Introducing Artificial Neural Networks as a Specific Enthalpy approximator for a course on introductory Thermodynamics

Aneet Dharmavaram Narendranath
Mechanical Engineering-Engineering Mechanics
Michigan Technological University
Houghton, MI, USA
dnaneet@mtu.edu

***Abstract*—In this innovative practice, work-in-progress paper, an example is provided through which mechanical engineering students can be instructed the heuristic creation of feedforward artificial neural networks (ANN), their training, validation and quantification of their accuracy, in the context of a thermodynamics course.**

As big data and machine learning continue to permeate and affect the viscera of society, new challenges and career opportunities emerge. Organizations such as NSF, McKinsey global institute, Gartner global newsroom, IBM, to name a few, have published projections on the global impact big data and machine learning on the job market and how these technologies are the "next frontier in innovation".

The example demonstrated here, may be introduced as a module in a traditional thermodynamics course. Using a validated ANN, the thermodynamic property of specific enthalpy of steam is evaluated, when given a thermodynamic state specification of temperature and pressure. The data used to train the neural network is generated using the equations of state provided in the IAPWS IF-97 industrial standard for water and steam. The effect of number and type of layers on the accuracy of the network and the effect of data pre-processing, on the accuracy of the network can be studied.

***Index Terms*—component, formatting, style, styling, insert**

I. Introduction

We continue to experience the advent and impact of artificial intelligence (AI) with current-day applications such as smartphone based assistants [3] or web search-engine technology [4] running many aspects of diurnal life. Machine learning (ML) is one of the prerequisites to create AI. It involves "learning" *input* $\rightarrow$ *output* mapping from a dataset of inputs and outputs and "fitting" a complex curve (or surface) as an approximation or to make predictions of future (spatio-temporal) states for static, numeric/non-numeric or time-series data. An artificial neural network (ANN) is one of the many "tools" that can be used or created towards machine learning and hence artificial intelligence.

The material presented in this paper will make the creation of simple artificial neural networks as function approximators, **more accessible to mechanical engineering students**, thus equipping them with one of the the building blocks of cutting-edge technologies that use AI, viz., self-driving vehicles (to name a few: [5], [6]), bionic technologies [3], next generation computing technology that may be used to solve complex optimization problems [7]. Neural networks can take advantage of the increased amount of data availability [36] towards intelligent design of complex systems.

II. Feedforward Neural Networks

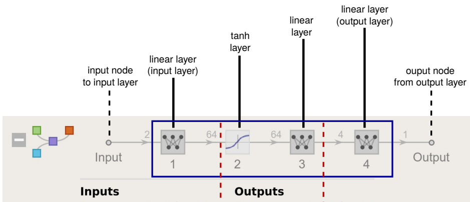
A feedfoward neural network that allows the flow of data in unidirectional fashion through its multilayered architecture is shown in figure 1a. Each layer performs a mathematical operation on the data fed to it, to fit an internal regression model that approximates the overall *input* $\rightarrow$ *output* mapping. Figure 1b shows the results of a neural network used as a simple function approximator, for the mapping $y = x^2$. This example could be followed with a "minute paper" or muddiest point technique or ungraded quiz type formative assessment to measure if students understand the use of a neural network as a function approximator.

The layers of an ANN may be connected heuristically and carry some mystery [8]. These layers can be linear mathematical operations coupled to layers of fuzzy, nonlinear operations. The *inputs* $\rightarrow$ *outputs* thermodynamic mapping of data used in this paper is shown in figure 2.

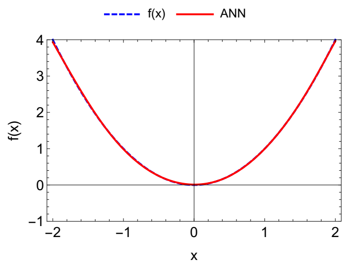
An ANN accepts input data at an input layer stage, has one or more hidden layers that may be heuristically chosen and an output layer which provides an approximation (or prediction). An ANN created in Wolfram Mathematica 12.0 with depiction of the internal layers is shown in figure 1. This representation shows a one-way movement of information and is called a *feedforward network*. The layers used in the thermodynamic approximator in this paper are the "linear layer" and the "Tanh layer" (a nonlinear layer to approximate nonlinear transitions).

