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MLP Temelli Yapay Zeka Modellerinde Çıktıları Etkileyen Giriş Veri Seti Niteliklerinin Model Mimarisine Göre Davranışlarının Araştırılması

Muhammer İLKUÇAR[*,a]

[a,*] *Muğla Sıtkı Koçman Üniversitesi, Fethiye İşletme Fakültesi, Yönetim Bilişim Sistemleri Bölümü, Muğla, 48300, Türkiye*

MAKALE BİLGİSİ

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***Anahtar Kelimeler*:**
Açıklanabilir Yapay Zeka
Sorumlu Yapay Zeka
Derin Yapay Sinir Ağları
Makine Öğrenmesi
SHAP

[*] ***Sorumlu Yazar***
e-posta:
muhammerilkucar@mu.edu.tr

ÖZET

Yapay zekanın yaygınlaşması ile birlikte açıklanabilirlik, yorumlanabilirlik, şeffaflık gibi konular, özellikle sağlık, savunma sanayi, güvenlik, hukuk gibi alanlarda çok daha önemli hale gelmiştir. Bu çalışmada; ileri beslemeli geri yayılımlı çok katmanlı Yapay Sinir Ağı (MLP: Multi Layer Perceptron) yapay zeka modellerinde giriş veri seti nitelik değerinin model çıkışına olan etkilerinin model mimarisi ile olan ilişkisi araştırılmıştır. Model giriş veri özniteliklerinin model tahminine katkıları SHAP (SHapley Additive exPlanations) yöntemi ile ölçülmüştür. MLP mimarisi değiştikçe giriş veri seti nitelik değerlerinin model çıkışına katkı oranları sıralaması da değişmektedir. Öznitelik etki sıralamasındaki değişimin çoğunlukla katkı düzeyleri birbirine görece yakın olan öznitelik değerleri için geçerli olduğu, etki oranı diğer özniteliklerden biraz farklı olan özniteliklerin etki sıralamasının MLP mimarisi ile çok fazla değişmediği gözlemlenmiştir. Bu sonuçlara göre MLP model mimarisinin Açıklanabilir Yapay Zeka'da da belli bir oranda etkili olduğu, modelin doğruluk değeri ile özniteliklerin önem oranları arasında anlamlı bir ilişki olmadığı sonucuna varılabilir.

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Analysis of the Behavior of The Input Data Set Attributes Affecting the Outputs in MLP Based Artificial Intelligence Models According to the Model

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[*] ***Corresponding Authors***
e-mail:
muhammerilkucar@mu.edu.tr

ABSTRACT

With the widespread use of artificial intelligence, explainability, interpretability, and transparency have become very important issues, especially in the health, defence, security, and law domains. In this study, the same datasets were used with different multilayer perceptron (MLP) architectures, and the effects of dataset attributes on MLP model output were analysed. The contributions of the model input data attributes to the model prediction were measured using the SHAP (SHapley Additive exPlanations) method. For the datasets, as the MLP architecture changed, the importance ranking levels of the input dataset attribute values also changed. It was observed that the change in the attribute influence ranking was mostly applicable and valid for attribute values whose contribution levels were relatively close to each other, and the influence ranking of the attributes whose influence ratio was slightly different from other attributes did not change significantly based on the MLP architecture. According to these results, it can be concluded that the model architecture also influences Explainable Artificial Intelligence results to a certain extent, and that there is no direct relationship between the model's accuracy and attribute importance ranking.

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1. *INTRODUCTION*

Artificial intelligence has permeated all facets of life and is steadily progressing towards becoming an essential component of our lives. Artificial intelligence models have achieved significant success in various domains such as categorization, clustering, prediction, etc. As a result, they have been effectively utilized in diverse sectors such as education, engineering, health, transportation, finance, media, art, etc. Recently, different Artificial intelligence (AI) applications have become widespread in both business and individual daily life, such as Generative Adversarial Networks (GAN) and Large Language Models (LLM). The widespread use of artificial intelligence has prompted concerns about its outputs, including their explainability, interpretability, dependability, trustworthiness, and ethical.

