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ShinyMICE: an Evaluation Suite for Multiple Imputation

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Abstract

This Research Report contains the Introduction and Methods section of the technical paper that will be submitted for publication in *Journal of Statistical Software*. ("There is no page limit, nor a limit on the number of figures or tables", see `https://www.jstatsoft.org/pages/view/authors`.) I have chosen to use the second format from the Research Report guidelines: "It is the first half of the thesis, i.e., there are no results included yet, but the report contains a full introduction including a literature review and a methods section that contains details about the data, instruments and or statistical procedures". The goal was to develop novel methodology and guidelines for evaluating multiple imputation methods, and implement these in an interactive evaluation framework for multiple imputation: **ShinyMICE**.

Keywords: multiple imputation, evaluation methodology, **ShinyMICE**, **mice**, R.

1. Introduction: Multiple Imputation Methodology

At some point, any scientist conducting statistical analyses will run into a missing data problem (Allison 2001). Missingness is problematic because statistical inference cannot be performed on incomplete data, and ad hoc solutions can yield wildly invalid results (Van Buuren 2018). To circumvent the ubiquitous problem of missing information, Rubin (1987) proposed the framework of multiple imputation (MI). MI is an iterative algorithmic procedure in which missing data points are 'guessed' (i.e. imputed) several times. The variability between the imputations validly reflects how much uncertainty in the inference is due to missing information–that is, if all statistical assumptions are met Rubin (1987).

With MI, many assumptions are made about the nature of the observed and missing parts of the data and their relation to the 'true' *data generating model* (Van Buuren 2018). Without proper evaluation of the imputations and the underlying assumptions, any drawn inference

may erroneously be deemed valid. Such evaluation measures are currently missing or underdeveloped in MI software, like the world leading R package **mice** (Van Buuren and Groothuis-Oudshoorn 2011). Therefore, I will answer the following question: 'Which measures are vital for evaluating the validity of multiply imputed data?'.

1.1. Features

The aim of this paper is to provide applied researchers an introduction to the interactive evaluation device **ShinyMICE**. The intended audience consists of empirical researchers and statisticians who (want to) use multiple imputation to solve missing data problems. Basic familiarity with multiple imputation methodology is assumed. For an accessible and comprehensive introduction to MI from an applied perspective, see Van Buuren (2018). For the theoretical foundation of MI, see Rubin (1987). All programming code used in this paper is available in the file 'XYZ.R' along with the manuscript, and on Github repository 'XYZ'.

1.2. Notation

The R **Shiny** application introduced in this paper is developed with the aim to integrate it into the **mice** environment. **ShinyMICE** therefore follows notation and conventions of Van Buuren and Groothuis-Oudshoorn (2011). For an overview of the deviations from the 'original' notation by Rubin (1987), see Van Buuren (2018).

Let Y denote an $n \times p$ matrix containing the data values on p variables for all n units in a sample. The collection of observed data values is denoted as Y_{obs}; the missing part of Y is refered to as Y_{mis}. Response indicator R shows whether a data value in Y is missing or observed. The relation between R, Y_{obs}, and Y_{mis} determines the missingness mechanism.

Terminology (MCAR, MAR, MNAR).

Blue points are observed, the red points are imputed.

2. Theoretical Background

- missingness mechanims, ignorability

"The practical importance of the distinction between MCAR, MAR and MNAR is that it clarifies the conditions under which we can accurately estimate the scientifically interesting parameters without the need to know ψ" (Van Buuren 2018, par. 2.2).

- Rubin's rules

- FCS vs. JM?

2.1. Theoretical Background from Thesis Proposal

The validity of the MI solution depends on numerous assumptions that cannot be verified from the observed data alone. So instead of statistical tests for assumptions, evaluation procedures have been developed. For the following assumptions, no reliable procedure has been proposed and/or implemented: 1) *ignorability* of the *missingness mechanism* (Rubin 1987); 2) *congeneality* of the imputation models (Meng 1994); and 3) *compatibility* of the MI modeling procedure (Rubin 1996).

