Application of Artificial Neural Networks for Optimizing Operating Conditions of a Chemical Process

Kathiravan Srinivasan, School of Information Technology and Engineering,
Vellore Institute of Technology, Vellore, India,
Ashish Garg, Vellore Institute of Technology, Vellore, India,
Bor-Yann Chen, National Ilan University, Yilan County, Taiwan (ROC),
Chang-Tang Chang, National Ilan University, Yilan County, Taiwan (ROC),
Aswani Kumar Cherukuri, Vellore Institute of Technology, Vellore, India,
Jennifer Pounjeba Philip Christopher, National Ilan University, Yilan County, Taiwan (ROC).

ABSTRACT

Considering that there are a significantly large number of variables and several steps, in a chemical process, modeling of such a method is non-trivial. Moreover, the process has a non-linear and transience dependence on the conditions. Artificial Neural Network (ANN) and Deep Learning methods based on ANNs have been widely recognized as one of the most influential modeling and learning techniques for nonlinear systems. The salient feature of ANN- based modeling is that the detailed mathematical information about the process steps is not pre-determined or fed to the system; instead, the learning takes place by using the training examples. Therefore, it is not surprising that ANN-based modeling is used for predicting the outcomes of chemical processes. Experimental data will be required to train the model and also to validate the predictions.

I. INTRODUCTION

It is imperative to model and predict chemical processes as it helps to reduce the number of experiments and prediction of better results beforehand which further saves a lot of time, energy and money to perform experiments. As the behavior of chemical processes is mostly non -linear, many processes like Response Surface Methodology (RSM) [1], and Taguchi's method are already used to study the chemical processes behavior; but the main drawback is that these methods need a proper design before making a prediction and deliver optimal results. In our study, we will be using a multilayer perceptron (MLP) which take the inputs as training data and learn from them by iterating over several times adjusting the value of weights and corresponding bias, and at each time correcting itself to generate a more optimal fit towards data. As is required by ANN -based schemes, a simulation matrix of input variables such as pressure, temperature, and so on. Moreover, the output variable, namely, the linear expansion will be generated from the experimental data. This way, two model layers, namely, the input layer consisting of multivariable nodes and the output layer consisting of the efficiency, will be conceptually created. The internal layers will be incorporated based on the complexity of the problem.

II. PROPOSED METHOD

The training of a neural network will be performed using Levenberg-Marquardt algorithm [2], also known as the damped least-squares method. It has been designed to work individually with loss functions that proceed to be the sum of squared errors. Further, it functions devoid of calculating the exact Hessian matrix. As an alternative, it works with the gradient vector and Jacobian matrix the foremost step is to cal -culate the loss, the gradient, and the Hessian approximation. Then the damping factor is adjusted to reduce the loss at each iteration.

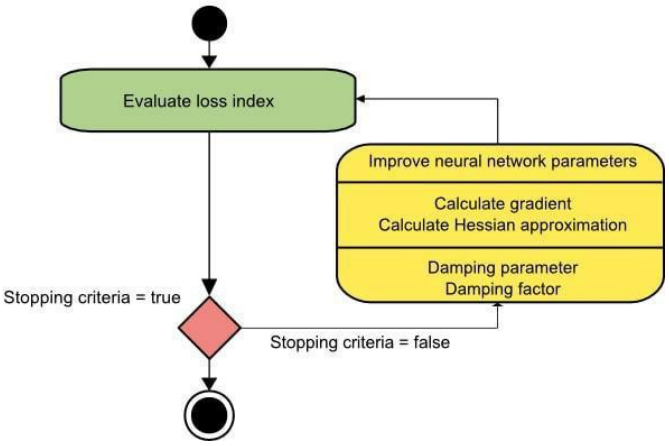

Fig 1: Working of the Levenberg-Marquardt algorithm

As the Levenberg-Marquardt algorithm is a method that is tailored for functions of the type sum-of-squared error. Also, it makes swift progress when training neural networks measured on that kind of errors. For massive datasets and neural networks, the Jacobian matrix becomes enormous and therefore require much memory, the use of it is not recommended, when we have big datasets, so it suits best for chemical process modeling with few sets of experimental data [3-6]

III.IMPLEMENTATION AND RESULTS

Typically, for proving the modeling power of artificial neural network using Levenberg-Marquardt as a learning algorithm; a linear expansion experimental design data of firecrackers [1] is taken into account. In this approach, the Streaming time, Drying temperature and gel setting time is regarded as an input parameter and linear expansion of a produced firecracker as an output variable. The stimulation is performed using the MATLAB software. The neural network with the configuration of three input neurons in input layer ten neurons in hidden layer and one output neuron in output layer were found best in the prediction of experimental results, the results of same can be found in Table 1 and Table 2.

Table 1: Experimental and Predicted Results

Experimental	Predicted
66.32	62.73
56.54	58.31
57.71	57.71
61.73	58.31
51.3	51.5
64.64	61.36
57.77	58.31
70.3	70.3
55.42	55.42
56.45	56.45
64.14	64.14
71.14	70.22
67.27	67.27
69.3	69.3
61.78	57.47
57.22	58.315

Table 2: Statistical Parameters of Prediction

Statistical Parameters	Values
R^2	0.90
RMSE	1.87
AE	1.8%

IV. Conclusion

The present study optimizes the gelatinization condition for linear expansion using Artificial Neural Networks. The Multi-layer neural network, (3-10-1) is chosen to develop accurate and complicated non-linear relationship with ANN and, in this case coefficient of determination (R^2) is found to be 0.90 as in (Table 2). This Table 2 shows a functional agreement of predicted data with experimental data, and it is also noticed that the predicted power of ANN with R^2=0.90 is better than RSM with R^2=0.86, hence for this case, ANN can be used for predictive modeling.

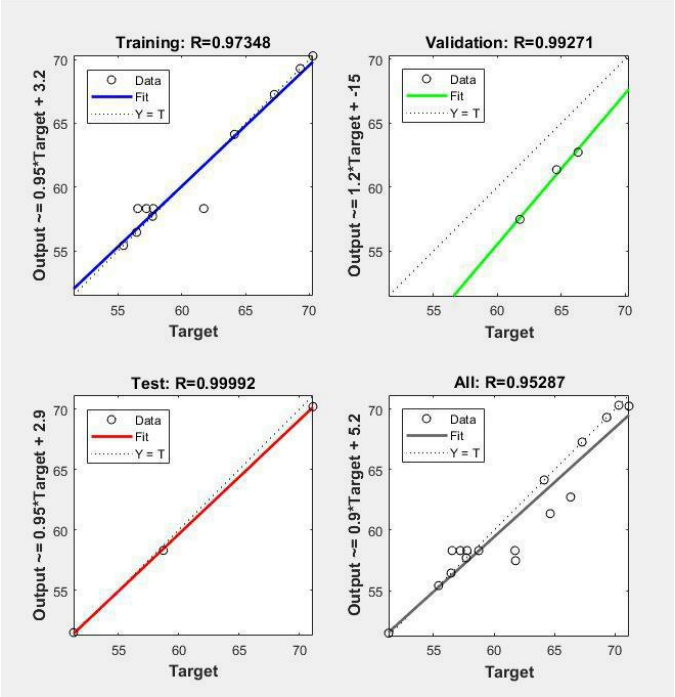

Fig 2: Simulation Results

V. References

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