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A Comparison of Multiple Imputation Methods in Multiple Imputation by Chained Equations for Longitudinal Continuous Data: A Simulation Study

Uzunlamasına Sürekli Veri İçin Zincirlenmiş Denklemlerle Çoklu Atama İçindeki Çoklu Atama Yöntemlerinin Karşılaştırılması: Bir Simülasyon Çalışması

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ABSTRACT Objective: Missing data is one of the main problems in longitudinal data. Imputation is one of the ways to solve this problem. Multiple imputation methods are preferred to single imputation methods because they explain the uncertainty around the true value and get almost unbiased estimates. In this study, we aim to compare 5 multiple imputation methods within multiple imputation by chained equations (MICE) for longitudinal continuous data. **Material and Methods:** We evaluated the performance of the 5 methods by generating data from multivariate distribution in R programming language. We deleted 10%, 20%, and 30% of the complete data under missing completely at random and missing at random. We simulated 1,000 repetitions. Our evaluation criterion is root mean squared error. **Results:** When there is a weak correlation in time points, MICE-random forest (MICE-RF) has the least biased results. When there is a strong correlation in time points, MICE-predictive mean matching (MICE-PMM) and MICE using linear regression with bootstrap (MICE-BOOT) have the least biased results. MICE-classification and regression trees and MICE using Bayesian linear regression have the most biased results. **Conclusion:** MICE-RF, MICE-PMM, and MICE-BOOT can be used for longitudinal continuous data with missing observations. Moreover, researchers can generate different multivariate distributions in simulation studies to determine the optimal method.

Keywords: Longitudinal data; missing data; missing completely at random; multiple imputation

ÖZET Amaç: Eksik veri, uzunlamasına veri analizinde temel sorunlardan biridir. Bu sorunu çözmek için bilinen yollardan biri atamadır. Çoklu atama yöntemleri, gerçek değer etrafındaki belirsizliği açıkladıkları ve neredeyse yansız tahminler elde ettikleri için tekli atama yöntemlerine tercih edilmektedir. Bu çalışmada, uzunlamasına veri için MICE içindeki 5 çoklu atama yönteminin karşılaştırılması amaçlanmaktadır. **Gereç ve Yöntemler:** Beş yöntemin performansı, R programlama dilinden çok değişkenli dağılım üreterek değerlendirilmiştir. Tamamen rastgele kayıp ve rastgele kayıp mekanizmaları altında tam verilerin %10, %20, %30'u silinmiştir. 1.000 tekrar yapılmıştır. Değerlendirme kriteri olarak karekök ortalama kare hata belirlenmiştir. **Bulgular:** Zaman noktaları arasında zayıf korelasyon varken, MICE-rastgele orman [random forest (RF)] (MICE-RF) en yansız sonuçlara sahiptir. Zaman noktaları arasında güçlü korelasyon varken, bootstrap ile doğrusal regresyon kullanan MICE [MICE using linear regression with bootstrap (MICE-BOOT)] ve MICE-tahmini ortalama eşleştirme [MICE-predictive mean matching (MICE-PMM)] en yansız sonuçlara sahiptir. MICE-sınıflandırma ve regresyon ağaçları ve Bayesian doğrusal regresyonu kullanan MICE en yanlı sonuçlara sahiptir. **Sonuç:** MICE-RF, MICE-PMM ve MICE-BOOT kayıp veriye sahip uzunlamasına veri için kullanılabilir. Ayrıca araştırmacılar, benzetim çalışmalarında farklı çok değişkenli dağılımlar üretebilirler.

Anahtar Kelimeler: Uzunlamasına veri; kayıp veri; tamamen rastgele kayıp; çoklu atama

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In clinical trials, researchers use longitudinal data to look at the influence of treatment on the disease process over time. However, there can be missing observations for several reasons in longitudinal data (e.g., people do not respond to specific questions in a survey, or the individual dies and drops out from the survey). There are 3 missing data mechanisms in the literature: missing completely at random (MCAR), missing at random (MAR), and missing not at random (MNAR).[1] In this study, we focus on MCAR and MAR. In MNAR, observed values of the variable yield biased estimates of the missing values. Moreover, there are 3 missing data patterns: univariate, monotone, and non-monotone. In a univariate pattern, only one variable has missing data. In a monotone pattern, once the subject drops out, he is not available again. If the pattern is not monotone, it is called non-monotone.[2]

