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

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## Abstract

Iterative imputation is a popular tool to accommodate missing data. While it is widely accepted that valid inferences can be obtained with this technique, these inferences all rely on algorithmic convergence. There is no consensus on how to evaluate the convergence properties of the method. This paper provides insight into identifying non-convergence of iterative imputation algorithms.

## Keywords

missing data, iterative imputation, non-convergence, mice

## Introduction

Anyone who analyzes person-data may run into a missing data problem. Missing data is not only ubiquitous, but treating it can also be tedious. If a dataset contains just one incomplete observation, statistical inferences are undefined and will not produce any results. To circumvent this, many statistical packages employ list-wise deletion by default (i.e., ignoring incomplete observations). Unfortunately, this *ad hoc* solution may yield wildly invalid results (Van Buuren 2018). An alternative is to *impute* (i.e., fill in) the missing values in the incomplete observations. Subsequently, statistical inferences can be performed on the completed dataset. By repeating this process several times, a distribution of plausible results may be obtained, which reflects the uncertainty in the data due to missingness. This technique is known as ‘multiple imputation’ (MI; Rubin 1976). MI has proven to be a powerful technique to yield unbiased and confidence

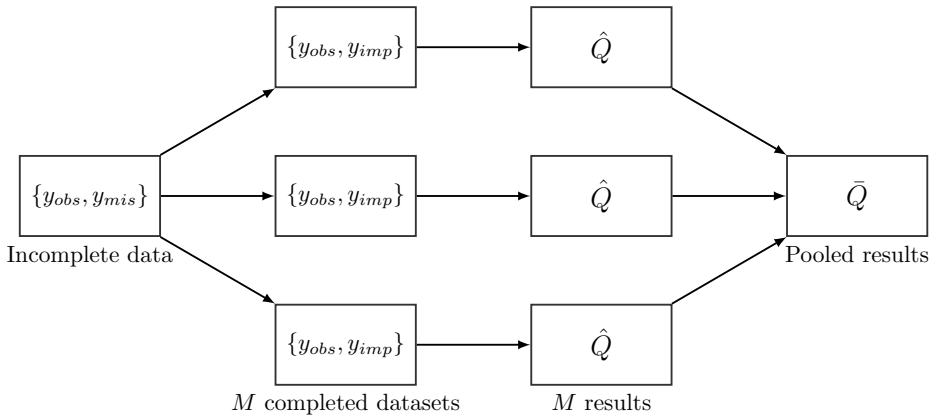
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**Figure 1.** Scheme of the main steps in multiple imputation.

valid estimates of the true—but missing—data inference under many circumstances (Van Buuren 2018).

Figure 1 provides an overview of the steps involved with MI—from incomplete data, to  $M$  multiply imputed datasets, to  $M$  estimated quantities of interest  $\hat{Q}$ s, to a single pooled estimate  $\bar{Q}$ . Missing data in dataset  $y$  is imputed  $M$  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 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  $\bar{Q}$ .

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 how to evaluate convergence 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.

Currently, the recommended practice for evaluating convergence in iterative imputation algorithms is to visually inspect imputations for signs of non-convergence. **Add that this refers to chain means and variances already? It’s insufficient that these are univariate, so multivariate state space of the algorithm may not be converged when univariates are ok. And Van Buuren (2018)’s suggestion to track**

user-defined statistics (e.g., regression coefficient) may be somewhat advanced for empirical researchers. Moreover, this is not model-independent, i.e., only apply to one substantive model, while one of the advantages of MI is that missing data problem and scientific problem are split. Then we can say 'we propose a novel...' and integrate this: Note that usually we only evaluate the convergence of univariate scalar summaries (e.g., chain means or variances). With these we cannot diagnose convergence of multivariable statistics (i.e., relations between scalar summaries). Van Buuren (2018, § 4.5.2) proposed to implement multivariable evaluation of the MICE algorithm through eigenvalue decomposition building on the work of MacKay and Mac Kay (2003). Eigenvalues of a covariance matrix are a measure of the data's covariance..

This method 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. Yet, monitoring convergence of iterative imputation algorithms diagnostically is challenging. Iterative imputation algorithms such as MICE are Markov chain Monte Carlo (MCMC) methods. In MCMC methods, 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 is not to establish the point at which convergence is reached, but to monitor signs of non-convergence (Hoff 2009). Several of such diagnostics exist for MCMC methods, but it is not known whether these are appropriate for iterative imputation algorithms.

