MISSING DATA IMPUTATION FOR SUPERVISED LEARNING

Abstract: This paper compares methods for imputing missing categorical data for classification tasks using random forests, decision trees, and artificial neural networks (ANNs). Researchers analyzing survey data typically choose decision trees or random forests for classification tasks, largely because these models do not require imputing missing data nor encoding categorical variables, unlike ANNs or other classifiers. We experiment on two benchmark datasets with missing categorical data, comparing classifiers trained on non-imputed (i.e., one-hot encoded) or differently-imputed data with different degrees of missing-data perturbation. The results show imputation methods can increase predictive accuracy in the presence of missing-data perturbation. Additionally, we find that for imputed models, missing-data perturbation can improve prediction accuracy by regularizing the training data.

Key words and phrases: artificial neural networks (ANNs), decision trees, imputation methods, missing data, prediction intervals, random forests, survey data

1. Introduction

Missing data is a common problem in survey-based political science research. 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 labeled training data in order to categorize new examples.[1] The ability of researchers to accurately fit a model model and yield unbiased estimates may be compromised by missing data. Nonresponse in surveys is typically handled by imputation methods, which are used to estimate a value for missing data. However, many popular imputation methods assume data missing at random (MAR), which occurs when the probability of missingness depends only on the observed data. Imputation methods that assume data are MAR when the data is in fact missing not at random (MNAR), when the probability of an example having a missing value depends on the missing data itself, can bias model estimates.

The objective of the present study is to compare the out-of-sample per-

[1] Applications of supervised learning in political science include studies of international and civil conflict(Beck et al., 2000; De Marchi et al., 2004; Hill and Jones, 2014; Muchlinski et al., 2016) and election fraud (Cantú and Saiegh, 2011; Montgomery et al., 2015). Recently, political scientists have employed supervised learning for estimating heterogeneous treatment effects, (Imai and Strauss, 2011; Green and Kern, 2012; Imai et al., 2013; Grimmer et al., 2014), text analysis (Quinn et al., 2010; Hopkins and King, 2010; Grimmer and Stewart, 2013; Lauderdale and Clark, 2014; Wilkerson et al., 2015), and record linkage (Giraud-Carrier et al., 2010).

formance of three popular machine learning classifiers — decision trees, random forests, and artificial neural networks (ANNs) — trained on differently-imputed or non-imputed (i.e., one-hot encoded) survey datasets that contain various degrees of missing-data perturbation. Researchers analyzing survey data typically choose decision trees or random forests for classification tasks, largely because these models do not require imputing missing data nor encoding categorical variables, unlike ANNs or other classifiers. The results of the present study will provide guidance to applied researchers on how to handle missing data for supervised learning tasks.

This manuscript is organized as follows: Section 2 describes missing data mechanisms and imputation methods; 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

In this section, we describe the missing data mechanisms underlying patterns of missing data common to survey datasets. We then review popular methods of handling missing data.

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, Chap. 1). 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 (De Leeuw et al., 2003).

Imputing missing values in situations where missing data hide values that are useful for classification tasks can help improve prediction accuracy. 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, Chap. 1), let $Y = y_{ij}$ be a $(n \times K)$ dataset with each row $y_i = (y_{i1}, \ldots, y_{iK})$ 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 missing completely at random (MCAR) if the probability of missingness is independent of the data, or $f(M|Y, \phi) = f(M|\phi)$ for all Y, ϕ, where ϕ denotes unknown parameters. The MAR assumption is less restrictive than MCAR in that the probability of missingness depends only on the observed data,

$f(M|Y,\phi) = f(M|Y_{\text{obs}},\phi)$ for all Y_{mis},ϕ. The MNAR assumption is that the probability of missingness may also depend on the unobserved data, $f(M|Y,\phi) = f(M|Y_{\text{mis}},\phi)$ for all Y_{mis},ϕ. Researchers typically assume data is MAR, which mitigates the identifiability problems of MNAR because the probability of missingness depends on data that are observed on all individuals (Tsiatis, 2007, Chap. 6).

2.2. Imputation methods

Complete-case analysis (i.e., discarding examples with missing values) wastes information and biases estimates unless the missing data are MCAR. Since there is no way to distinguish whether the missing data are MCAR or MNAR 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 replacement*, which substitutes missing values with the mean (for quantitative features) or mode (for qualitative features) of the feature vector, and *prediction 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 using ANNs with mean/mode imputation, regression models (logistic regression and multiple linear regression), andhot deck, finding 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

In this section, we describe our experiment on two benchmark datasets with missing categorical data, comparing three popular classifiers — ANNs, decision trees, and random forests— trained on either one-hot encoded or differently-imputed data with different degrees of MCAR perturbation.

