

# Explainability of Machine Learning Models under Missing Data

Tuan L. Vo\*, Thu Nguyen<sup>\*1a</sup>, Hugo L. Hammer<sup>b,a</sup>, Michael A. Riegler<sup>a,b</sup>,  
Pål Halvorsen<sup>a,b</sup>

<sup>a</sup>*SimulaMet, Oslo, Norway*

<sup>b</sup>*Oslo Metropolitan University, Oslo, Norway*

---

## Abstract

Missing data is a prevalent issue that can significantly impair model performance and interpretability. This paper briefly summarizes the development of the field of missing data with respect to Explainable Artificial Intelligence and experimentally investigates the effects of various imputation methods on the calculation of Shapley values, a popular technique for interpreting complex machine learning models. We compare different imputation strategies and assess their impact on feature importance and interaction as determined by Shapley values. Moreover, we also theoretically analyze the effects of missing values on Shapley values. Importantly, our findings reveal that the choice of imputation method can introduce biases that could lead to changes in the Shapley values, thereby affecting the interpretability of the model. Moreover, and that a lower test prediction mean square error (MSE) may not imply a lower MSE in Shapley values and vice versa. Also, while Xgboost is a method that could handle missing data directly, using Xgboost directly on missing data can seriously affect interpretability compared to imputing the data before training Xgboost. This study provides a comprehensive evaluation of imputation methods in the context of model interpretation, offering practical guidance for selecting appropriate techniques based on dataset characteristics and analysis objectives. The results underscore the importance of considering imputation effects to ensure robust and reliable insights from machine learning models.

*Keywords:* Missing Data, Imputation, Shapley Values

---

<sup>1</sup>\*denotes equal contribution

---

## 1. Introduction

Missing data is a common issue that can significantly affect model performance and interpretability. This problem can occur due to various reasons, such as data collection errors, privacy concerns, or intentional omission. Addressing missing data is crucial, and one effective approach is imputation, i.e., filling in the missing data points to create a more complete dataset for analysis, thereby improving the overall reliability of the results.

Various imputation methods exist, ranging from simple techniques like mean imputation to more sophisticated approaches such as multiple imputation by chained equations (MICE) and k-nearest neighbors (KNN). Each method has its strengths and weaknesses, influencing not only the performance of predictive models but also their interpretability. For example, in [1], the authors study the effects of missing data on the correlation heatmap and found out that the technique that computes a correlation matrix with the highest accuracy (in terms of RMSE) does not always produce correlation plots that closely resemble those derived from complete data. However, the effects of missing data on various aspects of explainable AI have not yet been fully studied.

Shapley values, a concept derived from cooperative game theory, have gained prominence as a robust method for interpreting complex models [2]. Shapley values attribute the contribution of each feature to the final prediction, offering insights into feature importance and interaction. However, the accuracy and reliability of Shapley values can be affected by the choice of the imputation method, as the imputed values can introduce biases or distortions. Despite the importance of this issue, little attention has been paid to the effect of imputation on the Shapley values of the downstream model. For example, in [3], the authors examine various imputation methods to choose the best one and then use Shapley values to explain the prediction of the downstream task. However, the effects of imputation methods on Shapley values have not been thoroughly examined.

This paper aims to explore the effects of various imputation methods on the calculation of Shapley values. By comparing different imputation strategies, we seek to understand how they influence the interpretability of machine learning models and the robustness of the insights derived from Shapley's values. The study provides a comprehensive evaluation of imputation methods

in the context of model interpretation, offering guidance for practitioners on selecting appropriate techniques for their specific datasets and objectives.

The rest of the paper is organized as follows. In Section 2, we briefly review works on explainable AI and missing data to gain insights into the development of missing data in relation to explainable AI and highlight open issues for future consideration. Next, in Section 3, we describe the methods being examined in this work. Following that, we theoretically analyze the effects of missing data on Shapley values in Section 4 and conduct and analyze the experiment results in Section 5. Finally, the paper concludes with a discussion of our findings and suggestions for future work in Section 6 and Section 7.

## 2. Missing data techniques and explainability

In this section, we review various missing data handling techniques and their explainability.

### 2.1. Explainable AI

Explainable Artificial Intelligence (XAI) has garnered significant attention in recent years due to its critical role in ensuring transparency, trustworthiness, and accountability in AI systems. As AI continues to be integrated into various domains, the need for models that can not only perform well but also provide human-understandable explanations for their predictions has become paramount.

A significant development in XAI is the emergence of intrinsic interpretability approaches. These involve designing models that are interpretable by nature. Decision trees [4], rule-based models [5], and linear models [6] are classical examples of intrinsically interpretable models. More recently, models such as Generalized Additive Models (GAMs) [7] and attention mechanisms in neural networks [8] have been explored for their ability to provide insights into the decision-making process. However, their explanation follows their specific explanation style, making it difficult to compare with other models that do not follow the same explanation schemes during model selection.

Recent advancements have also seen the integration of XAI with deep learning models. Techniques such as DeepSHAP [9] and Integrated Gradients [10] provide explanations for neural network predictions by attributing the output to the input features in a manner consistent with the model’s internal

workings. These methods bridge the gap between the high performance of deep learning models and the need for interpretability.

One prominent approach in XAI is the use of post-hoc explanation methods. These techniques, such as LIME (Local Interpretable Model-agnostic Explanations) [11] and SHAP (SHapley Additive exPlanations) [9], offer explanations by approximating the behavior of complex models locally around a given prediction. LIME creates local surrogate models that are interpretable, while SHAP leverages Shapley values from cooperative game theory to fairly distribute the contribution of each feature to the prediction. Both methods have been widely adopted due to their model-agnostic nature, allowing them to be applied to any black-box model.

Overall, compared to other techniques, the Shapley value offers several distinct advantages over other Explainable AI (XAI) techniques. Unlike methods that provide only local explanations or are limited to specific model architectures, the Shapley value delivers a unified and theoretically grounded approach applicable to any machine learning model. It ensures fairness by distributing the model’s output among the features based on their marginal contributions, offering a comprehensive and additive feature attribution that respects interaction effects. This fairness and consistency make Shapley values particularly valuable in high-stakes domains like medicine or finance [12, 13, 14, 15, 16, 17], where understanding the relative importance and interplay of various features is crucial for trust and accountability. Additionally, Shapley values provide a global interpretability framework, making it easier to understand the model’s behavior across different scenarios, thus enhancing transparency and facilitating more informed decision-making.

However, the robustness and reliability of these attributions can be significantly influenced by the treatment of missing data.

## 2.2. Missing data imputation techniques

The most common approach to handling missing values is to use imputation methods to fill in the gaps. Techniques such as matrix decomposition or matrix completion, including MGP [18], Polynomial Matrix Completion [19], ALS [20], and Nuclear Norm Minimization [21], allow for continuous data to be completed and subsequently analyzed using standard data analysis procedures. Additionally, regression or clustering-based methods, such as CBRL and CBRC [22], utilize Bayesian Ridge Regression and cluster-based local least square methods [23] for imputation. For large datasets, deep learning imputation techniques have gained popularity due to their performance

[24, 25, 26]. It’s important to note that different imputation methods may produce varying values for each missing entry, making the modeling of uncertainty for each missing value crucial. Bayesian and multiple imputation techniques, such as Bayesian principal component analysis-based imputation [27] and multiple imputations using Deep Denoising Autoencoders [28], are particularly useful in these scenarios. Furthermore, certain tree-based methods can naturally handle missing data through prediction, including missForest [29], the DMI algorithm [30], and DIFC [31]. Methods that can manage mixed data types have also emerged, such as SICE [32], FEMI [33], and HCMM-LD [34].

Although various missing data methods have been developed [35], most of them to date do not have a built-in explanation mechanism for imputed values, although how a value is imputed can have a profound impact on the performance and interpretability of downstream machine learning models. If one uses a prediction model such as a regression or classification model, then one can use Shapley values or some other XAI technique to explain the imputation of missing values. However, many times, one may want to use a more complicated imputation method that requires building regression or classification models and looping through the data multiple times to improve imputation accuracy.

Sometimes, the imputed values of some imputation techniques can be easily achieved even though the original algorithm does not provide an explanation. K-nearest neighbor imputation may offer some explanation of the imputed values based on the K-nearest neighbors. Next, since tree-based techniques are explainable, the explanation for tree-based imputation methods such as missForest [29] can be achieved by building a tree to explain the classification results. However, a potential ambiguity can be the prediction of one missing entry based on the imputed values of the other entries during the iteration process. Similar things apply to MICE imputation [36], a method for handling missing data through iterative predictions based on the relationships between observed and missing variables.

In recent years, more attention has been paid to the explainability of the imputation method under missing data. For example, [37] introduces DIMV, an imputation method that provides explainability and uncertainty of imputation via conditional distribution, or [1] analyzes the effects of various imputation and direct parameter estimation methods to the correlation plot. Next, Hans et al. [38] introduce an explainable imputation method that leverages association constraints within the data. However, up to our

knowledge, so far, there is no work on the effects of missing data on Shapley values.

### *2.3. Direct missing data handling techniques without imputation*

Different from the imputation approaches, methods that directly handle missing data can have clearer implications in terms of explainability.

Specifically, Nguyen et al. [35] introduced the EPEM algorithm to estimate the maximum likelihood estimates (MLEs) for multiple class monotone missing data when the covariance matrices of all classes are assumed to be equal. Additionally, DPER [39] addresses a more general case where missing data can occur in any feature by using pairs of features to estimate the entries in the mean and covariance matrices. The implication to model explainability of using direct parameter estimation methods, like EPEM and DPER, includes improved transparency and interpretability of the model’s behavior, as these methods provide clear estimates of means and covariances, which can be directly examined and understood. In fact, [1] analyzes the effects of various imputation and direct parameter estimation methods on the correlation plot, and finds that DPER is not only scalable but also better for this task than imputation techniques such as SOFT-IMPUTE [40], KNNI, GAIN [41], GINN [42], missForest [29].

Note that LSTM [43] can handle missing data directly. In fact, it is used the work of Ghazi et al. [44] to model disease progression while handling missing data in both the inputs and targets. Another work by Li et al. [45] proposed a technique for the bi-clustering problem that can manage missing data, enabling simultaneous partitioning of rows and columns of a rectangular data array into homogeneous subsets. Learning directly from the data may offer advantages in speed and reduced storage costs by eliminating the need for separate models for imputation and the target task.

Using techniques that directly handle missing data can significantly enhance model explainability. By learning directly from the data, the model avoids the added complexity of managing separate imputation and prediction models, simplifying the overall structure and making it easier to understand. Additionally, it helps avoid potential biases that can be introduced by filling in missing values, as in imputation methods.

### 3. Methods

In this paper, we will also examine the effects of various imputation techniques on Shapley values. Therefore, in this section, we will briefly summarize the basics of Shapley values, the types of plots, and the imputation techniques that will be used to examine Shapley values in the experiments.

#### 3.1. Shapley values

Shapley values, originally derived from cooperative game theory [46], have been adapted as a powerful tool for interpreting machine learning models [9]. They provide a systematic way to attribute the contribution of each feature to a model’s prediction, ensuring a fair distribution based on the interaction of features. Consider a machine learning model  $v$  that takes an input vector  $\mathbf{x} = (x_1, x_2, \dots, x_p)$  and produces a prediction  $v(\mathbf{x})$ . The Shapley value for the value  $x_i$  of corresponding feature  $f_i$  quantifies its contribution to the prediction  $v(\mathbf{x})$ . Formally, let  $P = \{1, 2, \dots, p\}$  be the complete index set of features and  $S$  a coalition of feature indices (a subset of  $P \setminus \{i\}$ ). For  $i = 1, 2, \dots, p$ , the Shapley value  $\phi_i$  for the feature value  $x_i$  is defined as

$$\phi_i = \sum_{S \subseteq P \setminus \{i\}} \frac{|S|!(p - |S| - 1)!}{p!} [v(S \cup \{i\}) - v(S)],$$

where  $|S|$  is the number of elements in subset  $S$ , and  $v(S \cup \{i\})$ ,  $v(S)$  is the model prediction using feature indices in  $S$  plus  $i^{th}$  feature and only in  $S$ , respectively. In the context of classification problems, the model outputs a probability distribution over classes. The Shapley values can be calculated for each class’s probability, providing insights into how each feature influences the likelihood of each class. Specifically, calculating Shapley values in classification problems can be broken down into the algorithm 1.

The types of plot that will be examined in this paper include:

- A Global Feature Importance plot is a visualization tool for examining the impact of individual features within a predictive model. More specifically, it highlights the features that contribute the most to the model’s predictions, enabling a deeper understanding of the model’s behavior. Here, the global importance of each feature is determined by calculating the mean absolute value of Shapley values of that feature across all the given samples.

---

**Algorithm 1 Shapley Value calculation**

---

**Input:** a classification model  $v$  that predicts the probabilities for each class based on a sample  $\mathbf{x} = (x_1, x_2, \dots, x_p)$  and  $P = \{1, 2, \dots, p\}$  represents the index set of all features.

**Output:** The Shapley value  $\phi_i$  for each feature value  $x_i$ , for  $i = 1, 2, \dots, p$ .

```
1: for  $S \subset P$  do
2:    $v(S) \leftarrow$  trained classification model  $v$  with index in  $S$ .
3: end for
4: for  $i \in P$  do
5:   for  $S \subset P \setminus \{i\}$  do
6:     Marginal Contribution $_{(i)} \leftarrow v(S \cup \{i\}) - v(S)$ .
7:     Weight( $S$ )  $\leftarrow \frac{|S|!(p-|S|-1)!}{p!}$ .
8:   end for
9:    $\phi_i \leftarrow \sum_{S \subseteq P \setminus \{i\}} \text{Weight}(S) \times \text{Marginal Contribution}_{(i)}$ .
10: end for
```

---

- A beeswarm plot is a useful visualization tool to depict the distribution and influence of individual feature contributions on the model's predictions, particularly when using Shapley values. It provides a detailed view of how each feature affects the output of a model across the entire dataset. By displaying each data point as a dot and arranging these dots to show the distribution of Shapley values for each feature, the beeswarm plot offers a comprehensive overview of feature importance and interaction effects. It allows for the identification of patterns and outliers, helping to understand the behavior of the model with respect to individual features. Additionally, the plot can reveal how specific features interact with others, providing insights into complex dependencies within the data.

