A COPULA-BASED VISUALIZATION TECHNIQUE FOR A NEURAL NETWORK

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ABSTRACT

Interpretability of machine learning is defined as the extent to which humans can comprehend the reason of a decision. However, a neural network is not considered interpretable due to the ambiguity in its decision-making process. Therefore, in this study, we propose a new algorithm that reveals which feature values the trained neural network considers important and which paths are mainly traced in the process of decision-making. In the proposed algorithm, the score estimated by the correlation coefficients between the neural network layers that can be calculated by applying the concept of a pair copula was defined. We compared the estimated score with the feature importance values of Random Forest, which is sometimes regarded as a highly interpretable algorithm, in the experiment and confirmed that the results were consistent with each other. This algorithm suggests an approach for compressing a neural network and its parameter tuning because the algorithm identifies the paths that contribute to the classification or prediction results.

Keywords Neural Network · Interpretability · Copula

1 Introduction

Interpretability of machine learning is being vigorously discussed currently. Deep learning has an overwhelming performance compared to other machine learning techniques in the field of image recognition such as generic object recognition. It is applied in a wide range of fields, but is hesitated to be introduced under the normal social conventions due to the difficulty of interpretability in some cases. As for autonomous driving technology, deep learning and deep Q-network [Mnih, 2015] bring the possibility of producing amazing results [Sallab, 2017]. However, the cause of accidents is unclear if traffic accidents occur due to incorrect recognition. This problem also happens in the clinical practice. When a doctor makes a diagnosis based on the machine learning predictions, patients are not able to accept the diagnosis if the predictions show the disease without appropriate reasons. On top of that, security problems in machine learning models against Adversarial Attack [Madry, 2018] break gradually to the surface. It is recommended at the political level that the process of machine learning decision-making is clear and that humans should employ machine learning predictions with a deep understanding of how they function [Goodman, 2017]. What is the interpretability or explainability of machine learning after all? A good reference [Molnar, 2019] defined the interpretability of machine learning as “Interpretability is the degree to which a human can understand the cause of a decision.” Based on this definition, the Linear Model and Decision Tree can be considered as interpretable because in the Linear Model, it becomes clear which parameters are more important while in the Decision Tree, there is no ambiguity in the process of if-then-else statement. A rule-based algorithm can also be termed interpretable. However, a neural network is not interpretable based on the definition given above because the process of decision-making is ambiguous although several novel approaches to clarify the process have been attempted. Among them are the sensitivity analysis method...
A well-known indicator of variable dependencies is the correlation coefficient. The correlation coefficient between $X$ variable 

$\rho_X$ 

If $X$ variable $Y$ has a correlation coefficient, a range of $\sigma_X$ and $\sigma_Y$ is known as a copula and it gives an alternative expression of the multivariate cumulative distribution functions, i.e., it can be used for scale-free measures of dependencies on distributions such that $C(F_1, \ldots, F_n)$ is the joint distribution with the marginal distributions as the variables. This means that the continuous multivariate marginal distributions are able to be decomposed into $F_1, \ldots, F_n$ that expresses the behavior of random variables and a copula $C$ that expresses the dependency structure of the random variables. A copula with joint probability distributions, in the case of two variables of Theorem 1, is sometimes called a ‘pair’ copula. A pair copula can be written as a graphical model. Bedford and Cooke et al. introduced a novel technique that homologizes them (Bedford, 2001).

2 PRELIMINARIES

In this section, the concepts of a copula, correlation, and the relationship between them are introduced to define the proposed algorithm.

2.1 Copula

Let $X_1, \ldots, X_n$ be random variables and $x_1, \ldots, x_n$ be their values. $F_i$ is the distribution function of the random variable $X_i$ for all $x_i$ in $\mathbb{R}$, therefore, $F_i = P(X_i \leq x_i)$. We focus on the multivariate cumulative joint distribution $F(x_1, \ldots, x_n)$ to consider the behavior of multiple random variables. There exists the following relationship between the joint distribution and the marginal distribution.

**Theorem 1. (Sklar, 1959)** Let $F_1(x_1), \ldots, F_n(x_n)$ be the marginal distributions of $F(x_1, \ldots, x_n)$. Then, there exists a functional $C$ such that

$F(x_1, \ldots, x_n) = C(F_1(x_1), \ldots, F_n(x_n)).$

If $F_i(x_i)$ are continuous, then $C$ is unique.