3.1. Benchmark datasets

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 $N = 48,842$ examples and 14 features (6 continuous and 8 categorical). The prediction task is to determine whether a person makes over $50,000 a year. The CVRs dataset contains $N = 435$ examples, each the voting record of a member of the 98th U.S. House of Representatives for 16 key roll call votes. The dataset contains 16 categorical features with three possible values: "yea", "nay", and missing. The prediction task is to classify party affiliation (Republican or Democrat). In contrast to the Adult dataset, in which only a few features are highly correlated, many of the roll call votes in the CVRs

dataset exhibit strong correlations (Figures SM-1 and SM-2).

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 examples with missing values (Kohavi, 1996). The CVRs dataset donor claims to achieve a 5-10% error rate using an incremental decision tree algorithm called STAGGER, although it is unknown to the authors what train-test split is used or how missing values are handled (Schlimmer, 1987; Schlimmer and Granger Jr, 1986).

3.2. Patterns of missing data

Uncovering missing data patterns in the datasets will help to identify possible missing data mechanisms and select appropriate imputation methods. Figure SM-3 analyzes patterns of missing data in the Adult dataset, in which 7% of the examples contain missing values. Missing data in the Adult dataset is due to item nonresponse, as missing values are concentrated in three of the categorical features — *Work class*, *Occupation*, and *Native country*— and no examples contain entirely missing data. It is unlikely that the data are MCAR because observations that are missing in *Work class* are also missing in *Occupation* (about 6% of examples have missing values in both). There is no way to determine from the observed

data whether the missing data are MAR or MNAR; the data are MNAR if the probability of missingness cannot be explained only by the observed data in the other predictors.

Missing values in the CVRs dataset are not simply unknown, but represent 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. Close to half of the CVRs data contains missing values, which are present in every feature (Figure SM-4). 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. The data are unlikely to be MCAR because 12% of the data are missing in just `South Africa` and less than 1% of examples are missing across all features. It is most likely in this case that the CVRs data are MNAR because the probability of missing a vote or voting present on one important bill should not theoretically be influenced by observed votes on other important bills.

3.3. Preprocessing

We perturb the training data so that the proportion of missing values in

the set of categorical features Y_{cat} follows $\delta = \{0.1, 0.2, 0.3, 0.4\}$ according to the MCAR mechanism

$$\Pr(M = 1 | Y_{\text{cat}}, \phi) = \delta \text{ for all } Y_{\text{cat}}. \tag{3.1}$$

While perturbation is used primarily to study the effect of larger amounts of missing data, we note that missing-data perturbation is a form of dropout noise that can be used to control overfitting during the training process (Wager et al., 2013).

After one-hot encoding the categorical variables in the training data, we implement each of the following imputation techniques, discussed in Section 2.2: k-NN, prediction model (logistic regression, random forests, or SVMs), mode replacement, and random replacement. We then standardize continuous features by subtracting the mean and dividing by the standard deviation of the feature. The test data is preprocessed in the same manner, with the exception that we do not perturb categorical features in the test data.[2]

3.4. Model training and assessment

We train three different classifiers on the preprocessed data: decision trees, random forests, and ANNs. The ANNs consists of four layers, each

[2]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.

of the two hidden layers having 1024 nodes, and updates with the adaptive learning rate method *Adadelta* (Zeiler, 2012). We explore the hyperparameter space — momentum schedule, dropout regularization, and learning rate — via Bayesian optimization (Snoek et al., 2012), which selects optimal models based on training error. Prediction intervals are obtained from the standard deviation of test set errors of ANNs trained with different convergences (Heskes et al., 1997).

Random forests and decision trees are trained with preselected hyperparameters. Prediction intervals follow from the variation created by varying the maximum depth of the decision trees, and for random forests, the number of trees and decision rule for the number of features to consider when looking for the best split.

3.5. Results

We assess the performance of the classifiers in terms of test set error rate on one-hot encoded or differently-imputed data and for various degrees of MCAR perturbation. The results on the Adult dataset and CVRs dataset are plotted in Figures 1 and 2, respectively. Error bars represent ± 1 standard deviation from the test error rate. One-hot-encoded decision trees beats the state-of-the-art on the CVRs dataset by over 2% (0.027 ± 0.006). The ANNs classifier trained on data imputed with k-NN yields the lowest

generalization error (0.144 ± 0.06) on the Adult dataset, which is slightly above the state-of-the-art for the dataset even with 10% of the categorical feature values perturbed. In comparison, a random forests classifier trained on non-perturbed and one-hot encoded data yields a test error rate of 0.152 ± 0.02. This comparison shows that the classifiers can overfit the data and, in the case of imputed models, perturbation improves prediction accuracy by regularizing the training data.