In this paper, we investigate how non-convergence in iterative imputation algorithms may be diagnosed, how well these methods perform, and at which point convergence may safely be assumed. For reasons of brevity, we only focus on the iterative imputation algorithm implemented in the popular `mice` package (Van Buuren and Groothuis-Oudshoorn 2011) in R (R Core Team 2020). The convergence properties of the MICE 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.

**Include sub-questions!** How can non-convergence be identified diagnostically? 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`)? **How severe is it when the algorithm has not converged? And what are guidelines for practice? Can the parameter of interest, estimand  $Q$ , be correct when the algorithm is not (yet) converged, and vice versa?** *(Maybe add these too? What are the effects of continued iterations on estimates, predictions and inferences? 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).)*

### Some notation

Let  $y$  denote an  $n \times k$  matrix containing the data values on  $k$  variables for all  $n$  units in a sample. The data value of unit  $i$  ( $i = 1, 2, \dots, n$ ) on variable  $j$  ( $j = 1, 2, \dots, k$ ) may be either observed or missing. **The number of units  $i$  with at least one missing data value can be divided by the total number of units  $n$  to obtain the ‘missingness proportion’  $p_{mis}$ .** 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:  $\theta$ s are scalar summaries of interest in the iterative algorithm (e.g., chain means; the average of the imputed values in each imputation chain).**

### Identifying non-convergence

The goal of imputation through e.g. FCS/MICE is to obtain a multivariate distribution by iterating over the sequence of univariate imputations. Traditionally, the inspection of the multivariate convergence is done by visually inspecting the univariate chain means and variances over the iterations, or by tracking the Rhat and autocorrelation. The downside to these approaches is that they either focus on the univariate state space, or primarily track the change over the iterations of a multivariate outcome conform the scientific model of interest. Focusing on the convergence of these outcome parameters may influence this procedure in the sense that the model of evaluation favors the model of interest. Ideally, one would like to evaluate a model-independent parameter that summarizes the multivariate nature of the data. We propose eigenvalue as such a parameter, because it...

Mixing and stationarity have historically been inspected visually, by evaluating traceplots of scalar summaries of interest ( $\theta$ s; e.g., chain means and chain variances). As [Van Buuren \(2018\)](#) describes, users can also specify a model-specific scalar summary (e.g., a regression coefficient). A user-specified scalar summary, however, is not universal to all complete data problems. Therefore, as inspired by ([MacKay and Mac Kay 2003](#)), we propose a  $\theta$  that summarizes the multivariate state space of the algorithm. Namely, the first eigenvalue of the variance-covariance matrix of the  $M$  completed datasets. **The first eigenvalue has the appealing property that is not dependent on the substantive model of interest.**

Since convergence of iterative imputation algorithms is in distribution, there is not a unique point at which the algorithm reaches a converged state. We can only evaluate scalar summaries of the multivariate state space of the algorithm,  $\theta$ s. The recommended scalar summaries to evaluate are chain means and chain variances. Additionally, researchers may “monitor some statistic of scientific interest” ([Van Buuren 2018](#), § 6.5.2). Because of the issues mentioned above, we propose a novel  $\theta$  to monitor: the first eigenvalue of the variance-covariance matrix of the completed data. Let  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_j$  be the eigenvalues of  $\Sigma$  in each of the  $M$  completed datasets  $y_{obs}, y_{imp}$ .  $\lambda_1$  is measure that summarises the covariances in the completed datasets.

There are two requirements for convergence of iterative algorithms: mixing and stationarity (Gelman et al. 2013). Without mixing, imputation chains do not intermingle nicely, **indicating that ...** Without stationarity, there is trending within imputation chains, which implies that further iterations would yield a different set of imputations.

