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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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known as 'multiple imputation' (MI; Rubin 1976), and requires an additional step to pool the results across imputations. 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? How many iterations are sufficient/needed to reach convergence? Are the default number of iterations sufficient (i.e., 5 in mice, 10 in SPSS and Stata, 30 in mi)? What are the effects of continued iterations on estimates, predictions and inferences? And finally, do the answers differ with varying missingness proportions?

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 ($m = 1, \dots, M$) and T is the number of iterations ($t = 1, \dots, T$). 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**

Convergence diagnostics

The two challenges for convergence of iterative algorithms are mixing and stationarity (Gelman et al. 2013), see Figure 1. 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 $\widehat{R}$ ('Gelman-Rubin statistic'; Gelman and Rubin 1992). With a recently proposed adaptation, $\widehat{R}$ 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 $\widehat{R}$ will be used.

Potential scale reduction factor

To define $\widehat{R}$, 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 θ 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 θ, and average these to obtain within-chain variance W.

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

We then estimate between-chain variance B as the variance of the collection of average θ 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 θ. $\widehat{R}$ 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 θ could be shrunken 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 $T \to \infty$. 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 θ-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 θ-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 θ-values of subsequent iterations diverge from one-another, which may increase the variance of θ 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. 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.**

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 ($\widehat{R} = 1$).

Simulation Hypothesis

This study evaluates whether $\widehat{R}$ 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 $\widehat{R}$ will over-estimate non-convergence of MI algorithms. The threshold of $\widehat{R} < 1.01$ will then be too stringent for diagnosing convergence. This over-estimation may, however, be diminished because $\widehat{R}$ 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 $\widehat{R}$. **(Add actual hypothesis: we thought that mice would converge sooner than $\widehat{R}$ would indicate that it did)** No hypothesis was formulated about the performance of AC as convergence diagnostic.

Simulation study

The convergence of `mice` 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.

```
# pseudo-code of simulation
simulate data
for (number of simulation runs from 1 to 1000)
  for (number of iterations from 1 to 100)
    create missingness
    impute the missingness
    compute convergence diagnostics
    perform analysis
    pool results
    compute simulation diagnostics
aggregate convergence and simulation diagnostics
```

(Add step for different missingness proportions.)

A finite population of $N = 1000$ is simulated to 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 data generating model is a multivariate normal distribution

$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ \epsilon \end{pmatrix} \sim N \left[\begin{pmatrix} 12 \\ 3 \\ 0.5 \\ 0 \end{pmatrix}, \begin{pmatrix} 4 & 4 & 1.8 & 0 \\ 4 & 16 & 4.8 & 0 \\ 1.8 & 4.8 & 9 & 0 \\ 0 & 0 & 0 & 100 \end{pmatrix} \right]$$

Outcome variable Y is subsequently calculated as

$$Y = 1 + 2X_1 + .5X_2 - X_3 + \epsilon.$$

(Add the function `mvtnorm::rmvnorm()` back in somewhere here? If yes, use citation("mvtnorm").)

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 $\widehat{R}$ 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` $= 1, 2, \ldots, 100$).

$\widehat{R}$ (**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, $\bar{Q}$. We use the function `mice::pool()` to estimate u bar (**check wat dat nou precies is!!**) according to Rubin's (1987) rules, and subsequently implement finite population pooling conform Vink and van Buuren (2014).