Today, in addition to the impressive performance of artificial intelligence models, the significance of notions such as responsibility, explainability, and justice is increasing [1]. The field of Explainable Artificial Intelligence (XAI) has emerged due to the influence of input data set qualities on the output of machine learning (ML) models, and the need for transparency, traceability, and explainability of the obtained results [2]. XAI is essential in all domains that employ artificial intelligence, but it holds particular significance in sectors such as healthcare, defence, security, and law [2,3]. Explainable Artificial Intelligence (XAI) is a crucial technology that enhances the dependability and transparency of AI systems, fostering user trust in these systems. For AI to be adopted by people, it must be explainable and reliable [4].

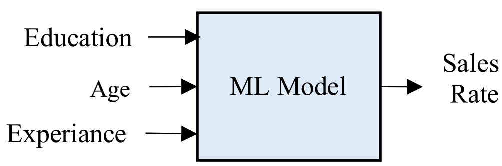
According to Saeed and Omlin [3], XAI can be useful in fields including digital forensics, 5G, and the Internet of Things. However, there are certain general issues with XAI design, development, application, explainability, and interpretability. In order to guarantee the fairness, transparency, and accountability of machine learning systems, Barredo Arrieta et al. [5] contend that XAI is crucial for the creation and application of ML models. A study of the literature on interpretable machine learning in the field of artificial intelligence in healthcare was carried out by Tjoa and Guan [6]. Došilović, Brčić and Hlupić [7] examine the most recent developments in the application of XAI in supervised machine learning and contend that XAI should take precedence given the growing concern over AI and the issue of trust. XAI methods can be applied to many machine learning algorithms. Thanks to XAI, the interpretability of machine learning algorithms increases. Deep learning algorithms are more difficult to explain and comprehend than algorithms like Decision Trees [8], Support Vector Machines [9,10], Logistic Regression [11], and Naive Bayes [12] classifiers. On the other hand, an artificial neural network have many parameters. The system is like a black box, especially in multilayer and deep artificial neural networks where the large number of layers and parameters makes them difficult to interpret.

In this study, the effects of network architecture and input data attributes on XAI results in MLP were examined.

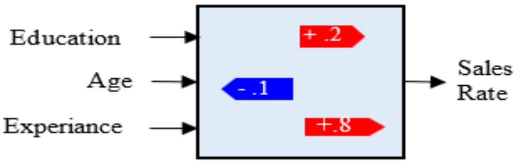
2. *MATERIALS AND METHODS)*

2.1. SHapley Additive exPlanations (SHAP) Method

SHapley Additive exPlanations (SHAP) Method is a method based on game theory [13] that reveals the contribution of each input feature to the model's output in machine learning [14]. Game theory examines situations where there is more than one player and each player's actions affect the decisions of the other players. In game theory, methods exist to measure how much each player contributes to the outcome of a game. In the SHAP method, the input attributes of the ML model can be viewed as players, and their contribution to the model's prediction (the game's outcome) can be measured. In this way, the outputs of the model will be more explainable by measuring which attributes affect the output of an ML model and how. It can also be observed which attributes of the input data set are more important and which are less important for the ML Model with SHAP. A simple SHAP model is shown in Figure 1 [15]. The ML Model has three input features (age, education, and experiences) and one output (sales rate) (Figure 1.a). The sales rate will be predicted for age, education, and experience inputs with the trained ML model. As seen in Figure 1.b, the "experience" feature makes a positive contribution to the "sales rate" output with 0.8, while the "age" feature makes a negative contribution with 0.1. While education and experience feature positive contributions to the sales rate estimate, age features provide negative contributions.



a)ML Model



(b) Explanation Model

Figure 1. Machine Learning model and explanation model (Makine öğrenmesi modeli ve açıklanabilir model).

3. *DATASET*

In the study two different datasets were used: Breast Cancer Wisconsin and Heart Disease [16]. Since these datasets are widely used in the literature, they were preferred for other researchers.

