Can We Trust Explanation! Evaluation of Model-Agnostic Explanation Techniques on Highly Imbalanced, Multiclass-Multioutput Classification Problem

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Abstract: Explainable AI (XAI) assist clinicians and researcher in understanding the rationale behind the predictions made by data-driven models which helps them to make informed decisions and trust the model's outputs. Providing accurate explanations for breast cancer treatment predictions in the context of highly imbalanced, multiclass-multioutput classification problem is extremely challenging. The aim of this study is to perform a comprehensive and detailed analysis of the explanations generated by post-hoc explanatory methods: Local Interpretable Model-agnostic Explanation (LIME) and SHaply Additive exPlanations (SHAP) for breast cancer treatment prediction using highly imbalanced oncologycal dataset. We introduced evaluation matrices including consistency, fidelity, alignment with established clinical guidelines and qualitative analysis to evaluate the effectiveness and faithfulness of these methods. By examining the strengths and limitations of LIME and SHAP, we aim to determine their suitability for supporting clinical decision making in multifaceted treatments and complex scenarios. Our findings provide important insights into the use of these explanation methods, highlighting the importance of transparent and robust predictive models. This experiment showed that SHAP perform better than LIME in term of fidelity and by providing more stable explanation that are better aligned with medical guidelines. This work provides guidance to practitioners and model developers in selecting the most suitable explanation technique to promote trust and enhance understanding in predictive healthcare models.

1 INTRODUCTION

In recent years, a drastic change and transformation has been observed in the healthcare industry with the advent of Machine Learning (ML) technologies. These machine learning (data-driven) techniques help to examine a vast amount of medical data, leading to more accurate diagnoses, personalized treatment strategies as well as better patient outcomes. However, the black box nature and complexity of many ML models, especially deep learning algorithms make them unsuitable for many applications particularly in healthcare where interpretability and trust are fundamentals. Hence, the need for interpretable and transparent models is growing critical among doctors and patients who must understand why automatic decisions were made in order to ensure model's fairness, accuracy and compliance with ethical standards.

Local Interpretable Model-agnostic Explanation (LIME) and SHapley Additive exPlanation (SHAP) are two popular methods used to explain the predictions made by ML models. LIME, proposed by Ribeiro et al. in 2016, explains the individual predictions by estimating the model around them. On the other hand, SHAP, introduced by Lundberg in 2018 inspired by cooperative game theory, uses the Shapley value to represent the contribution of each feature to prediction. There are some studies such as (Ribeiro et al., 2016) and (Kumar et al., 2020) that highlight the strengths and weaknesses of these explanatory methods in different fields. However, direct comparisons of both LIME and SHAP, especially in healthcare domains and considering their impact on clinical decision-making, are limited.

An ideal model explainer should contain the following key properties:

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- It should provide a qualitative understanding between the input feature and the model's response.
- For a similar instance, explanation must be consistent each time.
- A surrogate model should approximate the black-box model's behavior well.
- Explanation must be consistently aligned with established medical guidelines and with the expert recommendations.

The main goal of this research is to conduct an insightful and comprehensive comparison of the explanation provided by LIME and SHAP for breast cancer treatment prediction in a highly imbalanced oncological dataset. We aim to assess their performance in term of interpretability, fidelity, stability and relevance to the medical guidelines.

This research article is organized in following manner: Section 2 comprises a quick review of the technical background, where introductory concepts about the LIME and SHAP are presented. A detailed introduction to the system model is presented in Section 3. The discussion about the experiments and dataset is reported in Section 4 followed by the Section 5 where we analysed and discussed the results of the experiment. We summarize the paper in Section 6 with concluding remarks and by highlighting some future directions.

2 TECHNICAL BACKGROUND

This section provides a brief introduction to two popular model-agnostic explainable machine learning approaches: LIME and SHAP.

2.1 SHAP

SHAP (shapley additive explanations) is a framework (Meng et al., 2020), which is inspired by cooperative game theory and used for optimal credit allocation, uses the Shapley values to explain the outcome of any machine learning model. In cooperative game theory, a coalition game consist of N players and a function v which maps the subsets $S = 1,2,3,4,\ldots,N$ to a real value $v(s)$. The value function represents how much combined payoff a set of players can gain by "cooperating" as a set. The Shapley value is a procedure to split the total value of the collective coalition, $v(1,2,...,N)$, between each of the players. The marginal contribution $\Delta v(i,S)$ of player i with respect to a coalition S is defined as:

$$\Delta v(i,S) = v(S \cup \{i\}) - v(S) \qquad (1)$$

The Shapley value can be thought of as a weighted average of a player's marginal contribution to each possible subset of players. The Shapley value of player i is then:

$$\phi_v(i) = \frac{1}{N!}\sum_{\pi \in \Pi} \Delta v(i, S_{i,\pi}) \qquad (2)$$

Where Π is set of permutations of integers upto N and $\pi \in \Pi$. Above equation can be written as:

$$\phi_v(i) = \frac{1}{N!}\sum_{S \subseteq \{1,2,...,N\}} |S|!\,(N - |S| - 1)!\,\Delta v(i,S) \quad (3)$$

Numerous methods have been developed to use the Shapley value for determining feature importance. In a model with features $f(x_1, x_2, ..., x_d)$, these features from 1 to d can be considered as players in a game, where the payoff v represents a measure of how important or influential each subset of features is. The Shapley value $\phi_v(i)$ represents the "influence" of the feature i on the overall outcome.

