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COMPARING MISSING DATA IMPUTATION METHODS FOR SUPERVISED CLASSIFICATION

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Abstract: This paper compares methods for imputing missing categorical data for classification tasks using random forests, decision trees and neural networks. Researchers analyzing survey data typically choose decision trees or random forests for classification tasks, largely because these models, unlike neural networks and others, do not require imputing missing data nor encoding categorical variables. We start by investigating techniques for missing categorical data imputation and categorical data encoding. We experiment on two benchmark datasets with missing categorical data, comparing a neural network with decision trees and random forests classifiers trained on data imputed with different techniques and various levels of perturbation. We beat the state-of-the-art test error on both datasets and conclude from the results that the performance of the classifiers and imputation strategies generally depend on the nature and proportion of missing data.

Key words and phrases: missing data, survey data, imputation methods, neural networks, random forests, decision trees

1. Introduction

Missing data is a common problem in survey data in various domains, such as social science and marketing. Sources of missing data in surveys include nonresponse and attrition in longitudinal surveys. For supervised classification tasks, the objective is to fit a model on categorically labeled training data in order to categorize new examples. The ability of researchers to accurately fit a model model may be compromised by missing data, depending on the underlying missing data mechanism. In this paper, we focus on data that are nonmissing at random (NMAR), which occurs when the probability of an example having a missing value may depend on the missing data itself. There is an inherent nonidentifiability problem when the missing data mechanism is NMAR because we cannot observe the true value of missing data (Tsiatis, 2007). Item nonresponse in surveys is typically handled by imputation methods, which are used to estimate a value for missing data. However, imputation methods assume data missing at random (MAR), which occurs when the probability of missingness depends only on the observed data.

The objective of the present study is to compare the out-of-sample performance of three popular machine learning classifiers — decision trees, random forests, and neural networks — trained on either differently-imputed or

non-imputed survey datasets that contain various degrees of NMAR missing data. Decision trees and random forests are typically used for survey data because missing data must be pre-processed to be suited for models that require numerical input, such as neural networks. Imputation methods that assume data at MAR when the data is in fact NMAR can bias model estimates. The results of the study will provide guidance to applied researchers on how to handle missing data in survey datasets and which classifier to use.

This manuscript is organized as follows: Section 2 describes missing data mechanisms and describe methods imputing missing data; Section 3 describes our experiments on two benchmark datasets and discusses the results; Section 4 concludes and offers areas for future research.

2. Missing data and imputation methods

2.1. Missing data patterns and mechanisms

It is important to first distinguish between missing data patterns, which describe which values are observed and which are missing, and missing data mechanisms, which describe the the probability of missingness (Little and Rubin, 2014). Common missing data patterns in surveys typically include unit nonresponse, where a subset of participants do not complete the survey, and item nonresponse, where missing values are concentrated on particular

questions. In opinion polls, nonresponse may reflect either refusal to reveal a preference or lack of a preference.

It may be beneficial to impute missing values in situations where missing data hide values that are useful for classification tasks. Understanding the missing data mechanisms underlying patterns of missing data is crucial since properties of imputation methods depend on the nature of these mechanisms. Following the notation of Little and Rubin (2014), let $Y = y_{ij}$ be a $(n \times K)$ dataset with each example $y_i = (y_{i1}, \ldots, y_{ik})$ the set of y_{ij} values of feature Y_j for example i. Let Y_{obs} define observed values of Y and Y_{mis} define missing values. Define the missing data identity matrix $M = m_{ij}$, where $m_{ij} = 1$ if y_{ij} is missing and $m_{ij} = 0$ if y_{ij} is nonmissing. The missing data mechanism is called missing completely at random (MCAR) if the probability of missingness is independent of the data, or $f(M|Y, \phi) = f(M|\phi)$, where ϕ denotes unknown parameters. The MAR assumption is less restrictive than MCAR in that that the probability of missingness depends only on the observed data, $f(M|Y, \phi) = f(M|Y_{\text{obs}}, \phi)$. We are primarily interested in the NMAR assumption that the probability of missingness may also depend on the unobserved data,

$$f(M|Y, \phi) = f(M|Y_{\text{mis}}, \phi) \quad \forall\, Y_{\text{mis}}, \phi. \tag{2.1}$$

Researchers typically assume data is MAR, which mitigates the identifiability problems of NMAR because the probability of missingness depends on the features that are observed on all individuals (Tsiatis, 2007).