Overall, the results show imputation methods can increase predictive accuracy in the presence of missing-data perturbation. For both datasets, one-hot encoded models trained in the absence of perturbation do just as well as imputed models trained on non-perturbed data. In the case of the Adult dataset, imputation clearly improves accuracy in the presence of MCAR-perturbed data. In contrast, each of the three classifiers trained on the one-hot encoded CVRs dataset perform relatively well across different levels of perturbation. The general pattern of results hold when the classifiers are trained on MNAR-perturbed data (Figures SM-6 and SM-7).

4. Conclusion

This paper investigates the effects of missing data imputation and perturbation on classification tasks using supervised learning algorithms. We compare the predictive performance of ANNs against decision tree

and random forest classifiers trained on datasets with one-hot encoded or differently-imputed data. We assess performance in terms of test set error for different levels of MCAR-perturbed training data. We come close to beating the state-of-the-art test error on the Adult dataset using an ANNs classifier trained on data imputed with k-NN and outperform the state-of-the-art on the CVRs dataset by over 2% using one-hot encoded random forests.

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, ANNs trained on imputed data generally 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.

Future work could help identify the conditions under which missing-data perturbation might improve prediction accuracy by acting as a regularization technique. The results of the present study show that perturbation can help increase predictive accuracy for imputed models, but not one-hot encoded models. Future work might compare missing-data perturbation with dropout training, which changes to zero all the values of a random subset of features (Hinton et al., 2012; Maaten et al., 2013; Wang

and Manning, 2013).

Supplementary Materials

The online supplementary material contains descriptive plots of feature correlation and missing data patterns in the benchmark datasets; plots of Bayesian hyperparameter optimization for training ANNs; and test set error plots for classifiers trained on MNAR-perturbed data.

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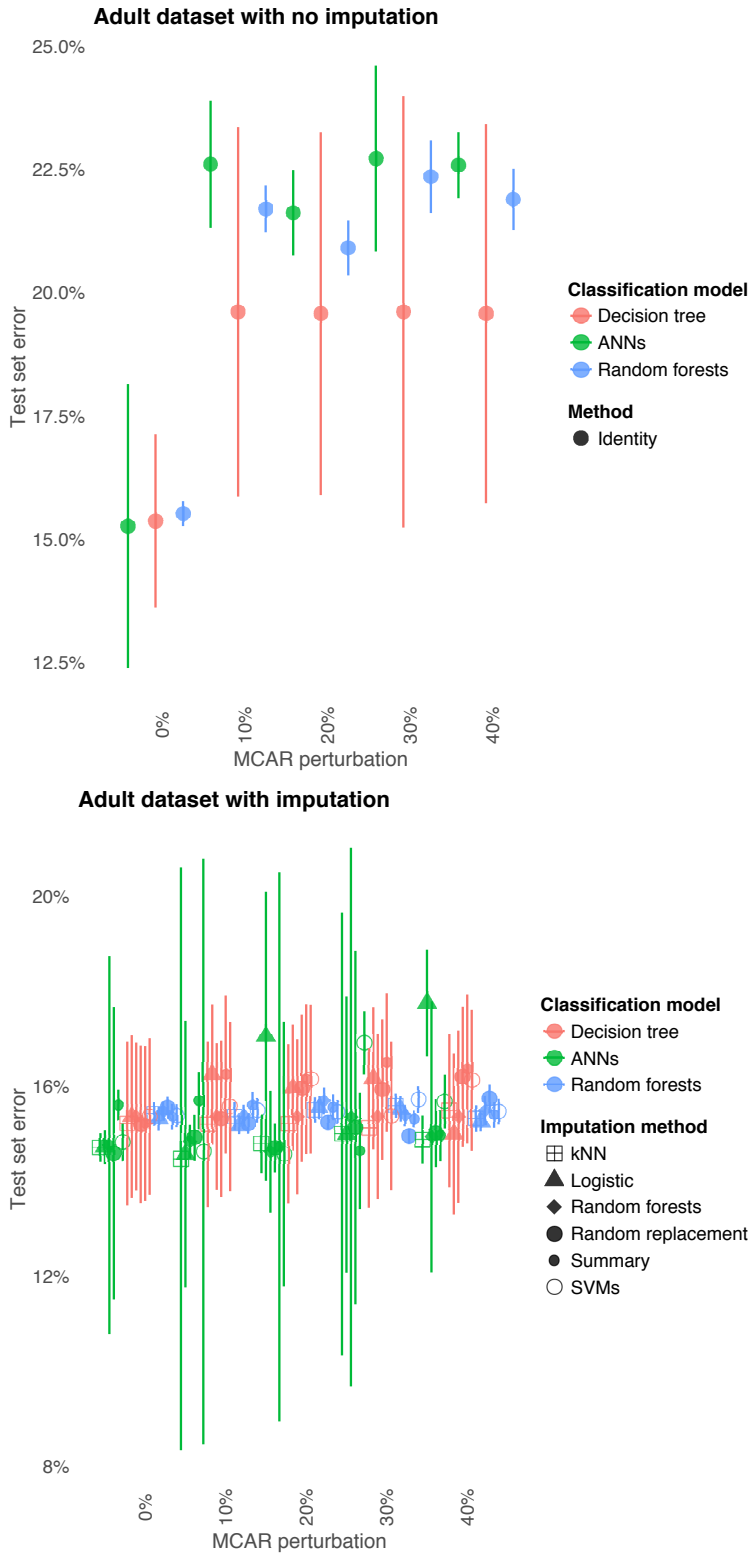

