Analysis of Misclassified Cases in a Metabolic Syndrome Prediction Model

Explain misclassification of a prediction model

Sejong Oh*
Department of Software Science, Dankook University, South Korea, sejongoh@dankook.ac.kr

Kyungmin Kim
Department of Software Science, Dankook University, South Korea, keung903@naver.com

Hyunseok Shin
Department of Computer Science, Dankook University, South Korea, shinhseok@dankook.ac.kr

Metabolic syndrome (MetS) refers to a phenomenon in which dangerous adult diseases, such as arteriosclerosis, hypertension, obesity, diabetes, and hyperlipidemia, occur simultaneously in one person. It has become one of the most common diseases. Recently, machine learning prediction models for MetS have been proposed to this end. Their prediction accuracies are under 0.9 and need to be improved further for a practical use in the medical field. In this study, we propose an analysis of misclassified cases in a MetS prediction model as a point of feature importance and interaction. We adopt a case-based feature importance/interaction approach for the analysis. The results help us understand the roles of features in the prediction model. Furthermore, this study can be used to improve the performance of prediction models.

CCS CONCEPTS • Machine learning • Machine learning approaches • Classification and regression tree

Additional Keywords and Phrases: Metabolic syndrome, Prediction model, Feature importance, Feature interaction

1 Introduction

Metabolic syndrome (MetS) is a cluster of medical conditions that occur together and increase the risk of heart disease, stroke, and Type 2 diabetes. These conditions include increased blood pressure, high blood sugar, excess body fat around the waist, and abnormal cholesterol or triglyceride levels [1]. The five risk factors and thresholds for MetS diagnosis are listed in Table 1 [2]. According to the Metabolic Syndrome Fact Sheet 2021 of Korea, 23% of adults aged ≤ 19 years and 27.7% of those aged ≤ 30 years had MetS between 2016–2018. Furthermore, approximately 50% of adults aged ≥65 years had MetS [3]. MetS has now become a global disease.

* Corresponding author.

Table 1: Five risk factors and thresholds for MetS diagnosis

MetS Risk Factor	Thresholds
Fasting Plasma Glucose	$\geq 100\ (mg/dl)$
Blood Pressure	Systolic ≥ 130 (mg/dl)
	or Diastolic ≥ 85 (mg/dl)
Triglycerides	$\geq 150\ (mg/dl)$
HDL- Cholesterol	Male: $< 40\ (mg/dl)$
	Female: $< 50\ (mg/dl)$
Waist Circumference	Male: $\geq 90\ cm$
	Female: $\geq 85\ cm$

Recently, machine learning skills have been used to predict MetS [4-8]. Classification algorithms can be used to predict MetS. Their prediction accuracies are between 0.8–0.9. In addition to the classification schemes, interpretation methods for machine learning prediction models have also been introduced [9-13]. Feature importance and interaction are well-known tools for observing a feature's role in prediction models [14-19]. Permutation-based feature importance analysis is a well-known method. If we want to know how much a feature F_x contributes to the predictive accuracy of a model, we can measure the prediction accuracy using all feature datasets (A) and using a modified dataset in which the values of F_x are permuted (B). Permutation refers to random shuffling. It removes the influence of a feature or features in a classification model. Therefore, A-B is used as the feature importance. If A-B is large, F_x is an important feature. Feature importance consists of feature power and feature interaction power. Feature power expresses the amount of information about a feature for the prediction task. Feature interaction power refers to the ability of a feature to interact with other features for the prediction task. Permutation-based feature importance cannot specify them.

Oh [20] suggested predictive case-based feature importance and interaction to reveal the role of features in a predictive model. Suppose we have a classification model for metabolic syndrome prediction and want to know the feature importance of F_x. We first prepare three types of datasets:

DS: entire training dataset that is used to build the classification model.
DS (F_x): all feature values are permuted (randomly shuffled), except for F_x in *DS*
DS (F_x(-)): feature values of F_x are permuted in *DS*

The next step is to obtain the prediction results using the above three datasets. Oh [20] correctly classified such cases into the following four groups.