### 3.2. Imputation techniques

In this section, we briefly summarize the missing data handling methods that we will examine for the effects on Shapley values. The methods being investigated consist of a method that can directly learn from missing data, such as XGBoost, to a simple imputation method as Mean Imputation, as well as the widely used or recently developed imputation techniques, such as

MICE, DIMV, missForest, and SOFT-IMPUTE. The details of the methods are as follows:

- **XGBoost** (Extreme Gradient Boosting) [47] is a powerful and efficient algorithm that belongs to the family of gradient boosting techniques. It builds an ensemble of decision trees, where each tree corrects errors made by the previous ones, enhancing predictive accuracy. XGBoost stands out for its speed and performance, employing advanced features like tree pruning, regularization, and parallel processing, which help in reducing overfitting and handling large-scale data. XGBoost can handle missing data directly.
- **Mean Imputation** is a classical technique used to handle missing data in a dataset. When some data points are missing, mean imputation replaces these missing values with the mean (average) of the available data for that particular variable. This method is straightforward and easy to implement, ensuring that all cases remain in the analysis and preserving the sample size.
- **Multiple Imputation by Chained Equations (MICE)** [36] is a technique for imputing missing data in datasets through regression. It considers the variability of missing values by crafting various imputed datasets. This technique entails sequentially modeling each inadequate variable based on other data variables, producing numerous imputations for each lacking value. The iteration ceases when the divergence among different entries falls below a set threshold. Through this approach, MICE preserves inter-variable connections and yields a stronger and more precise approximation of the missing values.
- **Conditional Distribution-based Imputation of Missing Values with Regularization (DIMV)** [37], is an innovative algorithm designed to handle missing data. This method works by determining the conditional distribution of a feature with missing entries, leveraging information from fully observed features. In addition, the DIMV algorithm is robust to the assumption of multivariate normal and does not require any label information. Therefore, it can be used for both supervised and unsupervised learning. DIMV can also explain the contribution of each feature to the imputation of a feature with a missing value in a regression coefficient-like manner. Moreover, the technique is robust to multicollinearity due to  $L_2$  norm regularization.

- **MissForest** [29] is an imputation method that leverages the predictive power of random forests to estimate missing values in datasets. In particular, it operates by iteratively predicting the missing values for each variable using the observed values and previously imputed values. This process continues until the imputations converge, minimizing the error between successive iterations. Moreover, missForest can handle both continuous and categorical data and capture complex interactions and non-linear relationships between variables, leading to more accurate imputations that make it versatile and suitable for various types of datasets.
- **SOFT-IMPUTE** [40] is an imputation technique based on matrix completion and low-rank approximation, particularly useful for handling missing data in large and sparse datasets. This method operates by iteratively replacing the missing entries with values that minimize the reconstruction error of the data matrix, using singular value decomposition (SVD). Furthermore, SOFT-IMPUTE alternates between imputing missing values and performing a soft-thresholding operation on the singular values of the data matrix. This process encourages the resulting matrix to be low-rank, effectively capturing the underlying structure of the data while filling in the missing entries.

#### 4. Theoretical analysis

In this section, we consider a simple linear regression model to show the effects of missing data in training and test data on the mean absolute Shapley values of a mean imputation method.

Assume we have a training data  $\mathcal{D} = (\mathbf{x}|\mathbf{y})$  which has  $n$  samples,  $\mathbf{x}$  is univariate input, and  $\mathbf{y}$  is a target. The corresponding missing data of  $\mathcal{D}$  is denoted by  $\mathcal{D}^* = (\mathbf{x}^*|\mathbf{y})$ . Here, we assume that only  $\mathbf{x}$  contain missing values and denote  $\text{Obs}(\mathbf{x})$  as the index set of observed samples in  $\mathbf{x}^*$ , i.e.,  $\text{Obs}(\mathbf{x}^*) = \{i \in \mathbb{N} : x_i \text{ is observed}\}$ . Moreover, we denote  $\mathcal{D}' = (\mathbf{x}'|\mathbf{y})$  as imputed data by using mean imputation. It means that

$$x'_i = \begin{cases} x_i, & \text{if } i \in \text{Obs}(\mathbf{x}^*) \\ \mathbb{E}[\mathbf{x}^*], & \text{if } i \notin \text{Obs}(\mathbf{x}^*) \end{cases}, \quad \text{for } i = 1, 2, \dots, n. \quad (1)$$

Now, suppose that the corresponding linear regression models on  $\mathcal{D}$  and  $\mathcal{D}'$

are

$$\begin{aligned} y &= \hat{f}(x) = \beta_0 + \beta_1 x, \\ y' &= \hat{f}(x') = \beta'_0 + \beta'_1 x', \end{aligned}$$

where

$$\begin{aligned} \beta_1 &= \frac{\text{Cov}(\mathbf{x}, \mathbf{y})}{\text{Var}(\mathbf{x})}, \\ \beta'_1 &= \frac{\text{Cov}(\mathbf{x}', \mathbf{y})}{\text{Var}(\mathbf{x}')}. \end{aligned}$$

We consider a test data  $\mathbf{z}$  which has  $m$  samples. It should be reminded that the test data  $\mathbf{z}$  could contain missing values (denoted by  $\mathbf{z}^*$ ) and the imputed version  $\mathbf{z}'$  is presented as

$$z'_j = \begin{cases} z_j, & \text{if } j \in \text{Obs}(\mathbf{z}^*) \\ \mathbb{E}[\mathbf{x}^*], & \text{if } j \notin \text{Obs}(\mathbf{z}^*) \end{cases}, \quad \text{for } j = 1, 2, \dots, m. \quad (2)$$

Then, we want to illustrate a global feature importance of  $\mathbf{x}$  and  $\mathbf{x}'$  on  $\mathbf{z}$  and  $\mathbf{z}'$  respectively by using mean absolute Shapley values, i.e.,

$$\begin{aligned} |\phi(\mathbf{z})| &= \frac{1}{m} \left( \sum_{j=1}^m |\phi(z_j)| \right), \\ |\phi'(\mathbf{z}')| &= \frac{1}{m} \left( \sum_{j=1}^m |\phi'(z'_j)| \right). \end{aligned}$$

where  $\phi(\mathbf{z})$  and  $\phi(\mathbf{z}')$  are the global feature importance on  $\mathbf{z}$  and  $\mathbf{z}'$  respectively;  $\phi(z_j)$  and  $\phi(z'_j)$  are the Shapley values on the prediction of sample  $z_j$  and  $z'_j$  respectively.

The following theorem shows that the global feature importance on  $\mathbf{z}'$  could be simplified.

**Theorem 1.** *The global feature importance of  $\mathbf{x}'$  on  $\mathbf{z}'$  can be simplified to*

$$|\phi'(\mathbf{z}')| = \frac{1}{m} \left( \sum_{j \in \text{Obs}(\mathbf{z}^*)} |\phi'(z'_j)| \right). \quad (3)$$

**Proof 1.** In [9], the Corollary 1, the Shapley value on the prediction of sample  $z'_j$  for  $j = 1, 2, \dots, m$  with the corresponding model on and  $\mathcal{D}'$  are defined as

$$\phi'(z'_j) = (z'_j - \mathbb{E}[\mathbf{x}'])\beta'_1.$$

Now, by using the mean imputation (2), if  $z_j$  is missing then  $z'_j = \mathbb{E}[\mathbf{x}^*]$ . Thus,

$$\phi'(z'_j) = (\mathbb{E}[\mathbf{x}^*] - \mathbb{E}[\mathbf{x}'])\beta'_1.$$

Moreover, it is worth noting that  $\mathbf{x}'$  is the version of mean imputation of  $\mathbf{x}^*$ , therefore  $\mathbb{E}[\mathbf{x}^*] = \mathbb{E}[\mathbf{x}']$ . This implies

$$\phi'(z'_j) = 0, \text{ for } j \notin \text{Obs}(\mathbf{z}^*).$$

The global feature importance of  $\mathbf{x}'$  on  $\mathbf{z}'$  is

$$\begin{aligned} |\phi'(\mathbf{z}')| &= \frac{1}{m} \left( \sum_{j=1}^m |\phi'(z'_j)| \right) \\ &= \frac{1}{m} \left( \sum_{j \in \text{Obs}(\mathbf{z}^*)} |\phi'(z'_j)| + \sum_{j \notin \text{Obs}(\mathbf{z}^*)} |\phi'(z'_j)| \right) \\ &= \frac{1}{m} \left( \sum_{j \in \text{Obs}(\mathbf{z}^*)} |\phi'(z'_j)| \right). \end{aligned}$$

Based on the theorem, we have the following analysis. First, when the missing rate of  $\mathbf{z}^*$  increases, the number of samples that have non-zero contributions in  $|\phi'(\mathbf{z}')|$  is decreased. We can find that  $|\phi'(\mathbf{z}')|$  would be small and less than  $|\phi(\mathbf{z})|$ . However, one important thing is that we cannot conclude that  $|\phi'(\mathbf{z}')|$  is always less than  $|\phi(\mathbf{z})|$ . The reason is that  $|\phi'(z'_j)|$  could be greater than  $|\phi(z_j)|$  for some  $j \in \text{Obs}(\mathbf{z}^*)$ . To be clearly, expanding the formulas  $\phi(z_j)$  and  $\phi'(z'_j)$  gives

$$\begin{aligned} |\phi(z_j)| &= |(z_j - \mathbb{E}[\mathbf{x}])\beta_1| = |z_j - \mathbb{E}[\mathbf{x}]| \cdot \frac{|\text{Cov}(\mathbf{x}, \mathbf{y})|}{\text{Var}(\mathbf{x})}, \\ |\phi'(z'_j)| &= |(z'_j - \mathbb{E}[\mathbf{x}'])\beta'_1| = |z'_j - \mathbb{E}[\mathbf{x}']| \cdot \frac{|\text{Cov}(\mathbf{x}', \mathbf{y})|}{\text{Var}(\mathbf{x}')}. \end{aligned}$$

Note that if  $j \in \text{Obs}(\mathbf{z}^*)$  then  $z'_j = z_j$  and if we suppose that  $\mathbb{E}[\mathbf{x}] \approx \mathbb{E}[\mathbf{x}']$ , then the difference between  $\phi(z_j)$  and  $\phi'(z'_j)$  comes from the remaining terms

$\frac{|\text{Cov}(\mathbf{x}, \mathbf{y})|}{\text{Var}(\mathbf{x})}$  and  $\frac{|\text{Cov}(\mathbf{x}', \mathbf{y})|}{\text{Var}(\mathbf{x}')}$ . Additionally, these terms depend on the missing rate in training data  $\mathbf{x}$  and  $\mathbf{x}'$ . In particular, because  $\mathbf{x}'$  is the imputed version of  $\mathbf{x}$  with mean imputation then  $\text{Var}(\mathbf{x}') \leq \text{Var}(\mathbf{x})$ . It means when the missing rate in training data increases, the term  $\frac{|\text{Cov}(\mathbf{x}', \mathbf{y})|}{\text{Var}(\mathbf{x}')}}$  could be greater than  $\frac{|\text{Cov}(\mathbf{x}, \mathbf{y})|}{\text{Var}(\mathbf{x})}$ . Thus,  $|\phi'(z'_j)|$  could be greater than  $|\phi(z_j)|$  for some  $j \in \text{Obs}(\mathbf{z}^*)$ . In summary, there is a different trend in global feature importance changes, this depends on the missing rates in training and test sets. A high missing rate in the test data can increase the global feature importance, but in the training data, it reduces that value.

Second, the distribution of those Shapley values on  $\mathbf{z}$  and  $\mathbf{z}'$  should have a zero mean. The evidence for that is

$$\begin{aligned}\mathbb{E}[\phi(z_j)] &= (\mathbb{E}[\mathbf{z}] - \mathbb{E}[\mathbf{x}])\beta_1, \\ \mathbb{E}[\phi(z'_j)] &= (\mathbb{E}[\mathbf{z}^*] - \mathbb{E}[\mathbf{x}'])\beta'_1.\end{aligned}$$

In practice,  $\mathbf{x}$  and  $\mathbf{z}$  are split from one data, thus it may have  $\mathbb{E}[\mathbf{z}] \approx \mathbb{E}[\mathbf{x}]$  and  $\mathbb{E}[\mathbf{z}^*] \approx \mathbb{E}[\mathbf{x}']$ . Therefore,  $\mathbb{E}[\phi(z_j)] \approx \mathbb{E}[\phi(z'_j)] \approx 0$ . One important thing is that this assumption may be true for other imputation methods. This is why we see the symmetry in beeswarm plots of original data and mean imputation.

## 5. Experiments

### 5.1. Experiment settings

In this study, we compare the Shapley values of the original data before missing data simulation with the Shapley values of XGBoost [47], a method that can be trained directly on missing data, and a two-step approach (imputation followed by regression). For the second alternative, during the imputation process, we test five methods: mean imputation, Multiple Imputation by Chained Equations (MICE) [36], conditional Distribution-based Imputation of Missing Values with Regularization (DIMV) [37], missForest [29], and SOFT-IMPUTE [40]. These methods are implemented with default settings using the *fancyimpute*<sup>2</sup>, *scikit-learn* [48], and *DIMV Imputation* packages<sup>3</sup>.