A. Wolfram Mathematica 12.0 and neural network creation

The author chose Wolfram Mathematica 12.0 given it's powerful symbolic algebra, calculus and ANN creation ecosystem [32]. The symbolic algebra capabilities of Mathematica allow minimum barrier to entry as opposed to traditional programming environments [9]. The ANN creation ecosystem in Mathematica (version 9 or greater) allows full access to aspects of operating with ANN, viz., data manipulation,



(a) ANN architecture of a feedforward network with an input layer, hidden layers and the output layer, constructed in the Wolfram Mathematica 12.0.



(b) Successful mapping of $y = x^2$ performed by an ANN. An example to motivate the utility of a neural network as a function approximator. This example could be followed by a formative-assessment technique.

Fig. 1: Mathematica representation of architecture of a neural network and it's successful utilization as a function approximator to approximate the function mapping $y = x^2$.

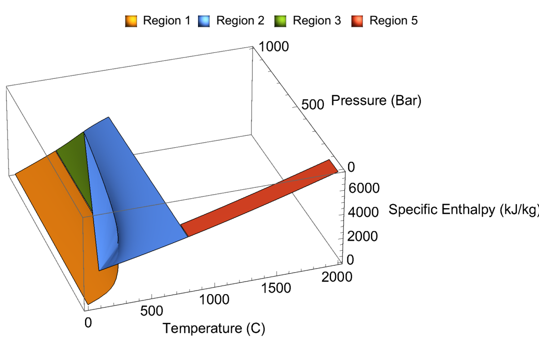


Fig. 2: ANN are trained to approximate the nonlinear mapping of (temperature, pressure)[inputs] $\rightarrow$ specific enthalpy[output] data. The data is organized into regions of similarity.

creation of and validation of neural networks without being inundated by the mathematics.

III. Literature Review

A. ANN in applied thermodynamics research

Some prominent examples of ANN in applied thermodynamics ([10]–[13], [15]–[17]) are on the evaluation of the coefficient of performance of refrigeration systems and the for the evaluation of thermophysical properties such as viscosity and thermal capacity. In all these cases, the ANN layers are assembled heuristically, in feedforward fashion. These analysis are limited to single equation-of-state problems or to approximate a thermodynamic efficiency calculation from thermophysical inputs.

B. ANN examples in engineering education

There exist pedagogic examples in non-mechanical engineering coursework, viz., hardware implementation of neural networks [22], a battery state of charge indicator using multi-layer, feedforward neural networks [23], replacement of logic circuit with ANN hardware for robotics [24], [27], load forecasting and fuzzy logic as relevant to power electronics and feedback control [25], [28], [29], use of ANN to teach matrix algebra [25] premised on character recognition much as is done in examples based on MNIST [30] or CIFAR [31] databases.

C. Pedagogic importance of this work in progress

Neural networks are practically being used to model complex processes and equipment ([33]–[35]) that rely on thermodynamic phenomenon. The example presented in this work in progress paper would prepare students to be aware that if first principles modeling is unable to accommodate a complex system's behavior, neural networks can be relied on to create an accurate model. However, accurate data sources, data organization skills, an experiential understanding of ANN creation and validation would be required.

Studies that demonstrate instructional examples of ANN for mechanical engineering students are few and far. There is one account of using a back-propagation ANN to optimize the *design for strength* of a structural member [20]. However this was with a single governing equations for the physics being simulated/predicted, unlike the multiple equations-of-state for steam in this paper. Additionally, the ANN outputs had error ($\geq 5\%$ w.r.t analytical solution) when a change of geometric properties was experienced. The optimization of the ANN was not an objective of this study.

There is one work of instructing neural networks in thermodynamics by predicting the output power of a gas turbine (with ideal gas) given inputs of pressure, temperature, operating time and flow rate [21] from experimental data. Both references, [20], [21] use the Excel package Neuralyst by Cheshire engineering corporation [26]. With the Neuralyst package, students need only focus on organization of data into a structured dataset. The creation and modification of the neural network framework is automatically handled by Neuralyst thus rendering the neural network a complete *black box* to students. The effort discussed in this paper is more of a *gray box* setting where students would need to organize the data and also heuristically create and iteratively modify a multi-layered architecture of an ANN to meet an accuracy goal.