1. A missingness mechanism is said to be ignorable when the probability to be missing does not depend on the missing data itself. Violation of this assumption can gravely affect inferences. Robustness of inferences to varying degrees of violation can be assessed with sensitivity analyses. Some practical guidelines exist (e.g., (Nguyen, Carlin, and Lee 2017)), but current MI software does not facilitate this methodology for empirical researchers.

2. Congeneal imputation models capture all required relations between observed and missing parts of the data. The extent to which this has been successful can be evaluated by plotting conditional distributions (Abayomi, Gelman, and Levy 2008). Such visualizations are available in MICE, but subsequent statistical tests to quantify the relations with covariates are not provided.

3. The third assumption is met when the MI algorithm converges to a stable distribution. However, conventional measures to diagnose convergence– e.g., Gelman and Rubin's 1992 statistic $\widehat{R}$ –are not applicable on multiply imputed data (Lacerda, Ardington, and Leibbrandt 2007). Therefore, empirical researchers have to rely on visual inspection procedures that are theoretically equivalent to $\widehat{R}$ (White, Royston, and Wood 2011). Visually assessing convergence is not only difficult to the untrained eye, it might also be futile. The convergence properties of MI algorithms lack scientific consensus (Takahashi 2017), and some default MICE techniques might not converge to stable distributions at all (Murray 2018). Moreover, convergence diagnostics for MI methods have not been systematically studied (Van Buuren 2018).

In short, the existing literature provides both possibilities and limitations to evaluating the validity of multiply imputed data. The goal of this research project is to develop novel methodology and guidelines for evaluating MI methods, and implement these in an interactive evaluation framework for multiple imputation. This framework will aid applied researchers in drawing valid inference from incomplete datasets.

3. Methods

3.1. Approach from Thesis Proposal

Initially, the research project will consist of an investigation into algorithmic convergence of MI algorithms. I will replicate Lacerda et al.'s simulation study on $\widehat{R}$ (Lacerda *et al.* 2007), and develop novel guidelines for assessing convergence. Ideally, I will integrate several diagnostics (e.g., $\widehat{R}$, *auto-correlation*, and *simulation error*) into a single summary indicator to flag non-convergence.

Subsequently, I will use R Shiny (Chang, Cheng, Allaire, Xie, and McPherson 2017) to implement the convergence indicator and existing evaluation measures in **ShinyMICE**, see Figure 1. The application will at least contain methodology for: sensitivity analyses; data visualizations (e.g., scatter-plots, densities, cross-tabulations); and statistical evaluation of relations between variables pre- versus post-imputation (i.e., χ^2 tests or t tests).

A working beta version of **ShinyMICE** will be considered a sufficient milestone to proceed with writing a technical paper on the methodology and the software. I will submit the paper

for publication in *Journal of Statistical Software*. Finally, **ShinyMICE** will be integrated into the existing MICE environment, and a vignette for applied researchers will be written.

The R code and documentation of this project will be open source (available on Github). Since the study does not require the use of unpublished empirical data, I expect that the FETC will grant the label exempt.

3.2. Sensitivity Analyses

What is already implemented?

- Current guideine: "Plot densities of both the observed and imputed values of all variables to see whether the imputations are reasonable. Differences in the densities between the observed and imputed values may suggest a problem that needs to be further checked" (Van Buuren and Groothuis-Oudshoorn 2011, p. 43).

What is not yet implemented, but exists?

- Robustness of inferences to varying degrees of violation can be assessed with sensitivity analyses. See (Nguyen *et al.* 2017) for guidelines.
- Forked MICE with MNAR sensitivity analyses

What is not implemented, and NA?

- Nothing within the scope of this thesis.

3.3. Data Visualization

What is already implemented?