Shapley sampling values (Štrumbelj and Kononenko, 2014) and SHAP values (Lundberg and Lee, 2017) are based on defining $v_{f,x}(S)$ as the conditional expected output of a model for a specific data point, considering only the features in the subset S that are known:

$$v_{f,x}(S) = \mathbb{E}[f(X) \mid X_S = x_S] = \mathbb{E}_{X_{\bar{S}}|X_S}[f(x_S, X_{\bar{S}})] \quad (4)$$

In above equation X_S: $\{X_i : i \in S\}$ is the set of random variable, and x_S is the set of values $\{x_i : i \in S\}$.

In KernelSHAP samples of the features in $\bar{S}$ are drawn from the marginal joint distribution of these variables. The estimated value function $\hat{v}_{f,x}(S)$

$$\hat{v}_{f,x}(S) = \mathbb{E}_D[f(x_S, X_{\bar{S}})] \qquad (5)$$

2.2 LIME

The LIME method interprets individual model predictions by locally approximating the model around a specific prediction. The local linear explanation model used by LIME, making it an additive feature attribution method.

Let f be the original prediction model (black-box model) to be explained and g the post-hoc explanation model. LIME defines the simplified inputs x' as "interpretable inputs", and the mapping $x = h_x(x')$ transforms the binary vector of interpretable inputs into the original input space. Different forms of the h_x mapping are applied based on the type of input space. For bag-of-words text features, h_x converts a vector of 1's and 0's (indicating presence or absence) into the original word count if the interpretable input is one, or zero if the interpretable input is zero.

For images, h_x considers the image as a collection of superpixels. It assigns a value of 1 to retain the original superpixel value, and 0 to replace the superpixel with the average of its neighbouring pixels (representing a missing superpixel). We focus on local methods aimed at explaining the prediction $f(x)$ for a given input x, as proposed in (Garreau and Luxburg, 2020). The prediction $f(z)$ can be approximated as:

$$f(z) \approx g(z) = \phi_0 + \sum_{i=1}^{M} \phi_i \cdot z_i$$

where: $g(z)$ is the interpretable model, ϕ_0 is the intercept, ϕ_i are the feature weights for the perturbed instances, z_i is perturbed instances.
LIME minimizes the following objective function:

$$\xi = \arg\min_{g \in G} L(f, g, \pi_{x'}) + \Omega(g) \tag{6}$$

Where f: original prediction model, x: original features, g: explanation model, π: proximity measure between an instance x and z (z is a perturbed instance) to define locality around x.

$L(.)$ is the measure of the unfaithfulness of g in approximating f in the locality defined by π. $\Omega(g)$ is a measure of model complexity of the explanation g. For example, if the explanation model is a decision tree, it can be the depth of the tree; in the case of linear explanation models, it can be the number of non-zero weights.

2.3 KernelSHAP (Linear LIME + Shapley Values)

KernelSHAP approximates Shapley values by solving a linear regression problem. KernelSHAP enhances the sample efficiency of model-agnostic estimations of SHAP values, by focusing on specific model types. Below we show how to find the loss function L, weighting kernel π_x'’ , and regularization term $\Omega(g)$ in equation 6 that recover the Shapley values.

$$\Omega(g) = 0, \tag{7}$$

$$\pi_{x'}(z') = \frac{(M-1)}{(Mchoose|z_0|)|z'|(M-|z'|)} \tag{8}$$

$$L(f, g, \pi_{x'}) = \sum_{z' \in Z} \left(f(h_x^{-1}(z')) - g(z')\right)^2 \pi_{x'}(z') \tag{9}$$

where $|z'|$ is the number of non-zero elements in z'.

3 APPROACH

Figure 1 illustrate the layout of the experiment. Prepossessing steps involve handling missing values, removing duplicates, and correcting errors, and feature selection is carried out in consultation with the expert. A detail description of these steps is presented in section-4. Randomforest is used as blackbox model which is trained on the medical dataset for the prediction of treatments for breast cancer patients. A Random Forest is an ensemble learning method (Azar et al., 2014). It works by constructing multiple decision trees during training. Each tree in the forest is built using a random subset of features and a random subset of the training data, which helps ensure that the trees are diverse and not excessively correlated. This randomness improves classification accuracy and gain better generalization ability (Parmar et al., 2019). Our use case involves predicting five treatment options, including surgery and four types of therapies ($Chemo, Target, Hormonal$ and $Radio$).

