

FUNCTIONAL RULE EXTRACTION METHOD FOR ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

The idea I propose in this paper is a method that is based on comprehensive functions for directed and undirected rule extraction from artificial neural network operations. Firstly, I defined comprehensive functions, then constructed a comprehensive multilayer network (denoted as N). Each activation function of N is parametrized to a comprehensive function. Following N construction, I extracted rules from the network by observing that the network output depends on probabilities of composite functions that are comprehensive functions. This functional rule extraction method applies to the perceptron and multilayer neural network. For any N model that is trained to predict some outcome given some event, that model behaviour can be expressed – using the functional rule extraction method – as a formal rule or informal rule obeyed by the network to predict that outcome. As example, figure 1 consist of a comprehensive physics function that is parameter for one of the network hidden activation functions. Using the functional rule extraction method, I deduced that the comprehensive multilayer network prediction depends on probability of that physics function and probabilities of other composite comprehensive functions in N . Additionally, functional rule extraction method can aid in applied settings for generation of equations of learned phenomena. This generation can be achieved by first training an N model toward predicting outcome of a phenomenon, then extracting the rules and assuming that probability values of the network comprehensive functions are constants. Finally, to simplify the generated equation, comprehensive functions with probability $p = 0$ can be omitted.

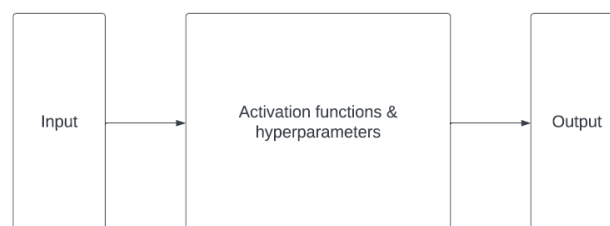
KEYWORDS

Rule extraction, comprehensive functions, neural network

1. INTRODUCTION

For decades, artificial neural network has been the most useful pattern recognition technique in various science and engineering areas like machine learning, computer vision, natural language processing, robotics, etc. [3, 1, 2]. Real world applications of this technique span vast number of industries, with increasing utilization across domains [11, 10, 7]. This immense utilization of artificial neural network stem from explosion of data and predictive power of models.

A standard model consist of input, activation functions, hyperparameters, and output. The input include training set and testing set, activation functions may be sigmoid, rectified linear unit, etc., [4] hyperparameters are used to control activation functions, and output is the model prediction.



The model undergo a training procedure that involve optimizing hyperparameter values until the model learn to output accurate predictions when given further training set as input. After the training procedure, the model is tested with a testing set to measure generalization capacity of the model. If it past the test, the model is fully ready for use by its user.

Although, this model may serve its user adequately, the user lack concrete understanding of any rule obeyed by the model to predict an output. [9] This lack of concrete understanding of the model rules resulted to the term “black-box network”, meaning that values of activation functions and hyperparameters are only numbers and they have no comprehensive relation to the probability distribution that the model learned. Without extracted rules, a user cannot prove that a model will make a right or wrong prediction at any given time. Before safely deploying a network model in a high-risk environment such as surgical robot in an operating room, autonomous vehicles on road highways, bots on trading system, etc., a user should be able to extract rules of the network model.

The functional rule extraction method explained in the following sections, is an efficient method for extracting rules from an N model consisting comprehensive functions. Rules extracted by this method can also be interpreted as equations of learned phenomena.

2. RELATED WORK

In earlier years, researchers have done a great deal of work in this area of rule extraction. S. M. Kamruzzaman and Ahmed Ryadh Hasan listed some of earlier work [12]. According to Kamruzzaman and Hasan, “R. Setiono and Huan Liu [13] presented a way to understand a Neural Network (NN). Understanding a NN is achieved by extracting rules with a three-phase algorithm: firstly, a weight decay backpropagation network is built so that important connections are reflected by their bigger weights; secondly, the network is pruned such that insignificant connections are deleted while its predictive accuracy is still maintained; and lastly, rules are extracted by recursively discretizing the hidden unit activation values.

