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IMPLEMENTATION OF MACHINE LEARNING ALGORITHMS FOR MODELING OF ESTERIFICATION REACTION IN CSTR

K. V. Ramesh, Department of Chemical Engineering, Andhra University, Visakhapatnam-530003, India. prof.kvramesh@andhrauniversity.edu.in;
K. Venkata Rao, Department of CSSE, Andhra University, Visakhapatnam-530003, India.

Abstract

In this paper experimental data of an esterification reaction carried out in a Continuous Stirred Tank Reactor (CSTR) have been subjected to regression analysis using machine learning algorithms. A ten layer neural network has been considered in the present study. Three algorithms viz., scaled conjugate gradient algorithm, Bayesian regularization algorithm and Levenberg-Marquardt algorithms were employed and found that the Levenberg-Marquardt algorithm has been applied with great success.

Keywords

Esterification, continuous stirred tank reactor, modeling, Levenberg-Marquardt algorithm

Introduction

The advent of digital computer and rapid developments in the computing software and hardware has contributed to phenomenal development in typical process industry applications. Among several pieces of equipment that form the process, a Continuous Stirred Tank Reactor (CSTR) is one of the most important equipments around which the entire process is usually constructed. As the name suggests, the CSTR is used to carry out chemical reactions and mostly liquid phase and liquid-solid reactions. For the purpose of illustration, in the present case, a liquid phase reaction has been considered because the data are accessible to the authors. The reaction is a second order esterification reaction in which propionic acid and butanol react and form butyl propionate and water in the presence of sulphuric acid catalyst. The experimental data for this reaction are taken from Kusuma[1]. The data consisted of four independent variables and one dependent variable. The dependent variable is the conversion and the independent variables are temperature, reaction time, catalyst concentration and reactant mole ratio. A total number of 200 data points were available for this case.

It is to be emphasized that the use of computational tools for effective handling of chemical engineering problems has gained wide attention of the researchers worldwide mainly in the recent two decades[2-5]. However, the studies handling the direct experimental data of chemical process equipment appears to be somewhat less common. In this regard, the authors investigated the application of three algorithms viz., scaled conjugate gradient algorithm[6], Bayesian regularization algorithm[7] and Levenberg-Marquardt algorithm[8,9] for performing regression on the experimental data of the present study.

Algorithmic Modeling

In the present investigation three algorithms have been employed for handling the experimental data. The first algorithm is Scaled Conjugate Gradient (SCG) Algorithm, the second one is Bayesian Regularization (BR) Algorithm and finally the Levenberg-Marquardt Algorithm. Figure 1 shows the neural network employed in the present study.

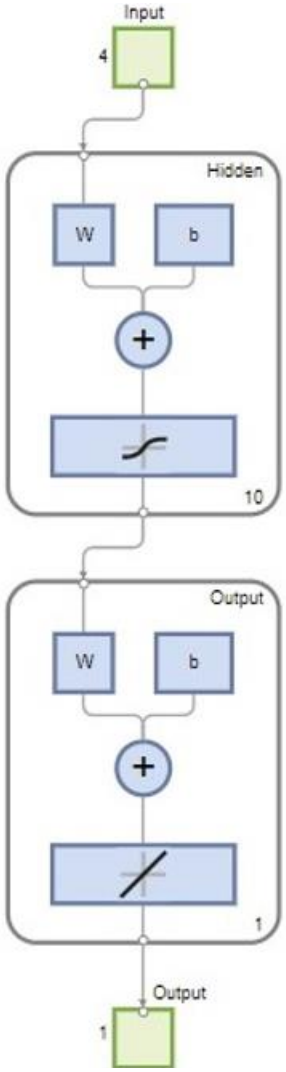

Fig.1. Two layer feedforward network with sigmoid hidden neurons and linear output neurons, suitable for regression tasks

Results and discussion

The data have been fit by using these algorithms and the results have been compiled and shown here in Table 1 for the sake of comparison. From a close examination of the data from this table reveals that the LM algorithm has been superior in fitting these data.

Table 1. Training results

	Observations	SCG		BR		LM	
		MSE	R	MSE	R	MSE	R
Training	140	0.0237	0.7246	0.0010	0.9886	0.0009	0.9896
Validation	30	0.0176	0.7335	NaN	NaN	0.0015	0.9850
Test	30	0.0265	0.7271	0.0020	0.9877	0.0034	0.9765
Additional test	200	-	-	-	-	0.0014	0.9856

Therefore, the results obtained with Levenberg-Marquardt algorithm had been presented in detail hereunder. Figure 2 shows the plots corresponding to the data fitting by LM algorithm. Figure 3 shows the error histogram and Figure 4 presents the validation diagram.