The most common method in longitudinal data is called listwise deletion. However, omitting missing data gives rise to a decline in statistical power and biased estimates. So, 2 main imputation approaches have been introduced in literature: single imputation and multiple imputation.[3] Multiple imputation methods have advantages over single imputation methods because they explain the uncertainty around the true value and get almost unbiased estimates. There are 2 multiple imputation approaches in longitudinal data. Joint modeling multivariate normal imputation includes parametric methods because it assumes normally distributed data. Fully conditional specification includes parametric and nonparametric methods because it does not depend on the assumption of normally distributed data. Multiple imputation by chained equations (MICE), also named fully conditional specification, is the way of implementing multiple imputation. The missing data are imputed on a variable-by-variable basis. Within the MICE method algorithm, imputation can be performed using a variety of parametric or nonparametric methods. In MICE, there are 5 multiple imputation methods for longitudinal continuous data with missing observations. The nonparametric methods are recursive partitioning (tree-based) methods and have been used to model big, complicated data in medicine and genetics.[4] The parametric methods assume normally distributed data. This study aims to determine the performance of 5 multiple imputation methods within MICE for incomplete longitudinal continuous data. In this study, we do not need ethical approval.

MATERIAL AND METHODS

MULTIPLE IMPUTATION METHODS IN MULTIPLE IMPUTATIONS BY CHAINED EQUATIONS

There are 2 general multiple imputation approaches to longitudinal data. These are joint modeling multivariate normal imputation and fully conditional specification. Joint modeling multivariate normal imputation includes parametric imputation methods because it assumes normally distributed data. Fully conditional specification includes parametric and nonparametric imputation methods because it does not rely on the assumption of normally distributed data. MICE are used for implementing multiple imputations and have been popular in recent years. In MICE, also named fully conditional specification, missing data are imputed on a variable by variable basis. There are 2 nonparametric and 3 parametric imputation methods in MICE. Nonparametric imputation methods are tree-based methods named MICE-classification and regression trees (MICE-CART) and MICE-random forest (MICE-RF). The 2 methods are based on recursive partitioning when the correlations among the variables exist. MICE-Predictive mean matching (MICE-PMM) is a parametric approach that identifies subjects with similar predictive means, then it samples one observed value from this group of similar subjects.[4] MICE using Bayesian linear regression (MICE-BAYES) and MICE using linear regression with bootstrap (MICE-BOOT) are parametric methods that explain the uncertainty around the true value.

MULTIPLE IMPUTATION BY CHAINED EQUATIONS-CLASSIFICATION AND REGRESSION TREES

The response variable can be categorical or continuous in this method. So, we refer to classification trees or regression trees, respectively.[5,6] MICE-CART creates only one tree as opposed to MICE-RF.[6] In MICE-CART, the minimum bucket is the minimum number of observations in any terminal node. We may risk overfitting our model by setting the minimum bucket to too small a value, such as 1. Therefore, we determined the minimum bucket as 5. For the implementation of MICE-CART, see [6].

MULTIPLE IMPUTATION BY CHAINED EQUATIONS-RANDOM FOREST

This method generates several trees as opposed to MICE-CART. Creating several trees decreases the variance and commonness of unstable trees.[5,6] Shah et al. showed that MICE-RF could be used when the response variable is continuous.[7] Simulations by Shah et al. suggested that the quality of the imputation for 10 and 100 trees is identical.[7] Therefore, we determined the number of trees to be 10 in this study. For the implementation of MICE-RF, see [6].

MULTIPLE IMPUTATION BY CHAINED EQUATIONS-PREDICTIVE MEAN MATCHING

MICE-PMM is a parametric method and is usually preferred over standard regression because it generates imputations from the data itself, which preserves data structure from the problems (e.g., skewness, imputing impossible values). The mice function uses PMM as the default parametric imputation method for continuous variables.[4,8] The number of donors is 5. For the implementation of MICE-PMM, see [2].

MULTIPLE IMPUTATION BY CHAINED EQUATIONS USING BAYESIAN LINEAR REGRESSION

$\dot{y} = \dot{B}_0 + X_{mis}\dot{B}_1 + \dot{\varepsilon}$, where $\dot{\varepsilon} \sim N(0, \dot{\sigma}^2)$ and given the data, $\dot{B}_0$, $\dot{B}_1$ and $\dot{\sigma}$ are random draws from their posterior distribution.[2] Box and Tiao explain the Bayesian theory by using the normal linear model.[9] For the implementation of MICE-BAYES, see [2].

