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# Missing the Point : Non-Convergence in Iterative Imputation Procedures

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## Abstract

**(Rewrite:)** Multiple imputation by chained equations (MICE) is a widely used tool to accommodate missing data. While empirical evidence supports the validity of inferences obtained using mice, there is no consensus on the convergence properties of the method. This paper provides insight into non-convergence of mice algorithms.

## Keywords

MICE; convergence

**Note for peer review: things written in bold are reminders for myself or things that I am unsure off still. Also, I just decided to change things majorly in my results section. So right now, the figures do not correspond to the text. Please only skim that section, because I am definitely going to rewrite it. Thanks already! - Hanne**

## Introduction

Missing data problems are ubiquitous and pervasive in the social and behavioral sciences. If a dataset contains just one missing value for a variable of interest, statistical inferences are undefined and will not produce any result. Incomplete observations are therefore ignored by default in many statistical packages (i.e., list-wise deletion is employed). Unfortunately, this *ad hoc* solution may yield wildly invalid results (Van Buuren 2018). An alternative is to ‘impute’ (i.e., fill in) every missing value in an incomplete dataset. With imputation techniques, one or several completed datasets are created, on which statistical inferences can be performed. The case with several completed datasets is

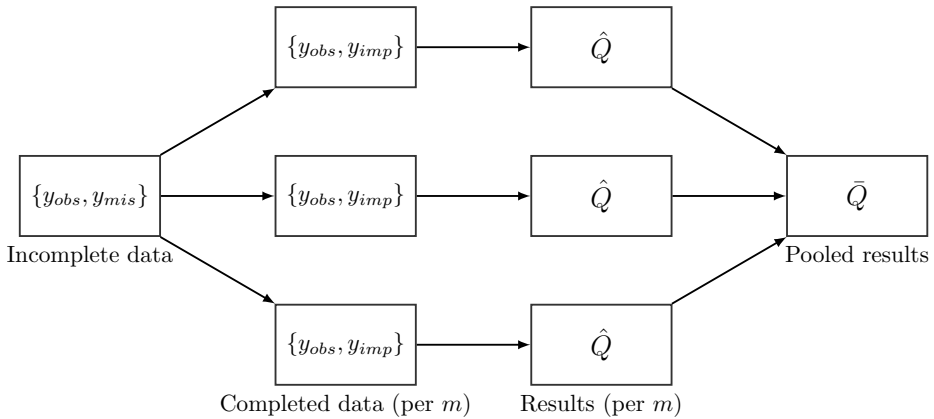
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**Figure 1.** Scheme of the main steps in multiple imputation.

known as ‘multiple imputation’ (MI; Rubin 1976), and requires an additional step to pool the results across imputations see figure 1??.

**Move this after notation??** Figure 1 provides an overview of the steps involved with MI—from incomplete data, to  $M$  completed datasets, to  $M$  estimated quantities of interest ( $\hat{Q}$ s), to a single pooled estimate  $\bar{Q}$ . Missing data in  $y$  is ‘imputed’ (i.e., filled in)  $M$  times. The imputed data ( $y_{imp}$ ) is combined with the observed data ( $y_{obs}$ ) to create  $M$  completed datasets. On each completed dataset, the analysis of scientific interest (the ‘substantive model’, or ‘complete data model’) is performed. The quantity of scientific interest (e.g., a regression coefficient) is denoted with  $Q$ . Since  $Q$  is estimated on each completed dataset,  $M$  separate  $\hat{Q}$ -values are obtained. These  $M$  values are combined into a single pooled estimate  $\bar{Q}$ . **ALSO: make clear that iteration happens within the first step.**