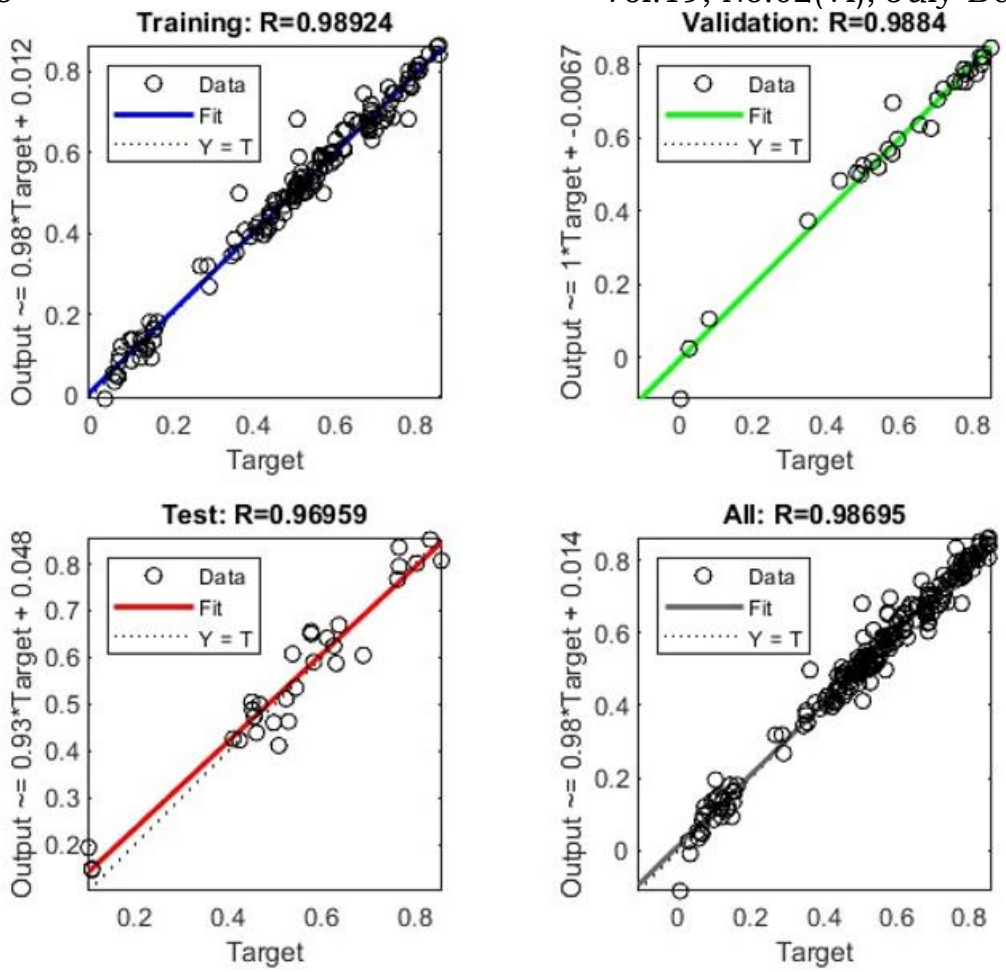

Fig.2. Data fit by Levenberg-Marquardt algorithm.