- Existing plot functions to evaluate relations between observed and missing parts of the data (**mice** functions `hist()`, `xyplot()`, and `stripplot()`).

What is not yet implemented, but exists?

- Improve plots using **lattice** package functionalities.
- Subsequent statistical tests to quantify the relations with covariates.
- Use evaluation of MI methods in SAS as example

What is not implemented, and NA?

- Nothing within the scope of this thesis.

3.4. Convergence Diagnostic

What is already implemented?

- Traceplots

What is not yet implemented, but exists?

- $\widehat{R}$, but too stringent (new) threshold, and assumption of overdispersed initial values of imputation chains not met.

- Autocorrelation. Schafer (1997, p. 129) wrote on worst linear statistic. We could calculate the autocorrelation of that statistic to know that the algorithm converged elsewhere too. See autocorr function plot in sas of worst linear function.

- Sensitivity analysis: Run algorithm several times and compare results.

What is not implemented, and NA?

- $\hat{R}$ threshold: Replicate simulation study and build a decision rule to solve the problem with $\hat{R}$.

- Stability of the solution: Possibly use the slope of means over iterations too to see whether there is trending. Or apply PCA on the imputed data and if that (the eigenvalues?) stays the same we know that the means and variances are stable as well, see McKay (?).

- MC error: MC error = SD/sqrt(number of iterations), where SD represents the variation across iterations. The MC error thus represents how much the means differ w.r.t. the iterations. MC error decreases as number of iterations increases. It should not be larger than 5% of the sample standard deviation.

4. Simulation study

4.1. Introduction

It is written as a (mini) thesis, with an introduction, methods section, some results (i.e., preliminary analyses, or pilot simulations), and a discussion of results. The length of the research report should be maximally 2500 words of text (without references list and or tables and figures). Please do not include appendices, and no more than 6 tables or figures. Table and Figure captions do not count towards the word limit. An abstract may be included, but is not necessary.

Missing data is ubiquitous. MICE can solve stuff. [Copy Thesis Proposal Introduction.]

Validity of inference MCMC algorithms threatned by non-convergence. Non-converegnce has two interpretations [look up source!!!]: mixing between chains and stability over iterations within chains. Diagnose non-convergence: $\widehat{R}$, autocorrelation, MC error, Geweke, the other one. However, existing methodology may not work on MI data. Focus on $\widehat{R}$.

The potential scale reduction factor tells us how much variance could be shrunken down by running the chains infinitely long. That tells us something about how dependent the chains are on the starting values. If there is no dependence on the initial values anymore, the chains have converged (in the mixing sense of the word).

As recommended by ... Rhat is computed as .... to be able to detect ... in the tails of the distribution.

Why is R hat not applicable on MI data? R hat is not appropriate because it assumes overdispersed initial values, which means that the initial values of the m imputation chains should be 'far away' from the distribution that the chains are converging to (the modus of

the distribution). With MI procedures, initial values are chosen such that ... or maybe even estimated from the observed data. This means that at most one initial value is necessary, but probably none at al. I should look this up. And, "if over-dispersion does not hold, σ^2_+ can be too low, which can lead to falsely diagnosing convergence." (Brooks and Gelman 1998, p 437). Empirical finding suggests otherwise: that R hat will not be smaller than 1.1 before iteration nr. 50. Therefore, the aim is to replicate empirical finding Lacerda et al.

Convergence can also be interpreted as stable over iterations, or non-recurring. Non-recurrence can be evaluated with autocorrelation. Autocorrelation shows how dependent subsequent draws of an imputation chain are on the previous value. If there is a lot of dependence, draws at e.g. iteration five are significantly correlated with the value of the first draw. Ideally, we want the chains to intermingle nicely, without trends witihin chains. Autocorrelation above the confidence level indicate dependence within chains.