G1: PRED(*DS*(F_x)) is correct, PRED(*DS*(F_x(-))) is incorrect
→ F_x contribution (for correct prediction)
G2: PRED(*DS*(F_x)) is incorrect, PRED(*DS* (F_x(-))) is correct
→ F_x(-) contribution (for correct prediction)
G3: PRED(*DS*(F_x)) is correct, PRED(*DS*(F_x(-))) is correct
→ Common contribution of F_x and F_x(-) (for correct prediction)
G4: PRED(*DS*(F_x)) is incorrect, PRED(*DS*(F_x(-))) is incorrect
→ Cooperative contribution of F_x and F_x(-) (for correct prediction)

PRED(*X*) is the predictive result that uses dataset *X*. From the grouping, feature interaction (*Int*) and importance (*Imp*) are defined by the following equations:

$$FS(F_x) = \text{feature power of } F_x = n(\text{G1}) \,/\, NI \qquad (1)$$

$$Int(F_x, F_x(-)) = \text{interaction between } F_x \text{ and } F_x(-) = n(G4) \,/\, NI \quad (2)$$
$$Imp(F_x) = \text{feature importance of } F_x = FS(F_x) + Int(F_x, F_x(-)) \quad (3)$$

In Equations (1) and (2), NI is the total number of cases (instances) in the dataset DS.

Oh [20] observed correctly classified cases from a given predictive model because a "correct classification" is important in predictive models. However, the observation of "misclassified cases" is also important if the classification accuracy is not as high as that of a MetS prediction model. In this study, we propose an observation method for misclassified cases. We modify Oh's method and consider negative feature importance and interaction. They are used to observe a feature's role in a misclassification.

2 Materials and Methods

We firstly built a predictive model using a MetS dataset. Simultaneously, we developed case-based negative feature importance and interaction (CBNFI) to observe misclassified cases of the model. Figure 1 shows the overall process of this study.

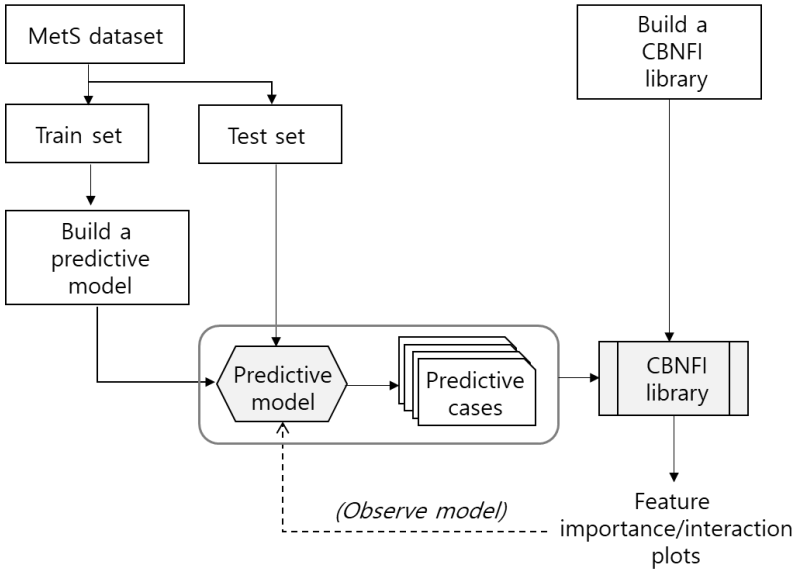

Figure 1: Overall process of this study

2.1 Dataset

This study was based on the "Health Examinee" dataset from the Korea Genome and Epidemiology Study conducted by the Korea Disease Control and Prevention Agency [21]. The dataset was collected from health examinees in major cities across the Republic of Korea according to a city-based cohort. The baseline survey was conducted in 2004 and 173,209 men and women over the age of 40 by 2013 participated in it. The final dataset for the study had 9,314 women subjects and down-sampled for a 1:1 balance between those with and without MetS. The final training and test sets had 7,450 and 1,864 cases, respectively. In addition, nine features were selected, and a new feature (BPWC) was synthesized from BP and WC features. Table 2 summarizes the dataset features.