MULTIPLE IMPUTATION BY CHAINED EQUATIONS USING LINEAR REGRESSION WITH BOOTSTRAP

$\dot{y} = \dot{B}_0 + X_{mis}\dot{B}_1 + \dot{\varepsilon}$, where $\dot{\varepsilon} \sim N(0, \dot{\sigma}^2)$ and $\dot{B}_0$, $\dot{B}_1$ and $\dot{\sigma}$ are the least squares estimates, and these estimates are computed from a bootstrap sample by taking from the observed data.[2] The bootstrap is a resampling method that estimates sampling variability in the data.[10] MICE-BAYES computes univariate imputations by drawing samples from the data, and integrates sampling variability into the parameters by taking the least squares estimates given the bootstrap sample.[11] For the implementation of MICE-BOOT, see [2].

SIMULATION STUDY

Different scenarios are constructed from a multivariate normal distribution with a 0 mean vector and variance-covariance matrix to determine the performance of the 5 methods for longitudinal continuous data with missing observations.

$$\mu=\begin{pmatrix}\mu_1\\ \mu_2\\ \mu_3\end{pmatrix},\ \Sigma=\begin{pmatrix}\sigma_1{}^2 & \sigma_1\sigma_2\rho_{12} & \sigma_1\sigma_3\rho_{13}\\ \sigma_1\sigma_2\rho_{12} & \sigma_2{}^2 & \sigma_2\sigma_3\rho_{23}\\ \sigma_1\sigma_3\rho_{13} & \sigma_2\sigma_3\rho_{23} & \sigma_3{}^2\end{pmatrix}$$

μ_1, μ_2 and μ_3 are means of the 3 measurement groups. ${\sigma_1}^2$, ${\sigma_2}^2$ and ${\sigma_3}^2$ are variances and ρ_{12}, ρ_{13} and ρ_{23} are correlation coefficients. We determined μ_1=μ_2=μ_3=0 for a 0 mean vector. We determined ρ_{12}=ρ_{13}=ρ_{23}=0.2 for weak correlation, ρ_{12}=ρ_{13}=ρ_{23}=0.5 for moderate correlation, ρ_{12}=ρ_{13}=ρ_{23}=0.8 for strong correlation, ρ_{12}=ρ_{13}=ρ_{23}=-0.2 for weak negative correlation. The variances of 3 groups will be kept equal to 1 without loss of generality. We assume compound symmetry for the covariance pattern. We determined n=100 for moderate sample size and n=50 for small sample size. Under MCAR, we deleted 10%, 20%, and 30% of the 3 groups. Under MAR, we used the mice package for deleting data. R is the matrix that stores the location of the missing data in the variables of X. ψ includes the parameters of the missing data model. The data X=(X_1, X_2, X_3) and the 3 variables have the correlation ρ between them. X_1, and X_2 have missing values and X_3 is fully observed.

$$\Pr(R_{X_1,X_2}=0) = \psi_0 + \frac{e^{X_1,X_2}}{1+e^{X_1,X_2}}\,\psi_{X_1,X_2} + \frac{e^{X_3)}}{1+e^{X_3}}\,\psi_{X_3)}$$

Where ψ = ($\psi_0, \psi_{X_1,X_2}, \psi_{X_3}$). ψ_{MAR}=(0, 0, 1)

logit (Pr(R_{X_1,X_2}=0)) = X_3, for MAR.[2]

We assume a non-monotone missing data pattern. Then, we applied the 5 imputation methods. For each scenario, we simulated 1,000 samples to evaluate the performance of the 5 methods. We used 3 R program packages.[12] We used the MASS package to generate multivariate normal distribution. Under MCAR, we used the missMethods package for deleting data. We used the mice package for imputing the 5 methods. Our evaluation criterion is root mean squared error (RMSE). RMSE displays the sample standard deviation of the difference between actual and estimated values as:

$$\text{RMSE}=\sqrt{\frac{\sum_{i=1}^{n}(X_i^{observed}-X_i^{imputed})^2}{n}} \quad (1)$$

n represents the number of measurements. $X_i^{observed}$ represents true value in the ith measurement and $X_i^{imputed}$ represents estimated value in the ith measurement.