Figure 1: Error rates on the Adult test set with (bottom) and without (top) missing data imputation, for various levels of MCAR-perturbed categorical training features (x-axis). Error bars represent one standard deviation from the test error prediction.

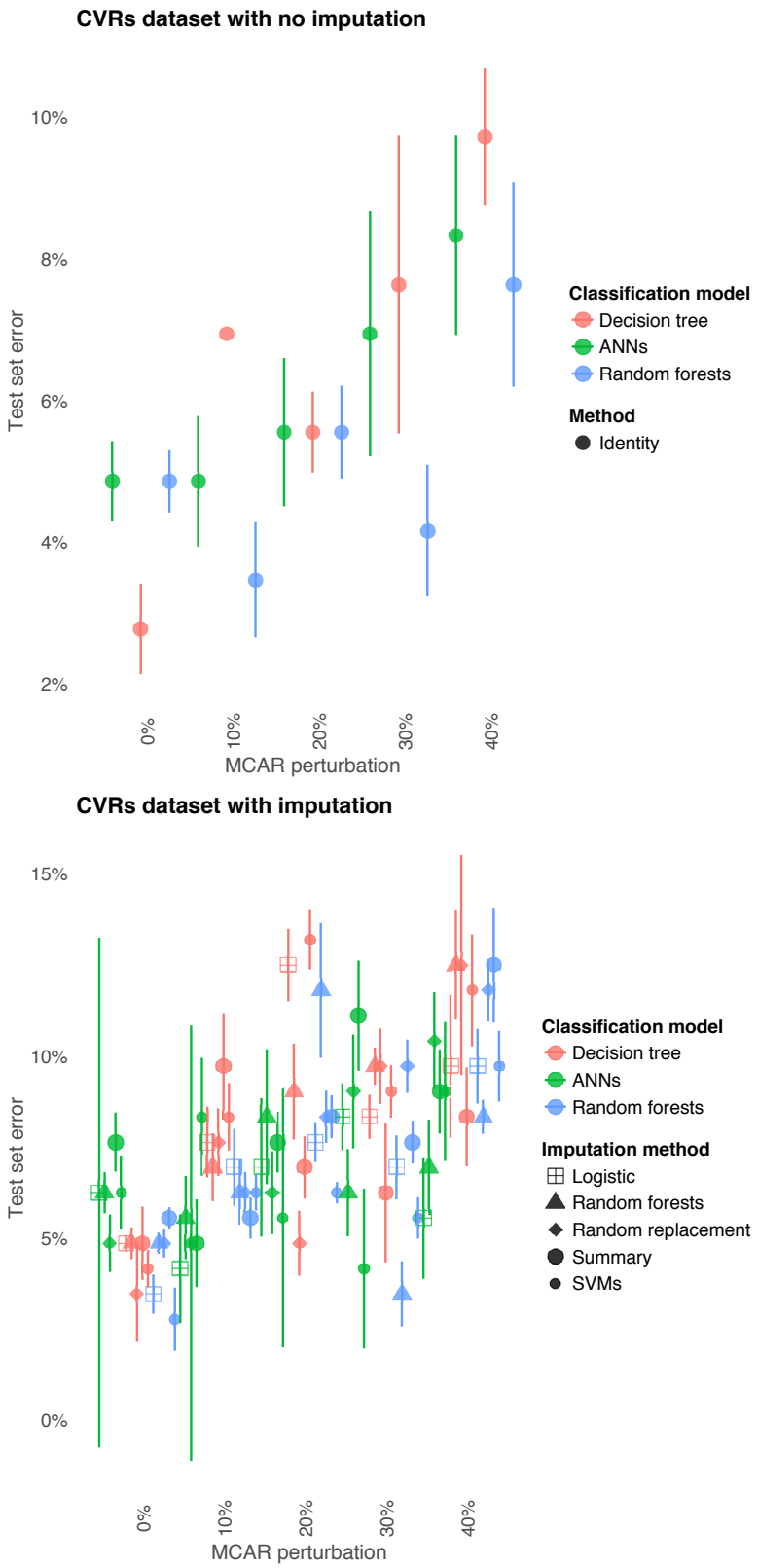

Figure 2: Error rates on the CVRs test set with (bottom) and without (top) missing data imputation.

See footnotes for Figure 1.

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