4.2. Simulation: Methodology

The aim is to evaluate whether the imputation procedure has converged. The primary research interest is in determining whether GR statistic Rhat is an appropriate convergence diagnostic, and if so, which level of stringency suits MI data. We can apply Rhat to the mean (or to the first two moments) of the variables of interest. The simulation diagnostics are as recommended by Stef van Buuren Van Buuren (2018). That is, average bias, average confidence interval width, and empirical coverage rate (coverage probability) across simulations. Also look at distributional characteristics, and plausibility of imputed values, see Vink.

Hypothesis based on Lacerda *et al.* (2007) is that the conventional acceptable level of Rhat is too strict for MI data. We expect that the simulation diagnostics will indicate proper imputations before Rhat will.

4.3. Simulation: Simulation Approach

In this study, 1000 MCMC simulations are performed. The simulation set-up consists of several steps, see pseudocode below. Simulation code is available in online appendix XYZ on Github.

```
# pseudocode of similation
simulate data with missingness
for (number of simulation runs from 1 to 1000)
  for (number of iterations from 1 to 100)
    impute the missingness
    compute convergence diagnostic
    perform analysis
    pool results
    compute simulation diagnostics
save convergence and simulation diagnostics
```

The simulated data is a finite population of $N = 1000$. The variables are dependent variable Y, independent variable X, and covariates Z_1 and Z_2. The quantity of scientific interest is the estimated regression coefficient of X on Y in linear regression model $Y \sim X + Z_1 + Z_2$. The data generating model of the predictors is a multivariate normal distribution with means

structure μ, and variance-covariance matrix Σ. Outcome variable Y is deduced from the predictor variables as follows:

$$\begin{pmatrix} X \\ Z_1 \\ Z_2 \\ \epsilon \end{pmatrix} \sim N \left[\begin{pmatrix} 12 \\ 3 \\ 0.5 \\ 0 \end{pmatrix}, \begin{pmatrix} 4 & 4 & 1.8 & 0 \\ 4 & 16 & 4.8 & 0 \\ 1.8 & 4.8 & 9 & 0 \\ 0 & 0 & 0 & 10 \end{pmatrix} \right]$$

$$Y = 2 \times X + 0.5 \times Z_1 - 1 \times Z_2 + \epsilon$$

After data generation, the complete data is 'amputed'. That is, the **mice** function `ampute()` is used to impose an MCAR missingness mechanism upon the data. The probability to be missing is the same for all cells, namely XYZ%. Table 1 shows a summary of the generated complete data, and the amputed data. The amputed data is the starting point of each of the 1000 simulations.

Missing data points are imputed with **mice** in R. All simulations are performed with imputation method 'norm' (Bayesian linear regression imputation), and five imputation chains. The number of iterations is varied over simulations ('maxit' argument between 1 and 100). For each number of iterations, simulation and convergence diagnostics are aggregated over 1000 MCMC simulations.

4.4. Simulation: Results

Results over 1000 simulations are presented in Table XYZ. Rhat is not perfect for MI data. The value shoudl theoretically not be smaller than one, yet it happened several times in this study. How could Rhat smaller than 1 occur? The number of simulations is smaller than in 'regular' MCMC processes. Therefore, the '$(n - 1/n)$' correction factor can influence the estimated potential scale reduction facotr. This downwards bias is in the opposite direction than expected.

And figure

4.5. Simulation Discussion

"The mixture-of-sequences variance, V, should stabilize as a function of n. (Before convergence, we expect σ^2 to decrease with n, only increasing if the sequences explore a new area of parameter space, which would imply that the original sequences were not overdispersed for the particular scalar summary being monitored.)" (Brooks and Gelman 1998, p 438).

We would like to have convergence measures for multivariable statistics (scalars?) of interest. This is, however, dependent of the complete data model. The eigenvector decomposition methof proposed by McKay (?) should be implemented. I could not find any resources to apply this method and it is outside the scope of this thesis to investigate how this apprach could be implemented.