Here, the functional $C$ is known as a copula and it gives an alternative expression of the multivariate cumulative distribution functions, i.e., it can be used for scale-free measures of dependencies on distributions such that $C(F_1, \ldots, F_n)$ is the joint distribution with the marginal distributions as the variables. This means that the continuous multivariate marginal distributions are able to be decomposed into $F_1, \ldots, F_n$ that expresses the behavior of random variables and a copula $C$ that expresses the dependency structure of the random variables. A copula with joint probability distributions, in the case of two variables of Theorem 1 is sometimes called a ‘pair’ copula. A pair copula can be written as a graphical model. Bedford and Cooke et al. introduced a novel technique that homologizes them (Bedford, 2001).

2.2 Correlation

A well-known indicator of variable dependencies is the correlation coefficient. The correlation coefficient between the random variables $X$ and $Y$ is defined as $\rho = \frac{E[(X-\mu_1)(Y-\mu_2)]}{\sigma_1 \sigma_2}$, where $\mu_1$ and $\mu_2$ are the means of $X$ and $Y$, respectively, while $\sigma_1$ and $\sigma_2$ are the standard deviations of $X$ and $Y$, respectively. If a joint probability distribution between two variables has a correlation coefficient, a range of $\rho$ satisfies $-1 \leq \rho \leq 1$. The joint probability distribution for $X$ and $Y$ has a linear correlation with an equation $y = a + bx$, $b > 0$, if $\rho = 1$. This means that $P(Y = a + bx) = 1$. Similarly, if $\rho = -1$, we get the same result except $b < 0$. If $\rho \neq \pm 1$, there is a line in the $xy$-plane where the joint probability for $X$ and $Y$ is concentrated with a width? Under certain constraints, this line actually exists. At this time, the $\rho$ can be regarded as a measure of strength which the joint probability for $X$ and $Y$ are concentrated on the line (Hogg, 2012). Clearly, linear correlation cannot represent dependencies that are non-linear. Rank correlation can be used to evade these kinds of problems that represent a dependency between the variables. Rank correlation is not a value of each variable itself but is a correlation based on a rank of each variable according to some criteria. In this study, we used the Kendall rank correlation coefficient (Kendall’s $\tau$) as the rank correlations. The population version of Kendall’s $\tau$ is defined as the probability of the concordance minus the probability of the distance:

$$\tau = P(\text{sgn}\{(X_1 - X_2)(Y_1 - Y_2)\} = 1) - P(\text{sgn}\{(X_1 - X_2)(Y_1 - Y_2)\} = -1)$$
If a pair of $\text{sgn}\{(X_1 - X_2)(Y_1 - Y_2)\} = 1$, then we call this relationship concordance and there is an increasing relationship between the random variables $X$ and $Y$. Otherwise, we call this relationship disconcordance and there is a decreasing relationship between the variables $X$ and $Y$. Furthermore, a range of Kendall’s $\tau$ is $-1 \leq \tau \leq 1$. Kendall’s $\tau$ can be expressed using a copula.

**Theorem 2.** [Nelsen, 2010] Let $\tau$ denote the difference between the probabilities of concordance and disconcordance of $(X_1, Y_1)$ and $(X_2, Y_2)$, then

$$\tau = 4 \int \int_{I^2} C_2(u, v) dC_1(u, v) - 1$$

where $C_1$ and $C_2$ are the copulas of $(X_1, Y_1)$ and $(X_2, Y_2)$, respectively. The unit square $I^2$ is the product $I \times I$ where $I = [0, 1]$.

In the next section, we explain how to visualize a neural network by using Kendall’s $\tau$.

## 3 ALGORITHM

A neural network having nodes and edges can be drawn as shown in Figure 1. Therefore, the correlation coefficients between the neural network layers can be calculated by applying the concept of a pair copula described in the previous section. The paths are obtained by connecting the input layer to the output layer in a forward direction. An example of the paths is denoted as red nodes and edges. The calculation result reveals which paths in a neural network are important for the classification or prediction calculation of the correlation coefficients. In this section, we propose a new algorithm that makes the decision-making of a neural network clear, known as the Copula-based Visualization Technique (CVT) for a neural network, as shown in Algorithm 1.

### Algorithm 1 CVT

1. Initial Setting:
   (a) Train a neural network
   (b) Compute all cumulative marginal distribution functions of any random variables
   (c) Compute the correlation matrices between distributions of the activation function values of all nodes using training samples
   (d) List all the paths. For example, see Figure !