2.2. Imputation methods

Complete-case analysis (i.e., simply discarding examples with missing values) is wasteful of information and will bias estimates unless the data are MCAR. Since there is no way to distinguish whether the missing data are MCAR or NMAR from the observed data, a natural strategy is to impute missing values and then proceed as if the imputed values are true values. Imputation methods that rely on explicit model assumptions include *mean or mode* imputation, which replaces missing values with the mean (for quantitative features) or mode (for qualitative features) of the feature vector, and *regression model* imputation, which replaces missing values with the predicted values from a regression of Y_{mis} on Y_{obs}. Explicit modeling methods assume the data are MAR while implicit modeling methods, which are algorithmic in nature and rely only on implicit assumptions, generally do not assume the underlying missing data mechanism. Implicit methods include *random replacement*, where an example with missing data is randomly replaced with another complete example randomly sampled, and *hot deck* imputation, where missing values are replaced by "similar"

nonmissing values. Hot deck imputation can be implemented by computing the k-nearest-neighbors (k-NN) of an example with missing data and assigning the mode of the k-neighbors to the missing data. (Batista and Monard, 2003) use this procedure and find k-NN imputation can outperform internal methods used by decision trees to treat missing data and summary statistic imputation. (Li et al., 2004) propose a hot deck imputation method based on fuzzy k-means.

(Silva-Ramírez et al., 2011) empirically compare imputation based on using artificial neural networks (ANNs) with mean/mode imputation, regression models (logistic regression and multiple linear regression), and hot deck, and find the ANNs model performs the best on datasets with categorical variables.

2.3. One-hot encoding for missing data

A natural strategy in dealing with missing data for supervised learning problems is one-hot encoding. Instead of imputing missing data, one-hot encoding creates a binary feature vector that indicates missing values. For categorical features, one-hot encoding simply treats a missing value symbol (e.g, "?") as a category when the categorical features are binarized. For continuous features, missing values are set to a constant value and a missingness indicator is added to the feature space. One-hot encoding for

missing data yields biased estimates when the features are correlated, which is often the case with survey data, even when data are MCAR (Jones, 1996).

3. Experiments

3.1. Benchmark data sets

We experiment on two benchmark datasets from the UCI Machine Learning Repository: the Adult dataset and Congressional Voting Records (CVRs) dataset (Lichman, 2013). The Adult dataset contains $N = 48,842$ observations and 14 features (6 continuous and 8 categorical). Missing values in this dataset are unknown survey responses. The prediction task is to determine whether a person makes over \$50,000 a year. The CVRs dataset contains $N = 435$ observations, each the voting record of a member of the 98^{th} U.S. House of Representatives for 16 key roll call votes identified by the Congressional Quarterly Almanac. Thus, the dataset contains 16 categorical features with three possible values: "yea", "nay", and missing. Missing values in this dataset are not simply unknown, but represents values other up-or-down votes, such as voted present, voted present to avoid conflict of interest, and did not vote or otherwise make a position known. The prediction task is to classify party affiliation (Republican or Democrat).

We randomly split each dataset 2/3 for training and 1/3 for testing. The state–of–the–art for the Adult dataset is a Naive Bayes classifier that

achieves a 14.05% generalization error after removing samples with missing values (Kohavi, 1996). The CVRs dataset donor claims to achieve a 90-95% accuracy using an incremental decision tree algorithm called STAGGER, although it is not known what train-test split is used or how missing values are handled (Schlimmer, 1987; Schlimmer and Granger Jr, 1986).

3.2. Patterns of missing values

Uncovering patterns of missing values in the dataset will help select strategies for imputing missing values. Figure 1 analyzes patterns of missing data in the Adult dataset, in which 7.4% of the observations contain missing values. Missing values occur in three of the categorical features: *Work class*, *Occupation*, and *Native country*. Since these the former two features are related, it is unlikely that these values are missing completely at random (MCAR); it is more likely, and much less desirable that the values are not missing at random (MNAR). The histogram (left) in Figure 2 shows *Work class* and *Occupation* each have about 5.6% of missing values, and *Native country* has about 1.7% missing values. The aggregation plot (right) shows 5.5% of samples are missing values for both *Work class* and *Occupation*. Less than 2% of samples are missing just *Native country* and less than 1% are missing all three features.