Thrun [14] describes a rule extraction algorithm, which analyzes the input-output behavior of a network using Validity Interval (VI) Analysis. VI-Analysis divides the activation range of each network unit into intervals, such that all network activation values must lie within the intervals. The boundaries of these intervals are obtained by solving linear programs. Two approaches of generating the rule conjectures (specific-to-general and general-to-specific), are described. The validity of these conjectures is checked with VI-analysis.

R. Setiono [15] proposes a rule extraction algorithm for extracting rules from pruned neural networks for breast cancer diagnosis. The author describes how the activation values of a hidden unit can be clustered such that only a finite and usually small number of discrete values need to be considered, while at the same time maintaining the network accuracy. A small number of different discrete activation values and a small number of connections from the inputs to the hidden units will yield a set of compact rules for a problem.

R. Setiono, W. K. Leow and Jack M. Zurada [16] describes a method called Rule Extraction from Function Approximating Neural Networks (REFANN) for extracting rules from trained neural networks for nonlinear regression. It is shown that REFANN produces rules that are almost as accurate as the original networks from which the rules are extracted. For some problems, there are sufficiently few rules that useful knowledge about the problem domain can be gained. REFANN works on a network with a single layer and one linear output unit.”

3. COMPREHENSIVE FUNCTION

A solution to problem of rule extraction is forming a comprehensive relationship between the learned probability distribution and the input. I will use the sigmoid function $A(X)$ to form a comprehensive relationship, although other activation function can be used.

$$A(X) = \frac{1}{1 + e^{-X}} = (1 + e^{-X})^{-1}$$

Definition 1: A **comprehensive function** is a function that has explanatory relationship within a set of composite functions.

3.1. Univariate Comprehensive Function

Definition 2: A **univariate comprehensive function** f_c (for the purpose of this paper) is a comprehensive function with parameter wx , such that $f_c: wx \rightarrow \mathbb{R}$.

Let X be a univariate comprehensive function $f_c(wx)$, then

$$A(f_c(wx)) = (1 + e^{-f_c(wx)})^{-1}$$

Some examples of univariate comprehensive function are:

1. Volume of a cube $V(s) = f_c(s) = s^3$
2. Trigonometry identity $T(a) = f_c(a) = \sin^2 a + \cos^2 a$

3.2. Multivariate Comprehensive Function

Definition 3: A **multivariate comprehensive function** f_c (for the purpose of this paper) is a comprehensive function with parameters w_1x_1, \dots, w_nx_n , such that $f_c: w_1x_1, \dots, w_nx_n \rightarrow \mathbb{R}$.

Some examples of multivariate comprehensive functions are:

1. Force $F(m, a) = f_c(m, a) = m \cdot a$
2. Quadratic formula $Q(a, b, c) = f_c(a, b, c) = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = (-b \pm \sqrt{b^2 - 4ac})(2a)^{-1}$

By definition 2, I deduce that from example 1 of the univariate case, $f_c(s) = f_c(wx)$ if and only if $s = wx$. This means that the activation function

$$A(f_c(wx)) = (1 + e^{-f_c(wx)})^{-1}$$

can be treated as

$$A(V(wx)) = (1 + e^{-[(wx)^3]})^{-1} \text{ iff } V(s) = V(wx)$$

Likewise, the second univariate example is treated as

$$A(T(wx)) = (1 + e^{-\sin^2 wx - \cos^2 wx})^{-1} \text{ iff } T(a) = T(wx)$$

$$o\left(A\left(Q\left(A(V(iw_1))w_5, A\left(F\left(A(V(iw_1))w_3, A(T(iw_2))w_4\right)\right)w_7, A(T(iw_2))w_6\right)\right)w_8\right)$$

$$= \left(1 + e^{-w_8} \left(1 + e^{-w_7 \left(1 + e^{-w_3 w_4 (1 + e^{-i w_1})^{-1} (1 + e^{-i w_2})^{-1}}\right)^{-1} \pm \sqrt{w_7 \left(1 + e^{-w_3 w_4 (1 + e^{-i w_1})^{-1} (1 + e^{-i w_2})^{-1}}\right)^2}^{-1} - 4 w_5 (1 + e^{-i w_1})^{-1} w_6 (1 + e^{-i w_2})^{-1} \left(w_5 (2 + 2 e^{-i w_1})^{-1}\right)^{-1}}\right)^{-1}\right)^{-1}$$