3.1. Breast Cancer Wisconsin Dataset

The Wisconsin Breast Cancer dataset [16] consists of 699 samples, 9 features and one diagnostic feature (label) (Table 1). In each feature, the tumour diameters of X-ray images taken from the breast are expressed numerically. According to these features, whether the tumour is benign or malignant is given as a label in the diagnostic feature. A diagnosis value of 2 means a benign tumour, and 4 means a malignant tumour. Of the data in the dataset, 241 samples belong to malignant tumours, while the remaining 458 samples are benign tumour samples. There are missing data for 16 samples in the Features6 column in the dataset. Missing data was filled with 0. Various techniques can be employed to replace missing values [17,18,19]. Filling the missing data with one of these strategies, rather than using zero, will have a favourable impact on the model's performance. However, the aim of this study was not to improve the performance of the model. For this reason, missing data in the dataset were simply filled with 0.

Table 1. Breast cancer dataset, features and diagnosis (label) sample data (Meme kanseri veri seti, teşhis (tiket) ve örnek veriler).

#	Feature_0	Feature_1	Feature_2	Feature_3	Feature_4	Feature-5	Feature_6	Feature_7	Feature_8	Diagnosis
0	5	4	4	5	7	10	3	2	1	2
1	3	1	1	1	2	2	3	1	1	2
2	6	8	8	1	3	4	3	7	1	2
3	4	1	1	3	2	1	3	1	1	2
4	8	10	10	8	7	10	9	7	1	4
…					…					…

3.2. Heart Disease Dataset

Table 2 displays the heart disease dataset [16], which consists of 13 features and a label indicating whether the person has heart disease or not. According to the findings, the diagnostic value was taken as 1 if the patient has heart disease and 0 if the patient does not have heart disease. The dataset consists of 1025 samples, all features are expressed numerically, and there are no missing data. In the dataset, 499 samples belong to patients with heart disease and 526 samples belong to patients without heart disease.

Table 2. Heart disease dataset, features and (label) diagnosis (Kalp hastalığı veri seti, nitelikleri ve teşhis/etiket).

Features	Explanation
Feature_0 (age)	Age in years
Feature_1 (sex)	Gender; 0:female; 1: male
Feature_2 (cp)	Chest pain type (1: atypical angina; 2: atypical angina; 3: non-anginal pain; 4: asymptomatic)
Feature_3 (trestbps)	Blood pressure at rest (mm Hg)-Tansion
Feature_4 (chol)	Serum kolestoral (mg/dl)
Feature_5 (fps)	fasting blood sugar > 120 mg/dl (1: true; 0: false)
Feature_6 (restech)	Resting electrocardiographic results
Feature_7 (thalach)	Maximum heart rate
Feature_8 (exang)	Exercise induced angina (1:Yes; 0: No)
Feature_9 (oldpeak)	ST depression caused by exercise relative to rest
Feature_10 (slope)	Hill exercise Slope of segment (ST)
Feature_11 (ca)	Number of large vessels colored by fluoroscopy (0-3)
Feature_12 (thal)	3:normal; 6: fixed defect; 7: reversible defect
Diagnostic	0: Not disease; 1: Disease

4. *RESULTS AND DISCUSSION*

In the study, MLP model training and SHAP tests with different architectures were performed for each data set. After training and testing Multi-Layers Artificial Neural Network (MLP) in different architectures with different data sets, the effects of the input data attributes in the model output and the importance levels of the input data attributes were observed by using the SHAP method. Thus, it was investigated whether the importance of the input data set attribute values according to their effects on the output varies with the MLP model architecture. In the study, the hyperparameters were kept constant for all MLP architectures and the effect of these parameters on the output was stabilized.

XAI techniques such as SHAP, DeepSHAP, DeepLIFT, DeepLIFT, CXplain, and LIME (Local Interpretable Model-agnostic Explanations) [15, 20, 21] are used as XAI techniques. SHAP is a game theory [22] approach to explaining the output of any machine learning model. It combines optimal credential location with local explanations using classical SHapley values from game theory and its related extensions. This technique graphically and statistically illustrates the importance of the features that affect the decisions of the AI system, the statistical information that affects the decisions of the AI system, and the factors that affect the decisions of the system [23]. XAI techniques can show different suitability according to the artificial intelligence machine learning model. They state that LIME is more suitable for Artificial Neural Networks and Random Forest algorithms, while SHAP is more suitable for boosting-based algorithms. Since the SHAP method uses all attributes of the entire dataset [20], the SHAP method is preferred as the XAI technique for MLP and Deep Learning Machine Learning algorithm in this study in order to see the importance of all factors determining the result. The common parameters used in all MLP architectures in the study are as follows:

- *Training dataset* : 70% of the data
- *Test dataset* : 30 % of the data
- *Validation dataset* : 1% of training dataset
- *Epoch* : 500
- *Early Stopping* : true
- *Batch size* : 1
- *Optimizer* : adam
- *Hidden layerS activation function* : ReLu
- *Output layerS activation function* : Sigmoid
- *Loss function* : BinaryCrossentropy
- *Performance metric* : Accuracy

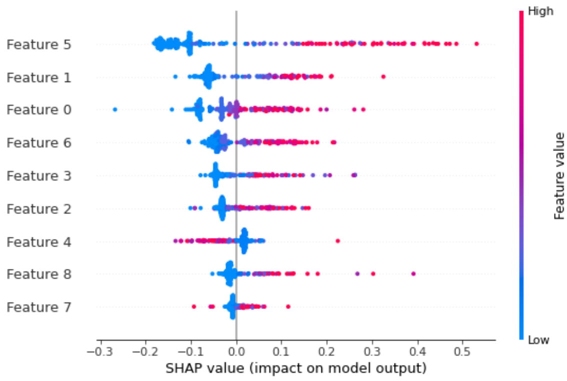
In order to the MLP algorithms to work better, the data was scaled in the range [0,1]. The model output is a binary classification (1: Patient, 0: Not Patient). Since the model output value is a continuous number between 0 and 1, it was converted to binary according to a certain threshold value. In this study, 0.5 was taken as the threshold. Accordingly, if the model output value was ≥ 0.5, it was considered as 1; in the other case, it was considered as 0. 70% of the data was reserved for training and 30% for testing. While training, 1% of the training data was used as validation data. The ReLu was used as the activation function for all hidden layers of the model. Since the output of the model will be binary classification, the output layer activation function is Sigmoid, and Binary Cross Entropy were used as the loss function. The model's optimization algorithm is *adam*, batch size 1, epoch 500, and no dropout used. With these hyperparameters, MLPs with different architectures were tested with two different data sets. In order to examine the effects of the input data set on the output with the MLP architecture, different architectures were selected. The architecture used 3, 4, 5, 6, and 7 layered architectures with high and close accuracy values. The number of nodes in the hidden layers was taken randomly between 5 and 50 as multiples of 5.

In the study, the accuracy score was used as the MLP model performance metric. Since the test data sets were balanced, the accuracy performance values reflect the success of the model. Since the study focused on XAI, the performance metrics such as precision, recall, f1 score, and r-square were not used. When the performance values of the MLP models in the study were compared with other studies conducted with the same data set in the literature [24-30], it was seen that the model was successful.