RESULTS

The principle of the analysis is given in Figure 1. Table 1 and Figure 2, Figure 3, and Figure 4 show the RMSE values of the 5 methods under MCAR. For the small sample size and weak negative correlation, MICE-RF yielded the least biased results, and MICE-BAYES had the most biased results. For weak positive correlation and the small sample size, MICE-RF gave the least biased results, and MICE-BAYES had the most biased results. For moderate positive correlation and the small sample size, MICE-PMM had the least biased results, and MICE-BAYES had the most biased results. For strong positive correlation and the small sample size, MICE-BOOT yielded the least biased results, and MICE-CART had the most biased results. For the moderate sample size and weak negative and weak positive correlations, MICE-RF gave the lowest RMSE, and MICE-BAYES had the highest RMSE. For the moderate sample size and moderate positive correlation, MICE-PMM gave the lowest RMSE, and MICE-BAYES had the highest RMSE. For the moderate sample size and strong positive correlation, MICE-BOOT yielded the lowest RMSE, and MICE-CART had the highest RMSE. Table 2 and Figure 5 show the RMSE values of the 5 methods under MAR. The results under MAR are similar to the results under MCAR.

TABLE 1: RMSE values of the 5 methods for different scenarios under MCAR

Parameter			Methods				
ρ	n	PM					
Small sample size			MICE-CART	MICE-RF	MICE-PMM	MICE-BAYES	MICE-BOOT
-0.2	50	10	0.42574	0.42140	0.42383	0.43789	0.43179
-0.2	50	20	0.61054	0.60912	0.61017	0.63809	0.62239
-0.2	50	30	0.75030	0.74934	0.74838	0.79397	0.77069
0.2	50	10	0.42929	0.42707	0.43225	0.44892	0.43860
0.2	50	20	0.61679	0.61131	0.62112	0.63976	0.63201
0.2	50	30	0.75296	0.75168	0.75782	0.79595	0.77694
0.5	50	10	0.37249	0.36985	0.36775	0.37984	0.37153
0.5	50	20	0.54104	0.54051	0.53772	0.55791	0.54033
0.5	50	30	0.68016	0.67672	0.67409	0.70093	0.68815
0.8	50	10	0.27042	0.26728	0.25804	0.25724	0.24766
0.8	50	20	0.41115	0.39823	0.38307	0.38090	0.37448
0.8	50	30	0.54400	0.52278	0.49938	0.50654	0.49316
Moderate sample size							
-0.2	100	10	0.42773	0.42073	0.42567	0.43097	0.42576
-0.2	100	20	0.60520	0.60348	0.60690	0.61785	0.61210
-0.2	100	30	0.74998	0.74894	0.75093	0.76866	0.75734
0.2	100	10	0.42926	0.42807	0.43190	0.43919	0.43449
0.2	100	20	0.61426	0.60768	0.61650	0.62750	0.61824
0.2	100	30	0.75735	0.75097	0.75719	0.77433	0.76331
0.5	100	10	0.37201	0.37284	0.36893	0.37429	0.37104
0.5	100	20	0.53678	0.53557	0.53566	0.54120	0.53724
0.5	100	30	0.67265	0.67085	0.66773	0.68005	0.67168
0.8	100	10	0.25991	0.25774	0.25165	0.25250	0.25099
0.8	100	20	0.38880	0.38640	0.37517	0.37720	0.37020
0.8	100	30	0.50742	0.50312	0.48438	0.48953	0.48133

RMSE: Root mean squared error; MCAR: Missing completely at random; PM: Percentage of missingness; MICE: Multiple imputation by chained equations; CART: Classification and regression trees; RF: Random forest; PMM: Predictive mean matching; BAYES: Using Bayesian linear regression; BOOT: Using linear regression with bootstrap

TABLE 2: RMSE values of the 5 methods for different scenarios under MAR

Parameter			Methods				
ρ	n	PM					
Small sample size			MICE-CART	MICE-RF	MICE-PMM	MICE-BAYES	MICE-BOOT
0.2	50	10	0.34811	0.34097	0.34590	0.36098	0.35828
0.2	50	20	0.49740	0.48915	0.49815	0.52957	0.51291
0.2	50	30	0.61124	0.60883	0.61346	0.65689	0.63603
0.5	50	10	0.30795	0.31095	0.30424	0.32027	0.31147
0.5	50	20	0.45093	0.44580	0.44248	0.46333	0.45213
0.5	50	30	0.55719	0.55510	0.54623	0.57789	0.56186
0.8	50	10	0.24869	0.22624	0.21873	0.21661	0.21006
0.8	50	20	0.37148	0.33810	0.32010	0.31735	0.30997
0.8	50	30	0.47447	0.42328	0.40465	0.40288	0.38953
Moderate sample size							
0.2	100	10	0.35197	0.34875	0.35451	0.36408	0.35484
0.2	100	20	0.50058	0.49676	0.50310	0.51383	0.50757
0.2	100	30	0.61485	0.61156	0.61724	0.63620	0.62820
0.5	100	10	0.31276	0.31334	0.30965	0.31894	0.31240
0.5	100	20	0.45169	0.44429	0.44470	0.45677	0.44788
0.5	100	30	0.55676	0.54912	0.54641	0.56187	0.55560
0.8	100	10	0.24014	0.22707	0.22203	0.21946	0.21572
0.8	100	20	0.34136	0.32997	0.31651	0.31701	0.31382
0.8	100	30	0.42441	0.40586	0.39342	0.39225	0.38447