We used the following data sets sourced from the Machine Learning Database Repository at the University of California, Irvine<sup>4</sup>. Detailed descriptions of the datasets are provided in Table 1.

Dataset	#Features	#Samples
California	9	20,640
Diabetes	8	768

Table 1: Descriptions of datasets used in the experiments

We simulate missing values by randomly generating the ratio of missing entries to total entries in the features, with missing rates ranging from 20% to 80% in 20% increments. The experiments are run on a Windows-based machine equipped with an AMD Ryzen 7 3700X 8-Core Processor running at 3.59 GHz, 16 GB of RAM, and a 64-bit operating system. Each experiment is repeated ten times, and then the results are averaged. The codes for the experiments are available at <https://github.com/simulamet-host/SHAP>.

### 5.2. Global feature importance plot

We present the Global Feature Importance plots across various missing rates for the California dataset in Figures 1, 2, 3 and 4, while the plots for the diabetes dataset are included in Appendix A. However, the key points

---

<sup>2</sup><https://github.com/iskandr/fancyimpute>

<sup>3</sup><https://github.com/maianhpuco/DIMVImputation>

<sup>4</sup><http://archive.ics.uci.edu/ml>

in the following inference on the California datasets can also be seen in the diabetes dataset.

Regardless of the missing rates, the global feature importance consistently highlights three main predictors of housing prices: Latitude, Longitude, and Median Income (MedInc). However, their orders seem to change compared to the plot on the original data. For example, at a missing rate of 0.2, the plot on the original data highlights Latitude the most, then Longitude, and then MedInc. However, all the remaining methods highlight MedInc the most.

Interestingly, across all missing rates, Xgboost produces the plots that deviate the most from the ground truth for the MedInc, Latitude, and Longitude features. Specifically, for the XGBoost model, besides presenting high mean absolute Shapley values for these three features with a range of (+0.28) to (+0.66), an interesting difference is observed where MedInc is recorded as more important than Latitude and Longitude, underscoring its critical role in predicting housing prices. Meanwhile, for the five imputation methods, those data have a similar distribution to the results on the original data but at lower, with a range of [+0.05; +0.22].

Additionally, the figures also show that when the missing rate increases from 20% to 40%, the Shapley values for these three comparison features generally decline, while XGBoost experiences an upward trend. The opposite pattern is seen when the missing rate rises to 60%. At the highest missing rate, there is a slight variation in these data, with an amplitude of about  $\pm 0.03$ .

### 5.3. Beeswarm plot analysis

#### 5.3.1. Beeswarm plot for the California datasets

The beeswarm plot for the California datasets at missing rates 0.2, 0.4, 0.6, and 0.8 are presented in Figures 5, 6, 7, 8, respectively. In these figures, we focus on three key features (Latitude, Longitude, and Median Income - MedInc) because the others show little impact.

XGBoost seems to be stable, MedInc consistently shows the highest Shapley values, ranging from (-0.5) to around (+1.5) across all missing rates, emphasizing its strong influence on the model outputs. The imputation methods show similar patterns with Shapley values for key features slightly reduced compared to the XGBoost model, but they still highlight the importance of Latitude, Longitude, and MedInc in the predictive modeling.

Considering the results at each missing rate, we observed similar distributions in the Shapley values for Latitude, Longitude, and MedInc on both the

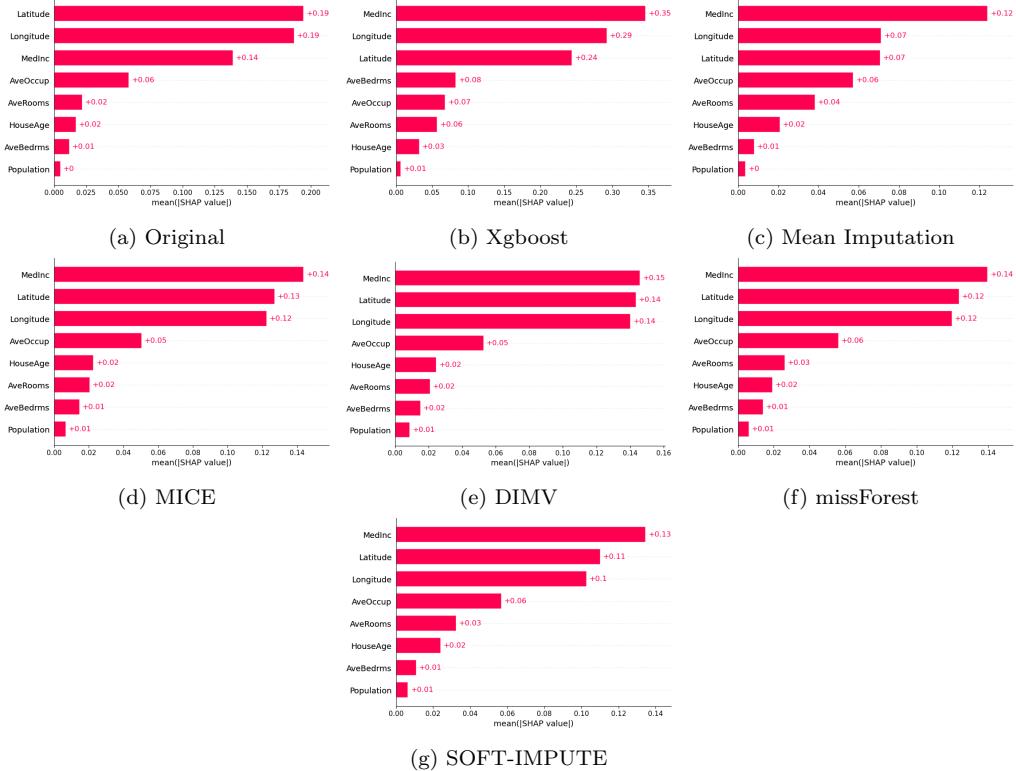


Figure 1: Global feature importance plot on the California dataset with the missing rate  $r = 0.2$

original and imputed data using various imputation methods, generally fluctuating around zero. However, XGBoost shows a distribution that is more skewed from zero. For example, at a missing rate of 20% in figure 5, the Shapley values in the original data for Latitude and Longitude range from  $(-0.75)$  to  $(+0.75)$ , and for MedInc from  $(-0.5)$  to  $(+0.7)$ . Likewise, the ranges for models with imputation methods are  $[-0.6; 0.6]$  and  $[-0.4; 0.6]$ , respectively, indicating that the imputation does not significantly alter the feature importance. Meanwhile, XGBoost displays a different distribution from  $(-1.0)$  to  $(+0.5)$  for Latitude and Longitude and a wider range from  $(-0.5)$  to  $(+1.5)$  for MedInc.

### 5.3.2. Beeswarm plot for the diabetes datasets

The beeswarm plot for the diabetes datasets at missing rates 0.2, 0.4, 0.6, and 0.8 are presented in Figures 9, 6, 11, 12, respectively. In these figures, the

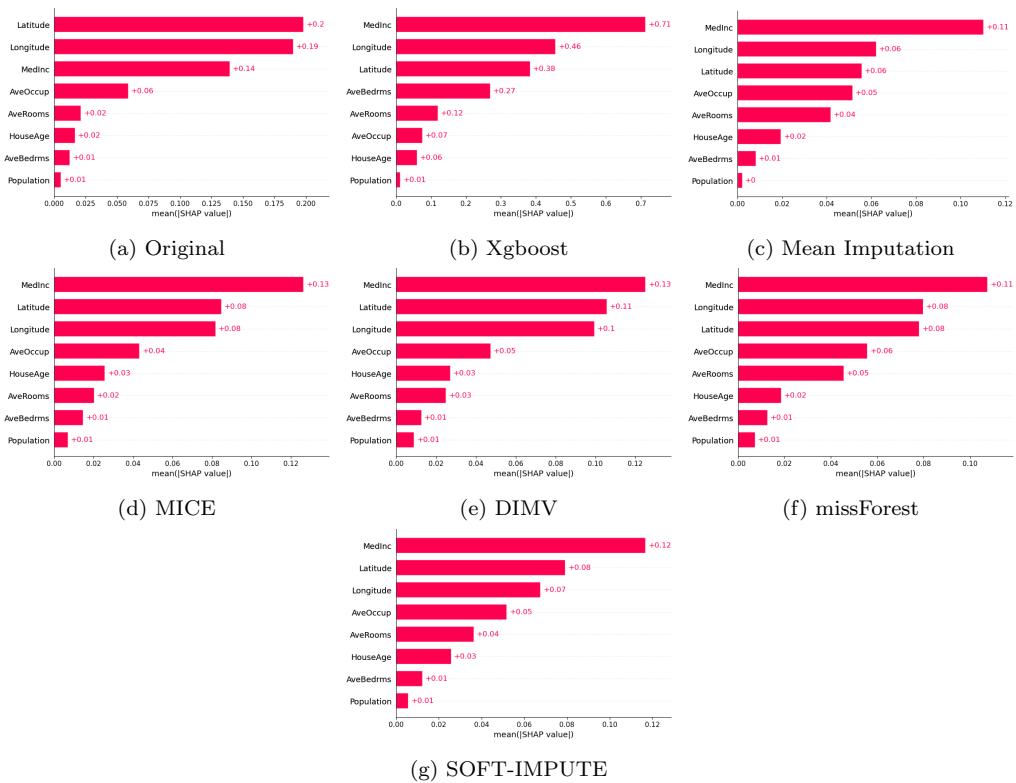


Figure 2: Global feature importance plot on the California dataset with the missing rate  $r = 0.4$

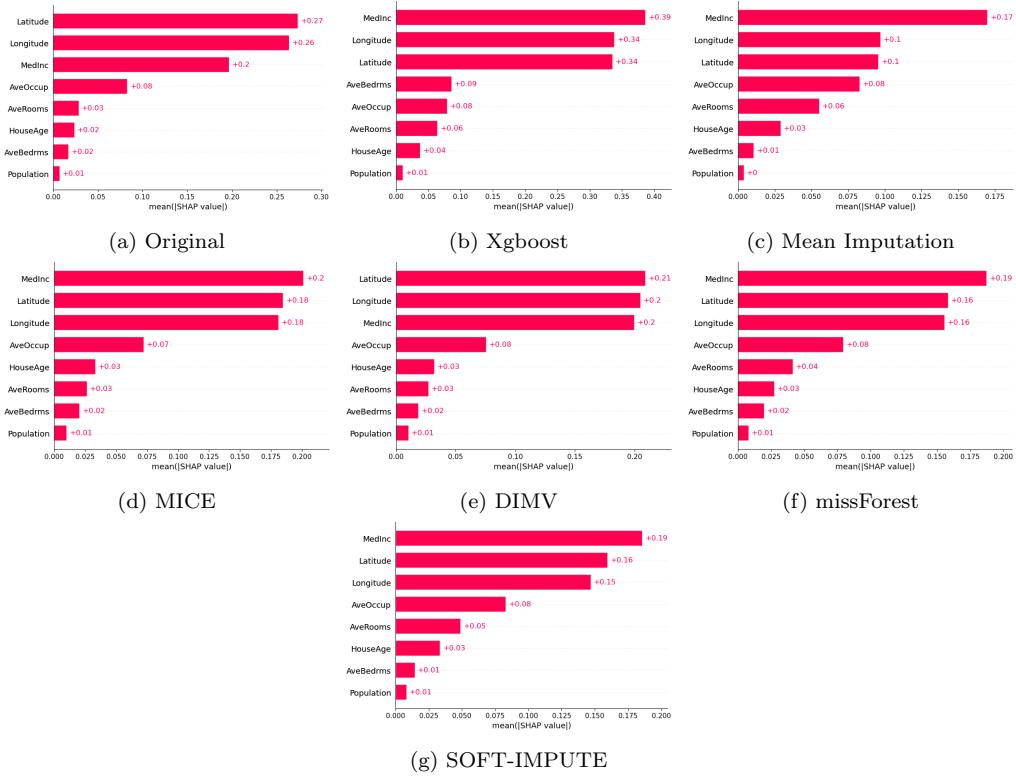


Figure 3: Global feature importance plot on the California dataset with the missing rate  $r = 0.6$

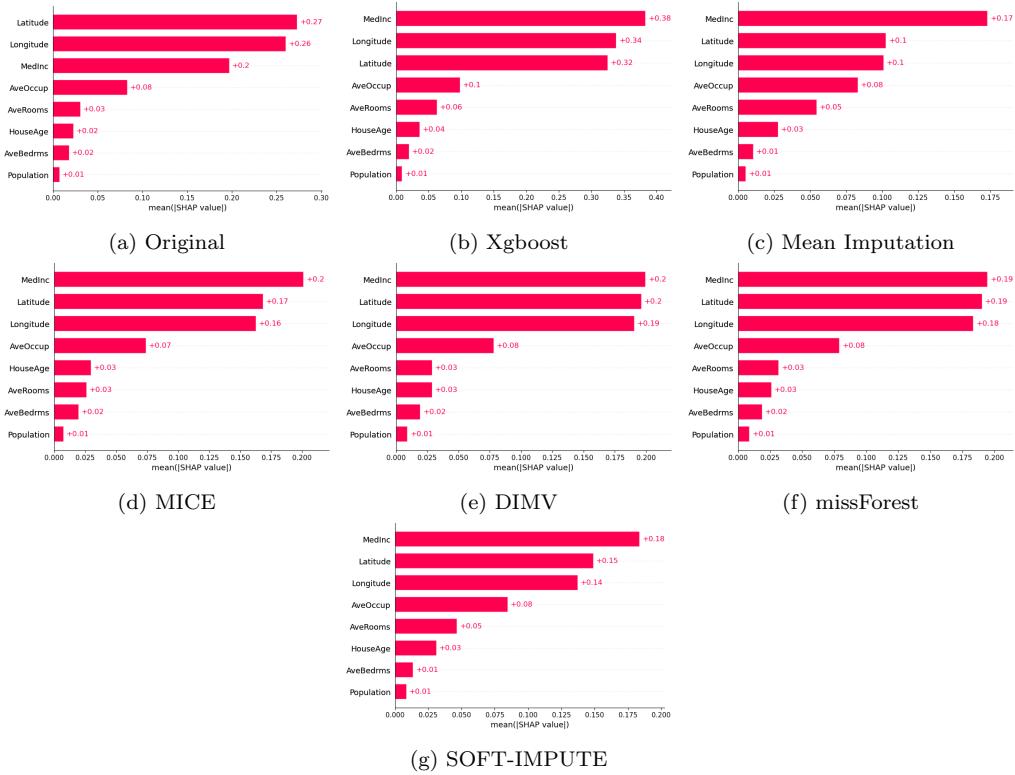


Figure 4: Global feature importance plot on the California dataset with the missing rate  $r = 0.8$

trend regarding the width of the Shapley values range is quite similar across the models, while reverse patterns can be observed in their distribution. When the missing rate increases, the range of Shapley values in the XGBoost model narrows down even though it starts with a width of approximately 0.9. Similarly, the range in the other models shows a slight reduction from about [-0.4; 0.4] at a 20% missing rate to [-0.2; 0.2] at the highest missing rate.