To illustrate what non-convergence looks like in MI, we reproduce the example from van Buuren (2018, § 6.5.2). Figure 2 shows the traceplot for one of the variables in the example. we see the average of the imputed values for a variable  $j$  in  $y_{imp}$ . The average imputed values in the left hand plot are about a magnitude 2 lower than the right hand plot. So non-convergence has a impact on the average imputed value for  $j$  in  $y_{imp,m}$ . This difference (presumably) translates to bias in the pooled estimate  $\bar{\mu}_j$  as well. And maybe also to higher order statistics, e.g. variances, covariances, etc. Therefore, it's important to converge. **Explain what we see, namely example by Van Buuren (2018) reproduced, showing the traceplots of chain means for some variable. The first plot is typical convergence of MICE, the second is pathological non-convergence because of a mis-specified imputation model. Each line is an imputation. In the first plot, the chains intermingle nicely and there is little to no trending. In the second plot, there is a lot of trending and some chains do not intermingle. Importantly, the chain means at the last iteration (the imputed value per  $m$ ) are very different between the two plots. The algorithm with the mis-specified model yields imputed values that are on average a magnitude two larger than those of the typically converged algorithm. This shows the importance of reaching converged states in iterative imputation algorithms.**

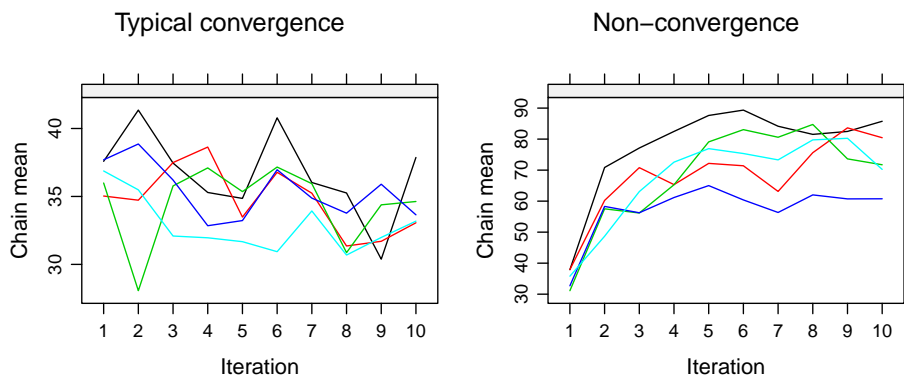
### Methods under evaluation

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, use we  $\hat{R}$  and  $AC$  to evaluate mixing and stationarity separately, as recommended by e.g., Cowles and Carlin (1996).

**Potential scale reduction factor** An updated version of  $\hat{R}$  has been proposed by Vehtari et al. (2019) (p. 5). **This version may be suitable for iterative imputation.** 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.



**Figure 2.** Typical convergence versus pathological non-convergence. Please note that this is the same data with a different imputation model, leading to different imputations (see the y axis!). Wel min of meer dezelfde origin op iteration 1.

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

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, or leave in**.  $\hat{R}$  is then obtained as a ratio between the over-estimated total variance and the within-chain variance:

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

We can interpret  $\hat{R}$  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  $\hat{R}$ -values will be close to one. High  $\hat{R}$ -values thus indicate non-convergence. The conventionally acceptable threshold for convergence was  $\hat{R} < 1.2$  (Gelman and Rubin 1992). More recently, Vehtari et al. (2019) proposed a more stringent threshold of  $\hat{R} < 1.01$ .

**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.

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

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. Negative  $AC$ -values indicate divergence within imputation chains. **Subsequent sampled values within each imputation chain are less alike.** 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. **Maybe remove:** Moreover, the magnitude of  $AC$ -values may be evaluated statistically, but that is outside of our scope.

### *In practice*

Before using them in the simulation, the two methods show at least be able to distinguish between the two algorithms plotted in Figure 2. From visual inspection we know that the typical convergence has some signs of non-mixing around iteration 2, and little trending. In the non-convergence situation, there is a lot of trending upto iteration 6, after which the chains reach a somewhat more stationary state. Mixing in this situation gets worse from the first iteration onward, and gradually gets better around iteration 7. To assess whether  $\hat{R}$  and  $AC$  may be appropriate non-convergence identifiers for iterative imputation algorithms, the following condition must hold: the methods indicate worse performance for the mis-specified model with pathological non-convergence (i.e., higher  $\hat{R}$ - and  $AC$ -values than the typical performance). And additionally the methods should reflect the increasing convergence in the typical convergence situation as the number of iterations goes up.