Computational details

The results in this paper were obtained using R 3.6.1 with the **mice** 3.6.0.9000 package. R

It.	Bias	Emp. SE	CI width	Cov. rate	Rhat	Autocorr.
1	-0.135	0.115	0.637	0.930		
2	-0.088	0.125	0.691	0.990	1.499	-0.500
3	-0.090	0.112	0.623	0.950	1.200	-0.658
4	-0.093	0.116	0.645	0.980	1.146	-0.738
5	-0.087	0.108	0.599	0.980	1.098	-0.711
6	-0.092	0.116	0.644	0.950	1.090	-0.674
7	-0.095	0.122	0.675	1.000	1.063	-0.588
8	-0.099	0.113	0.626	0.970	1.058	-0.523
9	-0.095	0.115	0.639	1.000	1.044	-0.519
10	-0.090	0.111	0.618	0.990	1.048	-0.414
15	-0.093	0.109	0.604	0.950	1.020	-0.339
20	-0.098	0.109	0.606	0.980	1.023	-0.234
25	-0.100	0.113	0.626	0.990	1.016	-0.091
30	-0.091	0.118	0.654	0.960	1.014	-0.153
40	-0.088	0.117	0.650	0.990	1.009	-0.070
50	-0.087	0.119	0.662	0.990	1.009	-0.029

itself and all packages used are available from the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/.

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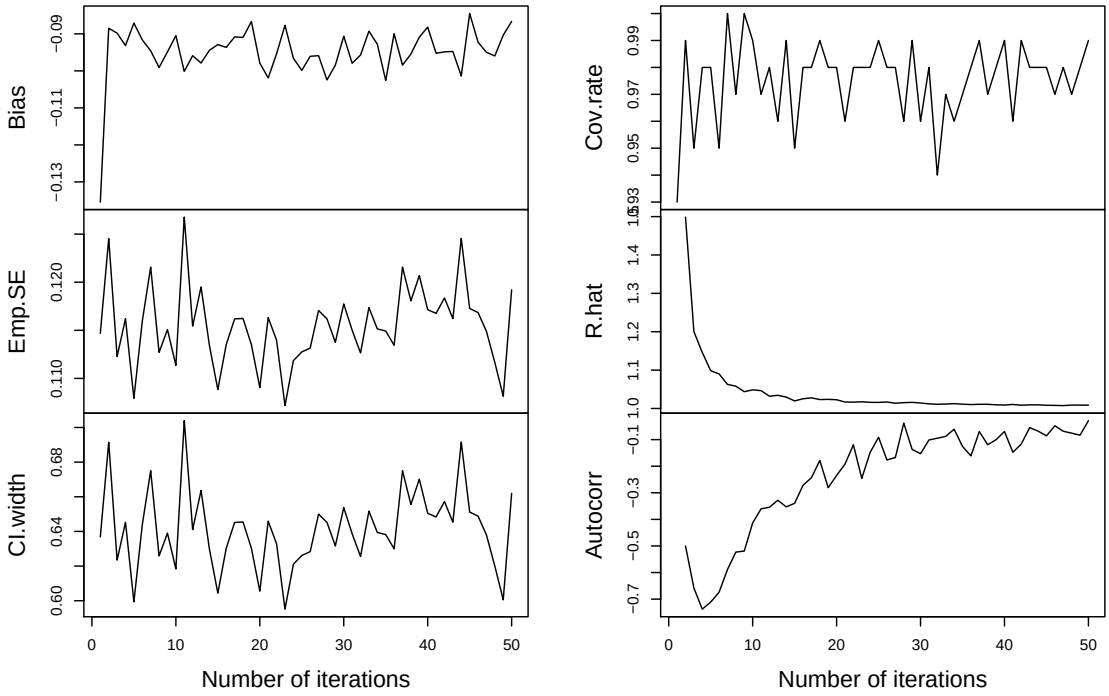

Figure 1: Simulation and convergence diagnostics over 1000 MCMC simulations.

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