Regarding the distribution of Shapley values, across all missing rates, the original and imputed data with imputation methods exhibit a relatively uniform distribution around the zero value. In contrast, the XGBoost model shows an increasingly skewed distribution as the missing rate rises. Notably, when the missing rate increases from 40% onwards, the Shapley values for features such as “bmi,” “bp,” “s5,” “age,” and “s6” tend to be positive, while the values for other features are negative. Another difference is that the SHAP value for the feature “s4” mostly shows positive values but turns negative when the missing rate reaches 80%.

#### 5.4. MSE analysis

$r$	criteria	Xgboost	MI	MICE	DIMV	missForest	SOFT
0.2	MSE	0.116	0.136	0.124	0.124	<b>0.089</b>	0.139
	MSE Shap	0.184	0.092	0.035	<b>0.028</b>	0.037	0.049
0.4	MSE	0.447	0.473	0.514	0.503	<b>0.445</b>	0.497
	MSE Shap	0.746	0.244	0.166	<b>0.139</b>	0.177	0.196
0.6	MSE	0.114	0.133	0.122	0.125	<b>0.089</b>	0.137
	MSE Shap	0.183	0.098	0.033	<b>0.026</b>	0.044	0.049
0.8	MSE	0.115	0.132	0.124	0.123	<b>0.090</b>	0.139
	MSE Shap	0.160	0.091	0.039	<b>0.030</b>	0.031	0.054

Table 2: MSE on the test set and MSE of Shapley values on the California dataset. Here, MI denotes Mean Imputation, and SOFT denotes SOFT-IMPUTE. The bold indicates the best performance.

The performance of various imputation methods was evaluated for the California dataset with different data missing rates in Table 2, and for the diabetes dataset in Table 3. Recall that here, the MSE is the MSE of the true label and predicted values on the test set. Also, MSE Shap is the MSE between the Shapley values of predicted and true labels on the test set as well.

From Table 2, one can see that across all missing data rates, missForest consistently achieved the lowest MSE values, indicating superior performance in terms of imputation accuracy. Specifically, for  $r = 0.2$ , missForest achieved an MSE of 0.089, significantly lower than the second-best method, Xgboost, with an MSE of 0.116. For higher missing data rates ( $r = 0.4, 0.6, 0.8$ ), missForest maintained its leading position with MSE values of 0.445, 0.089, and 0.090, respectively, outperforming other methods such as MI, MICE, and DIMV.

Also in Table 2, we can see that in terms of MSE Shapley values, DIMV demonstrated the best performance, indicating its robustness in maintaining the interpretability of the imputed data. For  $r = 0.2$ , DIMV achieved an MSE Shap of 0.028, outperforming MICE (0.035) and missForest (0.037). This trend continued across all missing data rates, with DIMV recording the lowest MSE Shap values of 0.139, 0.026, and 0.030 for  $r = 0.4, 0.6$ , and 0.8, respectively. We, therefore, observe that there are different imputation methods that perform the best in terms of prediction performance and in terms of explainability, underscoring the importance of selecting appropriate imputation methods based on specific criteria in the context of missing data analysis.

$r$	criteria	Xgboost	MI	MICE	DIMV	missForest	SOFT
0.2	MSE	0.209	0.199	<b>0.169</b>	0.177	0.174	0.187
	MSE Shap	0.058	0.020	<b>0.015</b>	0.016	0.018	0.017
0.4	MSE	0.293	0.284	0.307	<b>0.280</b>	0.298	0.285
	MSE Shap	0.127	0.028	0.029	<b>0.026</b>	0.030	<b>0.026</b>
0.6	MSE	0.407	<b>0.399</b>	0.423	<b>0.399</b>	0.480	0.407
	MSE Shap	0.156	<b>0.038</b>	0.041	<b>0.038</b>	0.042	0.039
0.8	MSE	0.527	<b>0.509</b>	0.569	0.549	0.683	0.562
	MSE Shap	0.215	<b>0.047</b>	0.051	0.052	0.059	0.050

Table 3: MSE on the test set and MSE of Shapley values on the diabetes dataset. Here, MI denotes Mean Imputation, and SOFT denotes SOFT-IMPUTE. The bold indicates the best performance.

Focusing on the results with the diabetes dataset in Table 3, overall, both MSE and MSE Shap experience a significant increase when the missing rate increases. In particular, MICE, MI, and DIMV were generally the most effective methods across different missing data rates, with MICE excelling at lower rates and MI and DIMV showing strong performance at higher rates.

For  $r = 0.2$ , MICE achieved the lowest MSE of 0.169, indicating better imputation accuracy among the evaluated methods. MI followed with an MSE of 0.199, while Xgboost had the highest MSE at 0.209. In terms of MSE Shapley values, MICE again performed best with an MSE Shap of 0.015, slightly better than MI at 0.020. At  $r = 0.4$ , DIMV demonstrated the best performance with an MSE of 0.280, outperforming MI (0.284) and SOFT-IMPUTE (0.285). The MSE Shapley values revealed that DIMV and SOFT-IMPUTE both achieved the lowest values of 0.026. For  $r = 0.6$ , both MI and DIMV achieved the lowest MSE and MSE Shap of 0.399 and 0.038, respectively, highlighting their effectiveness in handling higher rates of missing data. After that, MI still outperformed other methods with MSE and MSE Shap of 0.509 and 0.047, respectively, as missing rates increased to the highest.

Interestingly, from both Table 2 and Table 3, one can see that a lower MSE may not imply a lower MSE Shap and vice versa. For example, in Table 3, at a missing rate of 0.4, the MSE of MICE is 0.307, which is higher than the MSE of missForest (0.298). However, the MSE Shap of MICE is 0.029, which is lower than of missForest (0.030).

## 6. Discussion

In summary, from the present results and the deep analysis in the previous section, we can observe several interesting key insights.

The global feature importance plots and the beeswarm plots clearly show that different imputation methods lead to varying Shapley value distributions. This shows that the choice of the imputation method can significantly affect the interpretability of the model.

Across different missing rates, XGBoost, without imputation, seems to have the most significant changes in the Shapley values. While Xgboost can train and predict directly on data with missing values, the MSE between Shapley values of XgBoost and the Original is the highest in most of the experiments, and even higher implementing XgBoost Regression after filling in missing values by mean imputation.

As the missing rate increases from 20% to 80% percent, the differences between the imputation methods become more pronounced. This indicates that the choice of the imputation method becomes increasingly critical as the number of missing data increases.

The results for the California and diabetes datasets show some differences, suggesting that the impact of imputation methods may be data set dependent. This highlights the importance of considering the characteristics of the data set when choosing an imputation method.

The MSE plots show that methods with lower imputation MSE do not necessarily preserve Shapley values better (as measured by Shapley MSE). This suggests a potential trade-off between the accuracy of the imputation and the maintenance of the original importance structure of the feature.

Mean imputation tends to significantly alter the importance of features, especially at higher missing rates. MICE and DIMV often show similar patterns, possibly due to the fact that MICE is based on regression and DIMV is based on a conditional Gaussian formula. MissForest and SOFT-IMPUTE sometimes preserve feature rankings better than simpler methods, but this is not consistent across all scenarios.

The variability in results between methods and missing rates underscores the need to evaluate imputation effects when using Shapley values for model interpretation.

The following discussion is structured around our result and the specific pitfalls that may arise due to incomplete understanding of the relationship between missing data, imputation methods, and Shapley values. We high-

light how different approaches can lead to vastly different interpretations, how dataset characteristics and missing rates affect results, and the importance of considering both imputation accuracy and interpretability preservation.

**Pitfall 1: Assume the neutrality of the imputation method.** Our study reveals that different imputation methods can significantly alter Shapley values and, consequently, the interpretability of the model. For instance, mean imputation tends to distort feature importances, especially at higher missing rates, while methods like MICE and DIMV often show similar patterns. This underscores the importance of carefully considering the imputation method when using Shapley values for model explanation, as the choice can lead to vastly different interpretations of feature importance.

**Pitfall 2: Overlooking data set dependency.** We observed that the effects of imputation methods on Shapley values vary between data sets. For example, the California and diabetes datasets showed different patterns of importance of characteristics in different imputation methods. This highlights that dataset characteristics play a crucial role in determining the best imputation approach, and warns against applying a one-size-fits-all solution across different datasets.

**Pitfall 3: Ignoring the impact of missing rate.** Our results demonstrate that the impact of the choice of the imputation method becomes more pronounced as the missing rate increases. At lower missing rates, differences between methods are less stark, but as missing data increases, the choice of the imputation method becomes increasingly critical. This emphasizes the need for more careful consideration of imputation techniques when dealing with data sets with substantial missing data. In addition, a method may perform better than another one at low missing rates but perform worse than another one at high missing rates.

**Pitfall 4: Focussing solely on imputation accuracy.** We found a potential trade-off between the precision of the imputation and the preservation of the Shapley value. Methods that provide more accurate imputations do not necessarily better preserve the original Shapley values. This highlights a potential conflict between optimizing for prediction accuracy and maintaining interpretability and suggests that practitioners should consider both aspects when selecting an imputation method.

These pitfalls underscore the complex interaction between missing data handling, imputation methods, and model interpretability using Shapley values. Our findings highlight that there is no universal solution for handling missing data while preserving the interpretability of the model. Instead, the

choice of method should be context-dependent, considering factors such as data set characteristics, missing data rates, and the specific requirements of the analysis. Moreover, our results emphasize the need for a holistic approach that balances imputation accuracy with the preservation of feature-importance structures. As machine learning models continue to be applied in critical domains, understanding and addressing these pitfalls becomes important to ensuring reliable and interpretable results.

## 7. Conclusion

In this paper, we explore the impact of various imputation methods on the calculation of Shapley values for model interpretability. Our findings indicate that the choice of the imputation strategy can significantly influence the accuracy and reliability of Shapley values, thereby affecting the insights drawn from the machine learning models.

Our comparative analysis revealed that the chosen imputation method should align with the specific characteristics of the data set and the objectives of the analysis. Practitioners should carefully consider the trade-offs between computational efficiency and the potential for bias introduction when selecting an imputation method. The study underscores the necessity of evaluating the effects of imputation as a critical step in the preprocessing pipeline, especially when Shapley values are used for model interpretation.

Future work should focus on extending this analysis to a broader range of datasets and machine learning models to further validate our findings. In addition, the development of new imputation methods is tailored for specific types of data, model structures, and explainability, especially in relation to Shapley value interpretations. Also, more research needs to be done on the direction of handling missing data directly, as this helps to avoid noises and bias introduced to the model by imputation. By addressing these challenges, we can improve the reliability of model interpretations and support more informed decision-making in the application of machine learning.