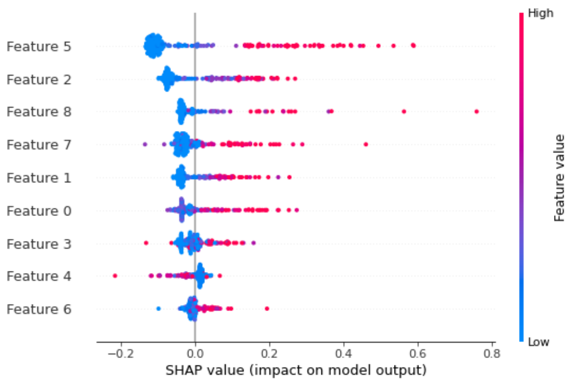
In Figure 2, for the Brest Cancer dataset, the model was trained separately using different MLP architectures, and the accuracy performance values and SHAP plots are shown. In the SHAP graphs, the effects of the dataset attributes of the model output (the importance of the attributes) can be seen graphically (Figure 2). For example, in Figure 2.a, the positive and negative effects of features on the outcome and the amount of these effects are shown in different colors. The color red indicates a positive effect, while blue indicates a negative effect. Also in the graph, the features are ranked according to their importance. For example, Feature5 is the most important feature while Feature7 is the least important feature. The accuracy values obtained for the different architectures and the importance ranks of the attributes (from important to unimportant) according to the SHAP graph results are given in Table 3. Upon examining Table 3 and Figure 2 show that the impact of the dataset attributes on the outcome also varies across the MLP architecture. For example, in Architecture 1, the importance ranking according to the effect of the attributes is 5-0-2-1-3-8-7-6-4, while in Architecture 4, the importance of the attributes ranking is 5-2-8-7-1-0-3-4-6. Here, Feature0 is ranked second from the beginning in Architecture 1, while in Architecture 4, it is ranked sixth from the beginning. Feature5 ranks first in all architectures, while the other features vary in importance (order) according to architecture. Since the importance rate of Feature5 is slightly different from the other features, it ranks first in all models. Since the importance ratios of other features are close to each other, it is seen that the ranking of importance ratios changes according to the model architecture. Examina the Table 3, it is seen that the ranking of the importance ratios of the features, changes even if they have the same accuracy value in different architectures. For example; although both Architecture1 and Architecture8 have an accuracy of 98%, the importance ranking of the attributes is different. Thus, it can be concluded that there is no relationship between the model's accuracy value and the importance ratios of the attributes.

Table 3. Listing the effects of breast cancer input dataset features of the output according to architecture (Meme kanseri girdi veri kümesi özelliklerinin model çıktısına etkilerinin mimariye göre listesi).

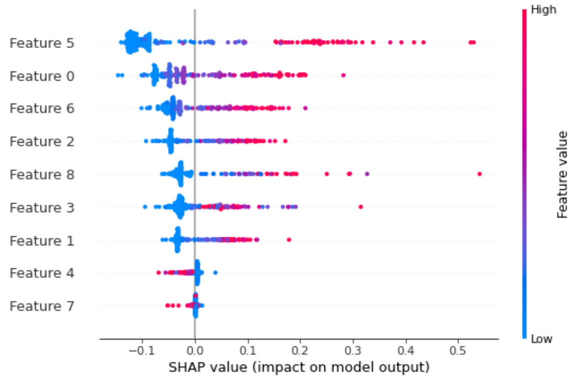
MLP Architecture	Accuracy	The importance of the input data set attributes according to their SHAP values, listed in descending order
9-5-10-5-1	0.98	5-0-2-1-3-8-7-6-4
9-5-10-10-1	0.98	5-1-2-3-6-7-0-8-4
9-5-5-1	0.95	5-0-6-2-8-3-1-4-7
9-10-5-1	0.97	5-2-8-7-1-0-3-4-6
9-10-15-1	0.96	5-1-0-6-3-2-4-8-7
9-15-1	0.98	5-2-0-6-1-3-8-7-4
9-45-1	0.98	5-0-2-6-3-1-8-7-4
9-15-10-10-15-1	0.98	5-1-0-2-6-3-8-4-7