Observe that each weight w_i (except w_1 and w_2 of the input) are weights of composite functions consisting of sigmoid functions and comprehensive functions. Since the extraction is concerned with rules compose of only comprehensive functions, the connection between the weights and sigmoid functions is not needed. Only connection between weights and comprehensive functions is needed in this rule extraction method. To disconnect weight from a sigmoid function and only reserve the weight connected to associated comprehensive function, while still preserving information from the sigmoid, I consider the weighted sigmoid below:

$$A(V)' = A(V)(w_3)$$

Let weighted volume $V' = (V)(p_3)$, where p_3 is probability of the volume V . Assuming that

$$V' = A(V)'$$

$$(V)(p_3) = A(V)(w_3)$$

$$p_3 = \frac{A(V)(w_3)}{V}$$

To now extract rule from the model, I extract the composites $r_i \in r, \forall i : 1 \leq i \leq 4$ of comprehensive functions (together with associated weights and probabilities) from figure 1 output expression:

$$\begin{aligned} r_1 &= (p_8) \left(-i^2 w_1 w_2 p_3 p_4 p_7 \pm \sqrt{(i^2 w_1 w_2 p_3 p_4)^2 p_7 - 4i^2 w_1 w_2 p_5 p_6} \right) (i w_1 p_5)^{-1} \\ r_2 &= (p_8) \left(-VT p_3 p_4 p_7 \pm \sqrt{(VT p_3 p_4)^2 p_7 - 4VT p_5 p_6} \right) (V p_5)^{-1} \\ r_3 &= (p_8) \left(-F p_7 \pm \sqrt{F^2 p_7 - 4VT p_5 p_6} \right) (V p_5)^{-1} \\ r_4 &= Q p_8 \end{aligned}$$

Definition 4: The product of all coefficients of a comprehensive function is the function probability.

The compositions r_1, r_2, r_3, r_4 are **formal rules** of the model in figure 1. An **informal rule** is worded statement of a formal rule. As shown, r_2 is a much complex rule than r_3 and r_4 . This complexity of r_2 result from explicitly stating complete probability distribution across comprehensive functions. Even the total sum of probability of each comprehensive function may not equal 1 for comprehension of r_2 . I normalize the sum to equal 1 by using softmax σ on all probabilities, mapping $\sigma(p_i) \rightarrow \rho_i$. The ρ_i symbol denote normalized probability.

$$\rho_i \leftarrow \sigma(p_i) = \frac{e^{p_i}}{\sum_{i=m}^n e^{p_i}}, \forall i: m \leq i \leq n$$

Here, $p_{i=m}$ is the first probability value and $p_{i=n}$ is the last probability value. Note that a formal rule can be used as equation of phenomenon which an N model has learned. The equation is correct if probabilities of comprehensive functions are not normalized, and if those probabilities

are constants. Any equation can be simplified by omitting comprehensive functions with probabilities that are equal to zero.

The formal rules r_2 , r_3 , and r_4 can be noted as **normal formal rules** below.

$$r_2 = (\rho_8) \left(-VT\rho_3\rho_4\rho_7 \pm \sqrt{(VT\rho_3\rho_4)^2\rho_7 - 4VT\rho_5\rho_6} \right) (V\rho_5)^{-1}$$

$$r_3 = (\rho_8) \left(-F\rho_7 \pm \sqrt{F^2\rho_7 - 4VT\rho_5\rho_6} \right) (V\rho_5)^{-1}$$

$$r_4 = Q\rho_8$$

A **normal informal rule** of r_3 is “The output of the network is based on rule that the probability ρ_8 of quadratic relationship between negative force at probability ρ_7 , square root of squared positive force at probability ρ_7 , square root of four negative cubic volume and trigonometry identity products at probability $\rho_5\rho_6$, and single cubic volume at probability ρ_5 , is true.”

Furthermore, rules can either be directed or undirected. Following the definitions of directed and undirected graphs [8], a **directed rule** is a rule that is obtained from a directed N model, while an **undirected rule** is a rule obtained from undirected N model. Figure 1 is example of a directed N model.

3. CONCLUSION

In this paper, I have shown that rules can be extracted from an N model, and such rules can be expressed as equations in formal form or worded statements in informal form. The two rule forms express the behaviour of an N model as well as equations of learned phenomena.

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