Figure 2 shows that 46% of the CVRs data contains missing values and

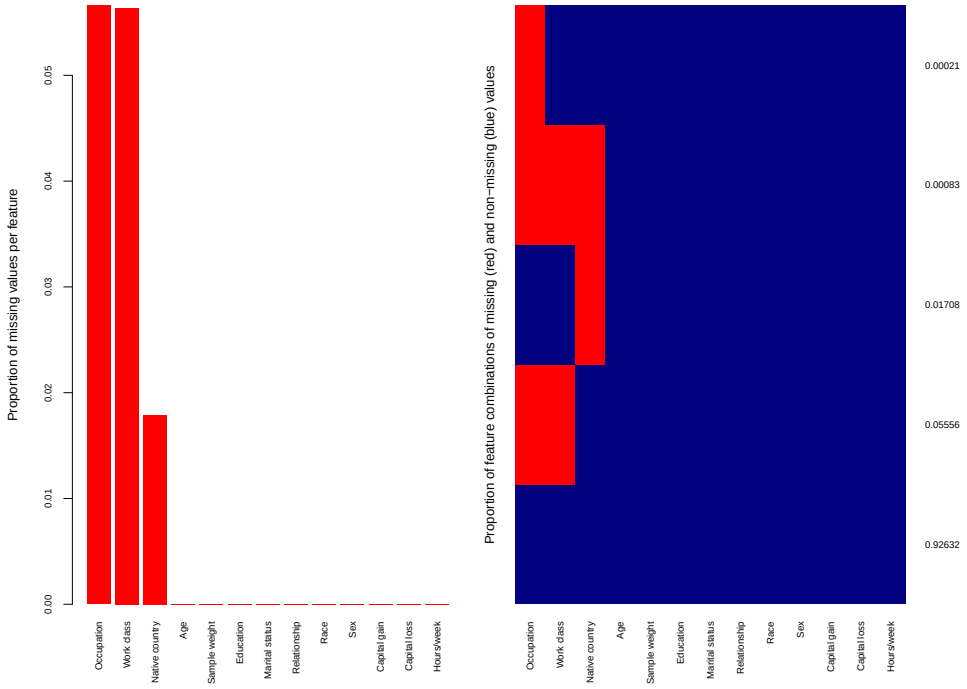

Figure 1: Histogram of proportion of missing values in each feature (Left) of Adult training set and aggregation plot of all existing combinations of missing and non-missing values in the samples (Right).

all features contain missing data. About a quarter of missing data is in `South Africa`, which was a controversial amendment to amend the Export Administration Act to bar U.S. exports to South Africa's apartheid regime. Twelve percent of missing data is in the feature `Water`, which is a water projects authorizations bill, and 7% of missing data rests in the feature `Exports`, which is a tariff bill.