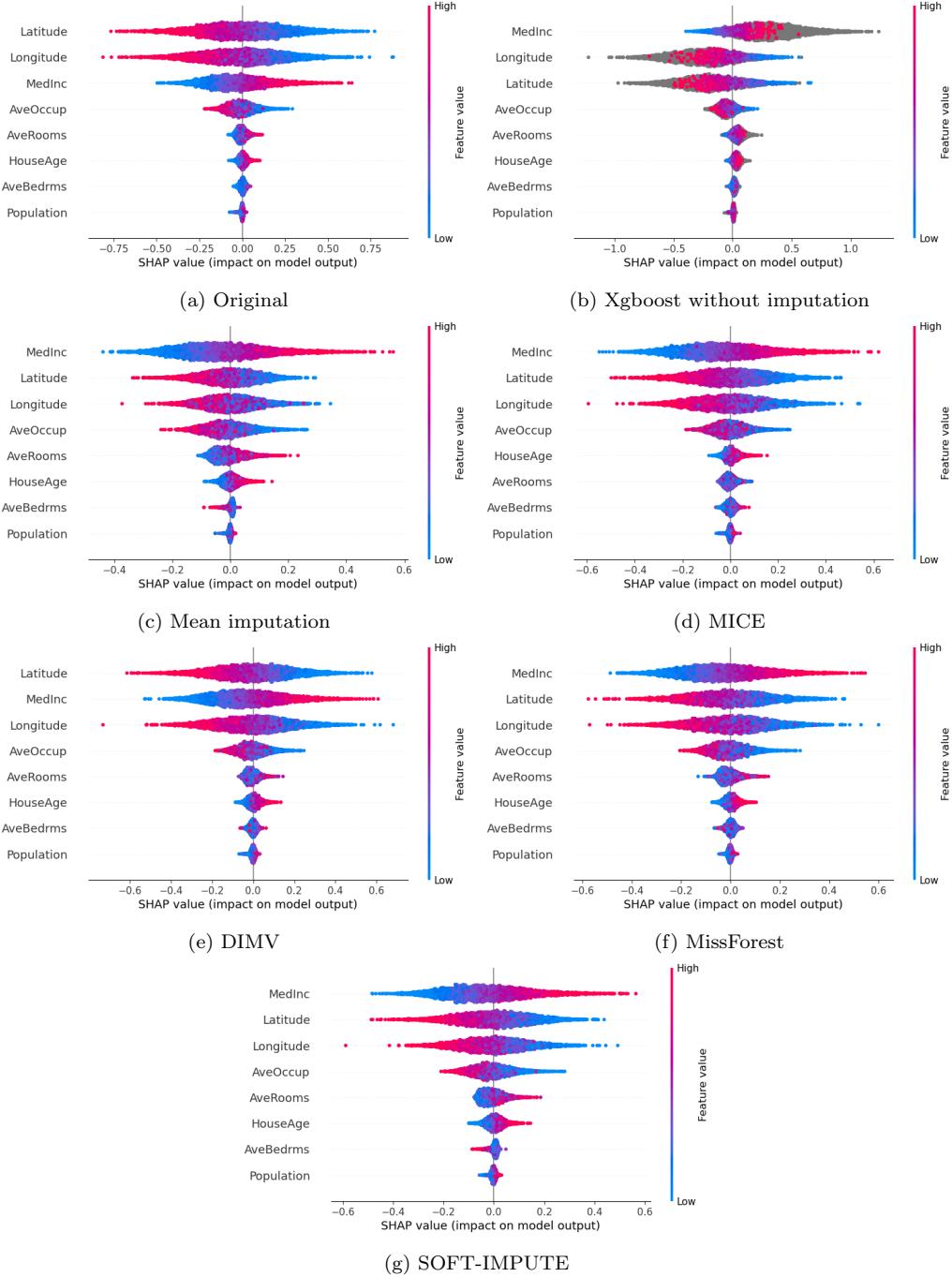


Figure 5: Beeswarm plots for the California dataset at missing rate  $r = 0.2$

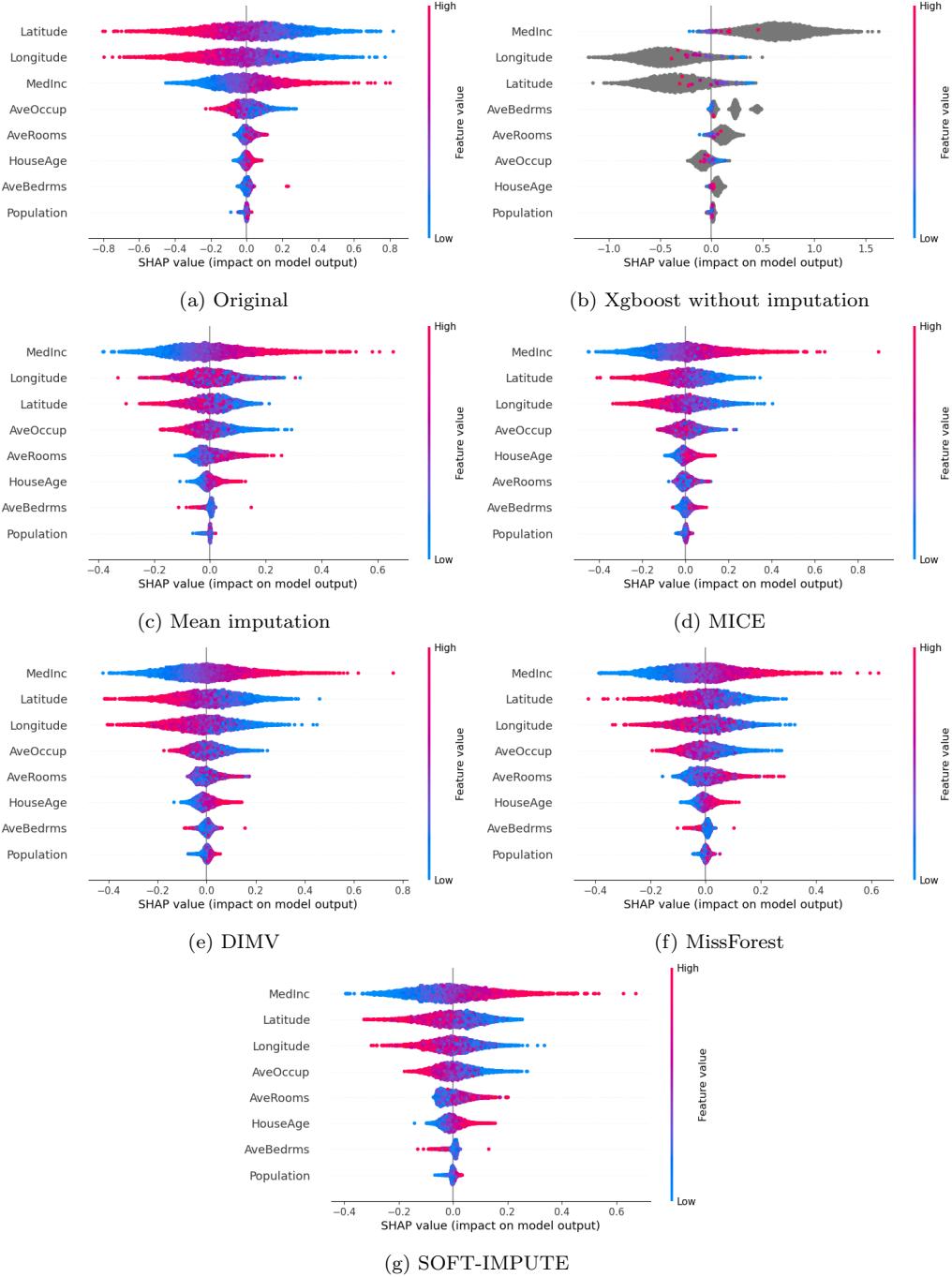


Figure 6: Beeswarm plots for the California dataset at missing rate  $r = 0.4$

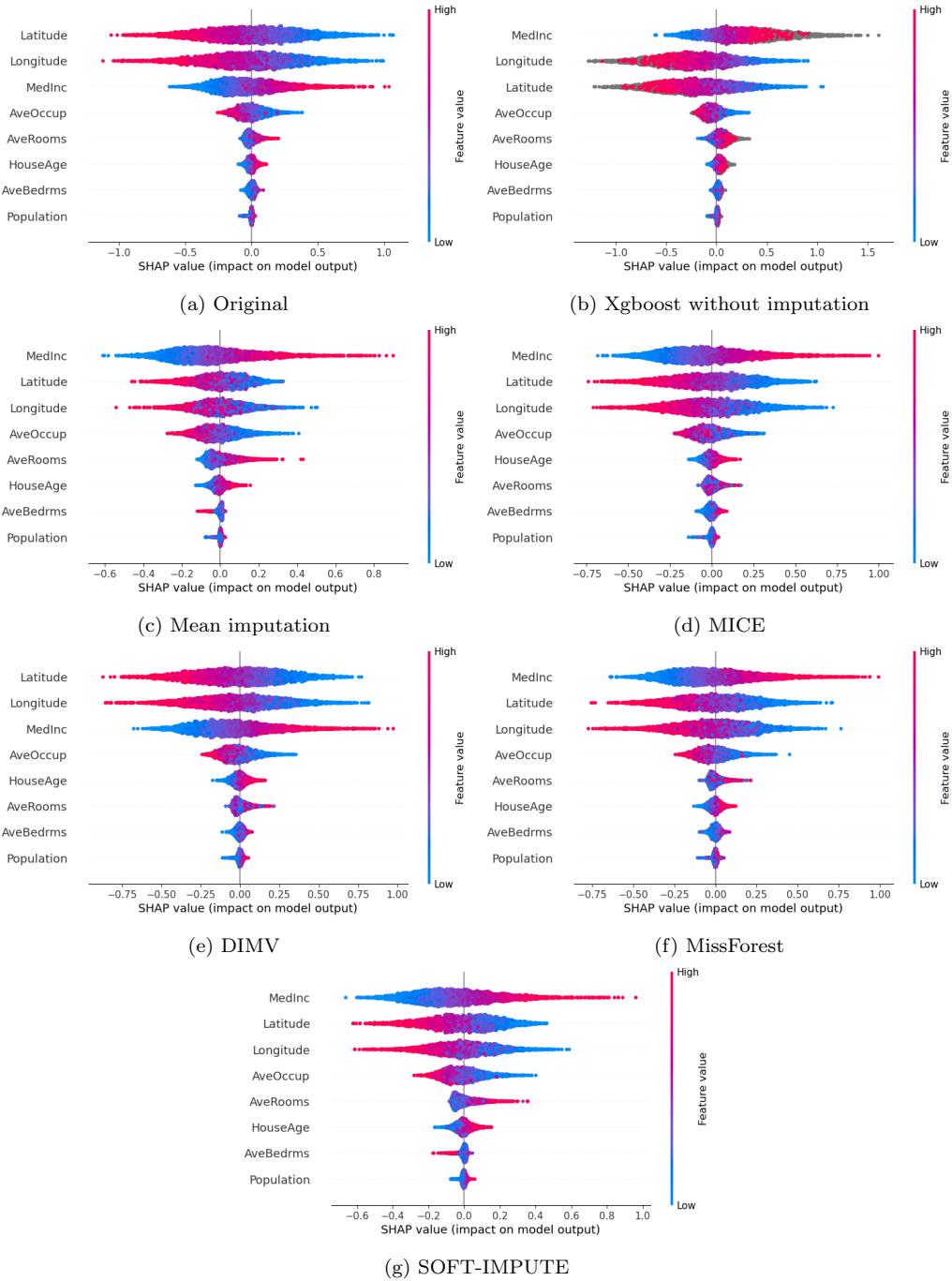


Figure 7: Beeswarm plots for the California dataset at missing rate  $r = 0.6$

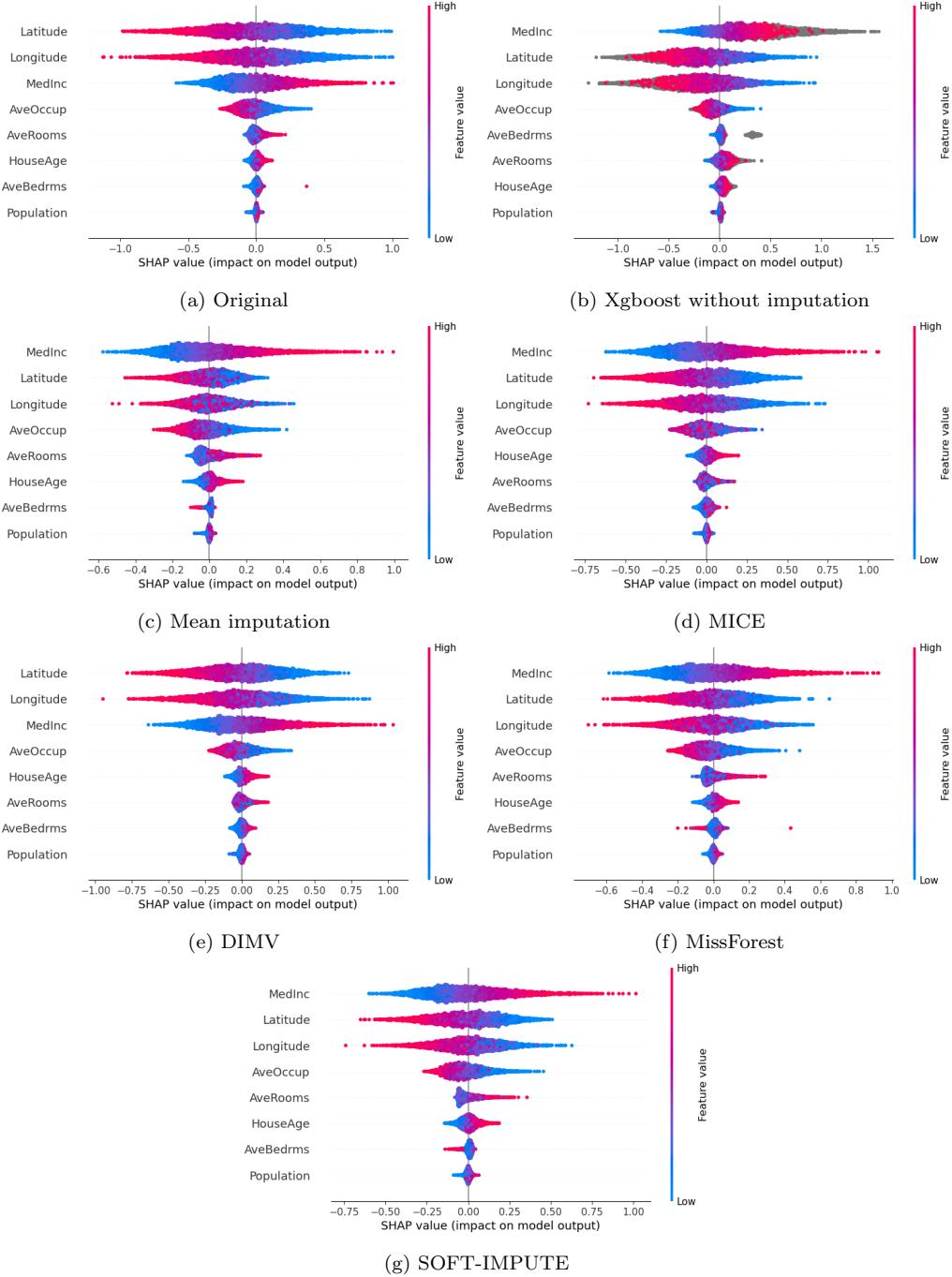


Figure 8: Beeswarm plots for the California dataset at missing rate  $r = 0.8$

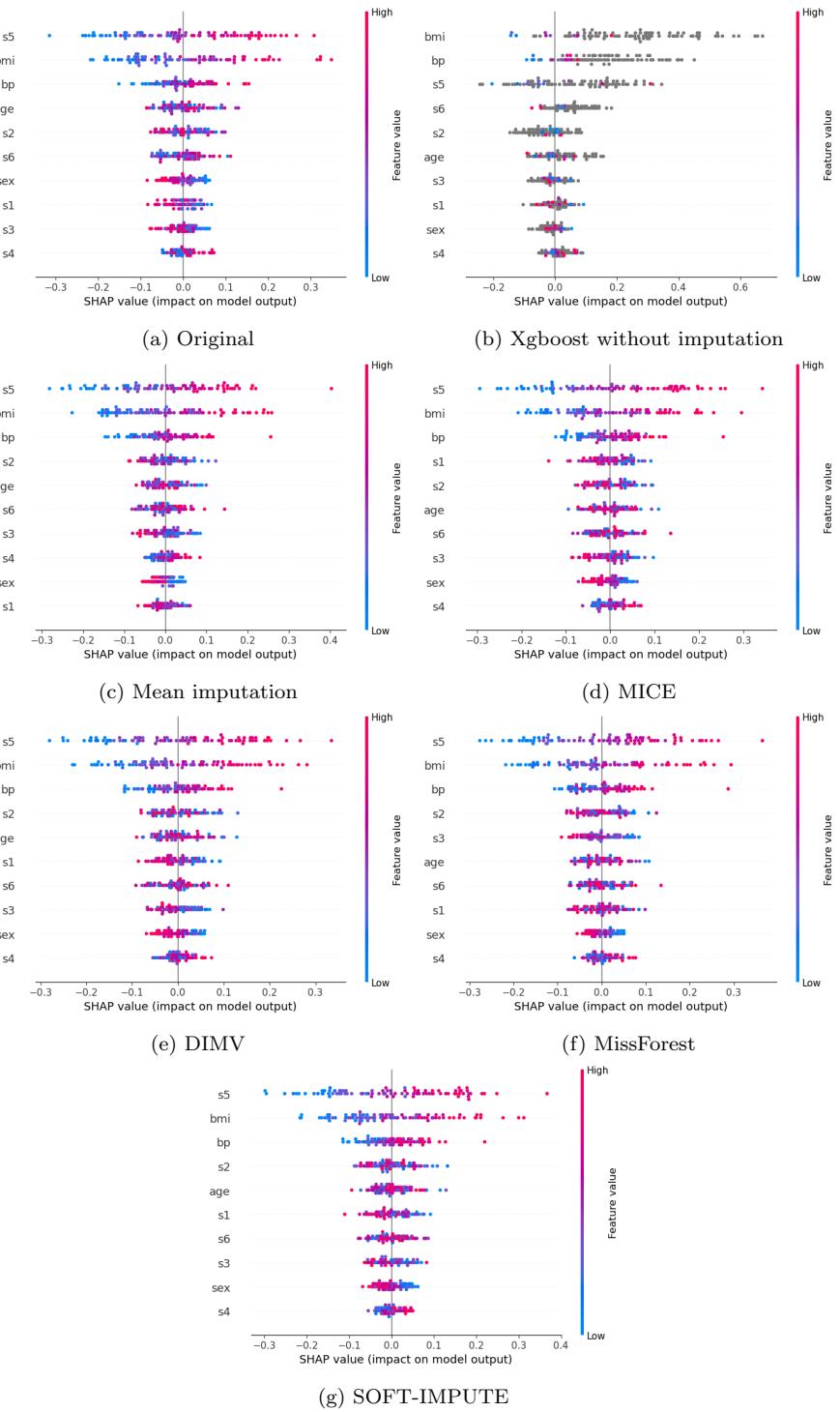


Figure 9: Beeswarm plots for the diabetes dataset at missing rate  $r = 0.2$

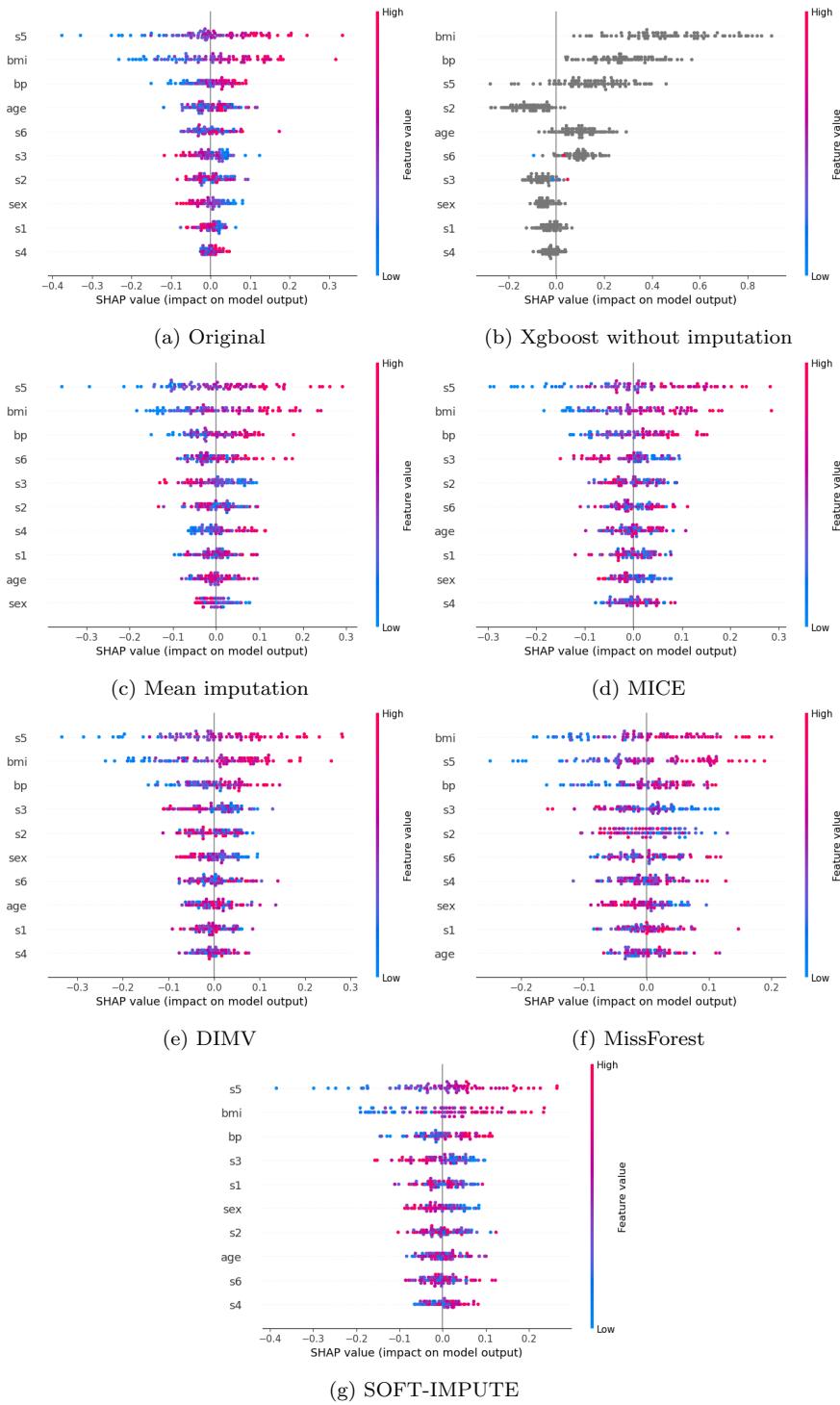


Figure 10: Beeswarm plots for the diabetes dataset at missing rate  $r = 0.4$

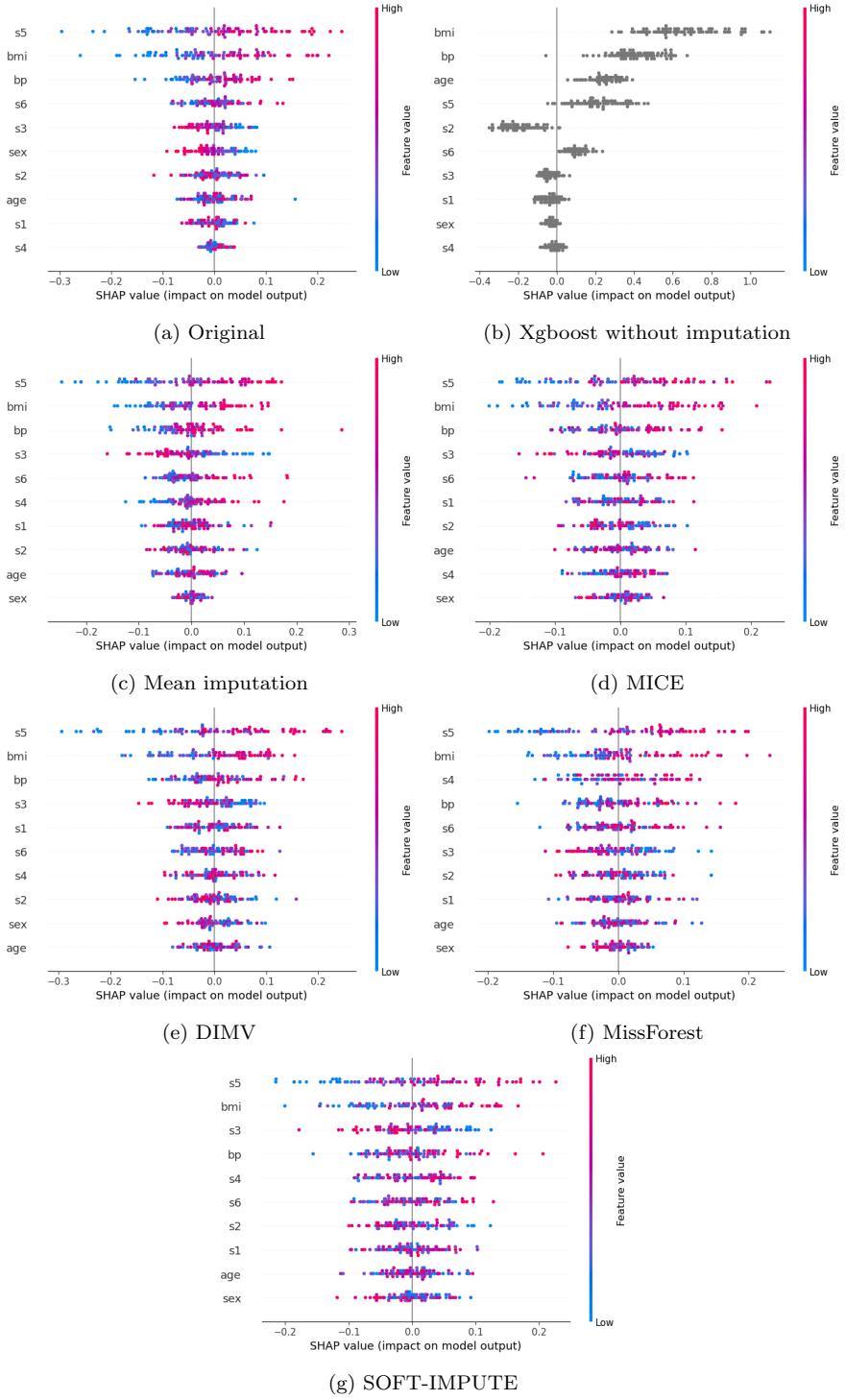


Figure 11: Beeswarm plots for the diabetes dataset at missing rate  $r = 0.6$

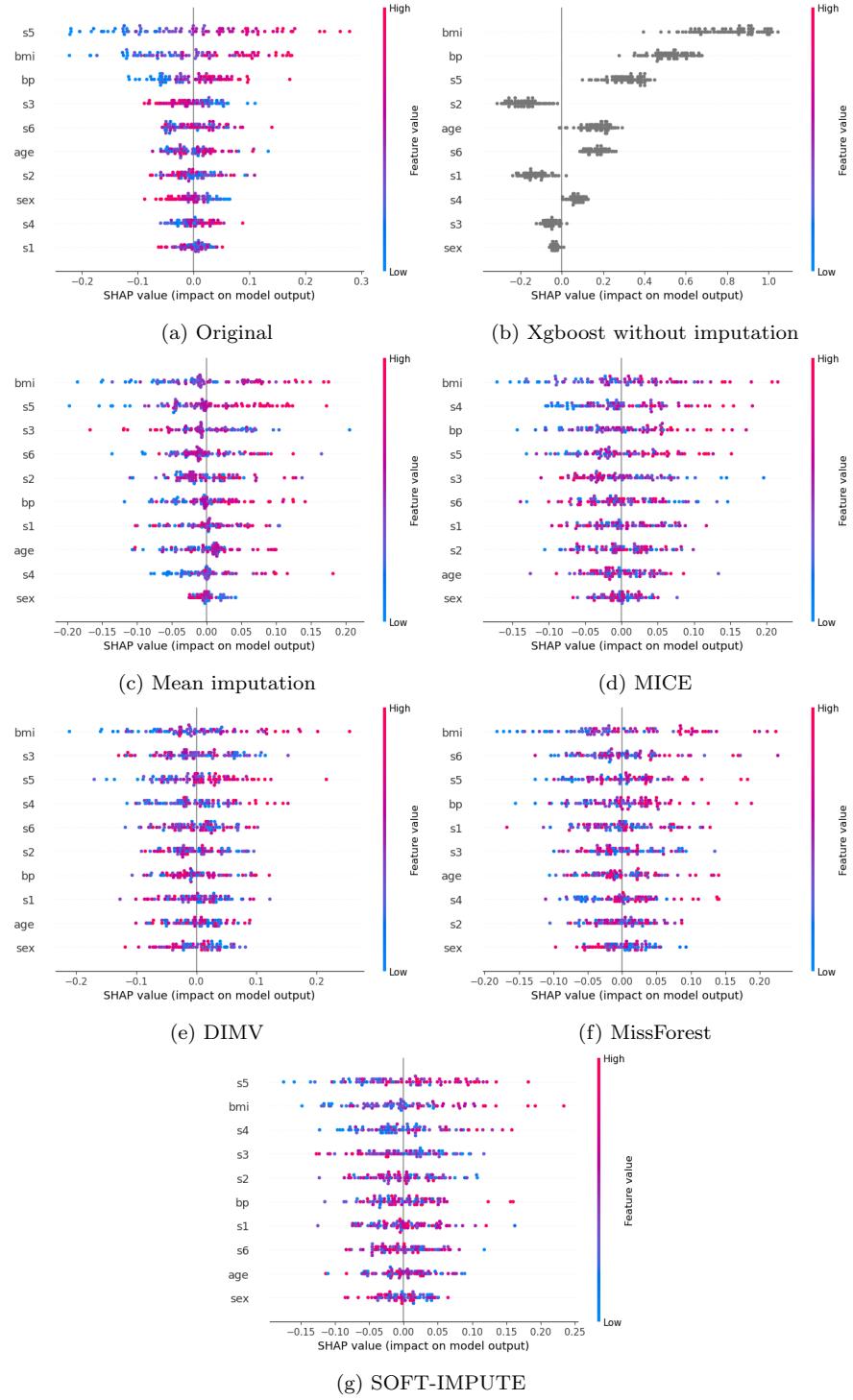


Figure 12: Beeswarm plots for the diabetes dataset at missing rate  $r = 0.8$

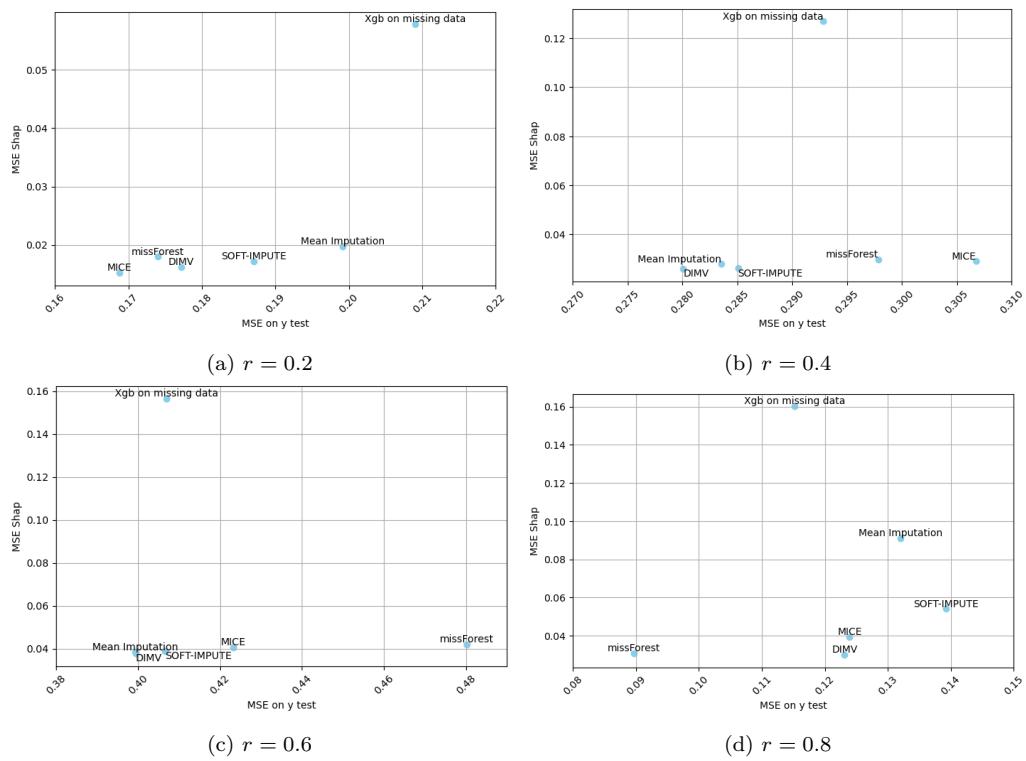


Figure 13: MSE versus Shapley MSE plots on the diabetes dataset

## References

- [1] N.-H. Pham, K.-L. Vo, M. A. Vu, T. Nguyen, M. A. Riegler, P. Halvorsen, B. T. Nguyen, Correlation visualization under missing values: a comparison between imputation and direct parameter estimation methods, in: International Conference on Multimedia Modeling, Springer, 2024, pp. 103–116.
- [2] C. Molnar, Interpretable Machine Learning, 2 ed., 2022. URL: <https://christophm.github.io/interpretable-ml-book>.
- [3] S. Lipovetsky, E. Nowakowska, Modeling with structurally missing data by ols and shapley value regressions, International Journal of Operations and Quantitative Management 19 (2013) 169–178.
- [4] J. R. Quinlan, Induction of decision trees, Machine learning 1 (1986) 81–106.
- [5] M. Kuhn, K. Johnson, M. Kuhn, K. Johnson, Classification trees and rule-based models, Applied predictive modeling (2013) 369–413.
- [6] T. Hastie, R. Tibshirani, J. H. Friedman, J. H. Friedman, The elements of statistical learning: data mining, inference, and prediction, volume 2, Springer, 2009.
- [7] T. J. Hastie, Generalized additive models, in: Statistical models in S, Routledge, 2017, pp. 249–307.
- [8] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, I. Polosukhin, Attention is all you need, Advances in neural information processing systems 30 (2017).
- [9] S. M. Lundberg, S.-I. Lee, A unified approach to interpreting model predictions, Advances in neural information processing systems 30 (2017).
- [10] M. Sundararajan, A. Taly, Q. Yan, Axiomatic attribution for deep networks, in: International conference on machine learning, PMLR, 2017, pp. 3319–3328.
- [11] M. T. Ribeiro, S. Singh, C. Guestrin, ” why should i trust you?” explaining the predictions of any classifier, in: Proceedings of the 22nd

ACM SIGKDD international conference on knowledge discovery and data mining, 2016, pp. 1135–1144.