2. Procedure:
   (a) Compute the Convolution of Correlation Coefficient (CCC). For example, CCC of red path in Figure ! is 
      $[x_1, \ldots, l_1(N), l_1(N + 1), \ldots, \text{pred}]$.
   (b) Compute the variance of CCC for a path with the same nodes and edges except the output nodes

In the initial setting, we are required to train a neural network, the cumulative marginal distribution function, correlation matrix, and paths. In the procedure step, we need to compute the variance of the convolution correlation coefficient: $\text{VaR}(\text{CCC})$.

This is the importance degree of each path for visualizing and understanding the neural network model. The variance of CCC expresses the path sensitivity. For example, we can arrange the ranking in a descending order of $\text{VaR}(\text{CCC})$. In general, it is not possible to understand how a model makes a judgment based only on weights in a neural network [Haufe, 2014; Kindermans, 2018]. For this reason, it is impossible to know how the feature value affects the classification or prediction result and which node is highly sensitive to the classification or prediction result only by looking at the weights.

## 4 VISUALIZATION OF A NEURAL NETWORK

The experiment with CVT to a neural network is described in this section. Subsection 4 presents the experimental setup such as the dataset and the calculation of the probability density functions (PDFs) and cumulative distribution functions (CDFs). Subsection 4.1 details the simultaneous visualization of the important feature values and the paths that are traced in the process of decision-making. This result presents our main contribution. The feature values obtained by CVT were ranked according to $\text{VaR}(\text{CCC})$ and were compared with the Random Forest result in Subsection 4.2.
the source codes to demonstrate this experiment are available at Github[1]. The Fisher’s Iris data set[2] included in the scikit-learn package[3] was used to train the neural network. The values of sepal length, sepal width, petal length, and petal width were used as the input feature values which defined x_0, x_1, x_2 and x_3, respectively. The labels of Setosa, Versicolor, Virginica were used as one-hot encoding vector. Here, Setosa is pred_0, Versicolor pred_1, Virginica pred_2. The structure of the trained neural network is illustrated in Figure 2 comprised of four nodes (red) in the input layer, six (blue) in the first hidden layer, six (blue) in the second hidden layers, and three (green) in the output layer. All the nodes in the hidden layers and the output layer express the values through the activation functions. Rectified Linear Unit (ReLU) was used as the activation function in the hidden layers and Softmax was used in the output function. This model is a standard neural network model. The data used for training was 120 samples out of 150 and the accuracy rate was approximately 97.5%.

CDFs are required to calculate the correlation coefficients as described in Section 2.1. Therefore, we first created histograms of the outputs of the nodes at the time of prediction. These histograms are equivalent to PDFs as shown in the left-side of Figure 3. Here, the PDFs at the input nodes were, in fact, the feature values. Next, we integrated them to obtain the CDFs as shown in the right-side of Figure 3. The Y-axis values of the CDFs histograms were used for this calculation.

[1] https://github.com/covit2019/analysis_codes
[2] http://archive.ics.uci.edu/ml/datasets/Iris
[3] https://scikit-learn.org/stable/auto_examples/datasets/plot_iris_dataset.html
Figure 3: Example of Conversion from a PDF (left) to a CDF (right) at Each Node

4.1 Calculation of Correlation Coefficients Between Neural Network Layers

As shown in Figure 4, the number of paths from the input to the second hidden layer (Hidden1) in the neural network is $4 \times 6 \times 6 = 144$ and each path is branched off to the three outputs. An example path from the 144 paths is drawn as a red line and the branch lines are drawn as blue dotted lines. Next, $\text{VaR}(\text{CCC})$ for each path was calculated using the CVT algorithm described in Section 3. The calculation of the correlation coefficients was executed by the noble C++ library: vinecopulib [Nagler, 2019]. Table 1 presents the top 10 important path ranking in a descending order of $\text{VaR}(\text{CCC})$. This table presents which paths are important for decision-making of the neural network from which the feature values $x_2$ and $x_3$ are especially important. Besides that, Figure 5 shows the visualization of all the paths. The importance defined as the sum of $\text{VaR}(\text{CCC})$ of paths through the edge is portrayed as a contrasting density, and the density corresponding to blue (less important) is set transparent to emphasize the important paths. The values listed in Table 1 are sometimes the same because the CDFs have discrete histograms. This problem can be avoided by making the bin size of the histograms finer or by using CDFs, which are estimated through function fitting.