RMSE: Root mean squared error; MAR: Missing at random; PM: Percentage of missingness; MICE: Multiple imputation by chained equations; CART: Classification and regression trees; RF: Random forest; PMM: Predictive mean matching; BAYES: Using Bayesian linear regression; BOOT: Using linear regression with bootstrap

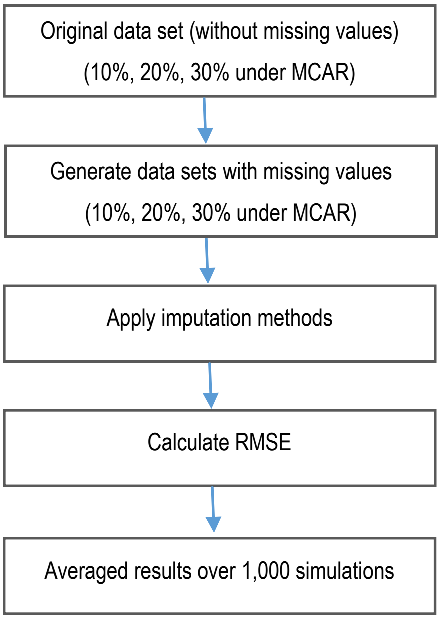

FIGURE 1: Principle of the analysis

MCAR: Missing completely at random; RMSE: Root mean squared error

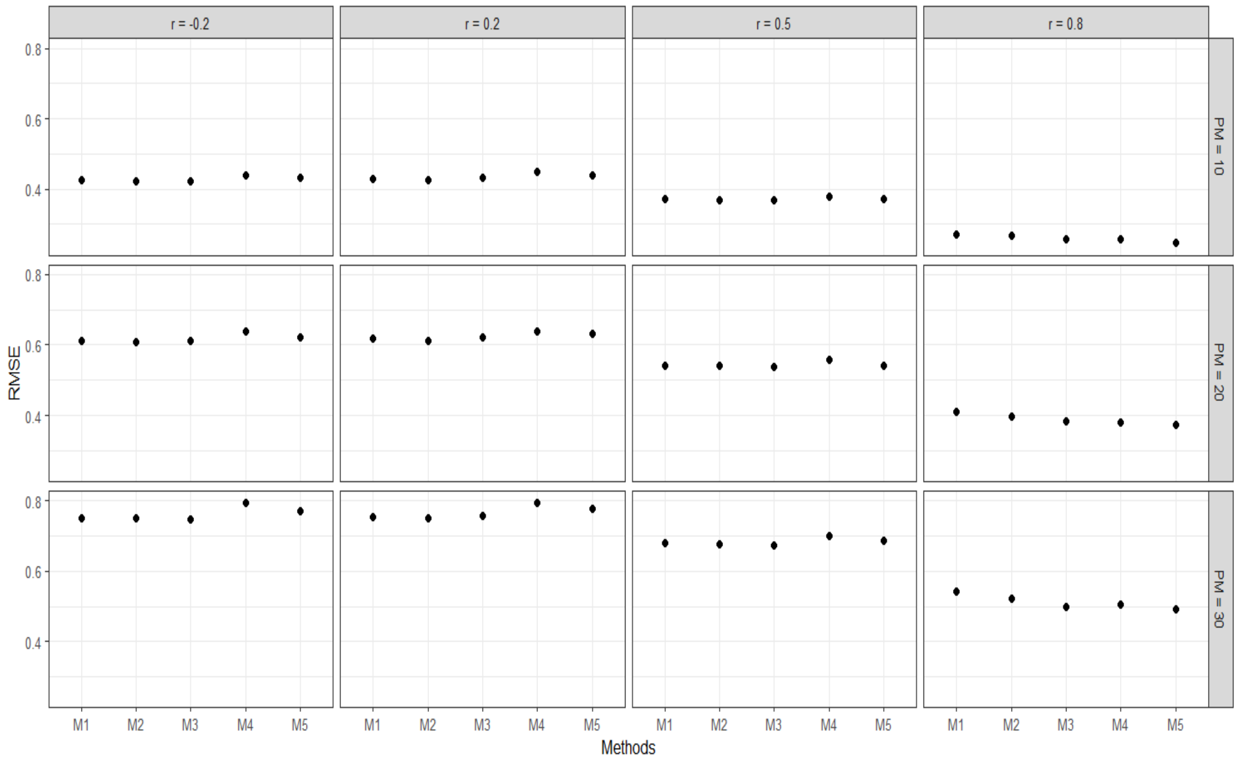

FIGURE 2: Performance of the 5 methods for 4 correlations, 3 percentage of missingness, and n=50 under MCAR

M1: MICE-CART; M2: MICE-RF; M3: MICE-PMM; M4: MICE-BAYES; M5: MICE-BOOT