By applying Rubin’s rules, the pooled result will reflect the uncertainty in the data due to missingness. Under many circumstances, this yields an unbiased and confidence valid estimate of the inference on the true—but missing—data (Van Buuren 2018). A popular method to obtain imputations is to use the ‘Multiple Imputation by Chained Equations’ algorithm, shorthand ‘MICE’ (Van Buuren and Groothuis-Oudshoorn 2011). MICE is an iterative algorithmic procedure to draw imputations from the posterior predictive distribution of the missing values. This introduces a potential threat to the validity of the imputations: what if the algorithm has not converged? Are the implications then to be trusted? And can we rely on the inference obtained on the completed data? These are all open questions, because the convergence properties of iterative imputation algorithms have not been systematically studied (Van Buuren 2018). Moreover, there is no scientific consensus on the convergence properties of MI algorithms (Takahashi 2017). Some default MICE techniques (e.g., ‘predictive mean modeling’) might not yield converged states at all (Murray 2018). Therefore, algorithmic convergence should be monitored carefully.

The recommended practice to monitor convergence is to visually inspect imputations for signs of non-convergence. This practice is insufficient on two counts: 1) it may be challenging to the untrained eye, and 2) only severely pathological cases of non-convergence may be diagnosed (Van Buuren 2018, § 6.5.2). Therefore, a quantitative, diagnostic evaluation of convergence would be preferred.

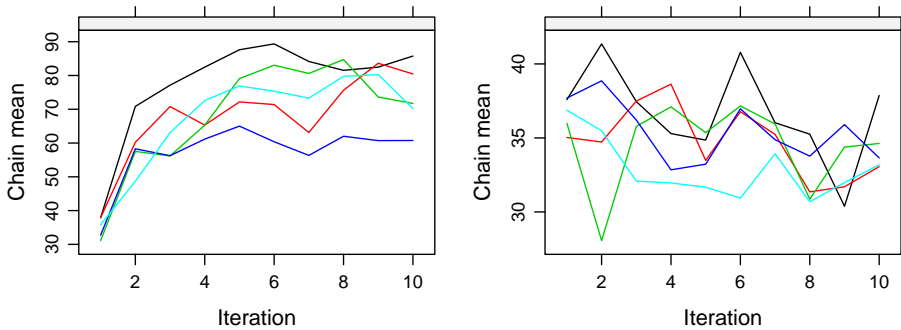
Iterative imputation algorithms such as MICE are Markov chain Monte Carlo (MCMC) methods, which means that convergence is not from a scalar to a point but from one distribution to another. The values generated by the algorithm (e.g., imputed values) will vary even after convergence. Therefore, the aim of convergence diagnostics for MCMC methods should not be to establish the point at which convergence is reached, but to monitor signs of non-convergence. Several convergence diagnostics for MCMC methods exist, but it is not known whether these are appropriate for MICE.

Main question: How can non-convergence be diagnosed? Sub-questions: Are common MCMC non-convergence diagnostics appropriate for MICE? And if so, which threshold should be used to diagnose non-convergence? How many iterations are sufficient/needed to be able to diagnose non-convergence? Are the default number of iterations sufficient (i.e., 5 in mice, 10 in SPSS and Stata, 30 in mi)? **(These are part of the methods, not RQ per se: What are the effects of continued iterations on estimates, predictions and inferences? And finally, do the answers differ with varying missingness proportions? That is, we vary the nr of iterations and the missingness proportion because we assume that the algorithm has not reached convergence at  $t = 1$ , and performs worse with moderate to high missingness (not so much with little or a LOT of missingness).)**

For reasons of brevity, we only focus on the MI algorithm implemented in the world-leading MI software: the R (R Core Team 2020) package `mice` (Van Buuren and Groothuis-Oudshoorn 2011). The convergence properties of this MI algorithm are investigated through model-based simulation. The results of this simulation study are guidelines for assessing convergence of MI algorithms, which will aid applied researchers in drawing valid inference from incomplete datasets.