| Path          | Setosa | Versicolour | Virginica | VaR(CCC) |
|---------------|--------|-------------|-----------|----------|
| $x_2, h0_5, h1_1$ | -0.00801 | 0.047293    | 0.69013   | 0.150615 |
| $x_2, h0_3, h1_1$ | -0.00801 | 0.047293    | 0.69013   | 0.150615 |
| $x_3, h0_3, h1_1$ | -0.00801 | 0.047293    | 0.69013   | 0.150615 |
| $x_3, h0_5, h1_1$ | -0.00801 | 0.047293    | 0.69013   | 0.150615 |
| $x_2, h0_5, h1_5$ | -0.00551 | 0.047878    | 0.69013   | 0.149875 |
| $x_2, h0_3, h1_5$ | -0.00551 | 0.047878    | 0.69013   | 0.149875 |
| $x_3, h0_5, h1_5$ | -0.00551 | 0.047878    | 0.69013   | 0.149875 |
| $x_3, h0_3, h1_5$ | -0.00551 | 0.047878    | 0.69013   | 0.149875 |
| $x_2, h0_3, h1_4$ | 0.0071334 | 0.074663    | 0.69013   | 0.126953 |
| $x_2, h0_5, h1_4$ | 0.0071334 | 0.074663    | 0.69013   | 0.126953 |

Figure 4: Example of Paths from Input Nodes to Output Nodes
4.2 Comparison with Random Forest

We compared the CVT results with those obtained by Random Forest for the validity of interpretability. Random Forest implemented in the scikit-learn package\(^4\) with the default parameters were used. The data used for training had 120 samples out of 150 and the accuracy rate was approximately 97%. This accuracy rate was extremely close to that of the neural network experimented in the previous subsection. Random Forest, which is sometimes regarded as one of the highly interpretable algorithms, can calculate the importance of the feature values. Therefore, we compared the Random Forest feature importance values with the following:

\[
E^{x_i}(\text{VaR}(\text{CCC}))
\]

where \(E^{x_i}(\cdot)\) is an operator that takes the expected value with respect to the feature values \(x_i\) and normalized to be compared. For example, \(E^{x_2}(\text{VaR}(\text{CCC}))\) means that the average of all paths begin with \(x_2\), i.e., that of the first row, the second, the fifth, ..., and so on as shown in Table 1. Figure 6 shows the result. It was not compared directly because the importance was calculated using different methods, but the results were consistent with each other. This means that CVT can derive the importance of feature values in a neural network.

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\(^4\) https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
5 RELATED WORKS

As summarized in the introduction, sensitivity analysis method [Zeiler, 2014; Smilkov, 2017] and reverse tracing method [Bach, 2015] have been studied intensively in the recent years. CVT is complementary to the aforementioned methods in terms of explaining the models as these methods do not address the problem of explaining important feature values and paths that contribute to the results of classification or prediction through all training data. In other words, CVT is not appropriate for measuring the effect and contribution of feature values of individuals when only a portion of the data is focused on. It is difficult to say which of these methods is better, and therefore, an appropriate method should be chosen based on the situation.

6 CONCLUSION AND FUTURE WORKS

In this study, we proposed a Copula-based Visualization Technique (CVT) for a neural network. CVT can easily visualize the decision-making process of a neural network using correlation coefficients. Information regarding the feature values that are considered to be important by the trained neural network and paths that are mainly traced in the process of decision-making are obtained by the proposed algorithm. The experimental result of the proposed algorithm was consistent with the importance values estimated using Random Forest. This suggests that CVT can be used for the interpretability of a neural network.

CVT was experimented using a simple neural network but can also be extended to other algorithms, including a deep neural network that can be considered as a graphical model. CVT can serve as a general method for machine learning interpretability. Kendall’s $\tau$ was used as the correlation coefficients, but other correlation coefficients, by all means, can also be used. Future works include the theoretical analysis and the use of other correlation coefficients for CVT. Additionally, CVT can suggest an approach for compressing a neural network as doing so helps in identifying the nodes and edges that contribute to the classification or prediction results. CVT can also use parameter tuning for the abovementioned reason. Additionally, CVT may be able to reveal the reasons for Adversarial Attack cheating a neural network, which can also be considered for future work.
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