MCAR: Missing completely at random; RMSE: Root mean squared error; PM: Percentage of missingness; MICE: Multiple imputation by chained equations; CART: Classification and regression trees; RF: Random forest; PMM: Predictive mean matching; BAYES: Using Bayesian linear regression; BOOT: Using linear regression with bootstrap

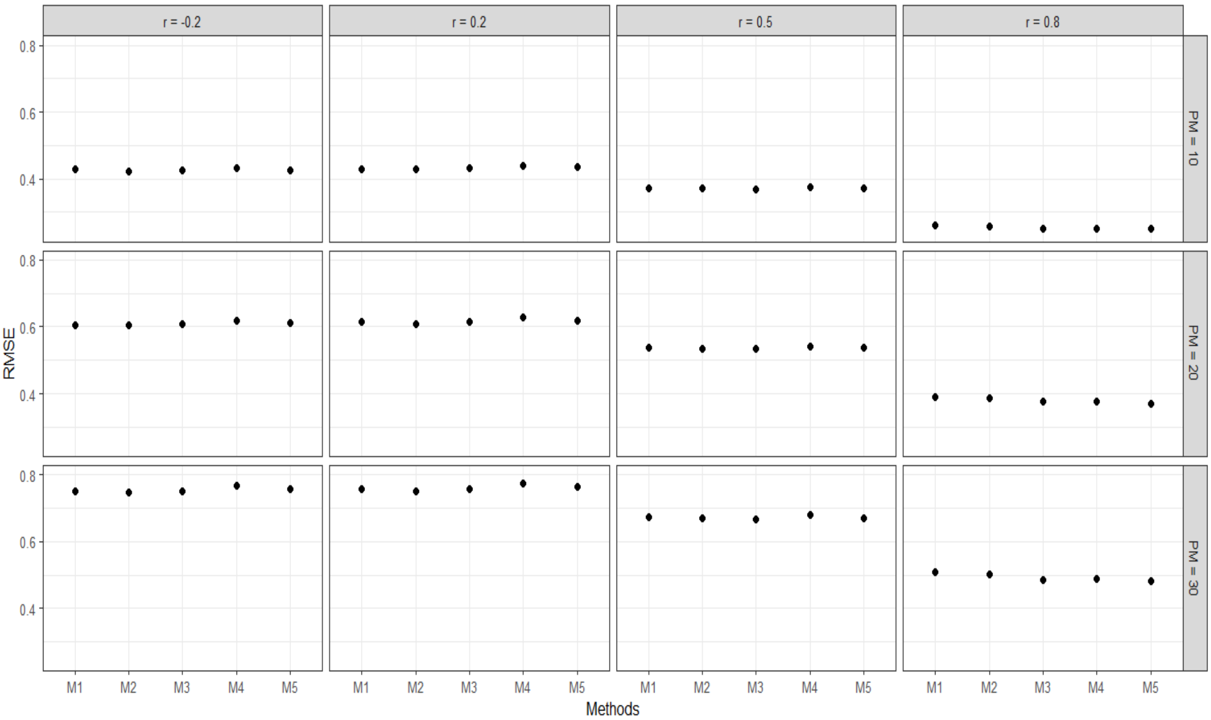

FIGURE 3: Performance of the 5 methods for 4 correlations, 3 percentage of missingness, and n=100 under MCAR
M1: MICE-CART; M2: MICE-RF; M3: MICE-PMM; M4: MICE-BAYES; M5: MICE-BOOT
MCAR: Missing completely at random; RMSE: Root mean squared error; PM: Percentage of missingness; MICE: Multiple imputation by chained equations; CART: Classification and regression trees; RF: Random forest; PMM: Predictive mean matching; BAYES: Using Bayesian linear regression; BOOT: Using linear regression with bootstrap