3.3. Imputation methods

We compare seven different imputation techniques within the following

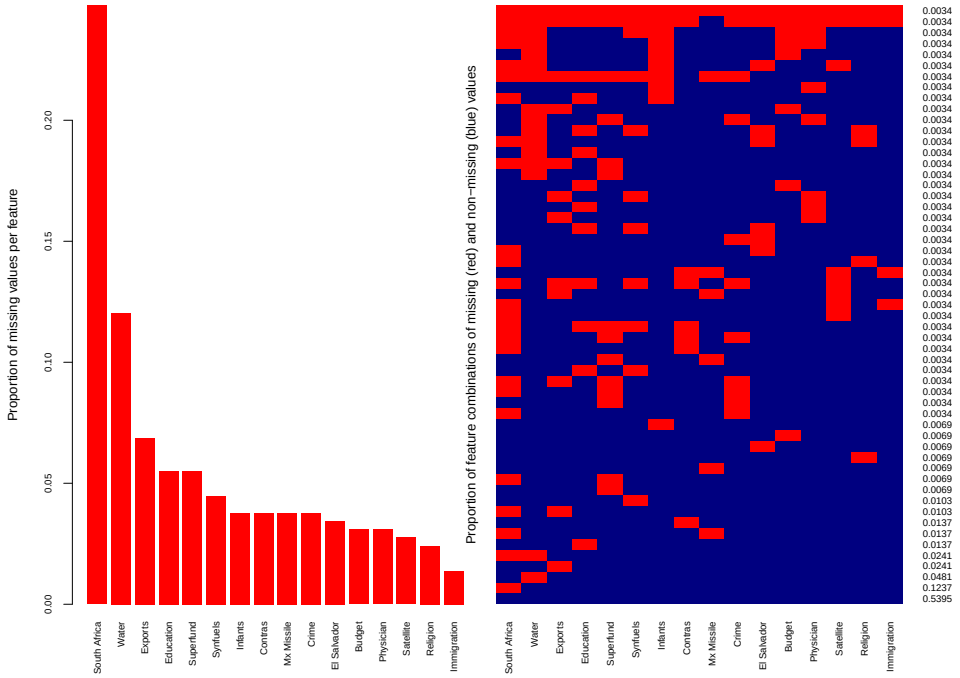

Figure 2: Histogram of proportion of missing values in each feature (Left) of CVRs training set and aggregation plot of all existing combinations of missing and non-missing values in the samples (Right).

five categories which are commonly found in the previous work on missing data imputation:

k-nearest-neighbors (k-NN) Compute the k-NN of the observation with missing data and assign the mode of the k-neighbors to the missing data.

Classification algorithm Train a classification algorithm — such as logistic regression, random forests or support vector machines (SVMs) — to classify missing data given existing data.

Random replacement The observation with missing data is randomly replaced with another complete observation randomly sampled.

Mode replacement Replace the missing data with the mode of the corresponding feature vector of the training set.

One-hot Create a binary feature vector to indicate which variable is present.

3.4. Preprocessing

The first step in preprocessing the training data is artificially increasing the number of missing values in order to study the effect of larger amounts of missing data. We accomplish this by perturbing the categorical training features by substituting nonmissing values with missing values so that each feature has a minimum missing data ratio, from 0-40%. For example if there 10 categorical features and 10 observations, a missing data ratio of 0.1 will perturb 10 values. Second, we implement one-hot encoding (-1,1) for the categorical variables. Third, we implement the imputation technique. Lastly, we standardize continuous features by subtracting the mean and dividing by the standard deviation of the feature. We preprocess the test data in the same manner, with the exception that there is no perturbation of test features.

When imputing the missing data with mode replacement, we use the training set mode. We also use the training set mean and standard deviation to standardize test set features.

3.5. Model training and hyperparameter selection

We train a four-layer neural network, with each of the two hidden layers having 1024 nodes. We use the adaptive learning rate method Adadelta (Zeiler, 2012) for the update rule. We explore the following hyperparameter space via Bayesian optimization (Snoek et al., 2012):

- Momentum schedule [0 to 1]
- Dropout regularization [No, Yes]
- Learning rate: [0.000001 to 0.01].

The goal of Bayesian optimization is to choose a point in the hyperparameter space that appropriately balances information gain and exploitation. Figure 3 shows the exploration of hyperparameter space during Bayesian optimization for both Adult and CVRs datasets. Each circle represents a candidate neural network classifier trained on a differently imputed and perturbed dataset. More circles appear in the plot for CVRs simply due to the fact that the training set is smaller. We see that most of the candidate models use dropout and have an initial learning rate close to the maximum of 0.01. The plurality of candidate models appear to either have momentum (1) or not (0). The candidate model with the lowest training error is selected for predicting on the test set.

3.6. Results

We assess the performance of the neural network classifier in terms of test set error rate in comparison with decision tree and random forests classifiers on differently imputed data and for various degrees of perturbation. We use one-hot encoding to represent missing data when no imputation method is used. The results on the Adult dataset and CVRs dataset are plotted in Figures 4 and 5, respectively. For the Adult dataset, the random forests classifier trained on data imputed with logistic regression yields the lowest generalization error (13.85% error), beating the state-of-the-art by 0.2%. In comparison, random forests trained on data with no missing data imputation matches the state-of-the-art (14.05%) and neural network trained on data imputed by random replacement performs considerably worse (14.37%). For the CVRs dataset, random forests trained on one-hot encoded data with up to 20% of the data perturbed beats the state-of-the-art by over 2% (2.77%). Neural networks trained on PCA-imputed data or no imputation also beat the state-of-the-art, with error rates of 3.47% and 4.16%, respectively.