In Figure 3A, the chain means from Figure 2 are plotted again, now together—as are the non-convergence diagnostics. Panel B shows  $\hat{R}$  as computed by implementing [Vehtari et al. \(2019\)](#)’s recommendations. As required,  $\hat{R}$  indicates less signs of non-convergence as the number of iterations goes up in the typical convergence situation. The superior performance of the typical convergence over the pathological non-convergence is less prominent, even flipped for  $t < 4$ . Panel C displays the  $AC$  as computed with the R function `stats::acf()`. When we look at this panel, we conclude something weird. The  $AC$ -values indicate equal performance (up-to  $t = 5$ ) for the typical convergence and the pathological non-convergence, while there is obvious trending in the latter. Moreover, the best convergence (as indicated by the lowest  $AC$ -value) is observed at  $t = 2$ , but looking at the chain means in panel A, there should be some signs of trending up-to iteration

number seven. After consulting the documentation on `stats::acf()` (R Core Team 2020), we conclude that this implementation of  $AC$  is not suitable for iterative imputation algorithms. There is a correction factor for a mathematical shortcut that works in the limit. According to Box et al. (2015), the function works when the number of iterations  $> 50$ . The default number of iterations in iterative imputation, however, is often much lower. Therefore, we compute  $AC$  manually, see panel D. The  $AC$  values in this plot do meet the requirements (...) and will therefore be used in the simulation study.

**acf is niet bedoeld om weinig iteraties te... niet een fout in acf, alleen hier niet van toepassing**

We assume that complete convergence, defined as  $\hat{R} = 1$  and  $AC = 0$ , will not be observed. Because even in the most converged state, the algorithm will show some signs of non-mixing and non-stationarity. Upon *sufficient* convergence, the imputation chains will intermingle such that the only difference between the chains is caused by the randomness induced by the algorithm ( $\hat{R} > 1$ ), and there may be some dependency between subsequent iterations of imputation chains ( $AC > 0$ ).

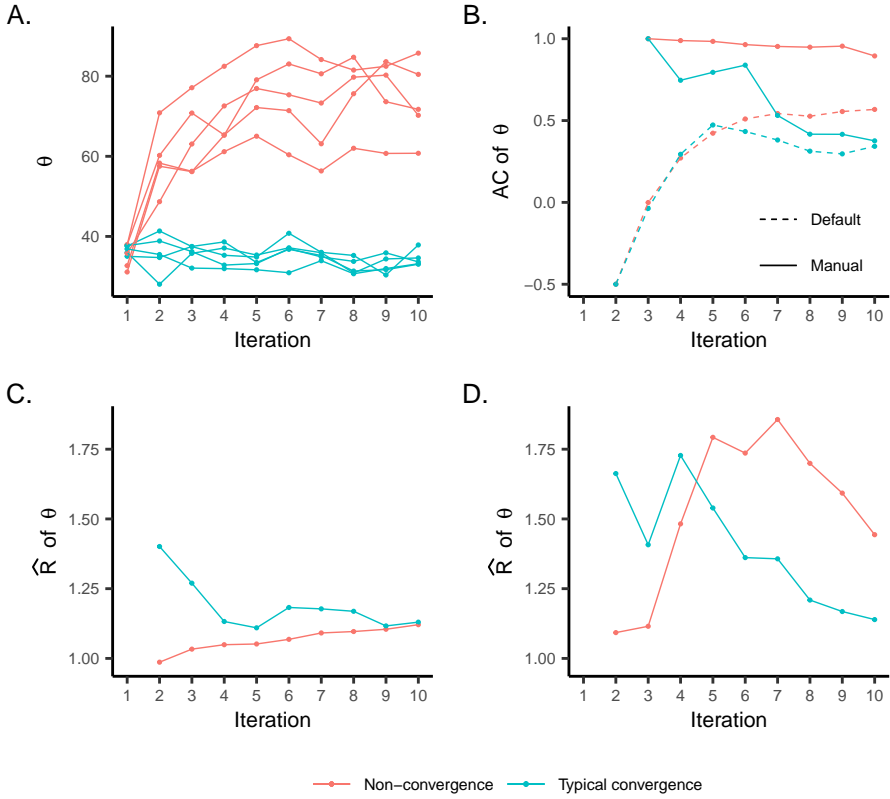
## Simulation study

The aim of the simulation study is to evaluate the impact of inducing non-convergence in the MICE algorithm on several quantities of scientific interest  $Q$ . Subsequently we will evaluate how well  $\hat{R}$  and  $AC$  perform in identifying the effects of non-convergence. And finally, we will formulate an informed advice on the requirements to safely assume *sufficient* convergence in practice. That is, we assume that the algorithm is *sufficiently* converged when each estimate  $\bar{Q}$  is an unbiased and confidence valid estimate of the corresponding estimand  $Q$ .