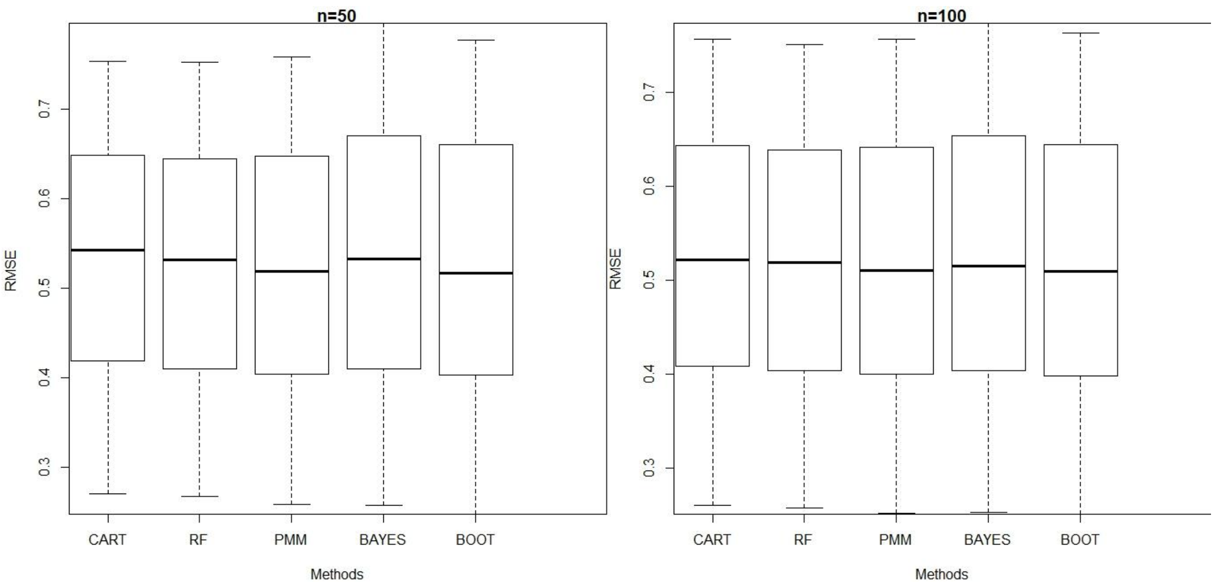

FIGURE 4: Boxplot of RMSE values for the 5 methods under MCAR
RMSE: Root mean squared error; MCAR: Missing completely at random; CART: Classification and regression trees; RF: Random forest; PMM: Predictive mean matching; BAYES: Using Bayesian linear regression; BOOT: Using linear regression with bootstrap