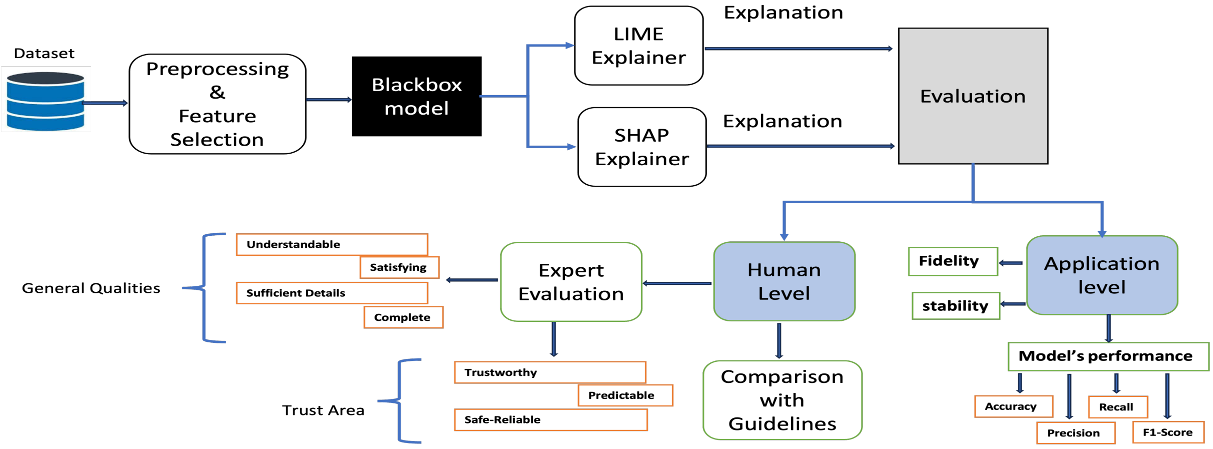


Figure 1: Evaluation of LIME and SHAP explainer through quantitative (Application-based) and qualitative (Human-based) assessments.

These therapies has further divided into four outputs/labels ($pre-surgery$, $Post-surgery$, *pre and post surgery and without surgery*) which make this problem multi-class multi-output problem. Two surrogate models (LIME and SHAP) are used to explain the predictions of the blackbox model. LIME provides local approximation to explain individual predictions. On the other hand SHAP uses sharply values from cooperative game theory to fairly distribute the contribution of each feature to the prediction.

The explanations from both LIME and SHAP are subjected to an extensive analysis. This process evaluates the effectiveness of each method in providing meaningful insights into the model's predictions. The evaluation is taken place onto two levels: Human-level and Application-level.

3.1 Application Level Evaluation

At application level, explanations are evaluated at following parameters:

3.1.1 Model's Performance

In this section we will present the evaluation matrices of black-box model. **Accuracy** measures the overall correctness of the model and is calculated as the ratio of correctly predicted instances to the total number of instances. **Precision** measures the accuracy of the positive predictions made by the model. It is calculated as the ratio of true-positive predictions to the sum of true-positive and false-positive predictions. **Recall** measures the model's ability to identify all relevant instances. It is calculated as the ratio of true positive predictions to the sum of true positives and false negatives. **F1-score** is the matrix which considers both precision and recall. It is harmonic mean of precision and recall, providing a balance between the two metrics.

3.1.2 Fidelity

Although post-hoc explanation methods (Guidotti et al., 2018) can be used to interpret black-box models, it is possible that the explanation generated is not always faithful to the decision-making of the original black box as the explanatory methods are different from the prediction methods. Hence, it is important to understand how well explainable methods can mimic the decision making process of black-box models (Messalas et al., 2019). Fidelity measures the similarity of prediction made by a black box and surrogate model.

Consider an input feature vector $x = (x_1, x_2, \dots, x_k)$, prediction probability for predicted class $Y(x)$ and Z as set of pertubations $z \in Z$. Mean absolute percentage error (MAPE), that computes the difference in the prediction probabilities of surogate model and black-box model, is used to measure the fidelity of explanations (Velmurugan et al., 2021).

$$\mathcal{F} = \frac{\sum_{1}^{|Z|} \frac{|Y(z)-Y(z)|}{Y(z)}}{|Z|} \tag{10}$$

Fidelity can also be computed by using R-squared:

$$R^2 = 1 - \frac{\sum_{i=1}^{k}(f(z^{(i)}) - g(z^{(i)}))^2}{\sum_{i=1}^{k}(f(z^{(i)}) - \bar{f})^2} \tag{11}$$

Where $f(z^{(i)})$ are predictions for perturbed samples from the complex model, $g(z(1))$ are predictions for perturbed samples from the surrogate model and $\bar{f}$ is the mean of the original model's predictions for the perturbed samples:

$$\bar{f} = \frac{1}{k}\sum_{i=1}^{k} f(z^{(i)}) \tag{12}$$

A high R^2 value close to 1 indicates high fidelity, meaning the surrogate model's predictions closely match those of the complex model.