## Notation

Let  $y$  denote an  $n \times p$  matrix containing the data values on  $p$  variables for all  $n$  units in a sample. The data value of unit  $i$  ( $i = 1, \dots, n$ ) on variable  $j$  ( $j = 1, \dots, p$ ) may be either observed or missing. The collection of observed data values in  $y$  is denoted by  $y_{obs}$ ; the missing part of  $y$  is referred to as  $y_{mis}$ . For each datapoint in  $y_{mis}$ , we sample  $M \times T$  times plausible values, where  $M$  is the number of imputations ( $m = 1, 2, \dots, M$ ) and  $T$  is the number of iterations ( $t = 1, 2, \dots, T$ ). The collection of samples between the initial value (at  $t = 1$ ) and the final imputed value (at  $t = T$ ) will be referred to as an ‘imputation chain’. **Add: missingness percentage = proportion of cases with one or more missing values, Q is quantity of scientific interest: “A scientific estimand  $Q$  is a quantity of scientific interest that we can calculate if we would observe the entire population” (Van Buuren 2018, par 2.3.1).**



**Figure 2.** Pathological non-convergence versus typical convergence.

## Convergence diagnostics

The two challenges for convergence of iterative algorithms are mixing and stationarity (Gelman et al. 2013), see Figure XYZ. Without mixing, imputation chains do not intermingle nicely. Without stationarity, there is trending within imputation chains. While the current practice is to inspect traceplots for signs of non-mixing and non-stationarity, diagnostic evaluation of these two challenges would be preferred. Non-stationarity within chains may be diagnosed with e.g., autocorrelation (*AC*; Schafer 1997; Gelman et al. 2013), numeric standard error ('MC error'; Geweke 1992), or Raftery and Lewis's (1991) procedure to determine the effect of trending on the precision of estimates. A widely used diagnostic to monitor mixing between chains is the potential scale reduction factor  $\hat{R}$  ('Gelman-Rubin statistic'; Gelman and Rubin 1992). With a recently proposed adaptation,  $\hat{R}$  might also serve to diagnose non-stationarity, but this has not yet been thoroughly investigated (Vehtari et al. 2019). Therefore, mixing and stationarity will be evaluated separately in this study. As recommended (e.g., Cowles and Carlin 1996, p. 898), *AC* and  $\hat{R}$  will be used.

## Potential scale reduction factor

To define  $\hat{R}$ , we follow notation by (Vehtari et al. 2019, p. 5). Let  $M$  be the total number of chains,  $T$  the number of iterations per chain, and  $\theta$  the scalar summary of interest (e.g., chain mean or chain variance). For each chain ( $m = 1, 2, \dots, M$ ), we estimate the variance of  $\theta$ , and average these to obtain within-chain variance  $W$ .

$$W = \frac{1}{M} \sum_{m=1}^M s_m^2, \text{ where } s_m^2 = \frac{1}{T-1} \sum_{t=1}^T \left( \theta^{(tm)} - \bar{\theta}^{(\cdot m)} \right)^2.$$

We then estimate between-chain variance  $B$  as the variance of the collection of average  $\theta$  per chain.

$$B = \frac{T}{M-1} \sum_{m=1}^M \left( \bar{\theta}^{(\cdot m)} - \bar{\theta}^{(\cdot \cdot)} \right)^2, \text{ where } \bar{\theta}^{(\cdot m)} = \frac{1}{T} \sum_{t=1}^T \theta^{(tm)}, \bar{\theta}^{(\cdot \cdot)} = \frac{1}{M} \sum_{m=1}^M \bar{\theta}^{(\cdot m)}.$$

From the between- and within-chain variances we compute a weighted average,  $\widehat{\text{var}}^+$ , which over-estimates the total variance of  $\theta$  **remove or explain why**.  $\widehat{R}$  is then obtained as a ratio between the over-estimated total variance and the within-chain variance:

$$\widehat{R} = \sqrt{\frac{\widehat{\text{var}}^+(\theta|y)}{W}}, \text{ where } \widehat{\text{var}}^+(\theta|y) = \frac{N-1}{N}W + \frac{1}{N}B.$$

