ECE/CS/ME 539 Introduction to Artificial Neural Networks

Project Progress Report

**Prediction of Thermodynamic Properties of Superheated Steam**

Team 13

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**ABSTRACT**

The goal of this project is to build an artificial neural network with multi-layer perceptron architecture (MLPNN) to predict the thermal dynamic properties of superheated steam. The performance of the MLPNN is assessed by comparing the SSE of the predicted values to those of equation of state (EOS) method and linear interpolation method on the same testing set. So far, we finished pre-processing the data, coded the EOS method and the linear interpolation method for comparison, and initiated the construction of the MLPNN. We are conforming perfectly to the proposed timeline, and we expect to finish the project as scheduled.

**Introduction**

**Overview**

The Gibb’s phase rule asserts that, for a pure compound, its set of thermodynamic properties (TP) are fully determined by specifying any two of the thermodynamic state variables. However, no model to date can calculate the TP of superheated steam (refer to as steam below), the most widely used industrial chemical, with satisfactory accuracy for engineering purposes. This project aims to capture the complex equation of state that governs the TP of steam using artificial neural networks.

**Motivations and Significance**

Industrial steam is primarily used in steam cracking of naphtha to produce light weight hydrocarbons, in steam turbine to generate electricity, and in heat transfer to control temperature. The efficiency of all three processes above depends heavily on the TP of steam, which are complex functions of operating conditions, typically specified as temperature and pressure. Therefore, accurate prediction of TP is fundamental to efficient operation.

**Related Works**

The traditional approach to TP prediction is empirical; the TP of steam is measured at a wide range of operating conditions and compiled into tables, and the TP at desired operating conditions is obtained by linearly interpolating within the table.

Chemists and physicists have developed numerous first-principle models for TP prediction, most of which are in the form of Equation of State (EOS). The most popular EOS includes Van der Waals EOS and Redlich-Kwong EOS. Despite the great advancement in EOS in the 20th century, its inaccuracy forbids the use of EOS in practical TP prediction.

The use of multi-layer perception neural network (MLPNN) in predicting TP of different substances has been demonstrated by a few researchers with promising degree of success [1] [2] [3]. However, to the best of the authors’ knowledge, no attempt has been made to apply deep MLPNN for prediction of TP of superheated steam. This work will serve as a first attempt to test the applicability of MLPNN in such task.

**Method**

**Data**

The TP of superheated steam was obtained from Ohio University as a csv file [4]. We pre-processed the data manually, so the processed data consists of six columns (temperature, pressure, volume, energy, enthalpy, and entropy) corresponding to the TP of superheated steam. 80% of this data was used for training, with the remaining 20% as testing set.

**Algorithm and Program**

The MLPNN was constructed using the Keras package in Python, the MLPNN consists of four layers, with 50, 25, 10, 4 neurons in each corresponding layer, and ReLU activation function. The MLPNN was trained using the training set as described above.

For comparison, the linear interpolation method was coded using standard interpolation techniques. Van-der Waals EOS was selected as a model for the EOS method due to its simplicity in coding, the derivation process for each TP can be found in Appendix A.

**Platform**

We chose Google Colab as the platform for coding and training the MLPNN, linear interpolation method, and EOS method. All the codes are available on Github [5].

**Performance Metric**

After training the MLPNN, all three methods are tested using the testing data set. A loss value is assigned to each prediction by computing the normalized sum of squared error between the predicted TP and the actual TP.

The normalization is done by subtracting the mean of training data from the predicted value and dividing the residue by the standard deviation of the training data. The same set of procedures is applied to the testing data. The normalized sum of squared error is then computed on the normalized predicted value and the normalized testing data.

The sum of loss values over the testing data set is used as an indication of performance to compare among the three methods for accuracy.

**Results**

The MLPNN is constructed and trained as disclosed in Method section. The sum of loss values over the testing set of each method is presented below in Table 1.

Table 1. Loss values of MLPNN, linear interpolation, and EOS method on the testing set

|  |  |  |  |
| --- | --- | --- | --- |
|  | MLPNN (this work) | Linear Interpolation | EOS |
| Loss | 109.51 | 1.29 | 20571.17 |

We see that the loss value on the testing set indicates that the un-optimized MLPNN is performing much better than the EOS method, however, it is still far from achieving the same performance as the state-of-art linear interpolation method

**Discussion**

The preliminary results suggests that the MLPNN is already outperforming the EOS method without any optimization. However, the MLPNN’s performance is two orders of magnitudes worse than the standard linear interpolation method, indicating that more work on fine tuning the MLPNN architecture and training hyper-parameters is needed to obtain the same level of performance.

**References**

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