3.1.3 Stability

The Stability Index (SI) compares the variables composition in the explanations $\mathcal{E}^1, \dots, \mathcal{E}^m$, that are generated multiple times for the same instance.
We consider the set of all possible combinations (two by two) $C_m^2(\mathcal{E}^1, \dots, \mathcal{E}^m)$ of the m explanations for the same instance. We define a measure of concordance among the two explanations:

$$\text{pair} = (\mathcal{E}_\alpha, \mathcal{E}_\beta) \tag{13}$$

$$V_\alpha = \{\text{feat} \in V : (\mathcal{E}_\alpha(\text{feat}) \neq 0\} \tag{14}$$

$$V_\beta = \{\text{feat} \in V : (\mathcal{E}_\beta(\text{feat}) \neq 0\} \tag{15}$$

$$\mathcal{C}_{pair} = |V_\alpha \cap V_\beta| \tag{16}$$

where V_α and V_β represent respectively the variables used in the explanations $\mathcal{E}_\alpha$ and $\mathcal{E}_\beta$. The concordance function $\mathcal{C}_{pair}$ returns an integer value, namely the cardinality of the intersection between V_α and V_β, ranging from 0 to p, p is the number of variables used by both V_α and V_β. For obtaining the VI index we evaluate the concordance over all the pairs in $C_m^2(\mathcal{E}^1, \dots, \mathcal{E}^m)$ and average them out.

$$VI = \frac{\sum_{1}^{k} \frac{\mathcal{C}_{pair}}{p}}{|C_m^2(\mathcal{E}^1, \dots, \mathcal{E}^m)|} \tag{17}$$

3.2 Human Level Evaluation

In order to evaluate the quality of the explanation generated using both LIME and SHAP, we compared them with medical guidelines and also carried out a human study.

3.2.1 Comparison with Guidelines

Medical guidelines are systematic statements that aid practitioners in decision-making. They are based on evidence and provide a framework for evaluating patients, diagnosing conditions, and recommending treatments.

Lets $\mathcal{M}$ is the complex machine learning model and x is the instance for which explanations are generated. Explanation $\mathcal{E}_{\mathcal{M}}$ generated by model $\mathcal{M}$ can be defined as:

$$\mathcal{E}_{\text{LIME}}(\mathbf{x}) = \{(f_i, w_i) : i = 1, 2, \ldots, n\} \tag{18}$$

$$\mathcal{E}_{\text{SHAP}}(\mathbf{x}) = \{(f_i, s_i) : i = 1, 2, \ldots, n\} \tag{19}$$

Where f_i is the i-th feature, w_i is its weight in the LIME explanation and s_i is SHAP value of i-th feature.

We define importance mapping function $\text{Imp}(f_i, \mathcal{E})$ as:

$$\text{Imp}(f_i, \mathcal{E}) = \begin{cases} w_i & \text{if } \mathcal{E} = \mathcal{E}_{\text{LIME}} \\ s_i & \text{if } \mathcal{E} = \mathcal{E}_{\text{SHAP}} \end{cases} \tag{20}$$

We define the $I_i(G, \mathcal{E})$ as indicator function:

$$I_i(G, \mathcal{E}) = \{(f_i, \text{Imp}(f_i, \mathcal{E}), G_i) \ : f_i \in G \tag{21}$$

$$I_i(G, \mathcal{E}) = \begin{cases} & \text{if } \text{Imp}(f_i, \mathcal{E}) > 0 \text{ and } G_i = \text{High} \\ 1 & \text{ or} \\ & \text{Imp}(f_i, \mathcal{E}) = 0 \text{ and } G_i = \text{Low} \\ & \\ 0 & Else \end{cases} \tag{22}$$

G is the set of medical guidelines, where $G_i \in \{High, Medium, Low\}$ represents the importance of feature i. Comparison index $\Gamma(G, \mathcal{E})$, that measures the concordance scores between explanations and medical guidelines, can be defined as:

$$\Gamma(\mathcal{E}, G) = \frac{1}{|G|} \sum_{i=1}^{|G|} I_i \tag{23}$$

A high value of $\Gamma(\mathcal{E}, G)$ close to 1 indicates that the explanations are completely matches the guidelines and vice versa.