We can interpret  $\widehat{R}$  as potential scale reduction factor since it indicates by how much the variance of  $\theta$  could be shrunk down if an infinite number of iterations per chain would be run (Gelman and Rubin 1992). This interpretation assumes that chains are ‘over-dispersed’ at  $t = 1$ , and reach convergence as  $T \rightarrow \infty$ . Over-dispersion implies that the initial values of the chains are ‘far away’ from the target distribution and each other. When all chains sample independent of their initial values, the mixing component of convergence is satisfied, and  $\widehat{R}$ -values will be close to one. High  $\widehat{R}$ -values thus indicate non-convergence. The conventionally acceptable threshold for convergence was  $\widehat{R} < 1.2$  (Gelman and Rubin 1992). More recently, Vehtari et al. (2019) proposed a more stringent threshold of  $\widehat{R} < 1.01$ .

### Autocorrelation

Following the same notation, we define autocorrelation as the correlation between two subsequent  $\theta$ -values within the same chain (Lynch 2007, p. 147). In this study we only consider  $AC$  at lag 1, i.e., the correlation between the  $t^{th}$  and  $t + 1^{th}$  iteration of the same chain.

$$AC = \left( \frac{T}{T-1} \right) \frac{\sum_{t=1}^{T-1} (\theta_t - \bar{\theta}^{(\cdot m)})(\theta_{t+1} - \bar{\theta}^{(\cdot m)})}{\sum_{t=1}^T (\theta_t - \bar{\theta}^{(\cdot m)})^2}.$$

We can interpret  $AC$ -values as a measure of stationarity. If  $AC$ -values are close to zero, there is no dependence between subsequent samples within imputation chains.

Positive  $AC$ -values indicate recurrence. If  $\theta$ -values of subsequent iterations are similar, trending may occur. Negative  $AC$ -values show no threat to the stationarity component of convergence. On the contrary even—negative  $AC$ -values indicate that  $\theta$ -values of subsequent iterations diverge from one-another, which may increase the variance of  $\theta$  and speed up convergence. As convergence diagnostic, the interest is therefore in positive  $AC$ -values. Moreover, the magnitude of  $AC$ -values may be evaluated statistically, but that is outside of this note’s scope.

Negative  $AC$ -values indicate divergence within imputation chains. **Subsequent sampled values within each imputation chain are less alike.**

In short, convergence is reached when there is no dependency between subsequent iterations of imputation chains ( $AC = 0$ ), and chains intermingle such that the only difference between the chains is caused by the randomness induced by the algorithm ( $\hat{R} = 1$ ).

### *Simulation Hypothesis*

This study evaluates whether  $\hat{R}$  and  $AC$  could diagnose convergence of multiple imputation algorithms. We assess the performance of the two convergence diagnostics against the recommended evaluation criteria for MI methods (i.e., average bias, average confidence interval width, and empirical coverage rate across simulations; Van Buuren 2018, § 2.5.2). That is, there is no baseline measure available to evaluate performance against.

Based on an empirical finding (Lacerda et al. 2007), we hypothesize that  $\hat{R}$  will over-estimate non-convergence of MI algorithms **explain why?**. The threshold of  $\hat{R} < 1.01$  will then be too stringent for diagnosing convergence. This over-estimation may, however, be diminished because  $\hat{R}$  can falsely diagnose convergence if initial values of the algorithm are not appropriately over-dispersed (Brooks and Gelman 1998, p. 437). In mice, initial values are chosen randomly from the observed data. Therefore, we cannot be certain that the initial values are over-dispersed. We expect this to have little effect on the hypothesized performance of  $\hat{R}$  **explain that the randomness induced by the MICE algorithm would take care of this??. (Add actual hypothesis: we thought that mice would converge sooner than  $\hat{R}$  would indicate that it did)** No hypothesis was formulated about the performance of  $AC$  as convergence diagnostic. **Added later: High  $AC$ -values are implausible in MI procedures. That is, the randomness induced by the MI algorithm effectively mitigates the risk of dependency within chains.**

### **Simulation study**

Research question when and how to diagnose non convergence?

