Multiple imputation using chained random forests: a preliminary study based on the empirical distribution of out-of-bag prediction errors

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Abstract

Missing data are common in data analyses in biomedical fields, and imputation methods based on random forests (RF) have become widely accepted, as the RF algorithm can achieve high accuracy without the need for specification of data distributions or relationships. However, the predictions from RF do not contain information about prediction uncertainty, which was unacceptable for multiple imputation. Available RF-based multiple imputation methods tried to do proper multiple imputation either by sampling directly from observations under predicting nodes without accounting for the prediction error or by making normality assumption about the prediction error distribution. In this study, a novel RF-based multiple imputation method was proposed by constructing conditional distributions the empirical distribution of out-of-bag prediction errors. The proposed method was compared with previous method with parametric assumptions about RF’s prediction errors and predictive mean matching based on simulation studies on data with presence of interaction term. The proposed non-parametric method can deliver valid multiple imputation results. The accompanying R package for this study is publicly available.

Keywords: Missing data; random forest; prediction error; multiple imputation

1 Introduction

Missing data have been a common nuisance in data analyses. To handle missing data problems, different imputation methods was proposed. For the past few years, with the fast development of machine learning methods, imputation methods based on machine learning algorithms have been proposed. Such imputation methods, specially imputation methods based on random forest (RF)\textsuperscript{1}, have drawn attentions from statisticians\textsuperscript{2} because of their abilities to handle data without the need to specify the distributions of the variables like most standard methods, and can handle complex relationships in the datasets automatically\textsuperscript{3} with high imputation accuracy\textsuperscript{4}.

However, such methods have incompatibility with traditional statistical methods. One major problem is that the predictions made by the RF algorithm does not contain information about the uncertainty of the predictions, which is unacceptable for multiple imputation. Using predictions from RF for imputation can cause less variability of imputations, narrower width of confidence intervals, and under coverage of confidence intervals\textsuperscript{5}. To get “proper” multiple imputation
results, researchers have tried to take the prediction uncertainty of RF into account and construct conditional distributions based on RF predictions. Shah et al. [5] assumed normality for RF prediction errors and used RF’s out-of-bag (OOB) mean squared error (MSE) as the estimate for the prediction error variance, while OOB MSE can be severely biased for estimating the variance for prediction errors [6, 7]. Doove et al. [8] sampled directly from observed values under the predicting nodes of RF without accounting for the prediction errors of RF.

Researchers have proposed different methods for describing the prediction uncertainty of RF, such as quantile regression forest by Meinshausen [9], jackknife and infinitesimal jackknife by Wager et al. [10], split conformal by Lei et al. [11]. Recently, Zhang et al. [12] used OOB prediction errors to form empirical error distribution of RF prediction for the construction of prediction intervals of RF, and this method can achieve valid results under certain conditions without additional repetitive computations. However, this empirical OOB prediction error distribution method relied on the number of trees grown in the RF model (less number of trees grown can lead to observations not out-of-bag for all the trees thus less valid observations in the empirical distribution), while for RF-based multiple imputation, often only a few trees (less than 20) were recommended by Shah et al. [5] It is not clear whether the empirical OOB error distribution can be used for constructing conditional distributions in multiple imputation.

In this paper, a novel RF-based multiple imputation method was proposed based on the empirical error distribution of RF and compared with previously established multiple imputation methods with normality assumption for RF prediction errors, as well as prediction mean matching (PMM), for data with presence of interaction term.

2 Methods

2.1 Empirical distribution of out-of-bag prediction errors

The original RF algorithm was proposed by Breiman [1], and afterwards Liaw et al. [13] provided an easy-to-use implementation in R named “randomForest”. As an ensemble learning method, RF used bootstrap aggregation (bagging) [14] to reduce the risk of overfitting and produce accurate predictions based on predictions from a number of random trees. For the process of constructing a random tree, the training set used was an independent bootstrap sample of the input dataset, and the unselected observations for a certain random tree is called the OOB sample for the tree. For a certain observation, predictions from the subset of RF that the observation is OOB, is called the OOB prediction, and the difference of input value and the OOB prediction is the OOB error. The empirical error distribution is from the individual OOB errors. The MSE of the OOB errors was used by Shah et al. [5] as the estimate of RF prediction error variance.