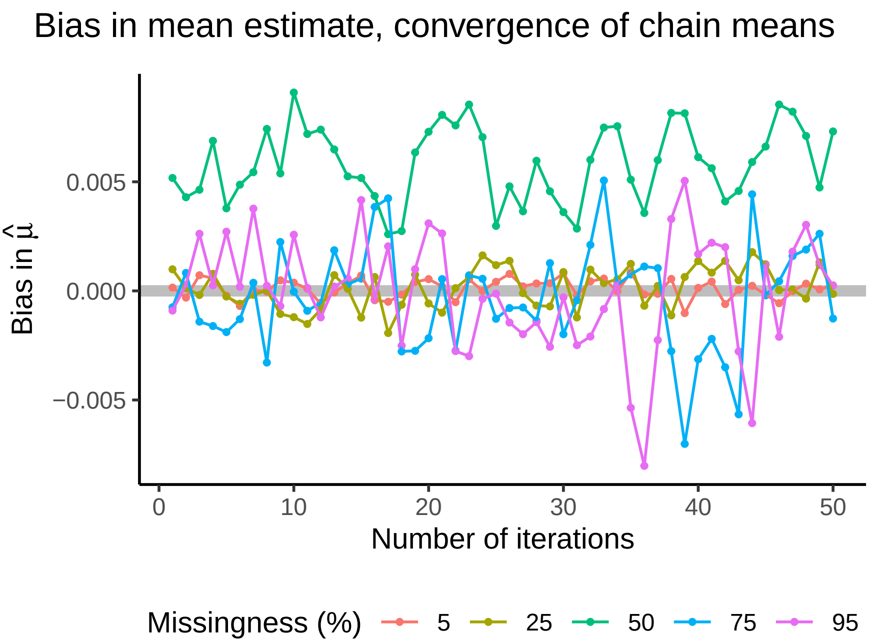
We compute bias as the difference between Q and $\bar{Q}$. Confidence interval width (CIW) is defined as the difference between the lower and upper bound of the 95% confidence interval (CI95%) around $\bar{Q}$. We compute the CI95% bounds as

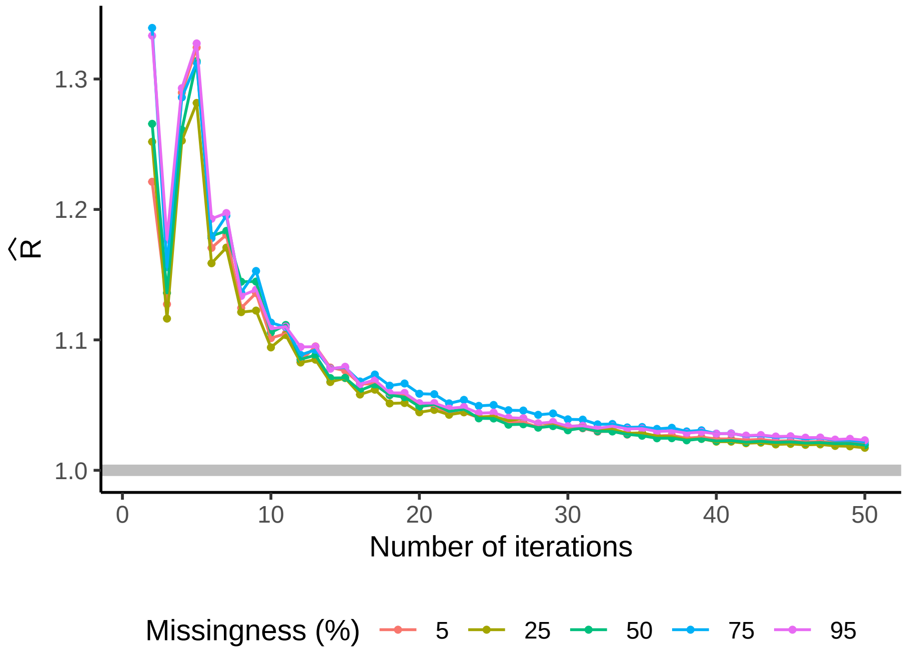
$$\bar{Q} \pm t_{(m-1)} \times SE_{\bar{Q}},$$

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 $\bar{Q}$.