QUESTION: How?

The two challenges of convergence are stationarity and mixing point. Mixing and stationarity can be evaluated visually. Common practice is to evaluate stationarity and mixing in trace plots for scalar summaries of interest. In mice these scalar summaries of interest are chain means and chain variances. As Van Buren describes users can also specify a model specific scalar summary (e.g., a regression coefficient). search a user specified scalar summary however is not universal to all complete data problems. Therefore as inspired by someone 2002 we will use introduce a scalar summary that summarizes the multivariate state space of the algorithm. In this study we use the first eigenvalue of the variance covariance matrix of the completed data set per imputation. The methods under evaluation are  $\hat{R}$  and  $AC$ . These will be computed for the three scalar summaries of interest: chain means, chain variances, and the first eigenvalue of the variance-covariance matrix across imputations.

The two methods will be evaluated with an estimand per scalar summary of interest. It is assumed that when the estimates are unbiased (and confidence valid), the algorithm is sufficiently converged. The  $\hat{R}$  and  $AC$  values with chain means as theta are evaluated against the bias in univariate mean estimates (**just for Y??**). Similarly, the performance measure for  $R_{hat}$  and  $AC$  applied to chain variances is the bias in estimated standard deviations. To evaluate the performance of  $R_{hat}$  and  $AC$  on the eigenvalues, we will use bias in R squared and in the estimated regression coefficient, the coverage rate of the CI95% of the regression estimate, and the CI length. **remove the term performance measure above and add that performance measures are bias in all estimands, and cov and CIL of regression coeff.**

#### ANSWER

In general there is more bias in the estimate in conditions with a higher proportion of missingness and or a lower number of iterations. As required the values of  $\hat{R}$  lower for conditions with a higher number of iterations. End somewhat higher 4 conditions with a higher percentage of missing data. However autocorrelation did not show a decrease with increase number of iterations. After replacing the ACF function with a manual calculation for autocorrelation the autocorrelation values were indeed decreasing with a higher number of iterations. Evaluation with the performance measures shows that are had an autocorrelation are conservative: signs of non-convergence in conditions where estimands are unbiased and or confidence valid. As expected complete convergence (as indicated by autocorrelation equals 0;  $\hat{R}$  equals 1) is not observed.

#### QUESTION: When?

Usually, convergence is diagnosed when  $R_{hat} < 1.2$  or 1.1 or 1.01. And a t-test is performed for  $AC$  values  $\neq 0$ . Performance measures are the same as above: unbiased, confidence valid estimates.

#### ANSWER

Our head is equal to 1.2 is not stringent enough because the performance measures  $R$  not unbiased and confidence fellas fell it 4 every condition in which  $\hat{R}$  is smaller than one point 2. At least, not when  $\hat{R}$  is smaller than one point two fur first occurs. The threshold  $\hat{R}$  is equal to one point one is somewhat conservative with respect to the performance measures. It seems OK.  $\hat{R}$  is equal to 1.01 is too stringent compared to the performance measures (**but may be necessary in more complex complete data models??**).

#### RECOMMENDATIONS

For empirical researchers: 1) Check trace plots for pathological non convergence and adjust imputation model if necessary. 2) use  $\hat{R}$  wait 1.1 ash threshold and autocorrelation with ? as threshold . Keep iterating until these thresholds are reached. 3) Do not use the R function ACF. Instead compute autocorrelations manually , see for example GitHub link. 4) Track your own scalar summary of interest. This is advanced but explained in Van Buren 2018. Compute  $\hat{R}$  and autocorrelation values for this scalar summary.