Table 2: Features in the dataset

No	Feature	Description
1	BP	blood pressure
2	WC	waist circumference
3	BPWC	BP×WC
4	whr	waist to hip ratio
5	bmi	body mass index
6	age	age of subject
7	pulse	pulse rate
8	BFP	percent body fat
9	bp_bi	blood pressure diagnosis (0:normal, 1:abnormal)
10	waist_bi	waist circumference diagnosis (0:normal, 1:abnormal)
11	mets	class label (0: normal, 1:MetS)

2.2 Metabolic syndrome predictive model

We used the XGBoost algorithm to build a prediction model. XGBoost is an ensemble-based classification algorithm that generates strong predictive models. We used five-fold cross-validation with five repeats to train the model and ensure variation in the data. A learning rate of 0.1 and a max depth of 6 were used as the training parameters. The parameters were selected according to proof of good performance. In addition, we used the softmax activation function. Table 3 summarizes the model's performance.

Table 3: Model performance

ACC (%)	B.ACC (%)	PPV (%)	NPV (%)	Sensitivity	Specificity
83.26	83.26	81.38	85.39	86.27	80.26

(ACC: accuracy, B.ACC: balanced accuracy, PPV: positive predictive value, NPV: negative predictive value)

Figure 2 shows a (positive) feature importance plot from the XGBoost model. A feature importance value expresses the effect of a feature on the correct prediction.

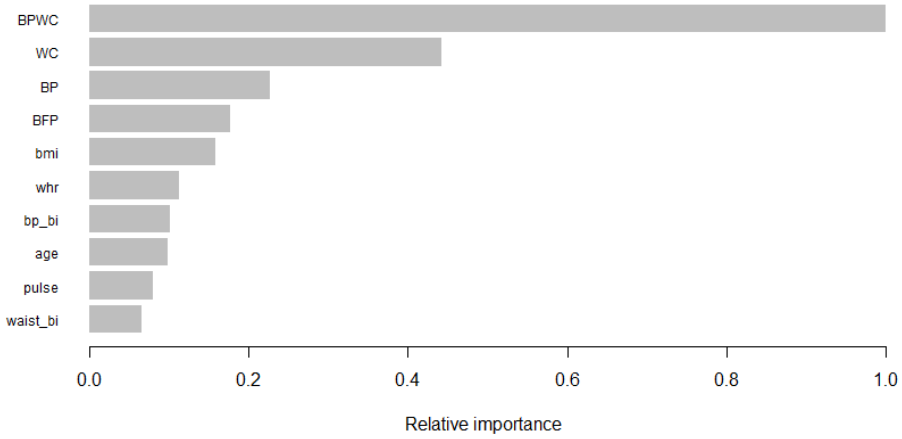

Figure 2: Case grouping for incorrectly predicted cases in *PRED*(*DS*)

2.3 Case-based negative feature importance and interaction

Our aim was to determine why misclassification occurs in MetS prediction. In this context, negative feature importance refers to the extent to which a particular feature contributes to a misclassification. Figure 3 shows the cases of misclassification, which can be categorized into four groups.

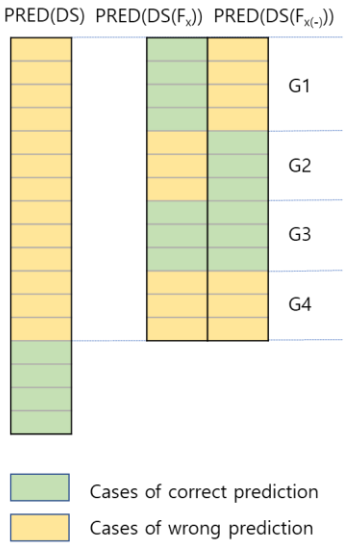

Figure 3: Case grouping for incorrectly predicted cases in *PRED*(*DS*)

G1: PRED($DS(F_x)$) is correct, PRED($DS(F_x(-))$) is incorrect

→ $F_x(-)$contribution (for correct misprediction)