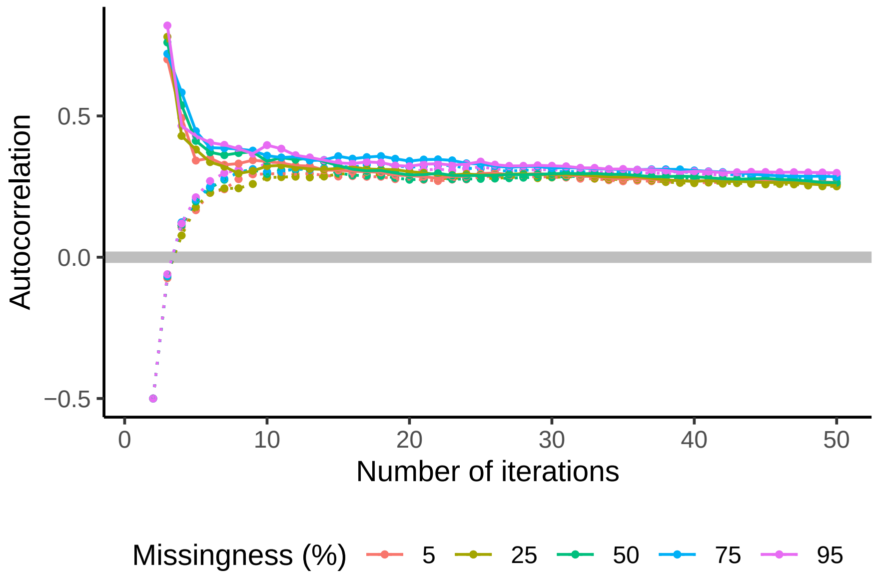
Results

(Add more info about figure legends and axes.)





Dotted lines are old AC computation, solid are new.



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, $\widehat{R}$ indicates that the mice algorithm does not reach a converged state ($\widehat{R}$ = 1) in any of the simulation conditions. Neither is the most recent recommended threshold reached ($\widehat{R} < 1.01$). The conventional $\widehat{R}$ 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 $T = 30$.

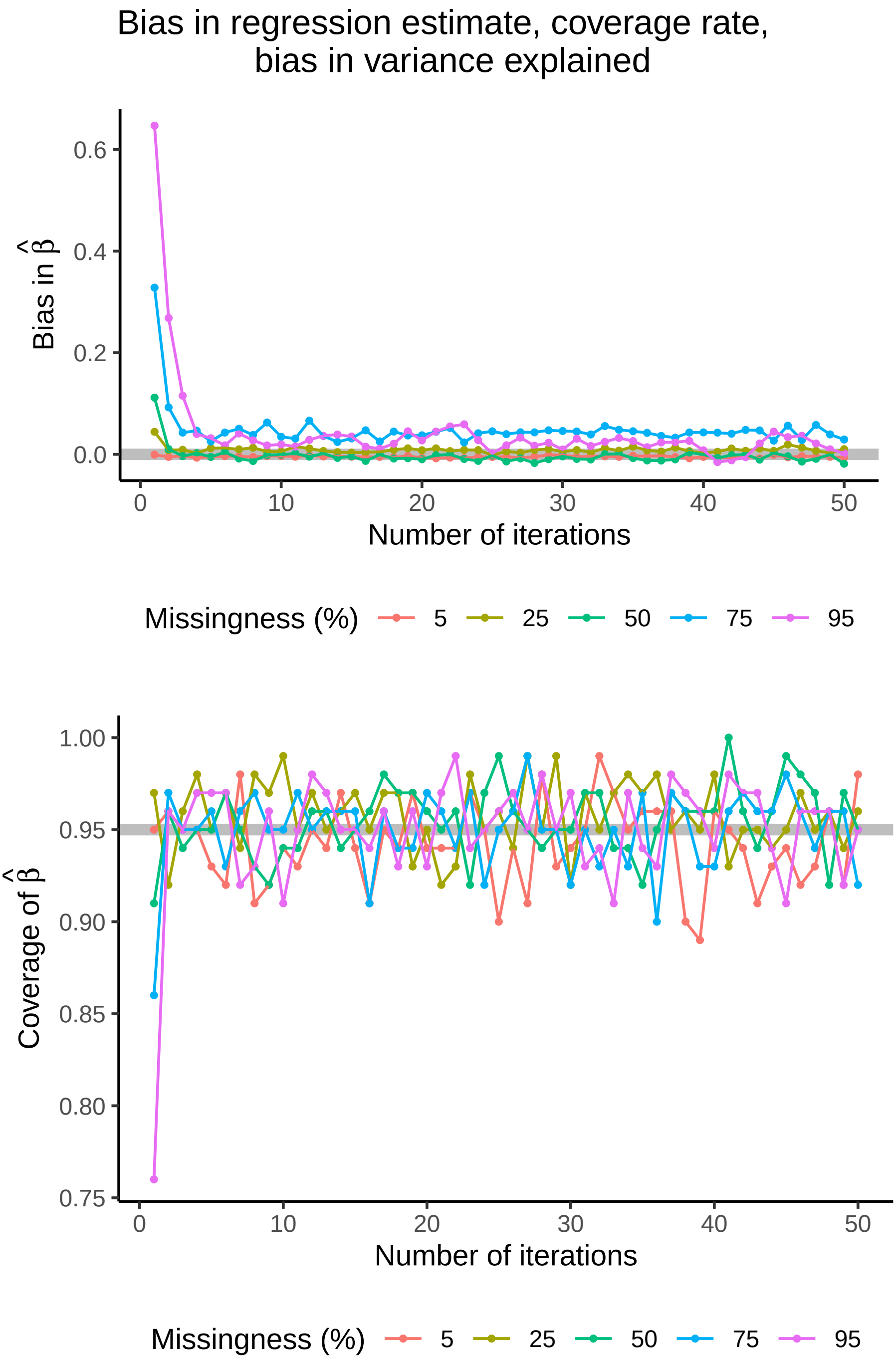
Auto-correlations indicate no sign of trending within imputation chains. In most simulation conditions AC is smaller than or about equal to zero. Across simulation conditions, however, the autocorrelation curve does not trend towards 0. Autocorrelation values plateau off at a value of around .1 . This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