#### LIMITATIONS/FUTURE RESEARCH

Pmm, M(N)AR, Empirical data, Vignette, ShinyMICE, AC across imputations, not iterations (unique for imp data??)

If I don't include it in my study, also: Significance of  $AC$  values; Estimate (PCA or reg. coeff.) versus  $R_{hat}$  and  $AC$  on the estimate

## Start methods section

**Add to this section: 1) explicit mention of simulation conditions; 2) emphasize that the plots are averages across repetitions, not within MICE; 3) sample effects due to single complete dataset** Convergence of the MICE algorithm is investigated through model-based simulation in R (version 3.6.3; [R Core Team 2020](#)). The simulation set-up is summarized in the pseudo-code below. The complete R script of the simulation study is available from [github.com/gerkovink/shinyMice](https://github.com/gerkovink/shinyMice).

```
# pseudo-code of simulation
1. simulate data
for (missingness proportions 5%, 25%, 50%, 75% and 95%)
  for (number of simulation runs from 1 to 1000)
    2. create missingness
    for (number of iterations from 1 to 100)
      3. impute missingness
      4. compute convergence diagnostics
      5. perform analysis of scientific interest
      6. pool results across imputations
      7. compute performance measures
    8. aggregate outcomes across simulation runs
9. combine outcomes of all missingness proportions
```

The aim of the simulation study is to evaluate the impact of inducing non-convergence by: 1) terminating the MICE algorithm at different imputation chain lengths ( $t = 1, 2, \dots, 100$ ), and 2) varying the missingness proportions ( $p_{miss} = .05, .25, .50, .75, .95$ ). The assumption underlying the different number of iterations is that the algorithm generally does reach convergence at  $t = 1$ , because the initial values are sampled randomly from the set of observed datapoints. **As the number of iterations goes up, the imputation chains will become independent of the initial values until the point at which an extra added iteration does not lead to a more converged state.** The second set of experimental conditions under consideration—the missingness proportions—are chosen to reflect the difficulty of the missingness problem. The inherent assumption is that low missingness proportions will lead to quick algorithmic convergence, since there is a lot of information in the observed data. Higher missingness proportions then cause slower convergence. However, if the fraction of missing information is very high, there is so little information in the data that the random component in the algorithm will take the overhand and a stable but very uncertain (high variance) point will be reached.

The data-generating mechanism is a multivariate normal distribution, representing person data on three independent variables (from an unspecified social scientific field of study). Let



$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \sim \mathcal{N} \left[ \begin{pmatrix} 12 \\ 3 \\ 0.5 \end{pmatrix}, \begin{pmatrix} 4 & 4 & 1.8 & 0 \\ 4 & 16 & 4.8 & 0 \\ 1.8 & 4.8 & 9 & 0 \end{pmatrix} \right].$$

For the purpose of this study, sampling variance is not of interest. Therefore, a single complete set may serve as comparative truth in all simulation runs (Vink). A finite population of  $N = 1000$  is simulated using the function `mvtnorm::rmvnorm()`. Subsequently, a fourth variable is constructed to serve as dependent variable in a multiple linear regression problem. Let

$$Y_i = 1 + 2X_{1i} + .5X_{2i} - X_{3i} + \epsilon_i,$$

where  $i = 1, 2, \dots, N$  and  $\epsilon \sim \mathcal{N}(0, 100)$ .

We consider four quantities of scientific interest (‘conceptual estimands’; Morris et al. 2019), namely ... solve a multiple linear regression problem, where dependent variable  $Y$  is regressed on independent variables  $X_1$ ,  $X_2$  and  $X_3$  (check notation with betas here, and add what the quantity/-ies of scientific interest is/are!):

$$Y \sim \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3.$$

The complete data is ‘amputed’ once for each simulation repetition with function `mice::ampute()`. **(change this to reflect current simulation set-up with 5, 25, 50, 75, and 95% of cases having missing data:** The missingness is univariate, and the probability to be missing is the same for all four variables, namely 20% (`prop = 0.8`, `mech = "MCAR"`). This leaves 20% of the rows completely observed). This study only considers only an MCAR missingness mechanism. Therefore, results may not be extrapolated to other missing data problems. Proper performance of the convergence diagnostics under MCAR is necessary but not sufficient to demonstrate appropriateness of  $\hat{R}$  and  $AC$  as convergence diagnostics. This is just a proof of concept.