Non-convergence will be induced by: 1) increasing the missingness proportion  $p_{mis}$  in dataset  $y$  incrementally, and 2) terminating the imputation algorithm at a varying number of iterations  $T$ . The first set of simulation conditions—the missingness proportions—is chosen to reflect the difficulty of the missingness problem. The underlying assumption is that low missingness proportions lead to quick algorithmic convergence, since there is a lot of information in the observed data. Higher missingness proportions should yield slower convergence. Unless, however, the fraction of missing information is so high that the random component in the imputation algorithm outweighs the information in the observed data. Then, convergence to a stable but highly variable state may be reached instantaneously. We assume that the incremental missingness proportions in our study will result in a corresponding increase in signs of non-convergence.

The assumption inherent to the second set of simulation conditions—the number of iterations—is that terminating the imputation algorithm too early causes non-convergence. Generally, the algorithm will not reach convergence if  $T = 1$ , because the imputed values in the first iteration (at  $t = 1$ ) depend on the initial values of the algorithm (which are sampled randomly from the set of observed datapoints). As the number of iterations increases, the imputation chains should become independent of the initial values, until the point at which adding an extra iteration does not lead to a more





**Figure 3.** Convergence diagnostics applied on the imputation algorithms of Figure 2.  $\theta$  = chain mean in  $y_{imp,m}$ .

converged state. We assume that we can induce non-convergence at least in conditions where  $T$  is smaller than the default number of iterations in `mice`,  $T = 5$ .

### Hypotheses

1. We expect that simulation conditions with a high missingness proportion  $p_{mis}$  and a low number of iterations  $T$  will result in biased, invalid estimates of the quantities of scientific interest,  $Q_s$ .
2. We hypothesize that  $\hat{R}$  and  $AC$  will correctly identify signs of non-convergence in those simulation conditions where the  $\hat{Q}_s$  are *not* unbiased and confidence valid estimates of the  $Q_s$ .
3. We hypothesize that the recommended thresholds to diagnose non-convergence with  $\hat{R}$  ( $\hat{R} > 1.2$ ,  $\hat{R} > 1.1$ , and  $\hat{R} > 1.01$ ) may be too stringent for iterative

imputation applications. In an empirical study, where  $\hat{R}$  was used to inform the required imputation chain length, it took as many as 50 iterations to overcome the conventional non-convergence threshold  $\hat{R} > 1.2$ . Yet, scientific estimates were insensitive to continued iteration after  $t > 5$  (Lacerda et al. 2007). We therefore suspect that  $\hat{R}$  may over-estimate signs of non-convergence in iterative imputation algorithms. In contrast to this, it may occur that the signs of non-convergence are under-estimated by  $\hat{R}$ , in exceptional cases where the initial values of the algorithm are not appropriately over-dispersed (Brooks and Gelman 1998, p. 437). In e.g. mice, initial values are chosen randomly from the observed data, hence we cannot be certain of over-dispersion in the initial values. In practice, we do not expect this to cause problems for identifying non-convergence with  $\hat{R}$ .

4. We expect that high  $AC$  values are implausible in iterative imputation algorithms with typical convergence. That is, after only a few iterations, the randomness induced by the algorithm will effectively mitigate the risk of dependency within chains.

## Set-up

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

**Data-generating mechanism.** In this study, sampling variance is not of interest. Therefore, a single complete dataset may serve as comparative truth in all simulation repetitions (Vink and van Buuren 2014). The data-generating mechanism is a multivariate normal distribution, representing person-data on three predictor variables in a multiple linear regression problem (from an unspecified social scientific field of study). Let the

predictor space be defined as

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

A finite population of  $N = 1000$  is simulated using the `mvtnorm` package (Genz and Bretz 2009). Subsequently, a fourth variable is constructed as outcome  $Y$ . For each unit  $i = 1, 2, \dots, N$ , let

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

where  $\epsilon \sim \mathcal{N}(0, 100)$ . From the complete set, we obtain the true values of each quantity of scientific interest  $Q$ .