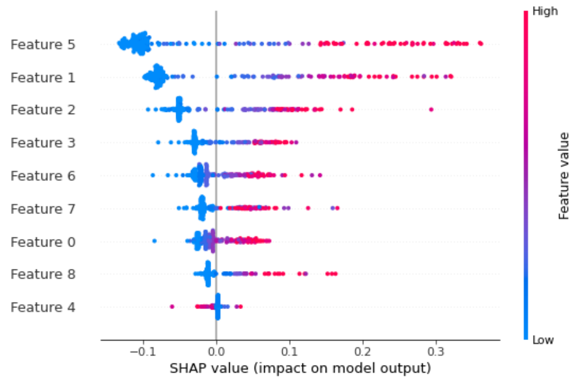
(a) MLP Architecture: 9-10-15-1



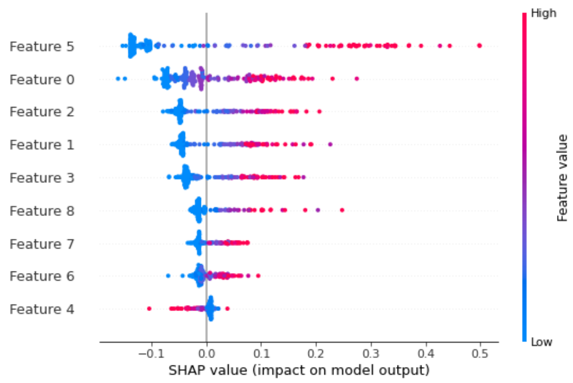
(b) MLP Architecture: 9-10-5-1



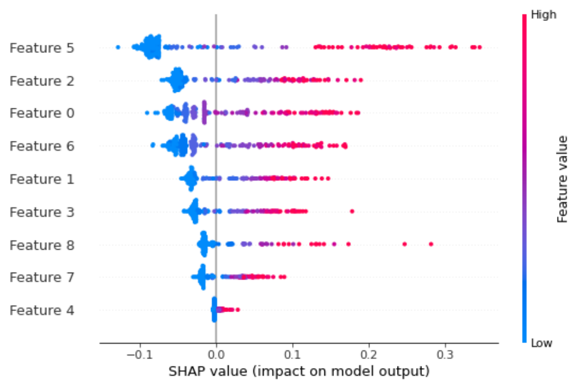
(c) MLP Architecture: 9-5-5-1



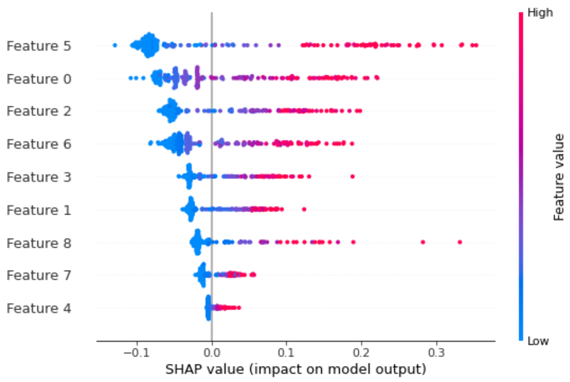
(d) MLP Architecture: 9-5-10-10-1



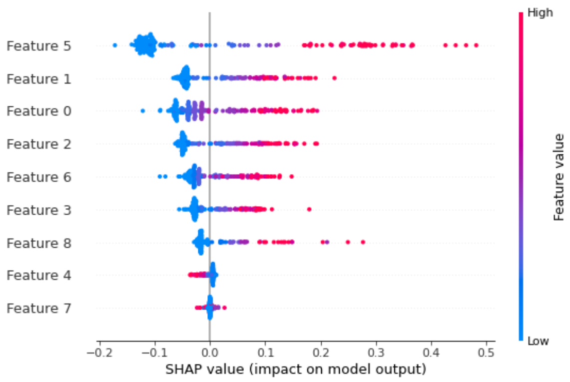
(e) MLP Architecture: 9-5-10-5-1



(f) MLP Architecture: 9-15-1



(g) MLP Architecture: 9-45-1



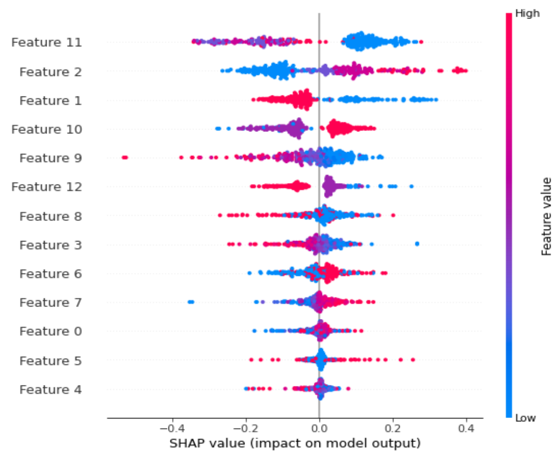
(h) MLP Architecture: 9-15-10-10-15-1

Figure 2. SHAP graphs of the breast cancer dataset obtained after MLP training for different architectures (Meme kanseri veri seti ile eğitilmiş, farklı mimarideki MLP'lerin, eğitim sonrasında elde edilen SHAP grafikleri).