3.2.2 Expert Evaluation

After the detailed description of the considered explanations, we focus now on the expert evaluation of explanations. We conducted survey which consists of two components: first, an introduction to the features as we converted categorical features to numerical features for training of black-box model. Second, we presented explanations from LIME and SHAP to the expert. We considered seven qualities: Understand, Satisfying, Sufficient Details, Complete, Trustworthy, Predictable and Safe-Reliable. The first four belong to the class of general qualities, because they apply universally to any explanation. While the later three are the members of the trust area, which is crucial for users to have confidence in the explanations. The clinician can evaluate the quality of the explanations by answering questions asked in the survey: giving an integer evaluation between 1 (very bad) and 10 (very good).

4 EXPERIMENT

This section first presents an overview of the dataset used during experiments, followed by a detail description of the steps taken to prepare the dataset for this study, including pre-processing, feature selection, and handling class-imbalance.

4.1 Dataset

The Integraal Kankercentrum Nederland (IKNL) is an organization dedicated to improving the quality of cancer care in the Netherlands, and is established to address the need for a coordinated and integrated approach to cancer prevention, treatment, and research. The synthetic dataset (Integraal Kankercentrum Nederland, 2021) retrieved from the IKNL comprises breast cancer data of a total of 60 thousand patients from 2010 to 2019. The data consists of 46 features, including five target variables, named chemo therapy,

Table 1: Distribution of targets.

Treatments	Modalities/Labels				
	No-therapy	Pre-surgical	Post-surgical	Pre- and post-surgical	Without surgery
Chemotherapy	39145	7187	11909	734	1025
Hormonal therapy	26977	664	26828	1433	4098
Radio therapy	20277	1532	36875	-	1316
Targeted therapy	50889	1490	3183	2834	1604
		Yes		No	
Surgery		5728		54272	

hormonal therapy, radiotherapy, targeted therapy and surgery.

The data exploration revealed a total of 58,377 women and 1,623 men, with an average age of 62 years, ranging from 18 to 105 years old.

The distribution of the patients over the classes of target variables can be seen in table 1.

4.2 Prepossessing

Features selection is carried out by incorporating expert knowledge. After consulting with a physician, several features were deleted from the dataframe which were irrelevant and have no influence on the treatment prediction, such as the *key_ID* of the patients and the *tumor*, the *year_of_incidence* or the *localisation* of the primary tumor (which is the same for every patient).

Moreover, to handle missing values, each row containing one or more missing values has been removed. Due to the complex intrinsic relationships between variables in the dataset, any fill-in method would result in implausible combinations.

Additionally, one-hot encoding was applied to convert categorical features into numerical form.

4.3 Class Imbalance Handling

Class imbalance between the target variables can be seen in the figure 2. Five targets/classes are shown along the x-axis. Each class has a number of outputs/labels that are represented in different colors. For example, *chemotherapy* has five output / labels (no therapy, pre-surgical, post-surgical, pre- and post-surgical, and without surgery). Each segment within the bars represents these labels by indicating the normalized value from 0 to 1. To solve this problem of class-imbalance, Synthetic Minority Oversampling TEchnique (SMOTE) (Fernández et al., 2018) is utilized. Where synthetic data is generated based on the distance between a minority data point and its nearest minority neighbor, thereby creating new synthetic data points between the two minority data points. The result is shown in the figure 3 where, for a particular *Class*, each segment within the bars has the same normalized value. Thus, the new dataset has the same number of instances for all the labels within the a specific class.

5 RESULT

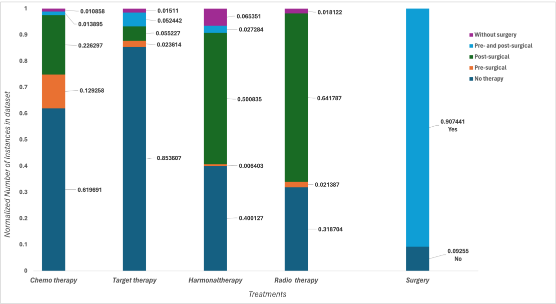


Figure 2: Class imbalance for targeted treatments.

The results presented in this section are obtained by running the experiments on MacBook M3 using Python version 3.11.5. Our main goal is to evaluate the explanations from the surrogate-models. We will present results of application level and human level evaluation in this section. SHAP and LIME provide a way of explaining how individual features contribute to the predictions of machine-learning models. The explanation plot provides a clear and interpretable visualization of the most critical features influencing the model's prediction for specific treatment. Figure4 shows the explanation for predicting ”chemo-therapy pre-surgery” treatment. The features here are ranked according to their importance. The most important feature is at the top, and vice-versa. In this figure, we stated only the features that support the prediction of ”pre-surgical chemotherapy”. A complete participation of features presented in figure5, where the other features are also included. Features in green colour support the prediction and features in red colour oppose this prediction.