- [12] D. Fryer, I. Strümke, H. Nguyen, Shapley values for feature selection: The good, the bad, and the axioms, *Ieee Access* 9 (2021) 144352–144360.
- [13] D. Watson, Rational shapley values, in: *Proceedings of the 2022 ACM Conference on Fairness, Accountability, and Transparency*, 2022, pp. 1083–1094.
- [14] A. Heuillet, F. Couthouis, N. Díaz-Rodríguez, Collective explainable ai: Explaining cooperative strategies and agent contribution in multiagent reinforcement learning with shapley values, *IEEE Computational Intelligence Magazine* 17 (2022) 59–71.
- [15] A. M. Storås, F. Fineide, M. Magnø, B. Thiede, X. Chen, I. Strümke, P. Halvorsen, H. Galtung, J. L. Jensen, T. P. Utheim, et al., Using machine learning model explanations to identify proteins related to severity of meibomian gland dysfunction, *Scientific Reports* 13 (2023) 22946.
- [16] A. M. Storås, I. Strümke, M. A. Riegler, P. Halvorsen, Explainability methods for machine learning systems for multimodal medical datasets: research proposal, in: *Proceedings of the 13th ACM Multimedia Systems Conference*, 2022, pp. 347–351.
- [17] T. Nguyen, A. M. Storås, V. Thambawita, S. A. Hicks, P. Halvorsen, M. A. Riegler, Multimedia datasets: challenges and future possibilities, in: *International Conference on Multimedia Modeling*, Springer, 2023, pp. 711–717.
- [18] B. Jafrasteh, D. Hernández-Lobato, S. P. Lubián-López, I. Benavente-Fernández, Gaussian processes for missing value imputation, *Knowledge-Based Systems* 273 (2023) 110603.
- [19] J. Fan, Y. Zhang, M. Udell, Polynomial matrix completion for missing data imputation and transductive learning, in: *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, (2020), pp. 3842–3849.
- [20] T. Hastie, R. Mazumder, J. D. Lee, R. Zadeh, Matrix completion and low-rank svd via fast alternating least squares, *The Journal of Machine Learning Research* 16 (2015) 3367–3402.

- [21] E. J. Candès, B. Recht, Exact matrix completion via convex optimization, *Foundations of Computational mathematics* 9 (2009) 717.
- [22] S. M Mostafa, A. S Eladimy, S. Hamad, H. Amano, Cbrl and cbrc: Novel algorithms for improving missing value imputation accuracy based on bayesian ridge regression, *Symmetry* 12 (2020) 1594.
- [23] P. Keerin, W. Kurutach, T. Boongoen, An improvement of missing value imputation in dna microarray data using cluster-based lls method, in: 2013 13th International Symposium on Communications and Information Technologies (ISCIT), IEEE, 2013, pp. 559–564.
- [24] S. J. Choudhury, N. R. Pal, Imputation of missing data with neural networks for classification, *Knowledge-Based Systems* 182 (2019) 104838.
- [25] A. Garg, D. Naryani, G. Aggarwal, S. Aggarwal, Dl-gsa: a deep learning metaheuristic approach to missing data imputation, in: International Conference on Sensing and Imaging, Springer, (2018), pp. 513–521.
- [26] K. Mohan, J. Pearl, Graphical models for processing missing data, *Journal of the American Statistical Association* (2021) 1–42.