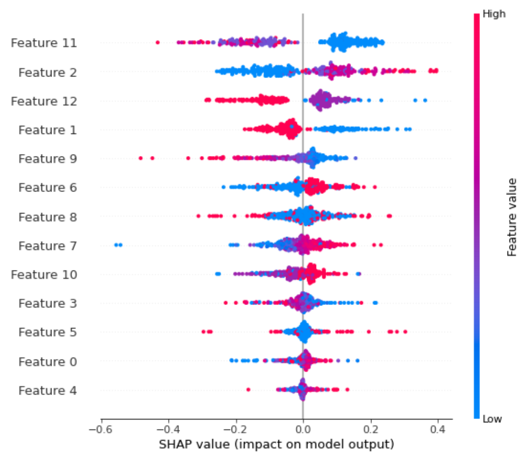
The effects of the attributes of the input dataset on the output for different MLP architectures of the heart disease dataset are given in Figure 3. The model architecture was not taken according to any rule. Different architectures were created by using different numbers of hidden layers and different numbers of nodes (units) in each hidden layer. Table 4 shows the structure of the architectures, model performance, and the effects of the dataset attributes on the output according to the model, ranked in descending order of importance. Examine Figure 3 and, the Table 4 are analyzed, it is seen that the ranking of the impact values of the dataset attribute values on the model output changes. For example, in Architecture 1, Feature10 is ranked fourth from the beginning, while in Architecture 5 it is ranked seventh. The importance of some features remained the same in all architectures. For example, Feature1 has maintained its first rank in all architectures. Examining the Figure 3, it can be seen that these features are relatively more important than other features. Feature4 ranks last in almost all models. This feature is the least important feature for all models.

Table 4. Listing the effects of the input dataset attributes on the output of the heart disease dataset according to different architectures (Kalp hastalığı veri kümesi özelliklerinin model çıktısına etkilerinin mimariye göre listesi)

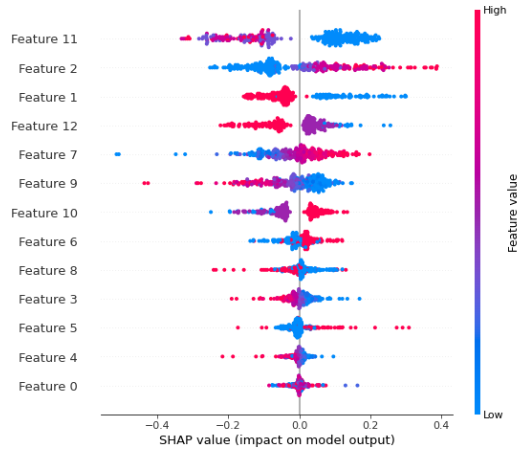
MLP Architecture	Accuracy	The rating of input data set qualities' contribution to the output
13-15-5-1	0.94	11-2-1-10-9-12-8-3-6-7-0-5-4
13-20-15-1	0.98	11-2-12-1-9-6-8-7-10-3-5-0-4
13-15-1	0.91	11-2-1-10-9-12-8-3-6-7-0-5-4
13-45-1	0.97	11-2-1-10-12-9-7-6-8-5-0-3-4
13-15-10-5-1	0.98	11-2-1-9-12-8-10-6-7-5-0-4-3
13-15-30-15-10-1	0.98	11-1-2-12-10-9-8-6-0-5-7-3-4