The material described in this paper includes: (1) use of industrial standard as a data source (2) creation of multi-layer neural networks (3) validation of multi-layer neural networks using an industrial standard (4) modification of multi-layer neural networks to meet an accuracy goal. Such a

comprehensive module on ANN is not available in the space of mechanical engineering curricula, per literature review.

IV. Identification of desired overall outcome: Example problem for summative assessment

From the principle of backward design [37], the overall outcome for students of learning this material is described via an example problem. As an example, given the mass flow rate of steam and input and output pressure and temperature for a steam turbine, students could be asked to use an ANN to evaluate the turbine's power output. To successfully complete this exercise, students would have to identify the region of the input data, choose the appropriate ANN, apply it to evaluate specific enthalpies of steam and then apply the first law of thermodynamics for an open system to calculate the power output. Students could be further asked to determine the accuracy of using their choice of ANN for this problem leading them to make quantitative comparisons with table data.

V. Learning objectives to meet overall outcome

The example in this paper allows for the inclusion of the following section learning objectives (SLO) when included as a "section" or "module":

(S1) Assembling and arranging (clustering) of data to improve accuracy of neural network.
(S2) Assessing the effect of training-validation data split (training on full data or on individual clusters of similarity) on accuracy of results.
(S3) Use of published industrial standard to create synthetic data for training a neural network.
(S4) Validation of this thermodynamic neural network using an industrial standard.
(S5) Improving the accuracy of a neural network by heuristically adding or removing layers.

Other SLOs may be identified and created (such as increasing data density to improve ANN accuracy). Not all these section learning objectives need to be imposed in a single course due to time constraints. In section IV, an example problem for summative assessment has been included.

VI. Instructional material to meet learning outcomes or to create "entry behaviours"

Entry behaviours [38] are fundamental skills that students (learners) should know to fulfill the SLOs before being able to answer the "big question" such as the example problem posed in section IV. Some of the instructional material to germinate these entry behaviours is described in the follow subsections. Examples structured around these entry behaviours and the mastery of this material through the evaluation of solution to the comprehensive problem may be assessed through homework assignments.

A. Assembly of data using industrial standard (S1, S3, S4)

The IAPWS IF-97 [19] industrial standard is used in this paper, to create the thermodynamic dataset of (T, P, h) (temperature, pressure, specific enthalpy). The dataset may be created using the *xsteam* [18] function which evaluates the thermodynamic state specific *equation of state* per the IF-97 standard. The *xsteam* package is available in several forms viz., MATLAB or Octave functions, MS-Excel or DLL file.

TABLE I: Sample of steam data organized as (T, P, r, h) which are temperature (Celcius), pressure (bar), region (number) specification and specific enthalpy (kJ/kg), respectively.

10	1	1	42.117
15	1	1	63.077
…	…	…	…
705	71	2	3899.798
710	71	2	3911.746
…	…	…	…

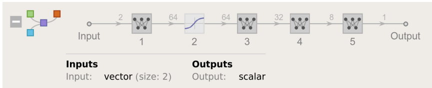
xsteam uses the (T, P) thermodynamic state specification to identify the state as being in one of four regions (fig 2). Once the region is identified per the IF-97 standard, the specific enthalpy (or other property such as specific entropy, speed of sound in the medium etc.) at that state is numerically evaluated.

The thermodynamic dataset in this paper is constructed by numerically sampling the entire (T, P) space in 5°C and 5 bar increments. The dataset collated using *xsteam* is ordered into 4 columnns: temperature (T, in Celcius), pressure (P, in bar), region specification (integer number) as per the IAPWS IF-97 standard and specific enthalpy (h, in kJ/kg). This is a dataset of 79800 rows and 4 columns representing temperatures incremented in 5 degrees from 0 to 2000 Celcius and pressures increment in 5 bar increments from 1 bar to 1000 bar (table I).