5.1 Results for Application Level Evaluation

5.1.1 Model's Performance

In this section, We evaluated the performance of black box model. Dataset divided into train and test data with a ratio of 80% and 20% respectively. We trained the Randomforst classifier and evaluated it's performance using four primary metrics, accuracy, precision, recall and F1-score. Results are shown in the table 2. It is evident that the classifier performs well for all treatment's prediction. Among them, the model

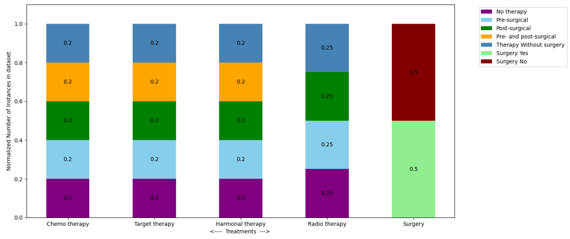
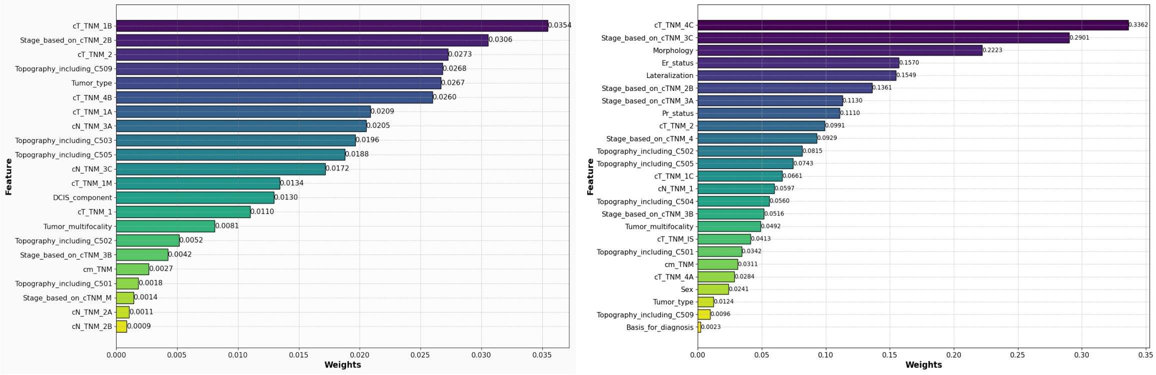


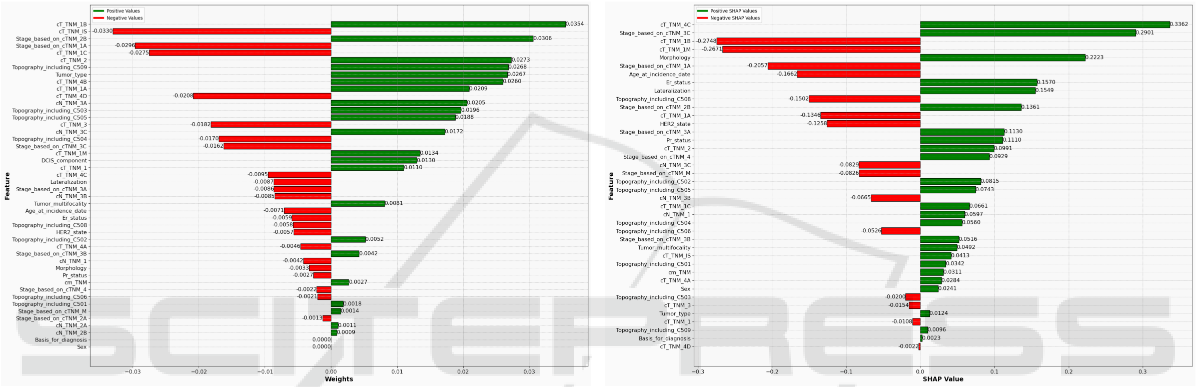
Figure 3: Balanced dataset after SMOTE.



(a) Top features for single label prediction (by LIME)

(b) Top features for single label prediction (by SHAP)

Figure 4: Top features, those supported the prediction of ***Pre-surgical Chemo Therapy***, by both LIME and SHAP.



(a) Summery of LIME explanation for single label prediction

(b) Summery of shap Explanation for single label prediction

Figure 5: Over all contribution of features (in-favour or opposite) for prediction of ***Pre-surgical Chemo Therapy*** provided by both LIME and SHAP.

performed better for *Hormonal-Therapy* where we obtained about 94% precision, F1 score, precision and recall scores. On the other hand, we have the lowest performance for *Radio therapy* which is about 76% for all evaluation metrics. This performance demonstrate that the model makes accurate prediction and effectively identifies relevant cases.