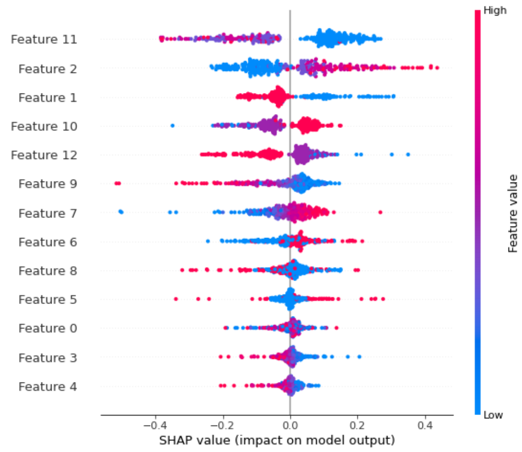
(a) MLP Architecture: 13-15-5-1



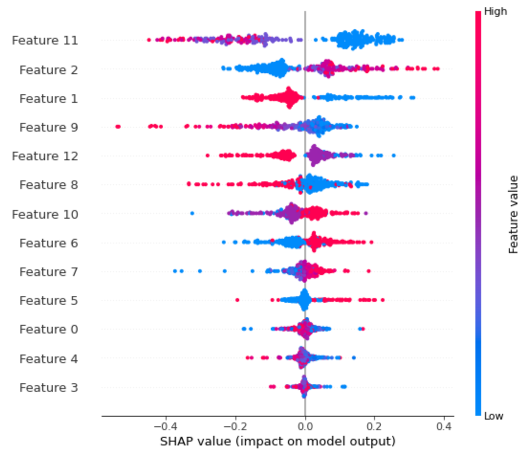
(b) MLP Architecture: 13-20-15-1



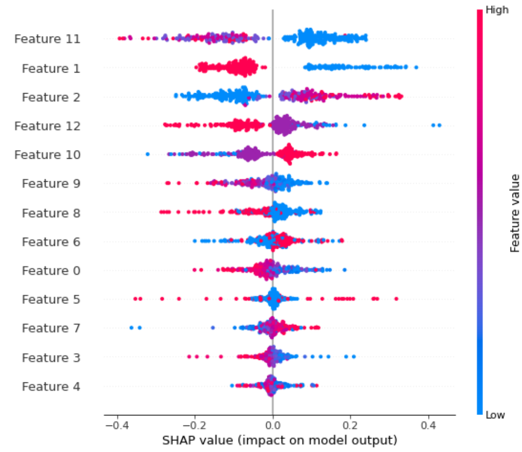
(c) MLP Architecture: 13-15-1



(d) MLP Architecture: 13-45-1



(e) MLP Architecture: 13-15-10-5-1



(f) MLP Architecture: 13-15-30-15-10-1

Figure 3. SHAP plots of the heart disease dataset obtained after MLP training for different architectures (Kalp hastalığı veri seti ile eğitilmiş, farklı mimarideki MLP'lerin, eğitim sonrasında elde edilen SHAP grafikleri).

5. *CONCLUSION*

In MLP systems, which contain too many parameters in artificial intelligence models and are seen as black-boxes, the explainability and interpretability of model outputs, the effects of the dataset on the output and the differences in the importance of dataset attributes according to MLP architecture were examined. Breast Cancer Wisconsin and Heart Disease datasets, which are frequently used in the literature, were used datasets. The reason for choosing this dataset is that issues such as explainability, interpretability, and transparency are much more important in the use of artificial intelligence in the health sector. Both datasets were trained and tested on MLP models with different architectures and the accuracy performance values of the models were measured. The SHAP method was used to track the impact and importance of the input dataset on the model output on the trained model. A test data set was used for the SHAP process. The graphs in Figure 2 and Figure 3 show the importance levels of the dataset attributes sequentially. The accuracy and importance of the dataset attributes obtained for both datasets are transferred to Table 3 and Table 4, respectively. When Figure 2 and Figure 3 and Table 2 and Table 3 are analyzed;

Input dataset features importance varies depending on the MLP architecture,

Different MLP architectures achieving similar accuracy can still produce different feature importance rankings, MLP models with the same architecture but different performance can yield different feature importance rankings,

The impact of attributes with relatively high importance is not much affected by the MLP architecture,

The relative ranking of features with similar importance levels is more likely to change between different architectures,

No direct relationship between the model accuracy performance value and the ranking of attribute influence (importance) values in artificial intelligence MLP methods,

It was observed that the relative importance of input features could be measured using SHAP for MLP models. Accordingly, it can be concluded that the architecture of the MLP models is also an issue that needs to be considered in terms of explainability, interpretability and transparency of the input-output relationship of artificial intelligence models.

The study can be extended by using, in MLP, the relationships of other hyper-parameters such as learning algorithm, activation functions, loss function, etc. to the effect rates of data attribute.

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