6921	0,0254
0,9969	1,0000	0,0756	0,4953	0,7273	0,8605	0,0031	0,9852	0,0148
0,6373	0,7333	0,1070	0,3972	0,3691	0,4128	0,0960	0,6816	0,0517
0,7427	0,8167	0,1967	0,5000	0,6832	0,8547	0,0740	0,8155	0,0012
0,6321	0,6333	0,2416	0,4486	0,6391	0,8198	0,0012	0,6776	0,0443
0,6640	0,6833	0,2147	0,4299	0,6336	0,8837	0,0193	0,7266	0,0433
0,6472	0,6667	0,2326	0,4439	0,6446	0,8488	0,0195	0,7009	0,0342
0,6485	0,8000	0,2192	0,4019	0,6336	0,8372	0,1515	0,7181	0,0819
0,7097	0,8200	0,2008	0,5243	0,6187	0,7360	0,1103	0,7575	0,0625
Average:						**0,0573**		**0,0356**

CONCLUSION

In conclusion it can be noted that the good results which have been achieved are due to the good possibilities of neural network solutions, used as a prediction tool in the study of associated parameters. The values of correlation coefficients between the different input parameters of the model, and between themselves and the resulting parameter examined by multiple correlation analysis could not confirm or deny the visible or theoretical relationship between the studied parameters. We examined the possibility of prediction of neural network solutions on examples that were not used during the training. Built neural model for network gives 2% less error than the error obtained by the standard ASTM - D4737 in order to predict the parameter Cetane number in production. This was achieved due to the densely saturated with various possible situations extract and the rich, and valuable from a scientific point of view set of 140 samples of fuel. In future research it is recommended that this experiment should be repeated with other neuron for network architectures that traditionally achieve good results, such as: Radial-Basis Network; Generalized Regression Network and Other. The aim would be both an assessment of their applicability and improvement of the model presented in the aspect of improving its accuracy. Subject of another scientific development could be a study of the feasibility of software for mathematical modeling, such as MATLAB, as a base to serve the development and implementation of software for the prediction of important indicators, including the cetane number of petroleum products in production conditions. And finally, to explore the possibility for constructing a model for the prediction of the cetane number on the basis of data from other indicators.

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Table. 4. Data used for the simulation of NN model

Appendix: Extract used for training of Neural Network model

ASTM D4737 (estimated)	ASTM D613 target (output)	Density 15 (input1)	ASTM 86_10 (input2)	ASTM D86_50 (input3)	ASTM D86_90 (input4)
0,5161	0,5683	0,2277	0,3364	0,4463	0,6570
0,6129	0,6533	0,1379	0,3178	0,4132	0,6802
0,6129	0,6833	0,2331	0,3785	0,6116	0,8081
0,5483	0,5967	0,1931	0,3037	0,4298	0,7326
0,5967	0,6233	0,2062	0,3458	0,5234	0,7791
0,4838	0,5750	0,3910	0,5794	0,6942	0,8023
0,5258	0,5250	0,0491	0,2383	0,1983	0,1802
0,6677	0,7167	0,2421	0,5374	0,6501	0,7965
0,6935	0,7250	0,2308	0,5701	0,6612	0,7326
0,4000	0,4250	0,1972	0,2664	0,2755	0,3256
0,0322	0,0333	0,6845	0,4299	0,4518	0,4360
0,0000	0,0000	1,0000	0,8037	0,8705	0,8721
0,0967	0,0667	0,7922	0,4673	0,5730	0,7558
0,6774	0,7167	0,2928	0,6542	0,7493	0,8314
0,5612	0,6200	0,3107	0,5000	0,6667	0,8140
0,6371	0,6550	0,2401	0,4673	0,6336	0,7849
0,5854	0,6167	0,2648	0,4766	0,6116	0,7326
0,6564	0,6850	0,2143	0,4720	0,5950	0,7267
0,4308	0,5583	0,0455	0,2523	0,1185	0,0000
0,4964	0,6550	0,1711	0,4393	0,3388	0,2326
0,5605	0,6733	0,2081	0,5327	0,4490	0,3488
0,6070	0,6933	0,2522	0,6262	0,5592	0,4651
0,6469	0,7467	0,2923	0,7196	0,6694	0,5465
0,7026	0,7550	0,3282	0,8131	0,7796	0,6977
0,8352	0,7333	0,3710	1,0000	1,0000	0,9302
0,4198	0,5517	0,0522	0,2523	0,1185	0,0000
0,5091	0,6550	0,1630	0,4393	0,3388	0,2326
0,5728	0,6767	0,2004	0,5327	0,4490	0,3488
0,6012	0,6917	0,2558	0,6262	0,5592	0,4651
0,6372	0,7183	0,2981	0,7196	0,6694	0,5465
0,6974	0,7250	0,3313	0,8131	0,7796	0,6977
0,7494	0,7350	0,3620	0,9065	0,8898	0,8140
0,8352	0,7183	0,3710	1,0000	1,0000	0,9302
0,4567	0,5483	0,0299	0,2523	0,1185	0,0000
0,4832	0,5917	0,0981	0,3458	0,2287	0,1163
0,5388	0,6267	0,1447	0,4393	0,3388	0,2326
0,5996	0,6567	0,1841	0,5327	0,4490	0,3488
0,6217	0,6867	0,2432	0,6262	0,5592	0,4651
0,6624	0,7117	0,2831	0,7196	0,6694	0,5465
0,7267	0,7250	0,3139	0,8131	0,7796	0,6977
0,7876	0,7400	0,3400	0,9065	0,8898	0,8140
0,4600	0,5067	0,0280	0,2523	0,1185	0,0000
0,5089	0,5617	0,0826	0,3458	0,2287	0,1163
0,5455	0,5983	0,1406	0,4393	0,3388	0,2326
0,5764	0,6350	0,1982	0,5327	0,4490	0,3488
0,5798	0,6550	0,2693	0,6262	0,5592	0,4651