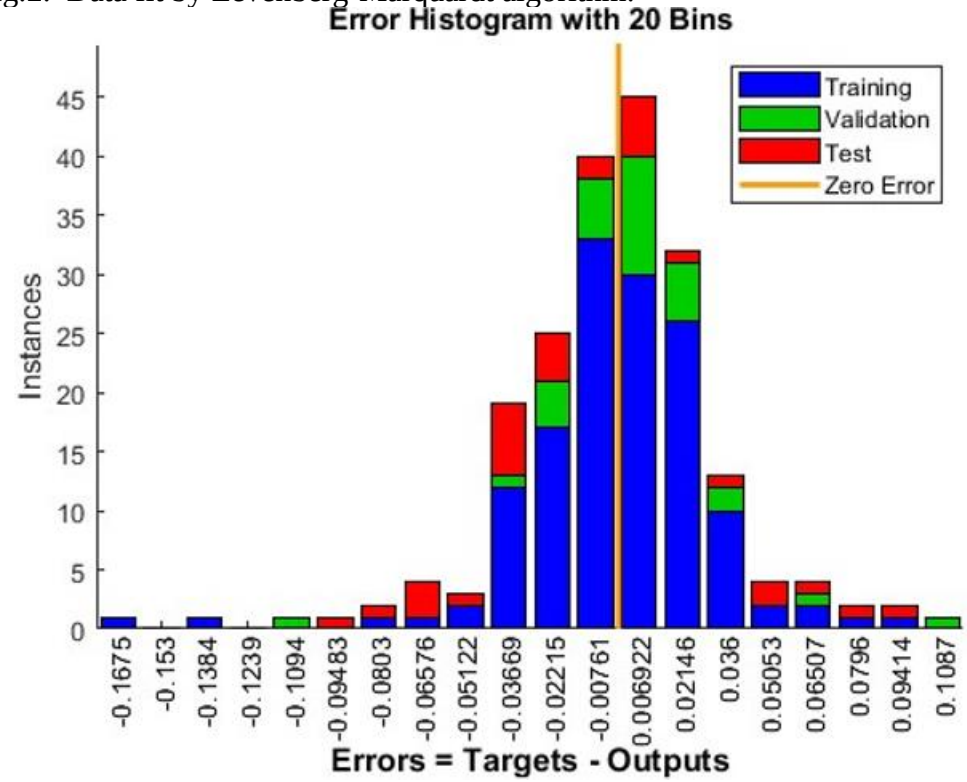

Fig.3. Error histogram

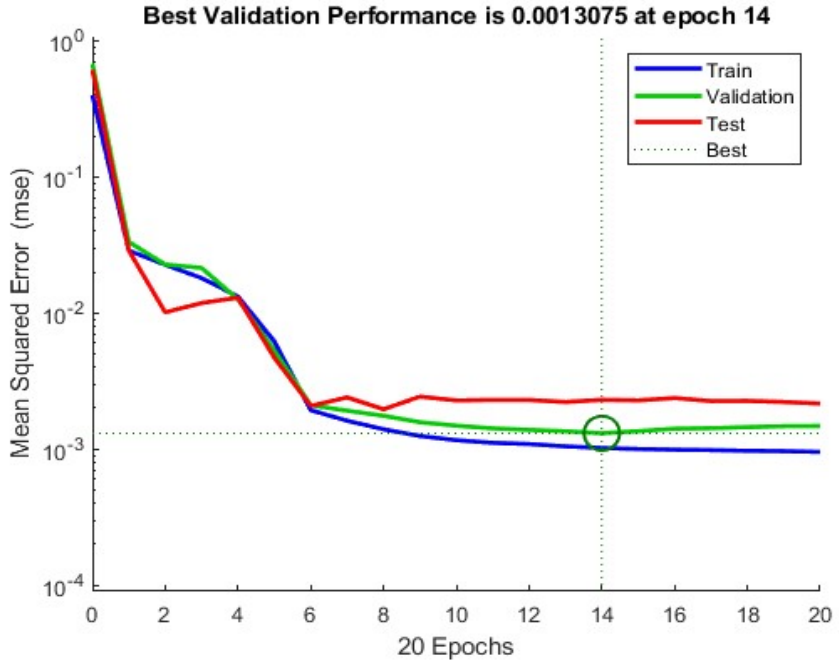

Fig.4. Validation diagram

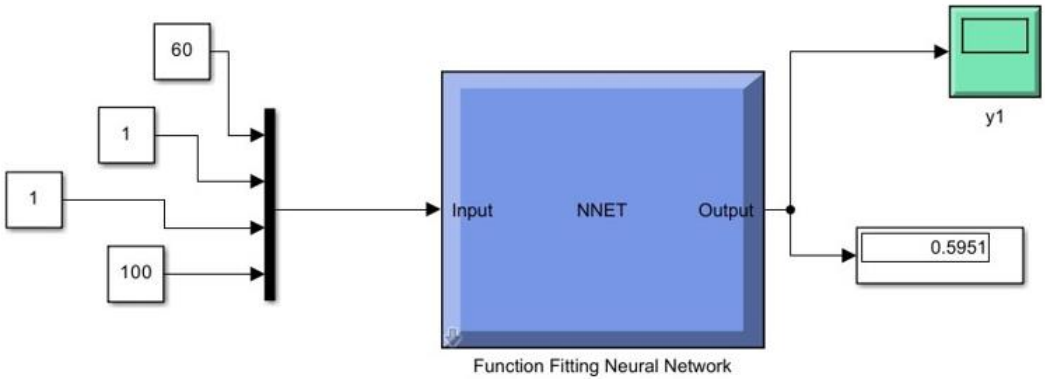

Fig.5. Function fitting neural network

Figure 5 shows the matlab simulink diagram containing the function fitting neural network. For example, by taking one case with inputs as 1, 1, 60 and 100 the output shown by the neural network is 0.5971 whereas the actual experimental value is 0.597. Similar findings were also noticed from randomly testing other data. The entire data tested thus have been plotted and shown in Figure 6.