G2: PRED($DS(F_x)$) is incorrect, PRED($DS(F_x(-))$) is correct

→ F_x contribution (for correct misprediction)

G3: PRED($DS(F_x)$) is correct, PRED($DS(F_x(-))$) is correct

→ Cooperative contribution of F_x and $F_x(-)$ (for correct misprediction)

G4: PRED($DS(F_x)$) is incorrect, PRED($DS(F_x(-))$) is incorrect

→ Common contribution of F_x and $F_x(-)$ (for correct misprediction)

From the grouping, the negative feature interaction (*IntN*) and importance (*ImpN*) are defined by the following equations:

$$IntN(F_x, F_x(-)) = \text{negative interaction between } F_x \text{ and } F_x(-) = n(\text{G3}) \,/\, NI \qquad (4)$$

$$ImpN(F_x) = n(\text{G2}) \,/\, NI + IntN(F_x, F_x(-)) \qquad (5)$$

3 Results and discussion

Figure 4 shows the negative feature importance in the MetS prediction model. As can be seen, BPWC has the greatest influence on misprediction, followed by BP, whr, and WC. An interesting point in Figure 4 is that the negative feature power is small, but the negative feature interaction is large in most features. Figure 5 and Figure

6 show the negative feature importance according to the classes of the predictive model. The negative feature importance in Class 0 (normal) and Class 1 (MetS) are similar to those of all classes. However, the ratios of feature power and interaction power are different in the two classes. For example, the ratio of the feature power of BPWS in Class 1 is smaller than that of Class 0, but the ratio of the interaction power of BPWS in Class 1 is larger than that of Class 0. We can observe that the order of negative importance differs between Classes 0 and 1. For example, BP is ranked 6th in Class 1 and 2nd in Class 0. This means the roles of the features are different when predicting Class 0 and when predicting Class 1.