**Scientific estimands.** We consider four types of  $Q$ s that are often of interest in empirical research. Namely, two descriptive statistics: the mean  $\mu_j$  and standard deviation  $\sigma_j$  of each variable  $j = Y, X_1, X_2, X_3$ . We also consider the regression coefficients of the predictors:  $\beta_1, \beta_2$ , and  $\beta_3$  in regression equation

$$Y' = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3,$$

where  $Y'$  is the expected value of the outcome. And finally, the proportion of variance explained by the set of predictors: coefficient of determination  $r^2 \times 100$  (**note that lower case  $r$  is used to avoid confusion with non-convergence diagnostic  $\hat{R}$** ). The true values of these scientific estimands are calculated with the R functions `base::mean()`, `stats::sd()`, and `stats::lm()` (R Core Team 2020). Each of these  $Q$ s is estimated with a corresponding  $\hat{Q}$ , after the complete dataset is first *amputed* (with a varying missingness proportion  $p_{mis}$ ) and subsequently imputed (with a varying number of iterations  $T$ ).

**Methods.** The complete dataset is amputed with the `mice` package (function `mice::ampute()`; Van Buuren and Groothuis-Oudshoorn 2011). All missingness is multivariate, and conform a ‘missing completely at random’ missingness mechanism (Rubin 1987). I.e., the probability to be missing is the same for all  $N \times k$  cells in  $y$ , conditional on the missingness proportion ( $p_{mis} = .05, .25, .5, .75, .95$ ).

Missing datapoints in  $y$  are imputed with the `mice()` function (Van Buuren and Groothuis-Oudshoorn 2011). All imputation procedures are performed with Bayesian linear regression imputation, and five imputation chains ( $M = 5$ ). The number of iterations varies between simulation conditions ( $T = 1, 2, \dots, 100$ ).

After each run of the `mice` algorithm, the function `mice::complete()` is used to combine the imputed data  $y_{imp,m}$  with the observed data  $y_{obs}$ , resulting in five completed datasets  $\{y_{obs}, y_{imp,m}\}$ , where  $m = 1, 2, \dots, 5$ .

- on the 5 imputations  $y_{imp,m}$ : get mean and var within imp chains as theta to compute conv diag -> then complete with `mice::complete()`

- on the 5 completed datasets  $\{y_{obs}, y_{imp,m}\}$ : 1) estimate Qhats for mu and sigma  $\rightarrow$  pool as mean()  $\rightarrow$  get Qbars of mu and sigma; 2) compute lambda as theta for conv diag; 3) perform lm to get Qhats for betas and  $r^2$   $\rightarrow$  use Qhats of beta as theta to compute conv diag  $\rightarrow$  pool Qhats of beta and  $r^2$  to get Qbars

The estimator for each  $Q$  is  $\bar{Q}$ —the pooled aggregate of the  $\hat{Q}$ s across imputations. To calculate the  $\bar{Q}$ s, we combine the observed data  $y_{obs}$  and the imputed data for each imputation  $y_{imp,m}$  with the function `mice::complete()`. Descriptive statistics are computed as the average across imputations for each variable ( $\mu_j$  and  $\sigma_j$ , where  $j = Y, X_1, X_2, X_3$ ). Estimated regression coefficients are obtained with the function `stats::lm()` for each imputation, and then pooled conform [Vink and van Buuren \(2014\)](#). The coefficient of determination is estimated for each imputation, and pooled using `mice::pool.r.squared()`.

For each run of the imputation algorithm, we compute non-convergence diagnostics  $\hat{R}$  and  $AC$ . We calculate  $\hat{R}$  by implementing Vehtari et al.'s (2019) recommendations, and  $AC$  as the correlation between the  $t^{th}$  and the  $(t + 1)^{th}$  iteration. The two methods are applied to four scalar summaries  $\theta$ : chain means (i.e., the mean in each  $y_{imp,m,j}$ ), chain variances (i.e., the variance in each  $y_{imp,m,j}$ ), a statistic of scientific interest  $\hat{Q}$  in each  $\{y_{obs}, y_{imp,m}\}$ , and the first eigenvalue of the variance-covariance matrix in each  $\{y_{obs}, y_{imp,m}\}$ ,  $\lambda_1$ .