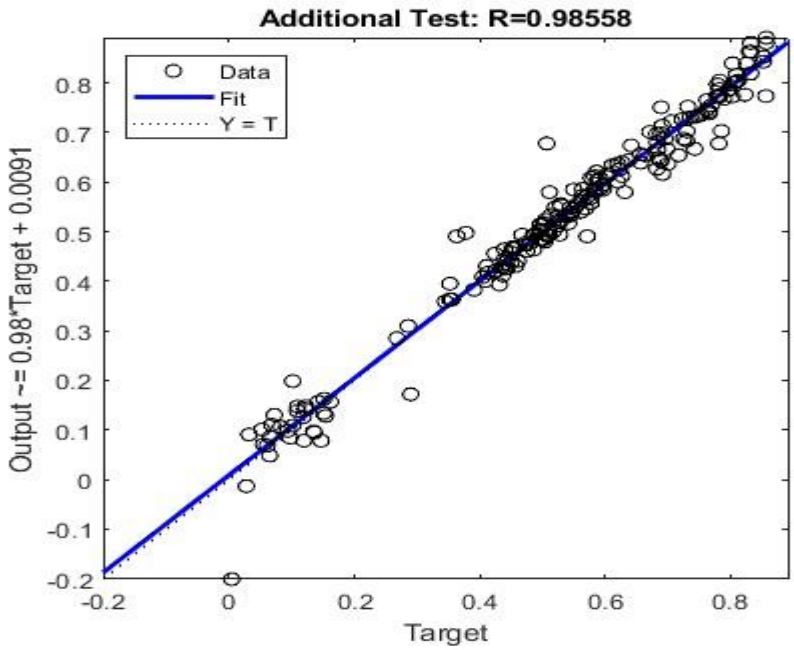

Fig.6. Experimental versus predicted data

It is observed from figure 6 that the entire experimental data have been fitted well with a mean squared error of 0.0014 and a correlation coefficient of 0.9856.

Conclusions

The following observations were made from the present study.

(i) Three algorithms viz., Scaled Conjugate Gradient Algorithm, Bayesian Regularization Algorithm Levenberg-Marquardt Algorithm have been employed to fit the experimental data of the esterification reaction..

(ii) It is found that the Levenberg-Marquardt algorithm has shown superior performance.

(iii) Entire data were validated with the neural network trained LM algorithm and found satisfactory results..

References

1. M. Kusuma, Formation of propionates: Kinetics and thermodynamics, Ph.D. thesis, Andhra University, Visakhapatnam, India (2023).
2. G.M.J. Raju, G.V.S. Sarma, K.V. Ramesh, C. Bhaskara Sarma, Mass transfer at the confining wall of an electrochemical cell with coaxially rotating composite promoter, *International Journal of Heat and Mass Transfer* 71, 682-690 (2014).
3. G. Vamsi Krishna, B. Sreenivasulu, N.S. Kirti, B. Ravali Sree, K.V. Ramesh, A numerical study on enhanced heat transfer in a lid driven cavity with and without fins, Proceedings of ICECA-2017 (IEEE), 609-614.
4. A. Sailaja, B. Sreenivasulu, B. Srinivas, K.V. Ramesh, Flow and heat transfer characteristics in a microchannel with asymmetric wall zeta potentials, Lecture Notes in Electrical Engineering, 521, 729-739 (2019).
5. B. Srinivas, P. Rohini Kumar, B. Sreenivasulu, K.V. Ramesh, An efficient method to design a series cascade controller using multi-objective optimization, Proceedings of ICECA-2017 (IEEE), 218-224.
6. J.S. Qin, Y. Liu, S. Tang, Partial least squares, steepest descent, and conjugate gradient for regularized predictive modeling, AIChE Journal, 69(4) e17992(2023)
7. M.C. Coleman, D.E. Block, Nonlinear experimental design using Bayesian regularized neural networks, 53(6) 1496-1509 (2007).
8. M. Zic, V. Subotic, S. Pereverzyev, I. Fajfar, Solving CNLS problems using Levenberg-Marquardt algorithm: A new fitting strategy cobinng limits and a symbolic Jacobian matrix, Journal of Electroanalytical Chemistry, 866, 114171(2020).
9. J. Bilski, J. Smolag, B. Kowalczyk, K. Grzanek, I. Izonin, Fast computational approach to the Levenberg-Marquardt algorithm for training feedforward neural networks, Journal of Artificial Intelligence and Soft Computing Research, 13(2) 45-61 (2023).