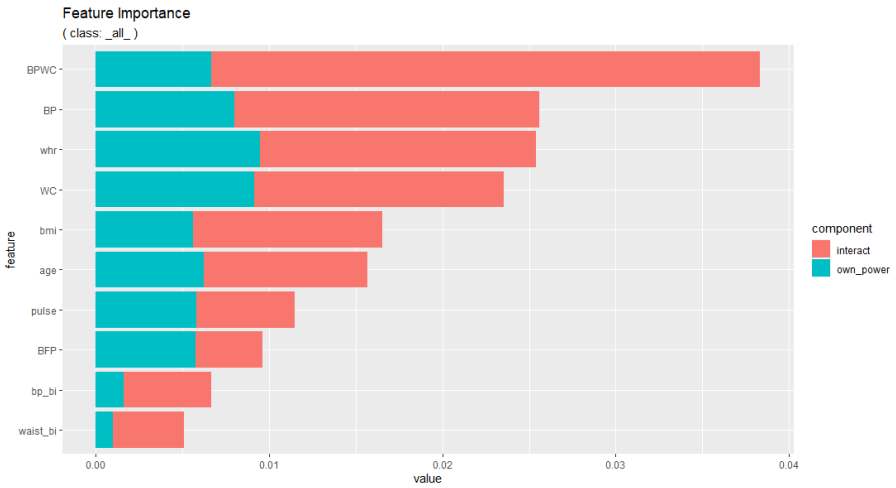

Figure 4: Negative feature importance in the predictive model

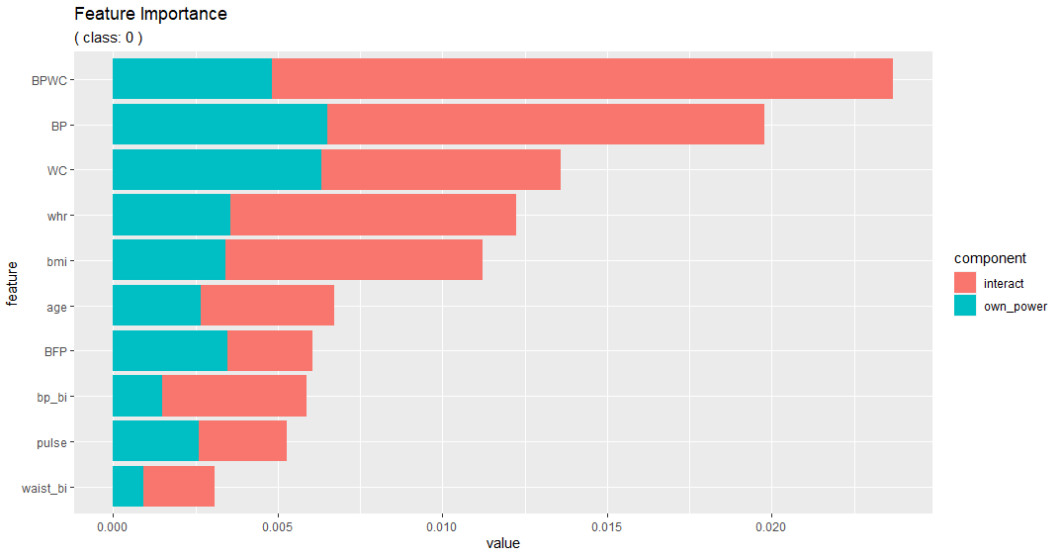

Figure 5: Negative feature importance according to the classes of the predictive model (Class 0 (normal))

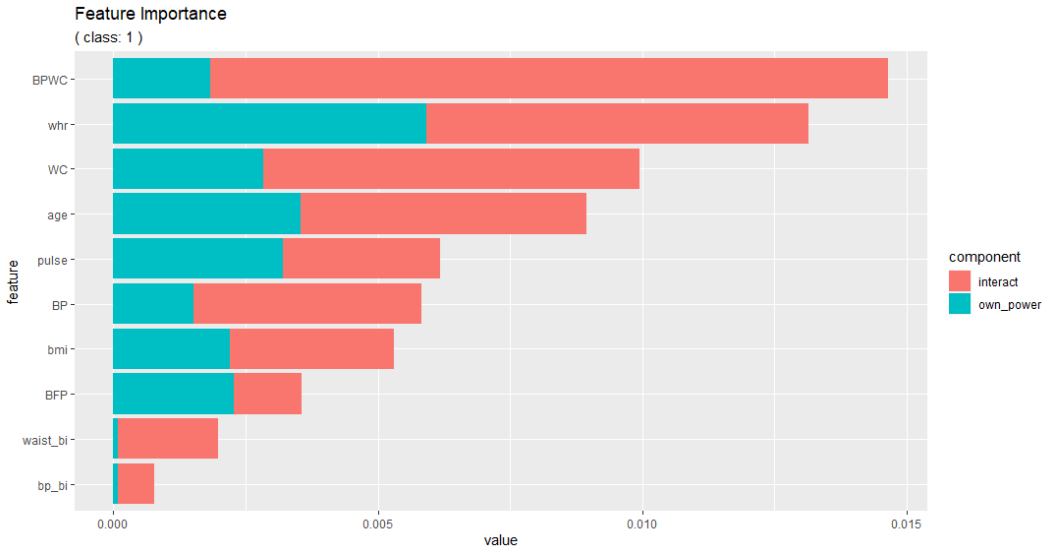

Figure 6: Negative feature importance according to the classes of the predictive model (Class 1 (MetS))

As BPWC is the most important feature for MetS prediction, it was necessary to observe its interaction with other features. Figure 7 shows a negative feature interaction graph between BPWC and the other features. BPWC strongly interacts with BP and WC because it is derived from BP and WC. In the case of BP-BPWC, the interaction is more active in Class 0; in the WC-BPWC case, it is Class 1. This is followed by whr and bmi in the next strongest interactions.