Overall, the performance of the classifiers and imputation strategies depend on the dataset and amount of missing data. For the Adult dataset, random forests classifiers trained on data imputed with other classifiers

(i.e., logistic regression, random forests, and SVMs) outperform other classifiers and imputation methods across different ratios of perturbed data. All classifiers trained on one-hot encoded data perform very poorly when the Adult dataset is perturbed. This is likely due to the fact that in the original, non-perturbed Adult dataset, missing values are concentrated in three features which may not be consequential for the prediction task. Perturbation exposes features that are more consequential to the prediction task to missing data.

Each of the three classifiers trained on one-hot encoded data perform well on the CVRs dataset. In this dataset, missing values represent potentially valuable information for the prediction task and can be more useful for the classifier than the imputed value for certain features. This is why it is not implausible that a classifier trained on perturbed, one-hot encoded data can have lower generalization error than a classifier trained on non-perturbed, one-hot encoded data.

4. Conclusion

Neural networks have become a popular machine learning algorithm in many domains, in part due to the ability of neural networks to "learn" how to engineer features. However, researchers analyzing survey data typically choose decision trees or random forests for prediction tasks because missing

data and categorical variables are not easy to handle with neural networks. This paper investigates techniques for handling missing data for training neural network classifiers.

We compare the predictive performance of a four-layer neural network against decision tree and random forest classifiers trained on datasets with differently imputed data. We assess performance in terms of test set error for different levels of perturbed training data, from 0% (no perturbation) to 40% perturbation. We beat the state-of-the-art test error on the Adult dataset by 0.2% using a random forests classifier trained on data imputed with logistic regression. Random forests trained on perturbed and one-hot encoded data outperforms the state-of-the-art on the CVRs dataset by over 2%.

We conclude from the results that the performance of the classifiers and imputation strategies generally depend on the nature and proportion of missing data. For the Adult dataset, random forests classifiers trained on data imputed with other classifiers outperform other classifiers and imputation methods across different ratios of perturbed data, while classifiers trained on one-hot encoded data perform very poorly on perturbed training data. This finding can be explained by the fact that missing values in the Adult dataset are concentrated in three features which may not be

consequential for the prediction task, and perturbation exposes features that are more consequential to the prediction task to missing data. For the CVRs dataset, each of the three classifiers trained on one-hot encoded data perform well across different levels of perturbation. This finding can be explained by the fact that missing values represent potentially valuable information for the prediction task in the CVRs data.

For future work, we will further explore the idea that missing data may have more predictive value than imputed data in certain domains. A related question is whether neural networks can outperform decision trees or random forests trained on one-hot encoded data by learning different types of missing values. For instance, can neural networks engineer features that reflect the different types of missing values in the CVRs data, where missing values represent any action other than an up-or-down vote (e.g., voted present)? Answers to these questions will help guide researchers in choosing which imputation strategies and classifiers to use for prediction problems in different domains.

Supplementary Materials

The code used for this project is available on Github (`https://github.com/rafaelvalle/MDI`).