- [27] V. Audigier, F. Husson, J. Josse, Multiple imputation for continuous variables using a bayesian principal component analysis, *Journal of statistical computation and simulation* 86 (2016) 2140–2156.
- [28] L. Gondara, K. Wang, Multiple imputation using deep denoising autoencoders, arXiv preprint arXiv:1705.02737 (2017).
- [29] D. J. Stekhoven, P. Bühlmann, Missforest-non-parametric missing value imputation for mixed-type data, *Bioinformatics* 28 (2012) 112–118.
- [30] M. G. Rahman, M. Z. Islam, Missing value imputation using decision trees and decision forests by splitting and merging records: Two novel techniques, *Knowledge-Based Systems* 53 (2013) 51–65.
- [31] S. Nikfalazar, C.-H. Yeh, S. Bedingfield, H. A. Khorshidi, Missing data imputation using decision trees and fuzzy clustering with iterative learning, *Knowledge and Information Systems* 62 (2020) 2419–2437.
- [32] S. I. Khan, A. S. M. L. Hoque, Sice: an improved missing data imputation technique, *Journal of big data* 7 (2020) 1–21.

- [33] M. G. Rahman, M. Z. Islam, Missing value imputation using a fuzzy clustering-based em approach, *Knowledge and Information Systems* 46 (2016) 389–422.
- [34] J. S. Murray, J. P. Reiter, Multiple imputation of missing categorical and continuous values via bayesian mixture models with local dependence, *Journal of the American Statistical Association* 111 (2016) 1466–1479.
- [35] T. Nguyen, D. H. Nguyen, H. Nguyen, B. T. Nguyen, B. A. Wade, Epem: Efficient parameter estimation for multiple class monotone missing data, *Information Sciences* 567 (2021) 1–22.
- [36] S. v. Buuren, K. Groothuis-Oudshoorn, mice: Multivariate imputation by chained equations in r, *Journal of statistical software* (2010) 1–68.
- [37] M. A. Vu, T. Nguyen, T. T. Do, N. Phan, P. Halvorsen, M. A. Riegler, B. T. Nguyen, Conditional expectation for missing data imputation, arXiv preprint arXiv:2302.00911 (2023).
- [38] S. Hans, D. Saha, A. Aggarwal, Explainable data imputation using constraints, in: Proceedings of the 6th Joint International Conference on Data Science & Management of Data (10th ACM IKDD CODS and 28th COMAD), 2023, pp. 128–132.
- [39] T. Nguyen, K. M. Nguyen-Duy, D. H. M. Nguyen, B. T. Nguyen, B. A. Wade, Dper: Direct parameter estimation for randomly missing data, *Knowledge-Based Systems* 240 (2022) 108082.
- [40] R. Mazumder, T. Hastie, R. Tibshirani, Spectral regularization algorithms for learning large incomplete matrices, *Journal of machine learning research* 11 (2010) 2287–2322.
- [41] J. Yoon, J. Jordon, M. van der Schaar, GAIN: missing data imputation using generative adversarial nets, CoRR abs/1806.02920 (2018). URL: <http://arxiv.org/abs/1806.02920>. arXiv:1806.02920.
- [42] I. Spinelli, S. Scardapane, A. Uncini, Missing data imputation with adversarially-trained graph convolutional networks, *Neural Networks* 129 (2020) 249–260.