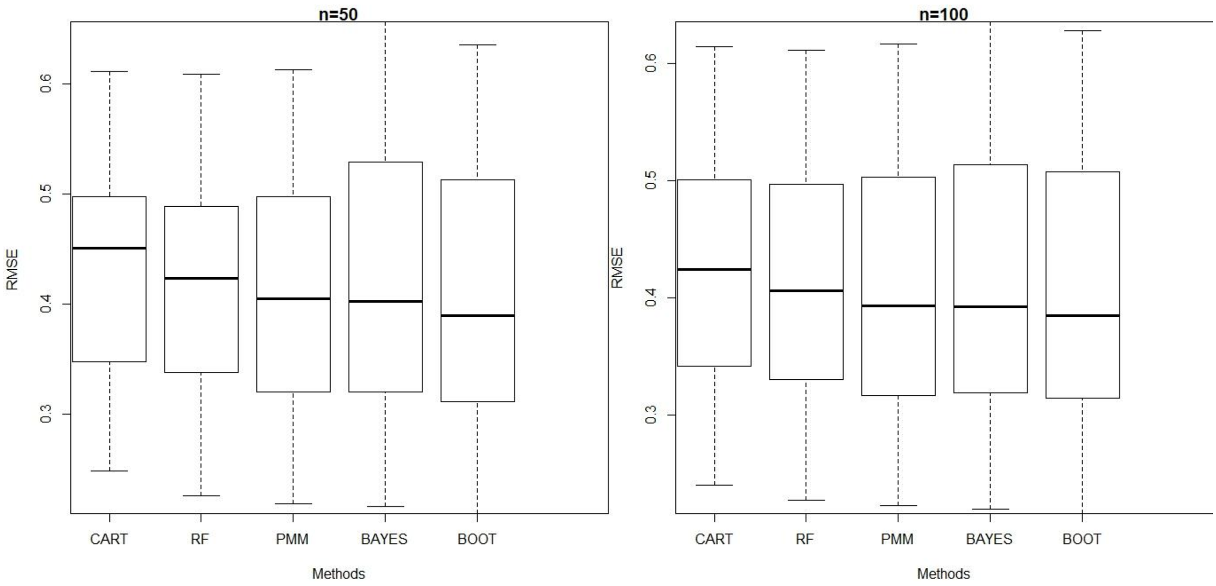

FIGURE 5: Boxplot of RMSE values for the 5 methods under MAR
RMSE: Root mean squared error; MAR: Missing at random; CART: Classification and regression trees; RF: Random forest; PMM: Predictive mean matching; BAYES: Using Bayesian linear regression; BOOT: Using linear regression with bootstrap

DISCUSSION

According to the simulation study results, MICE-CART and MICE-RF are more sensitive to the increasing correlation among the time points. As percentages of missingness increase, RMSE values increase. This result is normal as compared to the previous studies. For example, Goretzko compared MICE-RF and MICE-PMM for factor retention in exploratory factor analysis with missing data.[13] He determined that overall accuracy decreases as percentages of missingness increase. RMSE results are approximately close to each other for sample sizes 50 and 100. The tree-based methods are MICE-RF and MICE-CART. MICE-RF is superior to MICE-CART for all of the scenarios. In the literature, MICE-RF is a superior method among the tree-based methods. For example, Schwerter et al. determined that MICE-RF is the best method among the tree-based methods for drawing inference in empirical studies.[14] Javadi et al. compared MICE-CART and MICE-RF for handling missing binary outcome data in the presence of an interaction between a dummy and a continuous variable.[15] They found that MICE-RF has least biased results than MICE-CART. Shah et al. showed that MICE-RF can be used in continuous variables and compared the methods in the simulation study.[7] They determined that MICE-RF yielded least biased results than the parametric MICE methods. Slade and Naylor made a simulation study including MICE-CART, MICE-RF, and MICE-PMM in their study.[4] They found the least biased results in MICE-RF. The parametric imputation methods within MICE are MICE-PMM, MICE-BAYES, and MICE-BOOT. MICE-PMM has the least biased results for most of the scenarios among the parametric methods. Doove et al. determined that MICE-PMM is superior to MICE-BAYES in their study.[6]

CONCLUSION

This study aims at comparing the 5 multiple imputation methods within MICE for longitudinal continuous data with missing observations. Firstly, we gave general information about the 5 methods. Then, we made a simulation study by implementing different scenarios from multivariate normal distribution under the MCAR and MAR assumptions. MICE-RF can be used for weak correlations, and MICE-PMM can be used for moderate correlations among time points for incomplete longitudinal continuous data. MICE-BOOT can be used for strong correlations among time points. MICE-CART and MICE-BAYES are inferior to the other methods, and they should not be used for incomplete longitudinal continuous data. In the future, researchers can use different multivariate distributions for this issue. This study is limited to multivariate normal distribution.

Source of Finance

During this study, no financial or spiritual support was received neither from any pharmaceutical company that has a direct connection with the research subject, nor from a company that provides or produces medical instruments and materials which may negatively affect the evaluation process of this study.

Conflict of Interest

No conflicts of interest between the authors and/or family members of the scientific and medical committee members or members of the potential conflicts of interest, counseling, expertise, working conditions, share holding and similar situations in any firm.

Authorship Contributions

Idea/Concept: *Tuncay Yanarateş;* ***Design:*** *Tuncay Yanarateş;* ***Control/Supervision:*** *Tuncay Yanarateş;* ***Data Collection and/or Processing:*** *Tuncay Yanarateş;* ***Analysis and/or Interpretation:*** *Tuncay Yanarateş;* ***Literature Review:*** *Tuncay Yanarateş;* ***Writing the Article:*** *Tuncay Yanarateş;* ***Critical Review:*** *Tuncay Yanarateş, Erdem Karabulut;* ***References and Fundings:*** *Tuncay Yanarateş;* ***Materials:*** *Tuncay Yanarateş.*

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