5.1.2 Fidelity

Fidelity refers to how well the surrogate model approximates the predictions of the original complex model for a given instance. It can have values between 0 to 1. High fidelity indicates that the local surrogate model's predictions closely match those of the complex model for the instance being explained. We randomly selected 10 instances from the dataframe and assessed the fidelity of LIME and SHAP across 5 classes. The boxplot in Figure 6 illustrates the fidelity scores of both LIME and SHAP. The graph contains five pairs of box plots, each representing one of the treatment modalities. A horizontal line inside each box marks the median value. Overall, SHAP has higher fidelity than LIME. The fidelity scores of LIME for chemotherapy and radiotherapy were notably low. For target therapy, the mean fidelity scores of both LIME and SHAP were similar. Both explanation methods showed better results for surgery treatment prediction, which is a binary class.

Table 2: Performance of black-box model for breast cancer treatment prediction.

Treatments	Performance Metrics			
	Accuracy	F1 scores	Precision	Recall
Chemotherapy	0.801	0.800	0.804	0.801
Hormonal therapy	0.947	0.947	0.948	0.947
Radio therapy	0.764	0.763	0.763	0.764
Targeted therapy	0.815	0.813	0.815	0.815
Surgery	0.934	0.934	0.936	0.934

5.1.3 Stability

To evaluate stability, we aimed to determine if the explanations were consistent across the same instances

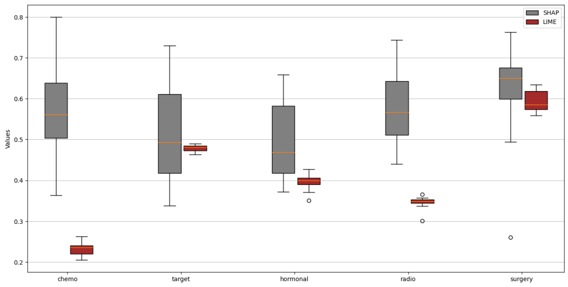


Figure 6: Fidelity score of LIME and SHAP over different treatments modalities.

when generated multiple times. We randomly selected 10 instances and, for each instance and each target class, generated explanations 5 times under the same model settings. We compared the feature compositions in these repeatedly generated explanations for each instance and class. Figure 7 presents the concordance of the top 5 features in the explanations for each treatment. SHAP demonstrated better stability compared to LIME in this multi-class, multi-output scenario. For some point, i.e. for target therapy and hormonal therapy, LIME has lower median and a slightly wider spread compared to SHAP.

5.2 Results for Human Level Evaluation

5.2.1 Comparison with Guideline

We have used the Oncoguide-2020 guidelines (Integraal Kankercentrum Nederland, 2020) about breast cancer developed by Integraal Kankercentrum Nederland (IKNL). For our primary treatment predictions, we extracted a portion of the relevant features from these guidelines, such as [*cT_TNM, cN_TNM, cM_TNM, Grade of tumor, Age, and HER2-status*]. Figure 8 illustrate the concordance scores of two explanation methods, SHAP and LIME, with medical treatment guidelines across five different treatment modalities: chemotherapy ('chemo'), targeted therapy ('target'), hormonal therapy ('hormonal'), radiotherapy ('radio'), and surgery ('surgery'). The concordance score measures how well the explanations from each method align with established medical guidelines. A higher concordance score is better, with an ideal value of 1.

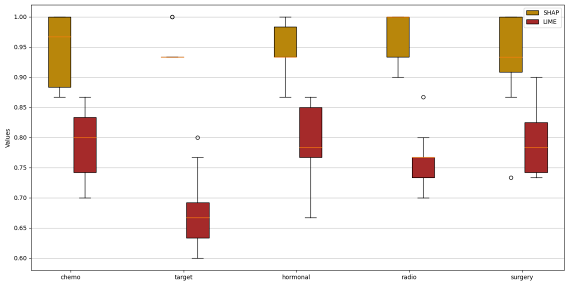


Figure 7: Stability score of LIME and SHAP for breast cancer treatment prediction.

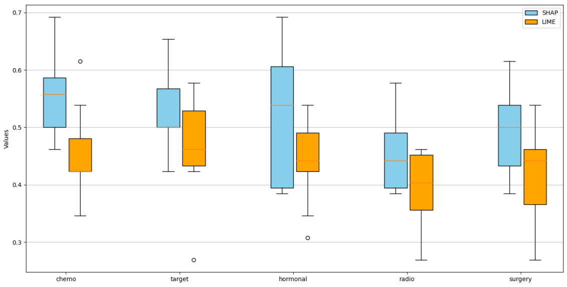


Figure 8: Comparison of explanations with IKNL-guideline.

The box-plot 8 shows that SHAP generally achieves higher median concordance scores across all treatment modalities compared to LIME. This suggests that SHAP explanations are more consistently aligned with medical guidelines. However, the variability within each method and modality indicates that there are specific cases where the concordance can vary significantly. This detailed visualization provides reliability and applicability of these explanation methods in clinical settings.