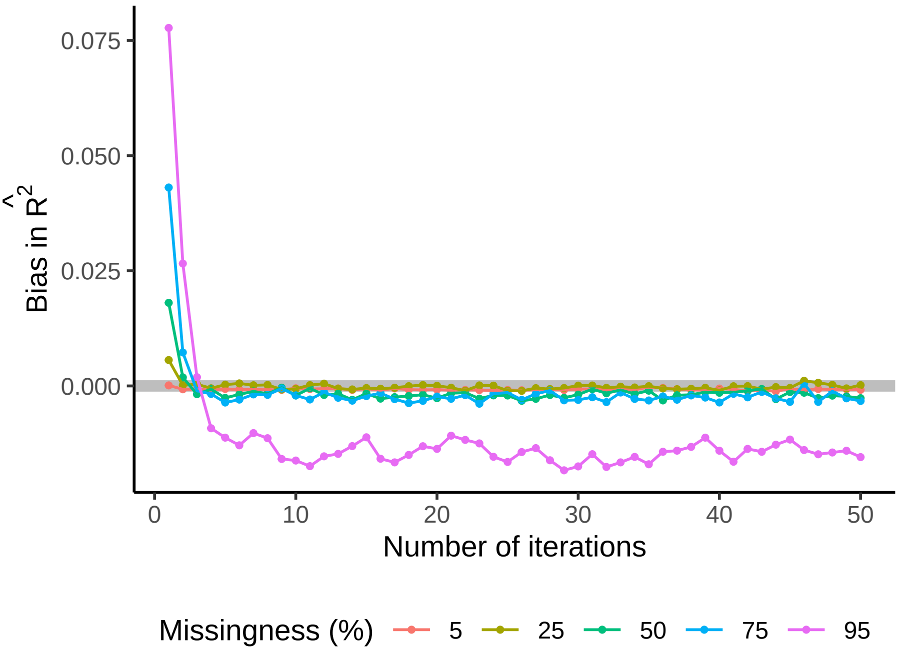
The $\widehat{R}$ and AC values for the imputation chain variances show equal trends and are therefore not discussed separately. Taken together, univariate estimates seem robust across simulation conditions. There is no clear effect of the number of iterations on the bias in these estimates, while the 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 underestimate estimated 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.


Bias in regression estimate, coverage rate,
bias in variance explained
Bias in β̂
0.6
0.4
0.2
0.0
0
10
20
30
40
50
Number of iterations
Missingness (%)
5
25
50
75
95
Coverage of β̂
1.00
0.95
0.90
0.85
0.80
0.75
0
10
20
30
40
50
Number of iterations
Missingness (%)
5
25
50
75
95



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 $\widehat{R}$ 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.**)
$\widehat{R}$ and autocorrelation indicate that algorithmic convergence may only be reached after twenty or even forty iterations, while unbiased, confidence valid estimates estimates may be obtained with as little as four iterations. These results are in agreement with the simulation hypothesis: $\widehat{R}$ 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' Qs (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 $\widehat{R} < 1.01$ 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 $\widehat{R}$-thresholds, the conventionally acceptable $\widehat{R} < 1.2$, 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 $\widehat{R} < 1.1$ 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 $\widehat{R} < 1.05$ may be implemented, since that is the level at which the $\widehat{R}$ 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` (`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 $\widehat{R}$ and AC. Under the current specifications, $T > 20$ would be more appropriate.

The observed dip in AC implies that default 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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