2.2 Multiple imputation using chained forests

Using the framework of MICE (multivariate imputation using chained equations), multiple imputation using chained forests is based on drawing data samples from conditional distributions constructed using RF, which can be summarized as:

First, initializing the simulation chains: the number of simulation chains equals to the number of imputations, and the missing part of the variable is replaced by random samples of the observed values of the variable.

Second, constructing conditional distributions based on RF: two distinct parts are formed based on whether the variable is missing, and the observed part is used as the input for training set of RF, and the missing part is used as the input for prediction set of RF. The bootstrap example of the training set is achieved from the input to account for the sampling variation. And the predictions from the prediction set was used to get the RF predictions. For continuous variables, the prediction errors of RF were accounted for by the empirical distribution of out-of-bag prediction errors. For categorical variables, the classes for predictions were assigned randomly according to the predicted probabilities.
For each of the simulation chains, the second step is performed iteratively multiple times, and the results from the last iteration were used. The software package “RfEmpImp” is now publicly available on GitHub [15].

2.3 Simulation studies

A series of simulations and analyses were carried out using R, version 3.6 (R Core Team, Vienna, Austria). Four sequential stages were involved:

1. Data generation: complete datasets were simulated based on pre-defined scenarios.
2. Amputation: the complete datasets were made incomplete based on specified rules.
3. Imputation: the missing values contained in the simulated datasets were filled in by missForest using different parallel strategies.
4. Analysis: Statistical analysis were performed on both the original complete datasets and the corresponding imputed datasets, and comparisons were made.

2.3.1 Data generation

Altogether, a total 1000 simulated datasets containing 2000 observations each were generated based on following settings.

\[
X \sim \text{Normal}(2, 1) \\
Z \sim \text{Normal}(2, 1) \\
Y = X - XZ + Z + \epsilon, \epsilon \sim \text{Normal}(0, 1)
\]

2.3.2 Amputation

Missing data mechanisms can be classified into three categories [16]. When data are MCAR, the probability of being missing is the same for all cases. When data are MAR, the probability of being missing is only related to (some of) the observed data. If neither MCAR nor MAR holds, then data are missing not at random (MNAR). While MCAR is simple to consider, most of the missing data methods use MAR assumption. Amputation functions provided by the “mice” R package [17, 18] were used in this study to generate missing values. Both missing completely at random (MCAR) and missing at random (MAR) patterns were used in this study. MCAR patterns were introduced by setting \(X\) and \(XZ\) to be missing with probability of each observation being missing was set to 50%. MAR patterns were introduced by setting \(X\) and \(XZ\) to be missing depending on \(Y\). Specifically, the probability of each observation being missing was set to 50% according to a standard right-tailed logistic function on \(Y\); thus the probability of the covariates being missing is higher for observations with higher values of \(Y\).

2.3.3 Imputation

Multiple imputation was performed using “mice” [17] R package. For each of the amputed dataset, RF-based imputation using empirical OOB error distribution (“Empirical”), RF-based imputation using normality assumption (“Normal”), and PMM were performed. Ten imputations were performed for each dataset and each imputation method, and the number of iterations restricted to 10 [5]. The PMM method is a semi-parametric imputation method recommended as the default method for handling missing data in continuous variables by the “mice” R package. For each variable, PMM calculates the predicted regression values for its non-missing and missing observations. It then fills in a missing value by randomly selecting one from the “donors” (non-missing observations whose predicted values are closest to the predicted value for the missing observation). The purpose of the regression in PMM is to construct a metric for matching observations with missing values to similar observations with observed values that can be used for imputation.
2.3.4 Analysis

Performance comparisons were made among the two RF-based imputation methods (“Empirical” and “Normal”), PMM imputation, and results from corresponding original data (“Original”), based on following statistics [19]: Comparisons were made between the two parallel strategies, along with the original sequential algorithm, based on:

1. the relative bias of the coefficient estimate:

\[
\frac{(\hat{\beta}_p - \beta_p)}{\beta_p}, \quad p = 1 \text{ or } 2
\]

corresponding to the intercept (if any), \(X_1\) or \(X_2\).

2. width of 95% confidence intervals (CIs);

3. coverage of 95% CIs.

An imputation method with superior performance can be generally characterized by smaller relative bias, width of 95% CIs closer to original data, coverage of CIs closer to 95%.