5.3 Expert Evaluation

We generated explanation on randomly chosen samples from the dataset and asked expert/clinician to judge the explanations and give score to these explanation. On the basis of proposed qualities, expert can give score between 1(very bad) and 10 (vary good) to each explanation. The graph 9 illustrate the aggregated average performance score of two methods, LIME and SHAP, across multiple instances. The graph highlights that SHAP is generally preferred by experts over LIME for explaining prediction tasks related to various breast cancer treatments.

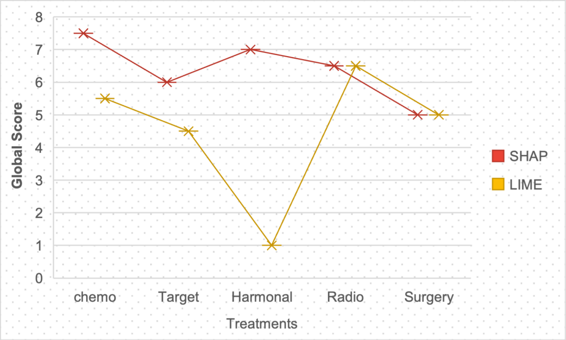


Figure 9: Aggregated score from expert evaluation for different treatments.

SHAP's consistent performance makes it a more suitable choice for scenarios where explanation and reliability is crucial.

This survey helps us to measure the credibility and reliability of the explanation and also helps us to assess the extent to which the explanation meets the expectations and needs of the experts.

6 CONCLUSIONS & FUTURE WORK

In this paper we have presented a comprehensive and detailed analysis of the explanation produced by post-hoc explanations methods LIME and SHAP, for predicting breast cancer treatments using highly imbalanced IKNL systhetic dataset. We evaluated these explanation on stability, fidelity, and their alignment with established medical guidelines and expert evaluations.

Our experiments showed that SHAP outperformed LIME in terms of fidelity for this problem. This advantage is likely due to SHAP's game theory foundation and the use of Shapley values, which provide a unique solution for feature importance allocation. This robust nature of SHAP enhances the accuracy, consistency, and reliability of explanations. On the other hand, LIME offers local explanations by modifying the input data and fitting a simplified model to approximate the original model's behavior around specific instances.

In terms of stability, which measures the consistency of explanations across the same instances over multiple runs, SHAP produced more stable explanations compared to LIME for local predictions. However, SHAP can be more expensive considering computations as there is a trade off between speed and stability.

Comparing the human-level interpretation, SHAP explanations were more consistently aligned with medical guidelines and with the expert evaluation than LIME. This could be attributed to LIME's reliance on random sampling, which can introduce variability across different runs.

For robust and dependable explanations, particularly in contexts demanding high fidelity, SHAP is a more reliable option for interpreting machine learning models.

In the healthcare industry, XAI is used very frequently in clinical decision models to ensure transparency and trustworthy analytics. It is applied to manage clinical diagnosis (Zhang et al., 2022), drug delivery (Jiménez-Luna et al., 2020), disease classification and treatment recommendations (Mellem et al., 2021) (Shah et al., 2023) and other purposes.

LIME and SHAP are widely recognized as leading model-agnostic XAI techniques. This study shows that SHAP outperforms LIME in both qualitative and quantitative assessments. However, these (LIME and SHAP) are not the only model-agnostic XIA (Xu et al., 2019) approaches available. Let us compare them to other techniques by examining their limitations and advantages:

- For simple models, partial dependency plots (PDPs) and individual conditional expectation plots (ICE) may be suitable. For complex models, LIME or SHAP might be more appropriate.
- If you need detailed explanations for individual predictions, LIME is usually a good choice. For global insights, SHAP, PDPs and sensitivity analysis are suitable.
- SHAP can be computationally expensive, especially for large datasets. LIME and PDPs are generally more efficient.

In our experiment, we utilized features listed in the current IKNL medical guidelines, although the model was trained on numerous other features. In future studies:

- we can incorporate guidelines from additional sources, including the American Cancer Society (ACM) (Oeffinger et al., 2015) and National Institute for Health and Care Excellence (NICE) (Murray et al., 2009) to ensure clinical relevance and accuracy.
- we can use other black-box ML models, i.e. deep neural network (DNN) (Samek et al., 2016), extreme learning machines (ELM) (Shah et al., 2019) and deep reinforcement learning (DRL) (Arulkumaran et al., 2017) to assess their impact on the outcomes, generalizability, and robustness.
- we can also compare LIME and SHAP explanations with those from interpretable models such as Explainable Boosting Machine (EBM) (Chen et al., 2021) and Bayesian Networks (BN) (Scanagatta et al., 2019).

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