Missing datapoints are imputed with the function `mice::mice()`. All MI procedures are performed with Bayesian linear regression imputation (`method = "norm"`), and five imputation chains (`m = 5`). The number of iterations varies between simulation conditions (`maxit = 1, 2, \dots, 100`).

$\hat{R}$  (of what?? i.e., chain means and chain variances of each variable) is computed by implementing Vehtari et al.’s (2019) recommendations.  $AC$  (of what? and how is  $AC$  aggregated across imputations? i.e., mean in latest sim) is computed with function `stats::acf()`.

To estimate the quantity of scientific interest,  $Q$ , we perform multiple linear regression on each completed dataset with the function `stats::lm()`. We obtain an estimated regression coefficient per imputation, which are pooled into a single estimate,  $\hat{Q}$ . We use the function `mice::pool()` to estimate  $\bar{u}$  (check definition!) according to Rubin’s

(1987) rules, and subsequently implement finite population pooling conform Vink and van Buuren (2014).

We compute bias as the difference between  $Q$  and  $\bar{Q}$ . Confidence interval width (CIW) is defined as the difference between the lower and upper bound of the 95% confidence interval (CI95%) around  $\bar{Q}$ . We compute the CI95% bounds as

$$\bar{Q} \pm t_{(m-1)} \times SE_{\bar{Q}},$$

where  $t_{(m-1)}$  is the quantile of a  $t$ -distribution with  $m - 1$  degrees of freedom, and  $SE_{\bar{Q}}$  is the square root of the pooled variance estimate. **Why track CIW?** Underestimating the variance of  $\bar{Q}$  may yield spurious inferences. From bias and CIW, we calculate empirical coverage rates. Coverage rate is the proportion of simulations in which  $Q$  is between the bounds of the CI95% around  $\bar{Q}$ .

## Results

(Add more info about figure legends and axes.)

### *Univariate estimates and convergence diagnostics*

The bias in the estimates of the variable means show little to no difference between simulation conditions. It doesn't seem to matter how many iterations you use in the mice algorithm, the estimates are unbiased. Similarly, the bias in the estimated variances is more or less stable across simulation conditions. These univariate quantities appear to be unaffected by the number of iterations.

When applied to the imputation chain means,  $\hat{R}$  indicates that the mice algorithm does not reach a converged state ( $\hat{R} = 1$ ) in any of the simulation conditions. Neither is the most recent recommended threshold reached ( $\hat{R} < 1.01$ ). The conventional  $\hat{R}$  threshold of 1.2 is reached in simulation conditions  $T = 3$  and  $T > 6$ . (With the default number of iterations (maxit = 5), this dip in Rhat values would be spotted, so it is no problem.) The point at which an extra iteration does not seem to improve the Rhat value is around  $T = 30$ .

Auto-correlations indicate no sign of trending within imputation chains. In most simulation conditions  $AC$  is smaller than or about equal to zero. Across simulation conditions, however, the autocorrelation curve does not trend towards 0. Autocorrelation values plateau off at a value of around .1. This is a small positive autocorrelation, which would indicate some trending within chains.

The  $\hat{R}$  and  $AC$  values for the imputation chain variances show equal trends and are therefore not discussed separately. Taken together, univariate estimates seem robust across simulation conditions. There is no clear effect of the number of iterations on the bias in these estimates, while the convergence diagnostics indicate that the algorithm did not reach a completely converged state (yet).