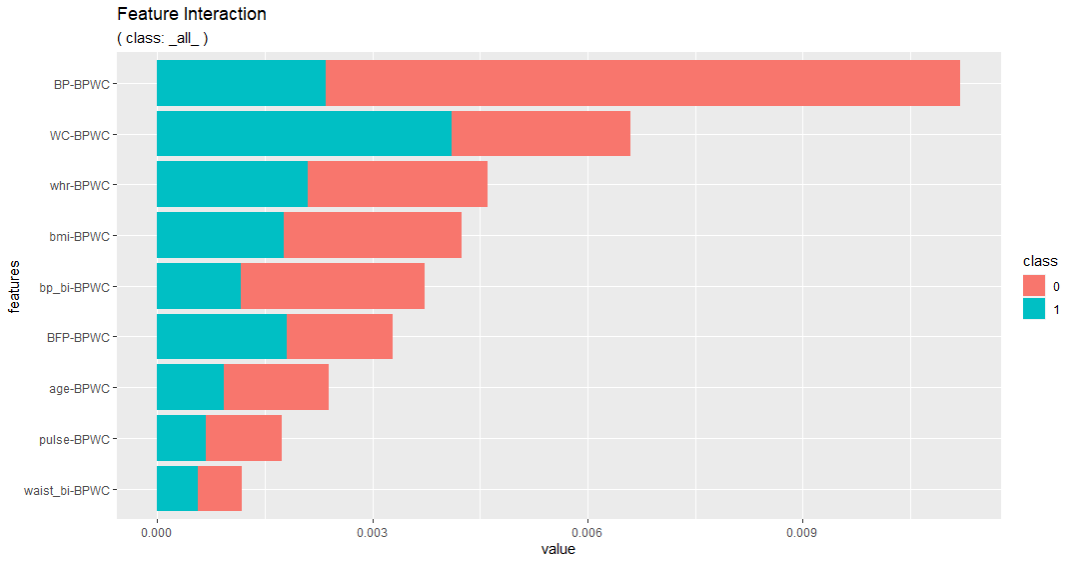

Figure 7: Negative feature interaction between BPWC and other features (0: normal, 1: MetS)

BPWC is a synthesized feature from BP and WC, but its influence is greater than that of BP and WC. This shows that feature synthesis should be strongly considered when developing a prediction model. The results of the experiment show the portions of negative feature power and interaction power for the features. In MetS prediction, we confirmed that feature interaction is more important than feature power. In the future, we may attempt to identify other features to reduce negative interactions.

ACKNOWLEDGMENTS

Data in this study were obtained from the Korean Genome and Epidemiology Study (KoGES; 4851-302), National Institute of Health, Korea Disease Control and Prevention Agency, Republic of Korea. This research was supported by the MSIT (Ministry of Science, ICT), Korea, under the High-Potential Individuals Global Training Program (2021-0-01531) supervised by the Institute for Information & Communications Technology Planning & Evaluation (IITP).