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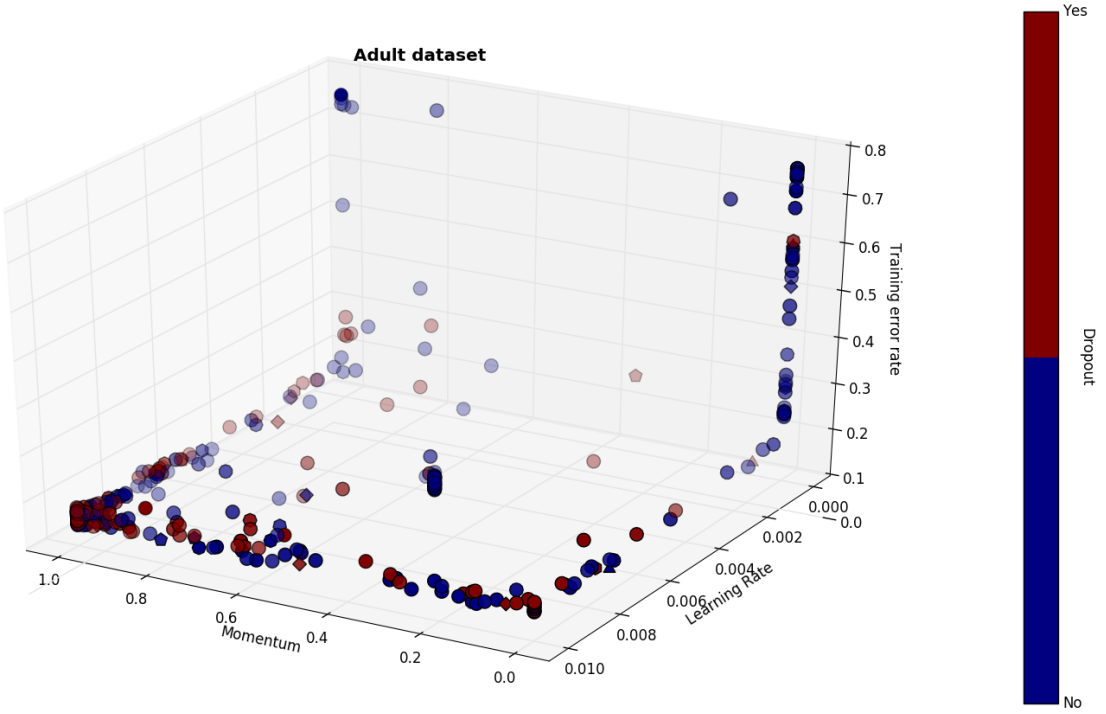
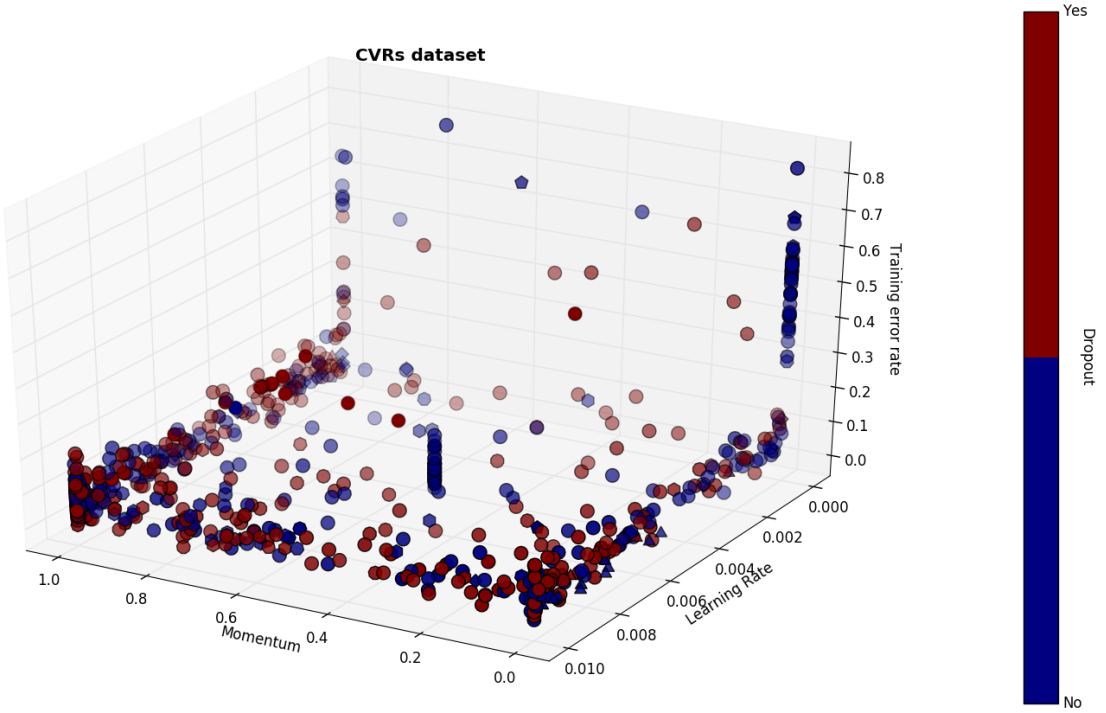