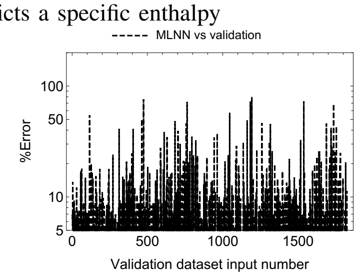
The *xsteam* evaluation of water and steam properties, given a thermodynamic state is similar to the mechanics of looking-up thermodynamic data from steam tables. Given a thermodynamic state, one ascertains what "region" of the tables the state belongs to: saturated liquid, subcooled liquid, sat. vapour, superheated vapour, sat. liquid-vapour mixture etc. Then using the appropriate section of tables, the desired thermodynamic quantity is read or interpolated. The regions of steam that this paper will focus on are shown in figure 2. This is a multidimensional dataset divided into non-intersecting regions.

B. Multi-layer feedforward Network to approximate specific enthalpy of steam

1) Training-validation data split: training on full data (S2): A heuristically created multilayer neural network (MLNN) is trained on a random sampling (to avoid mapping bias) of 97% of the IAPWS dataset representing regions 1,2,3,5. The training consists of feeding this MLNN the $(T, P) \to h$ mapping, thus allowing the ANN to learn the weights and biases within. The remaining 3% is used for validation of the trained neural network by using the (T, P) inputs from the validation set, thus providing an approximation $\hat{h}$ and comparing this with the specific enthalpy h for each (T, P) input in the validation set by calculating a percentage error (absolute value), viz., $|(\hat{h} - h)/h| \times 100$. The author has

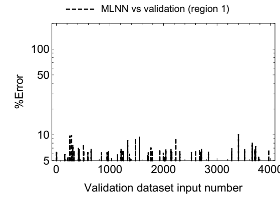


(a) Mathematica representation of MLNN. It requires an input of (T,P) and predicts a specific enthalpy

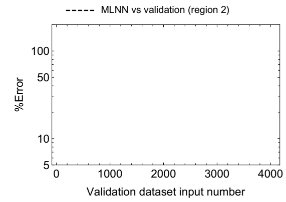


(b) Percentage error between the MLNN and validation dataset.

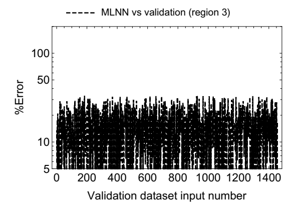
Fig. 3: A multilayer neural network trained on 97% of the IAPWS specific enthalpy data and it's error with respect to the 3% validation set. The X-axis shows that randomized validation data is input into the ANN in sequential fashion.



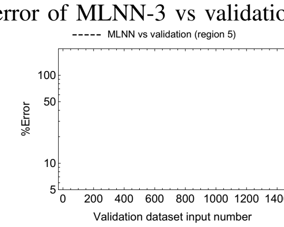
(a) Percentage error of MLNN-1 vs validation data in region 1



(b) Percentage error of MLNN-2 vs validation data in region 2.



(c) Percentage error of MLNN-3 vs validation data in region 3.



(d) Percentage error of MLNN-5 vs validation data in region 5.

Fig. 4: The multilayer neural network trained on 95% of the IAPWS region distributed data. Region 3 has the worst predictions, followed by region 1. The approximation error in region 2 and 5 is less than 5%.

experimented with other training-validation splits from 70%-30% to 97%-3%. The 97%-3% split provides the highest possible accuracy. The accuracy goal is set to be specific enthalpy prediction error of less than 5%. The error in MLNN when compared to the $(T, P) \rightarrow h$ mapping in the validation dataset is shown in figure 3.

2) Training-validation data split: Multiple ANN trained on different regions (S2): This MLNN may be trained on each region separately (MLNN-1 to MLNN-5) with a 70%-30% training-validation split. This MLNN trained on the 4 zones separately results in a higher accuracy of specific enthalpy approximation and requires a shorter time to train. The four percentage error plots for the region 1,2,3 and 5 are shown in figure 4. Note that in the percentage error plots, the lower limit on the y-axis is 5%. Meaning, any percentage error plot that is devoid of data points suggests that the prediction error was better than the goal of 5%.