REFERENCES

<bib id="bib1"><number>[1]</number>Mayo clinic, https://www.mayoclinic.org/diseases-conditions/metabolic-syndrome/symptoms-causes/syc-20351916</bib>
<bib id="bib2"><number>[2]</number>S. M. Grundy et al., “Diagnosis and management of the metabolic syndrome: an American Heart Association/National Heart, Lung, and Blood Institute Scientific Statement,” Circulation, vol. 112, no. 17, pp. 2735–2752, Oct. 2005, doi: 10.1161/CIRCULATIONAHA.105.169404.</bib>
<bib id="bib3"><number>[3]</number>Huh, J. H., Kang, D. R., Kim, J. Y., & Koh, K. K. (2021). Metabolic syndrome fact sheet 2021: executive report. CardioMetabolic Syndrome Journal, 1.</bib>
<bib id="bib4"><number>[4]</number>Yu, C. S., Lin, Y. J., Lin, C. H., Wang, S. T., Lin, S. Y., Lin, S. H., ... & Chang, S. S. (2020). Predicting metabolic syndrome with machine learning models using a decision tree algorithm: retrospective cohort study. JMIR medical informatics, 8(3), e17110.</bib>
<bib id="bib5"><number>[5]</number>Perveen, S., Shahbaz, M., Keshavjee, K., & Guergachi, A. (2018). Metabolic syndrome and development of diabetes mellitus: predictive modeling based on machine learning techniques. IEEE Access, 7, 1365-1375.</bib>
<bib id="bib6"><number>[6]</number>Gutiérrez-Esparza, G. O., Infante Vázquez, O., Vallejo, M., & Hernández-Torruco, J. (2020). Prediction of metabolic syndrome in a Mexican population applying machine learning algorithms. Symmetry, 12(4), 581.</bib>
<bib id="bib7"><number>[7]</number>Karimi-Alavijeh, F., Jalili, S., & Sadeghi, M. (2016). Predicting metabolic syndrome using decision tree and support vector machine methods. ARYA atherosclerosis, 12(3), 146.</bib>
<bib id="bib8"><number>[8]</number>Hosseini-Esfahani, F., Alafchi, B., Cheraghi, Z., Doosti-Irani, A., Mirmiran, P., Khalili, D., & Azizi, F. (2021). Using machine learning techniques to predict factors contributing to the incidence of metabolic syndrome in tehran: Cohort study. JMIR public health and surveillance, 7(9), e27304.</bib>
<bib id="bib9"><number>[9]</number>Molnar, C. (2020). Interpretable machine learning. Lulu. com.</bib>
<bib id="bib10"><number>[10]</number>Du, M., Liu, N., & Hu, X. (2019). Techniques for interpretable machine learning. Communications of the ACM, 63(1), 68-77.</bib>
<bib id="bib11"><number>[11]</number>Doshi-Velez, F., & Kim, B. (2017). Towards a rigorous science of interpretable machine learning. arXiv preprint arXiv:1702.08608.</bib>
<bib id="bib12"><number>[12]</number>Ahmad, M. A., Eckert, C., & Teredesai, A. (2018, August). Interpretable machine learning in healthcare. In Proceedings of the 2018 ACM international conference on bioinformatics, computational biology, and health informatics (pp. 559-560).</bib>
<bib id="bib13"><number>[13]</number>Murdoch, W. J., Singh, C., Kumbier, K., Abbasi-Asl, R., & Yu, B. (2019). Interpretable machine learning: definitions, methods, and applications. arXiv preprint arXiv:1901.04592.</bib>
<bib id="bib14"><number>[14]</number>Hooker, S., Erhan, D., Kindermans, P. J., & Kim, B. (2018). Evaluating feature importance estimates.</bib>
<bib id="bib15"><number>[15]</number>Zien, A., Krämer, N., Sonnenburg, S., & Rätsch, G. (2009, September). The feature importance ranking measure. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases (pp. 694-709). Springer, Berlin, Heidelberg.</bib>
<bib id="bib16"><number>[16]</number>Altmann, A., Toloşi, L., Sander, O., & Lengauer, T. (2010). Permutation importance: a corrected feature importance measure. Bioinformatics, 26(10), 1340-1347.</bib>
<bib id="bib17"><number>[17]</number>Casalicchio, G., Molnar, C., & Bischl, B. (2018, September). Visualizing the feature importance for black box models. In Joint European Conference on Machine Learning and Knowledge Discovery in Databases (pp. 655-670). Springer, Cham.</bib>
<bib id="bib18"><number>[18]</number>Tsang, M., Rambhatla, S., & Liu, Y. (2020). How does this interaction affect me? interpretable attribution for feature interactions. Advances in neural information processing systems, 33, 6147-6159.</bib>
<bib id="bib19"><number>[19]</number>Tang, X., Dai, Y., & Xiang, Y. (2019). Feature selection based on feature interactions with application to text categorization. Expert Systems with Applications, 120, 207-216.</bib>
<bib id="bib20"><number>[20]</number>Oh, S. (2022). Predictive Case-based Feature Importance and Interaction. Information Sciences.</bib>
<bib id="bib21"><number>[21]</number>Y. Kim, B.-G. Han, and KoGES group, “Cohort Profile: The Korean Genome and Epidemiology Study (KoGES) Consortium,” Int. J. Epidemiol., vol. 46, no. 2, p. e20, Apr. 2017, doi: 10.1093/ije/dyv316.</bib>