Adult dataset
Training error rate
Momentum
Learning Rate
Dropout
Yes
No


CVRs dataset
Training error rate
Momentum
Learning Rate
Dropout
Yes
No

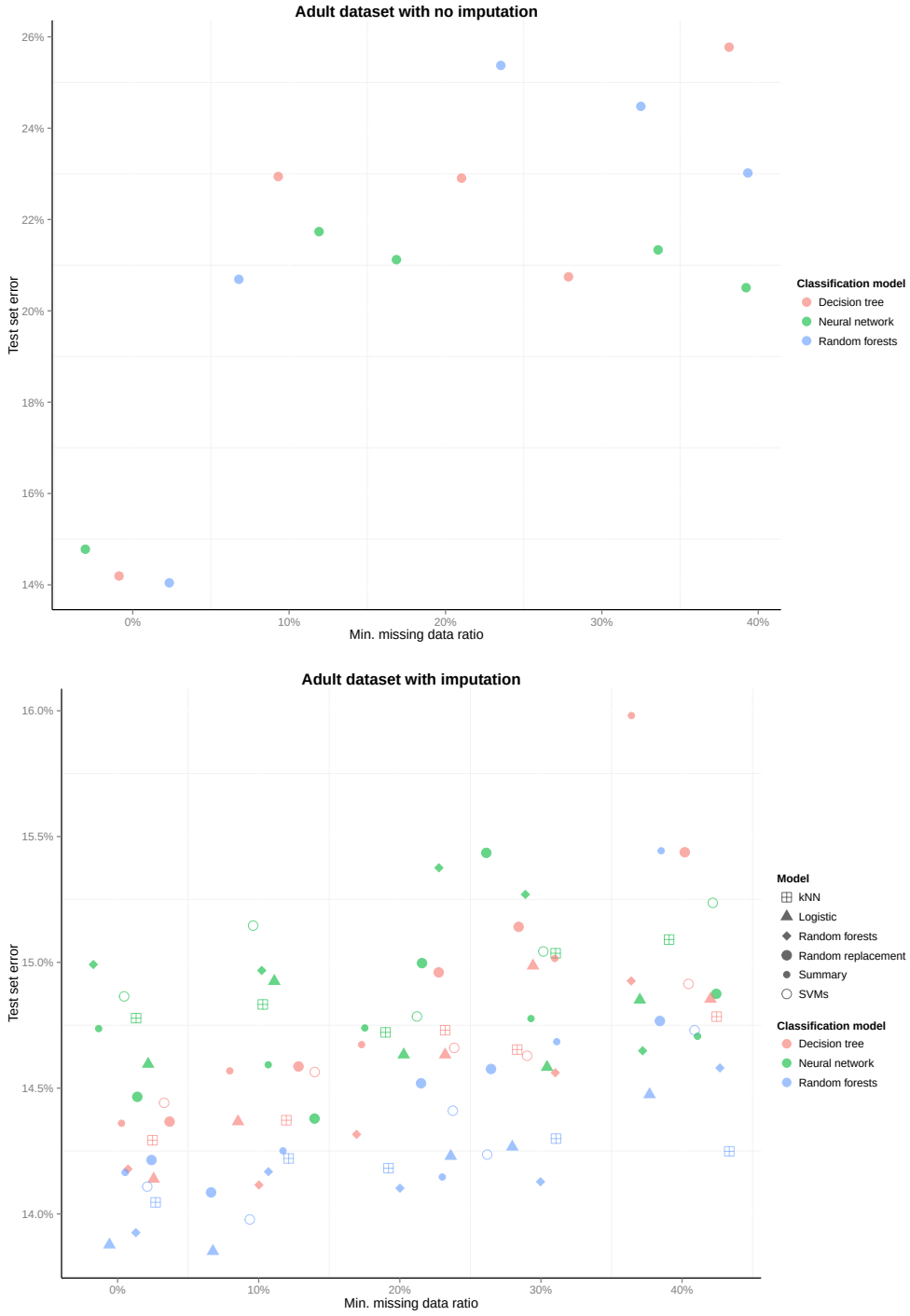


Figure 4: Error rates on the Adult test set with (bottom) and without (top) missing data imputation, for various levels of perturbed training features (x-axis). One-hot encoding is used to represent missing data in the absence of imputation. The decision tree and random forests classifiers are trained with maximum depths of 8 and 16, respectively.