3) Improving the accuracy of ANN by heuristically modifying number of layers (S5): Region 3 has the worst prediction with the error$\geq$ 5%. This can be ascribed to dataset for region 3 being the least dense leading to inadequate training per the universal approximation theorem [1].

VII. Assessment plan

The assessment plan will involve formative and summative assessment steps to measure student mastery of the various skills to successfully complete a design problem of the form in section § IV. This plan is illustrated in figure 5.

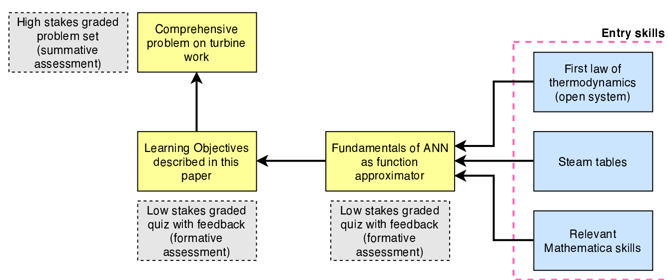


Fig. 5: Assessment plan for module on ANN described in this paper.

VIII. Summary

In this innovative practice, WIP paper, a neural network approximator for specific enthlapy of steam is described. This may be included as a section or module in a traditional course in thermodynamics. Using the idea of backward design, a comprehensive example problem to test students' mastery on neural network application for steam turbine power calculation is provided and possible section (or module) learning objectives are defined along with some instructional material towards ensuring that students fulfill the learning objectives.

REFERENCES

[1] Hornik K, Maxwell S, Halbert W. Multilayer feedforward networks are universal approximators. *Neural networks*, 2.5 (1989): 359-366.

[2] Shifrin, Leonid. Mathematica programming: an advanced introduction. *Creative Commons* (2008).

[3] Popenici SA and Kerr S. Exploring the impact of artificial intelligence on teaching and learning in higher education. *Research and Practice in Technology Enhanced Learning* 2017, 12(1): 22.

[4] Luckin R. Towards artificial intelligence-based assessment systems. *Nature Human Behaviour* 2017; 1(0028).

[5] Hillier P, Wright B and Damen P. Readiness for self-driving vehicles in australia. In *Workshop Report, February, ARRB Group Ltd. Retrieved from http://advi. org. au/wp-content/uploads/2016/04/Workshop-Report-Readiness-for-Self-Driving-Vehicles-in-Australia. pdf.*

[6] Sun Y, Olaru D, Smith B et al. Road to autonomous vehicles in australia: an exploratory literature review. *Road & Transport Research: A Journal of Australian and New Zealand Research and Practice* 2017; 26(1): 34.

[7] Jones N. Computing: The quantum company. *Nature News* 2013; 498(7454): 286.

[8] Francis L. The basics of neural networks demystified. *Contingencies* 2001; 11(12): 56–61.

[9] Chowdhury FN. Interdisciplinary course on neural networks at the graduate level. *Proceedings of the American Society for Engineering Education, 2002 ASEE Annual Conference*, 1997; 2: 1.

[10] Sencan A. Artificial intelligent methods for thermodynamic evaluation of ammonia–water refrigeration systems. *Energy Conversion and Management* 2006; 47(18-19): 3319–3332.

[11] Sencan A, Köse İİ and Selbaş R. Prediction of thermophysical properties of mixed refrigerants using artificial neural network. *Energy conversion and management* 2011; 52(2): 958–974.

[12] Sun DW. Thermodynamic design data and optimum design maps for absorption refrigeration systems. *Applied thermal engineering* 1997; 17(3): 211–221.

[13] Lashkarbolooki M, Hezave AZ and Ayatollahi S. Artificial neural network as an applicable tool to predict the binary heat capacity of mixtures containing ionic liquids. *Fluid Phase Equilibria* 2012; 324: 102–107.

[14] Lashkarblooki M, Hezave AZ, Al-Ajmi AM. Viscosity prediction of ternary mixtures containing ils using multi-layer perceptron artificial neural network. *Fluid Phase Equilibria* 2012; 326: 15–20.

[15] Golzar K, Amjad-Iranagh S and Modarress H. Prediction of thermophysical properties for binary mixtures of common ionic liquids with water or alcohol at several temperatures and atmospheric pressure by means of artificial neural network. *Industrial & Engineering Chemistry Research* 2014; 53(17): 7247–7262.