## Multivariate estimates

There is a clear bias in the regression estimates in simulation conditions where the number of iterations is smaller than four. In simulation conditions where  $T > 5$  there is little to no bias in the estimated regression coefficients. In most simulation conditions nominal coverage is obtained (i.e., coverage rates of .95) for the confidence intervals around the regression coefficients. Conditions with only one or two iterations show some under-coverage. Since confidence interval width is stable across conditions, the under-coverage may be attributed to the bias in the estimated regression coefficients.

If we look at the estimated proportion of explained variance in outcome variable  $Y$  we see that the coefficient of determination is underestimated in conditions where the number of iterations is equal to two or less, and slightly overestimated in conditions where the number of iterations is equal to three or more.

In short, we see that the minimum number of iterations required to obtain unbiased, confidence valid regression estimates is 5. This value, however, is dependent on the percentage of missing values. E.g., with 95% of cases having missing data we need at least seven iterations to obtain unbiased results.

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## Discussion

This note shows that convergence diagnostics  $\hat{R}$  and  $AC$  may diagnose convergence of multiple imputation algorithms, but their performance differs from conventional applications to iterative algorithmic procedures. **(nope! it shows that MICE can lead to correct outcomes when they have not converged according to two common conv diags. This may be due to the measures (e.g., assumption of overdisp) or due to the Qs (lm reg coeff, not higher dimensional/more complex RQs). Add what %miss has to do with it.)**

$\hat{R}$  and autocorrelation indicate that algorithmic convergence may only be reached after twenty or even forty iterations, while unbiased, confidence valid estimates may be obtained with as little as four iterations. These results are in agreement with the simulation hypothesis:  $\hat{R}$  over-estimates the severity of non-convergence when applied to MI procedures. %This may be due to the quantity of scientific interest chosen. More ‘complicated’  $Q$ s (e.g., higher order effects or variance components) might show bias, under- or over-coverage at higher  $T$ .

According to this simulation study, the recently proposed threshold of  $\hat{R} < 1.01$  may be too stringent for MI algorithms. **(This is only one of the goals: to give applied researchers a diagnostic to indicate that they should keep iterating. The other is the default in mice and other software packages, and yet another is ... i forgot)** Under the relatively easy missing data problem of the current study, the threshold was not reached. The other extreme of the  $\hat{R}$ -thresholds, the conventionally acceptable  $\hat{R} < 1.2$ , may be too lenient for MI procedures. Applying this threshold to the current data, lead to falsely diagnosing convergence at  $T = 3$  **(because it goes up after, not because it is not converged enough)**. It appears that the widely used threshold of  $\hat{R} < 1.1$  suits MI algorithms the best. We might, however, also formulate a new threshold, specifically

for the evaluation of MI algorithms. The current study suggests that  $\hat{R} < 1.05$  may be implemented, since that is the level at which the  $\hat{R}$  stabilize (around  $T = 20$ ) (**Not necessary for this Q, but maybe for more complicated Qs**).

The negative  $AC$ -values obtained in this study show no threat of non-stationarity. However, initial dip in  $AC$ -values may have implications for the default number of iterations in mice ( $\text{maxit} = 5$ ). Terminating the algorithm at  $T = 5$  may not be the most appropriate, since this lead to the worst convergence (**nope, only for Rh, not AC**), as indicated by  $\hat{R}$  and  $AC$ . Under the current specifications,  $T > 20$  would be more appropriate.

The observed dip in  $AC$  implies that default  $\text{maxit}$  value of five iterations is the worst possible number of iterations. Moreover, the results of this study imply that assessing the stationarity component of convergence with  $AC$  might be redundant.

Further research is needed to investigate their performance under clear violation of convergence, e.g. dependency between predictors (predictors with very high correlations). Until then, we have only shown that the convergence diagnostics can diagnose non-convergence of MI algorithms that trend towards a converged state. Also for future research, look at developing a convergence diagnostic for substantive models, and implement a Wald test for  $AC = 0$ .

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