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**

We investigated the potential of artificial neural network in predicting the thermal dynamic properties (TP) of superheated steam in this project. We developed a multilayer perceptron neural network (MLPNN) and a decision tree regressor ensemble (DTRE), and compared their performance to the more classical prediction equation of state (EOS) method and linear interpolation method. The optimized MLPNN scored a sum of squared error (SSE) on the testing set of 5.5, the DTRE scored an SSE of 34, while the linear interpolation method scored an SSE of 0.24, which was more than an order of magnitude better than both artificial neural networks. The outperformance of DTRE by MLPNN suggests that the underlying network architecture plays an important role in achieving high accuracies. We recommend future works to focus on exploring different neural network models, which may yield a model that is sufficiently close to the true model of TP of superheated steam, and capable of offering us physical insights into other substances.

**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, Redlich-Kwong EOS and CPA EOS [1]. Despite the great advancement in EOS in the 20th century, its inaccuracy forbids the use of EOS in practical TP prediction.

The use of artificial neural network in predicting TP of different substances has been demonstrated by a few researchers with promising degree of success, most of which are based on multi-layer perceptron neural network (MLPNN) [1] [2] [3]. However, to the best of the authors’ knowledge, no attempt has been made to apply decision tree regressor ensemble (DTRE) to predict TP of steam. This work will serve as a first attempt to test the applicability of DTRE in such task.

**Method**

**Data**

The TP of superheated steam was obtained from NIST via Indian Institute of Technology Bombay as a pdf file [4]. The dataset consists of 1600 measurements of steam TP containing pressure, temperature, specific volume, specific energy, specific enthalpy, and specific entropy. We pre-processed the data manually to convert the data in the pdf file into a csv file that can be used directly for training and evaluation; 80% of this data was used for training, with the remaining 20% used as testing set.

Since industrial operating conditions are often specified as temperature and pressure, the temperature and pressure of steam are used as features, with the remaining TP as labels. We performed feature normalization based on the training set to boost convergence in training. Specifically, each TP is normalized by subtracting the mean and dividing by the standard deviation of that TP in the training set.

**Algorithm and Program**

The MLPNN was constructed using the Keras package in Python, which consists of three layers with 21, 10, 4 neurons in each layer, with ReLU activation function. The size of the MLPNN was deliberately minimized to avoid overfitting, due to the small size of dataset. The structure reported above was determined using a weighted sum of squared error as metric, which is explained in Performance Metric in more details.

The DTRE was constructed using the Sci-kit learn package in Python, which consists of 2 decision tree regressors each of depth 4. The structure of the DTRE was optimized based on weighted sum of squared error as the MLPNN.

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. Although more accurate EOS in prediction of TP has been reported in literature, not enough details were disclosed to allow for efficient adaption to this work for comparison.

**Platform**

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

**Performance Metric**

For determination of the optimal artificial neural network structure, we compared the performance of each network structure on the testing set using a weighted sum of squared error (SSE) defined as

Where the SSE in the equation refers to the error between the predicted TP (volume, energy, enthalpy, and entropy) and the actual TP. The number of parameters was included to penalize the potential of overfitting. The structure with the smallest weighted SSE was deemed the optimum structure.

For comparison across different models, we selected the regular SSE on the testing set to serve as a performance indicator. The method with the smallest SSE was deemed as the most accurate method.

**Results**

Figure 1 below shows an example of how we determined the optimum number of neurons in the first layer of the MLPNN.

Chart, line chart

Description automatically generated

Figure . Computed weighted SSE on validation set versus the number of neurons in the first layer of the MLPNN.

The smallest weighted SSE is achieved with 21 neurons in the first layer, and was deemed as the optimal number of neurons in the first layer. Other optimal structural parameters for MLPNN and DTRE were determined in a similar fashion.

The performance of the various methods implemented are summarized as sum of loss values below in Table 1.

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | MLPNN | DTRE | Linear Interpolation | EOS |
| Loss | 5.5 | 34 | 0.24 | 368 |

The loss value on the testing set indicates that both MLPNN and DTRE outperforms the EOS method but falls short of the linear interpolation method. The loss values also suggest that the MLPNN method is seven times as accurate as the DTRE method.

**Discussion**

We see that the loss values vary by orders of magnitude, where the worst method, Van der Waals EOS, performing four orders of magnitude worse than the best method, linear interpolation. This result explains why linear interpolation remains engineers’ most preferred method of predicting TP of steam, as it is the simplest yet the most accurate method.

Although the structure and the training hyperparameter of the MLPNN and the DTRE have been optimized, their performance is still one to two orders of magnitude worse than the simple linear interpolation method, which explains the limited interest in using artificial neural network in this area of application.

It is worth discussing the reason why MLPNN outperforms DTRE so much. One possible could be the number of parameters, as MLPNN has 338 parameters, versus 180 parameters in DTRE. Another possibility is that the true model of the TP of steam is more closely approximated by MLPNN compared to DTRE, which naturally leads to better performance. We recommend future workers in this area to explore different types of artificial neural network architectures, which may lead us to arrive at a model that is sufficiently close to the true model of steam’s TP, that we can use to improve our understanding of the underlying physics of TP.

**References**

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**Appendix A.** Thermodynamic properties using Van der Waals equation of state calculation notes

There are four thermodynamic properties we need to calculate from equation of state: volume, energy, enthalpy, and entropy. Since no analytical solution exist for calculation of these properties as function of temperature and pressure, we need to work with the differentials of these four thermodynamic properties as a function of differential temperature and differential pressure.

The Van der Waals EOS is

The differential of volume as a function of temperature and pressure can be calculated using the relation

Define

Then

And we get

Which allows us to approximate

And likewise for volume with respect to temperature.

The energy can be calculated analytically from the definition of enthalpy

The differential of enthalpy, is given by

By definition

Which is known, for the other derivative term, we can use an alternative form of differential of enthalpy and Maxwell’s relation to get

Since we already know the differential of V with respect to T above, we can calculate H as

For the differentials of entropy, we need to revisit the differential of enthalpy, we see that

For the dependence on pressure, we can use Maxwell’s relation to get

We have listed all the equations needed to calculate the thermodynamic properties of steam using Van der Waals EOS. The parameters that appeared in the EOS, for the case of steam, are