[16] Torrecilla JS, Rodríguez F, Bravo JL et al. Optimising an artificial neural network for predicting the melting point of ionic liquids. *Physical Chemistry Chemical Physics* 2008; 10(38): 5826–5831.

[17] Kalogirou SA. Applications of artificial neural-networks for energy systems. *Applied energy* 2000; 67(1-2): 17–35.

[18] Holmgren M. X steam for matlab. *www x-eng com, accessed October* 2006; 21: 2006.

[19] Wagner W., Kruse A. Properties of Water and Steam, IAPWS-IF97: The Industrial Standard IAPWS-IF97 for the Thermodynamic Properties and Supplementary Equations for Other Properties. *Springer-Verlag*: Berlin, 1998.

[20] Haque ME An Artificial Neural Network Model for Preliminary Design of Reinforced Concrete Beam-Column. *Proceedings of the American Society for Engineering Education, 2002 ASEE Annual Conference*, 2002; 2306: 16–19

[21] Cole WE. Neural Network Modeling of a Power Generation Gas Turbine. *Proceedings of the American Society for Engineering Education, 2002 ASEE Annual Conference*, 1997

[22] Pack, D., & Soda, K., Simple Hardware Implementation Of Neural Networks For Instruction In Analog Electronics *Proceedings of the American Society for Engineering Education, 2002 ASEE Annual Conference*, 2004

[23] Hess, H. L., William, E. J. Student Project to Develop a Neural Network-based State of Charge Indicator for Primary Batteries, *ASEE Annual Conference and Exposition*, 2016; 25923–

[24] Wunderlich, J., Simulation Vs. Real Time Control; With Applications To Robotics And Neural Networks, *ASEE Annual Conference*, 2001

[25] Heydt, G., Karady, G., Tylavsky, D., Holbert, K., Power Zone: Artificial Intelligence Educational Modules For Power Engineering, *ASEE Annual Conference*, 2001

[26] Shih, Y., Neuralyst users guide. *Cheshire Engineering Corporation*, Pasadena, v1, 4.

[27] Clement, W.I. Use of Neural Networks in an Undergraduate Robotics Course. *Proceedings of IEEE Frontiers in Education Conference - FIE*,1993; 705–709.

[28] S. Karaki and R. Chedid, Artificial neural networks: a new approach for treating electrical engineering problems, *Proceedings of 1994 IEEE Frontiers in Education Conference - FIE*, 1994; pp. 567-572.

[29] Jurado, F ; Castro, M ; Carpio, J ; Rivilla, I, Experience with neural networks and fuzzy logic in an electrical engineering control course *31st Annual Frontiers in Education Conference. Impact on Engineering and Science Education.)*, 2001; 3, pp.S1E–8 databases

[30] Yann, L.; Corinna, C., Christopher, J., The MNIST database of handwritten digits, http://yhann.lecun.com/exdb/mnist,1998

[31] Krizhevsky, Alex and Hinton, Geoffrey, Learning multiple layers of features from tiny images, 2009

[32] https://reference.wolfram.com/language/guide/NeuralNetworks.html

[33] MacMurray, Joel, and David Himmelblau, Identification of a packed distillation column for control via artificial neural networks. In 1993 American Control Conference, pp. 1455-1459. IEEE, 1993.

[34] Uhrig, Robert E, Potential application of neural networks to the operation of nuclear power plants. Nuclear Safety 32, no. 1 (1991): 68-79.

[35] Shiraishi, Hitoshi, Susan L. Ipri, and Dan Cho, CMAC neural network for fuel-injection control. In 1993 American Control Conference, pp. 1773-1778. IEEE, 1993.

[36] LeCun, Yann, Yoshua Bengio, and Geoffrey Hinton., Deep learning. nature 521, no. 7553 (2015): 436-444.

[37] Wiggins, G., and J. McTighe. Understanding by design. Alexandria, VA: ASCD.-849-E-Learn (2018): 15-18.

[38] Dick, Walter, Lou Carey, and J. O. Carey. The systematic design of instruction. 6th. New York: Longmann (2001).