3 Results

3.1 Linear regression with interaction term

Figure 1: Relative bias of coefficient estimates of \(X\) and \(XZ\) when data were (a) MCAR or (c) MAR; width of confidence intervals of coefficient estimates of \(X\) and \(XZ\) when data were (b) MCAR or (d) MAR for linear regression with interaction of positive coefficient for \(X\) and negative coefficient for \(XZ\).
(1) MCAR data with positive coefficient for interaction and negative coefficient for X (Fig. 1ab). For relative bias of coefficient estimates of X, PMM imputation can lead to upward bias (median=0.1%, -0.1%, -0.1%, -0.1%, 3.0%, for“Original”, “Complete”, “Empirical”, “Normal”, and “PMM”, respectively). For CI width of X’s coefficients estimates, all methods can lead to increased CI width (median=0.09, 0.12, 0.14, 0.14, 0.11). For CI coverage of X’s coefficients estimates, PMM can lead to less coverage rate than other methods (percent=95.0%, 95.5%, 97.6%, 97.0%, 78.9%). For relative bias of coefficient estimates of XZ, overall, the bias was small (median=0.1%, 0.1%, 1.0%, 1.1%, -0.5%). For CI width of XZ’s coefficients estimates, RF-based methods can lead to increased CI width (median=0.05, 0.07, 0.08, 0.08, 0.07). For CI coverage of XZ’s coefficients estimates, all methods can lead to reasonable CI coverage, and RF-based methods can have higher CI coverage (percent=94.9%, 95.7%, 94.7%, 93.7%, 92.0%).

(2) MAR data with positive coefficient for interaction and negative coefficient for X (Fig. 1cd). For relative bias of coefficient estimates of X, complete-case analysis can lead to downward biased results, while RF-based methods can lead to slightly upward biased results (median=0.0%, -13.5%, 0.6%, 0.7%, 2.0%). For CI width of X’s coefficients estimates, RF-based methods can lead to increased CI width (median=0.09, 0.13, 0.16, 0.16, 0.11). For CI coverage of X’s coefficients estimates, complete-case analysis can lead to poor CI coverage, and RF-based methods can lead to high CI coverage, higher than that from PMM imputation (percent=94.7%, 2.6%, 97.3%, 97.7%, 83.6%). For relative bias of coefficient estimates of XZ, RF-based methods can lead to nearly unbiased results, while PMM imputation can lead to slight upward bias, and complete-case analysis can lead to downward bias(median=0.0%, -8.1%, 0.3%, 0.3%, 1.0%). For CI width of XZ’s coefficients estimates, RF-based methods can lead to increased CI width (median=0.05, 0.07, 0.08, 0.08, 0.06). For CI coverage of XZ’s coefficients estimates, RF-based methods can lead to high CI coverage, PMM imputation can lead to under-coverage, while CI coverage from complete-case analysis was near zero (percent=95.6%, 1.0%, 97.8%, 98.5%, 86.7%).

4 Discussion

In this study, a novel RF-based imputation method was proposed and compared with existing methods, results showed that the proposed method can produce valid multiple imputation results and can provide less biased results for certain scenarios. So, the normality assumption about RF’s prediction errors can be relaxed.

Compared with existing RF-based multiple imputation methods, the proposed method did not make parametric assumptions about the RF prediction errors. As a data-driven method, the prediction errors of RF can be also data-dependent, so strong parametric assumptions about RF prediction errors may not be valid. Also, the OOB MSE has been reported to be a biased estimate of the variance of RF prediction errors. The simulated scenarios in this study is somewhat simplistic for real-word analyses, and the number of trees (10 trees in RF) used was small to avoid over-fitting when training RF models. However, as the empirical distribution of OOB prediction errors depends on the number of trees constructed, the parameter of tree numbers may need further investigation for practical implementation for multiple imputation. In the study, the RF model building process was accelerated using parallel computing [20] (time consumption of RF-based methods is about 1.4x of PMM for simulated datasets in this study), however, whether changes can be caused by different RF software packages may need further discussion.

In this study, the simulations generated a relatively high proportion of missing data to accentuate the effects of missing data on the results, although lowering the proportion of missing data to 25% did not materially alter the main findings, while the complete-case analysis can produce slightly less biased results. In order to be consistent with previous studies, we used only 10 imputations with 10 iterations for comparisons, but for practical use, more stable pooled estimates may be achieved with more imputations and iterations.
5 Conclusions

The proposed RF-based multiple imputation method based on the empirical distribution of out-of-bag prediction errors can provide valid imputation results even with only a small number of trees built in the model.

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