0,6804	0,7033	0,2725	0,7196	0,6694	0,5465
0,7508	0,7217	0,2999	0,8131	0,7796	0,6977
0,7214	0,7367	0,3786	0,9065	0,8898	0,8140
0,4464	0,5200	0,0360	0,2523	0,1185	0,0000
0,5455	0,5683	0,1406	0,4393	0,3388	0,2326
0,5838	0,6283	0,1937	0,5327	0,4490	0,3488
0,5976	0,6433	0,2580	0,6262	0,5592	0,4651
0,6750	0,6933	0,2757	0,7196	0,6694	0,5465
0,7438	0,7000	0,3040	0,8131	0,7796	0,6977
0,7380	0,7100	0,3687	0,9065	0,8898	0,8140
0,5322	0,5800	0,0854	0,2056	0,2534	0,3140
0,6612	0,6733	0,3107	0,6168	0,8099	1,0000
0,5322	0,5550	0,0603	0,2196	0,2314	0,1977
0,6451	0,6117	0,2551	0,5467	0,6391	0,7616
0,6612	0,6750	0,3031	0,6215	0,7658	0,8547
0,5322	0,6000	0,0693	0,2430	0,2479	0,2093
0,6290	0,6750	0,2192	0,5234	0,5675	0,5407
0,7258	0,6583	0,3210	0,7523	0,8430	0,8953
0,6129	0,6167	0,4494	0,8692	0,9311	0,9419
0,5161	0,6250	0,0630	0,2150	0,2204	0,1860
0,5322	0,6667	0,0630	0,2523	0,2259	0,1919
0,6129	0,6833	0,2452	0,4813	0,6061	0,7093
0,6290	0,6633	0,2272	0,4953	0,5840	0,6860
0,6774	0,6833	0,3219	0,6869	0,8044	0,8837
0,7096	0,6500	0,2950	0,6729	0,7934	0,8663
0,5739	0,6333	0,1972	0,3178	0,4738	0,8081
0,1136	0,0500	0,5435	0,3738	0,4187	0,3895
0,3954	0,5333	0,0000	0,0000	0,0000	0,2791
0,5781	0,6667	0,4296	0,7897	0,8595	0,8895
0,4894	0,5333	0,3651	0,3832	0,7934	0,9360
0,5935	0,7117	0,1918	0,3178	0,5355	0,7558
0,2354	0,3050	0,6298	0,6079	0,7906	0,8378
0,3645	0,4483	0,4081	0,4332	0,7102	0,8151
0,4193	0,5150	0,3569	0,3668	0,6744	0,8047
0,2806	0,3867	0,4534	0,3210	0,6187	0,7797
0,3709	0,4583	0,3358	0,3126	0,5967	0,7645
0,3403	0,4100	0,3910	0,3720	0,6474	0,7849
0,4080	0,4683	0,3309	0,3523	0,6165	0,7762
0,4629	0,5067	0,2865	0,3210	0,5802	0,7634
0,2903	0,3683	0,4938	0,4360	0,7344	0,8203
0,6375	0,6767	0,2407	0,4766	0,6336	0,7616
0,8656	0,9183	0,1204	0,5841	0,6061	0,6395
0,6192	0,6317	0,2941	0,5467	0,7052	0,8605
0,5251	0,6200	0,3704	0,5607	0,7328	0,8605
0,4346	0,4667	0,4557	0,6028	0,7438	0,8547
0,3466	0,4550	0,5544	0,6449	0,7658	0,8779
0,1841	0,3017	0,7043	0,7103	0,8044	0,8895
0,5206	0,5833	0,3682	0,6028	0,6722	0,7674
0,6889	0,7667	0,1474	0,4252	0,5014	0,7209
0,7402	0,7833	0,2201	0,5397	0,7245	0,8779
0,7194	0,7833	0,2999	0,6636	0,8623	0,9797
0,7214	0,8000	0,3345	0,7500	0,9091	0,9942

0,3047	0,3333	0,4911	0,5047	0,6006	0,6657
0,3692	0,4000	0,4409	0,5187	0,6116	0,6802
0,4416	0,5000	0,3870	0,5304	0,6198	0,6919
0,5258	0,5667	0,3314	0,5467	0,6364	0,6977
0,3853	0,4050	0,2623	0,1729	0,3140	0,6163
0,4532	0,4950	0,1927	0,1776	0,3085	0,6105
0,5311	0,5800	0,1254	0,1776	0,3085	0,6047
0,3812	0,4167	0,3507	0,2243	0,4793	0,7558
0,4523	0,4850	0,2829	0,2336	0,4738	0,7558
0,5319	0,5767	0,2147	0,2290	0,4738	0,7558
0,3266	0,4183	0,4619	0,3411	0,6667	0,8256
0,3953	0,4967	0,4144	0,3879	0,6667	0,8372
0,5026	0,5700	0,3318	0,3785	0,6997	0,8314
0,5228	0,5917	0,2784	0,4346	0,5455	0,6628
0,6802	0,7850	0,1743	0,3364	0,6061	0,9186
0,6865	0,7333	0,2057	0,4346	0,6556	0,9709
0,6907	0,7117	0,0711	0,2383	0,4298	0,8547
0,7310	0,7833	0,1653	0,4159	0,6336	0,9419
0,7511	0,8167	0,1339	0,4019	0,5950	0,9360
0,8014	0,8717	0,0935	0,3879	0,5730	0,8895