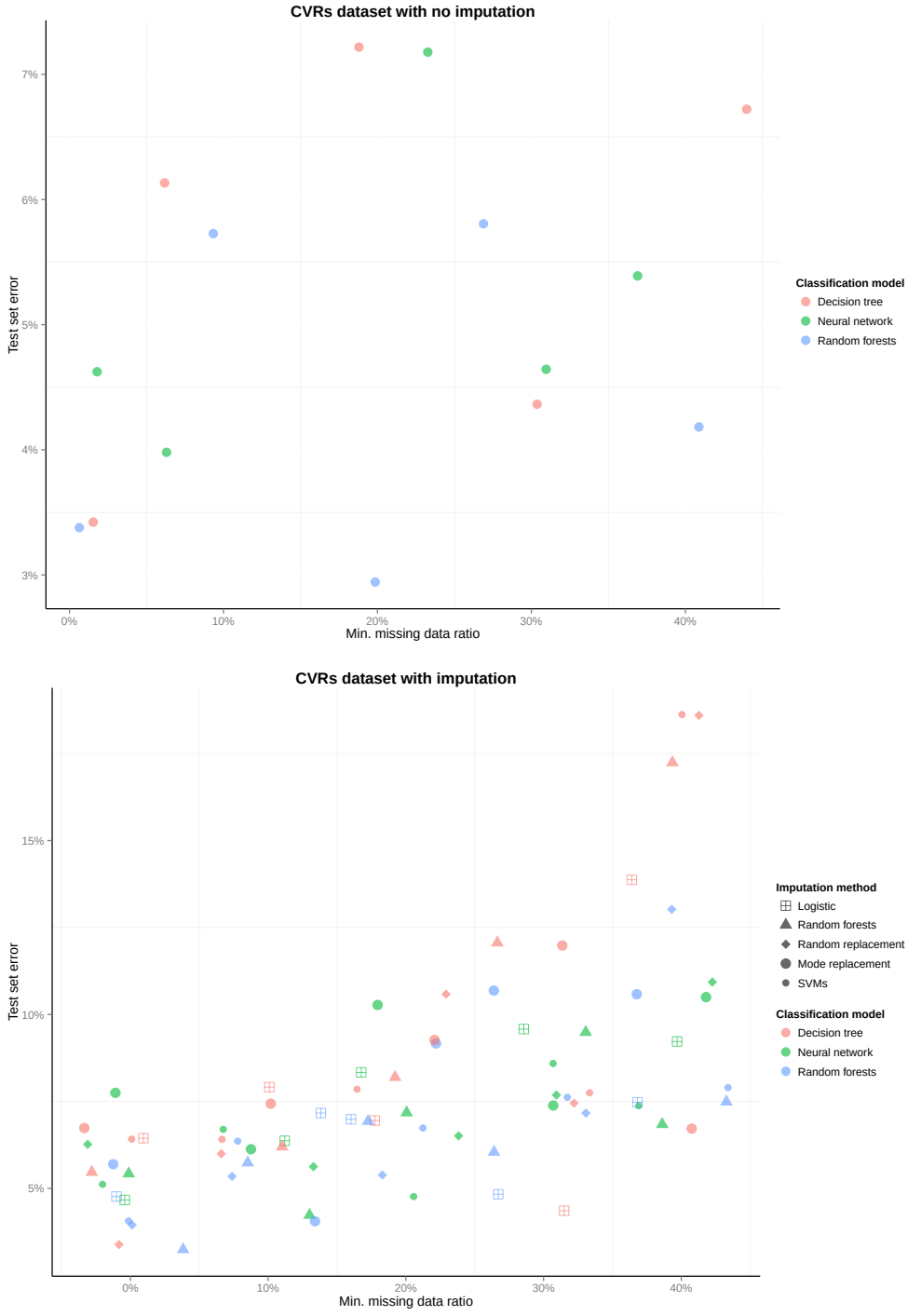


Figure 5: Error rates on the CVRs test set with (bottom) and without (top) missing data imputation.

See footnotes for Figure 4.

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