- [43] S. Hochreiter, J. Schmidhuber, Long short-term memory, *Neural computation* 9 (1997) 1735–1780.
- [44] M. M. Ghazi, M. Nielsen, A. Pai, M. J. Cardoso, M. Modat, S. Ourselin, L. Sørensen, Robust training of recurrent neural networks to handle missing data for disease progression modeling, arXiv preprint arXiv:1808.05500 (2018).
- [45] J. Li, J. Reisner, H. Pham, S. Olafsson, S. Vardeman, Biclustering with missing data, *Information Sciences* 510 (2020) 304–316.
- [46] L. S. Shapley, A value for n-person games, in: H. W. Kuhn, A. W. Tucker (Eds.), *Contributions to the Theory of Games II*, Princeton University Press, Princeton, 1953, pp. 307–317.
- [47] T. Chen, C. Guestrin, Xgboost: A scalable tree boosting system, in: *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining*, 2016, pp. 785–794.
- [48] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, E. Duchesnay, Scikit-learn: Machine learning in Python, *Journal of Machine Learning Research* 12 (2011) 2825–2830.

## Appendix A. Global feature importance plots on the diabetes dataset

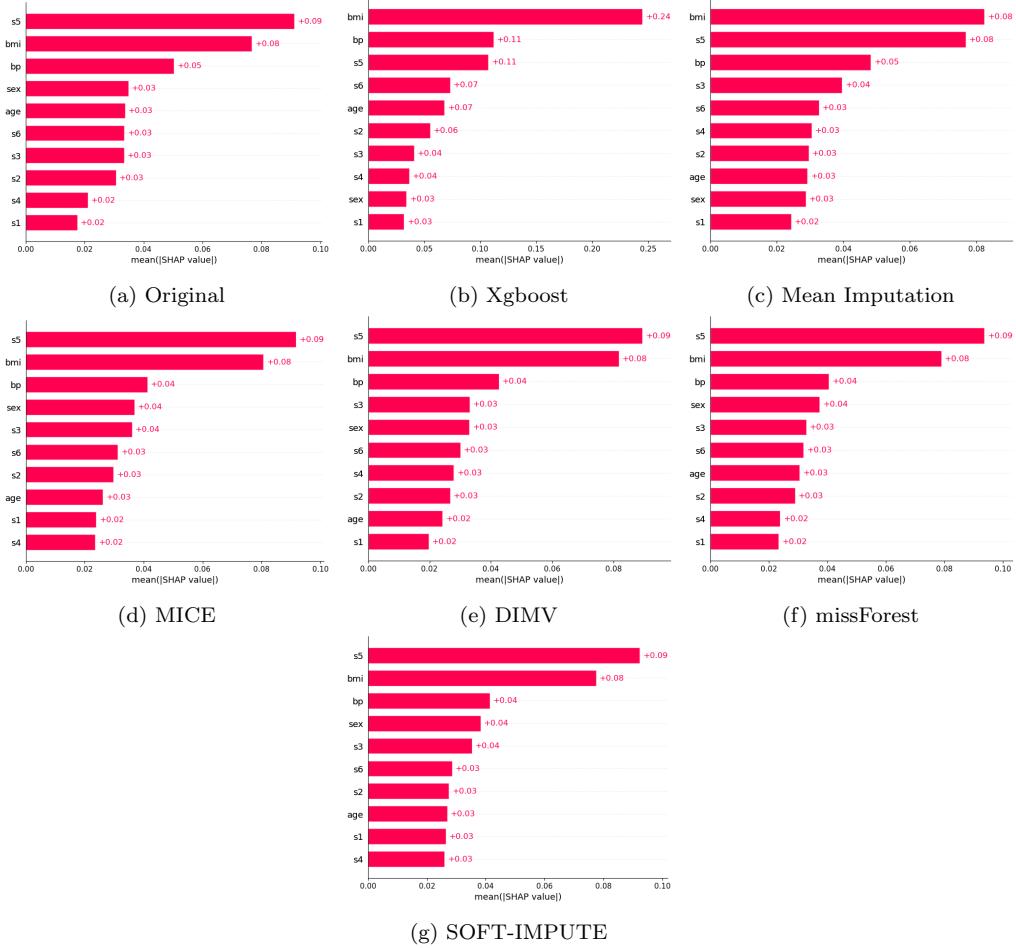


Figure A.14: Global feature importance plot on the diabetes dataset with the missing rate  $r = 0.2$

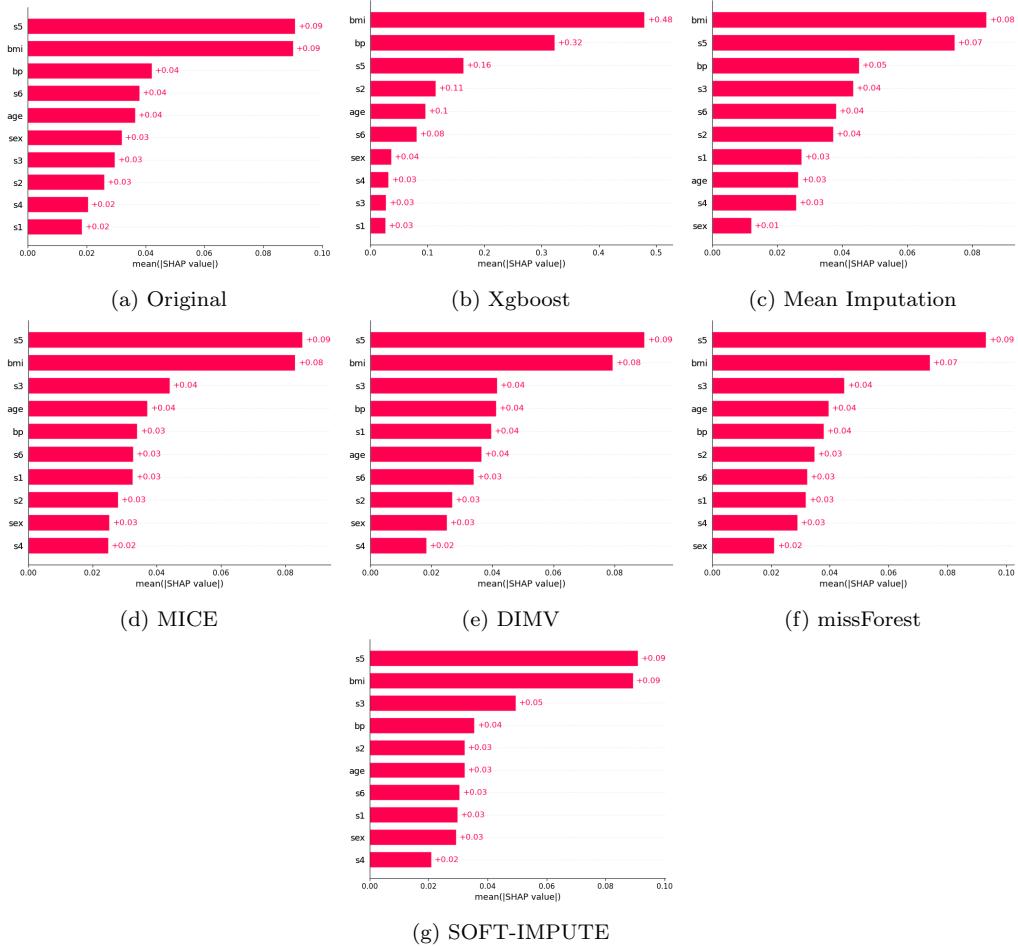


Figure A.15: Global feature importance plot on the diabetes dataset with the missing rate  $r = 0.4$

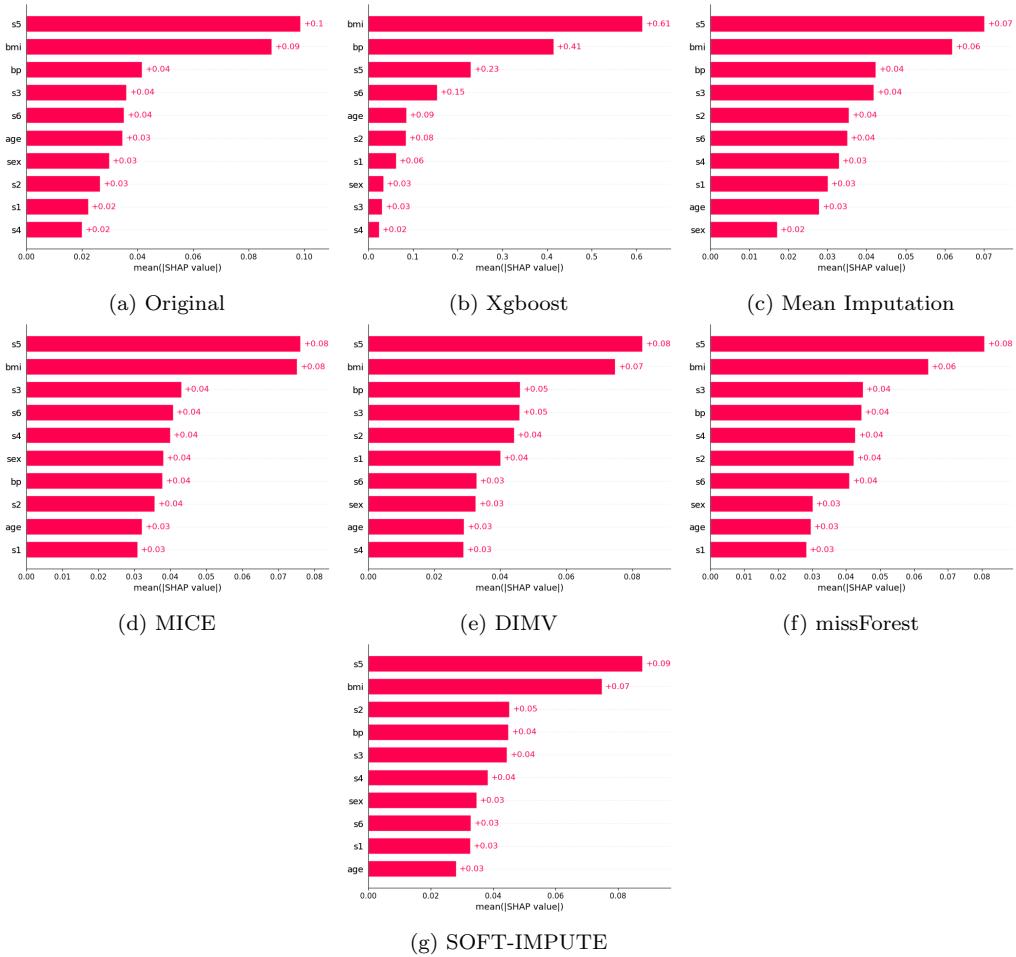


Figure A.16: Global feature importance plot on the diabetes dataset with the missing rate  $r = 0.6$

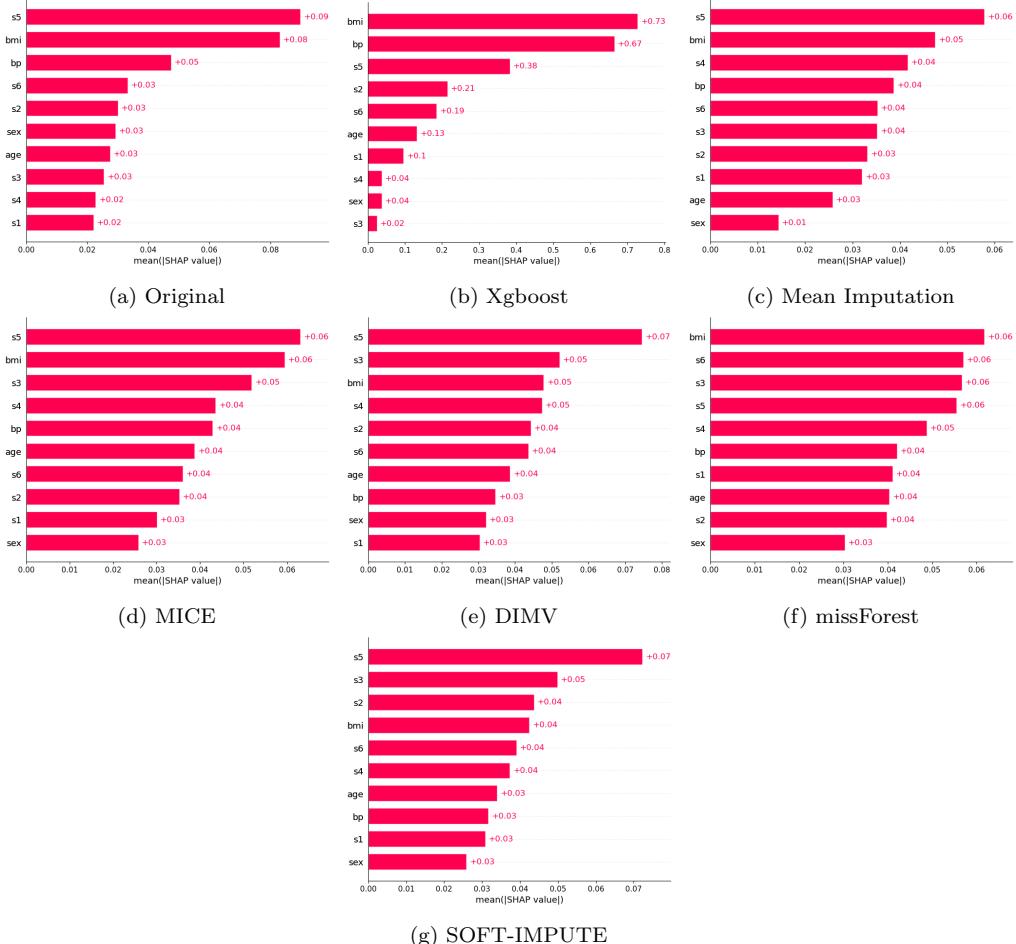


Figure A.17: Global feature importance plot on the diabetes dataset with the missing rate  $r = 0.8$