The  $\hat{R}$  and  $AC$  values with chain means as  $\theta$ s are evaluated against the bias in univariate mean estimates. Similarly, the performance measure for  $\hat{R}$  and  $AC$  applied to chain variances is the bias in estimated standard deviations. To evaluate the performance of  $\hat{R}$  and  $AC$  on the eigenvalues, we will use bias in the coefficient of determination,  $R^2$ . Additionally, we will evaluate the estimated regression coefficients, the coverage rate of the CI95% of the regression estimates, and the CI length (see **definitions in old Methods**). **remove the term performance measure here and add an extra paragraph to define performance measures as bias in all estimands, and coverage rate and CI length of regression coefficients.**

**Performance measures.** The impact of inducing non-convergence in the iterative imputation algorithm is assessed by comparing  $\bar{Q}$ s with  $Q$ s. For each  $Q$ , we compute bias as  $\bar{Q} - Q$ . For the regression coefficients  $Q = \beta_{1,2,3}$ , we also compute the empirical coverage rate (CR). CR is defined as the percentage of simulation repetitions in which the 95% confidence interval (CI) around  $\bar{Q}$  covers the true estimand  $Q$ . Let

$$CI = \bar{Q} \pm t_{(M-1)} \times SE_{\bar{Q}},$$

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. Since under-estimating the variance of  $\bar{Q}$  may yield spurious inferences, we also inspect CI width (CIW): the difference between the lower and upper bound of the 95% confidence interval around  $\bar{Q}$ .

The performance of two methods is evaluated against the bias and confidence validity of the estimated  $Q$ s.

## Results

We want to know what the effect is of inducing non-conv of the bias in all  $Q$ s and the confidence validity of the betas. So we plot the bias for each  $Q$  against the number of iterations in the condition and the missingness proportion in the condition. We look at averages across simulation repetitions. Then, we want to know if conditions in which the  $Q$ s are affected by non-convergence (on average) are also identified by the conv diag. We do this by looking at the bias in  $Q$  against the

**Add to this section: 1) emphasize that the plots are averages across repetitions, not within MICE; 2) sample effects due to single complete dataset.**

For reasons of brevity, we only discuss the convergence diagnostics for the  $Q$  with the worst performance in terms of bias. For the descriptive statistics, the magnitude of the bias was the largest in  $Y$  (i.e.,  $j = Y$  in  $\mu_j$  and  $\sigma_j$ ). For the  $Q = \beta_j$ ,  $j = 2$  showed the worst performance (i.e., the effect of  $X_1$  on  $Y$ ).

As expected, conditions with a higher proportion of missingness and/or a lower number of iterations show more signs of non-convergence, as indicated by more extreme bias in the estimated  $Q$ s. Roughly speaking this means that MICE is indeed not converged as  $t = 1$ , and converges gradually as  $t$  increases. The point at which an additional iteration does not lead to an improvement of the estimates depends on the difficulty of the missingness problem—between XYZ and XYZ. This means that the algorithm has converged sufficiently (**under the current specifications**).

As required for a method to diagnose non-convergence, the values of  $\hat{R}$  follow a trend similar to the performance measures.  $\hat{R}$  values are generally lower in conditions with a higher number of iterations, and somewhat higher in conditions with a higher percentage of missing data. Autocorrelation values were indeed decreasing with a higher number of iterations.

Evaluation with the performance measures shows that  $\hat{R}$  and autocorrelation are conservative: they indicate signs of non-convergence in conditions where  $\bar{Q}$ s are unbiased and or confidence valid estimates of  $Q$ .

### *Old Results section*

**(Add more info about figure legends and axes.)**

### *Univariate estimates and convergence diagnostics*

The bias in the estimates of the variable means shows 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 ( $\hat{R} < 1.01$ ). **This is only for 75% missingness:** The conventional  $\hat{R}$  threshold of 1.2 is reached in simulation conditions

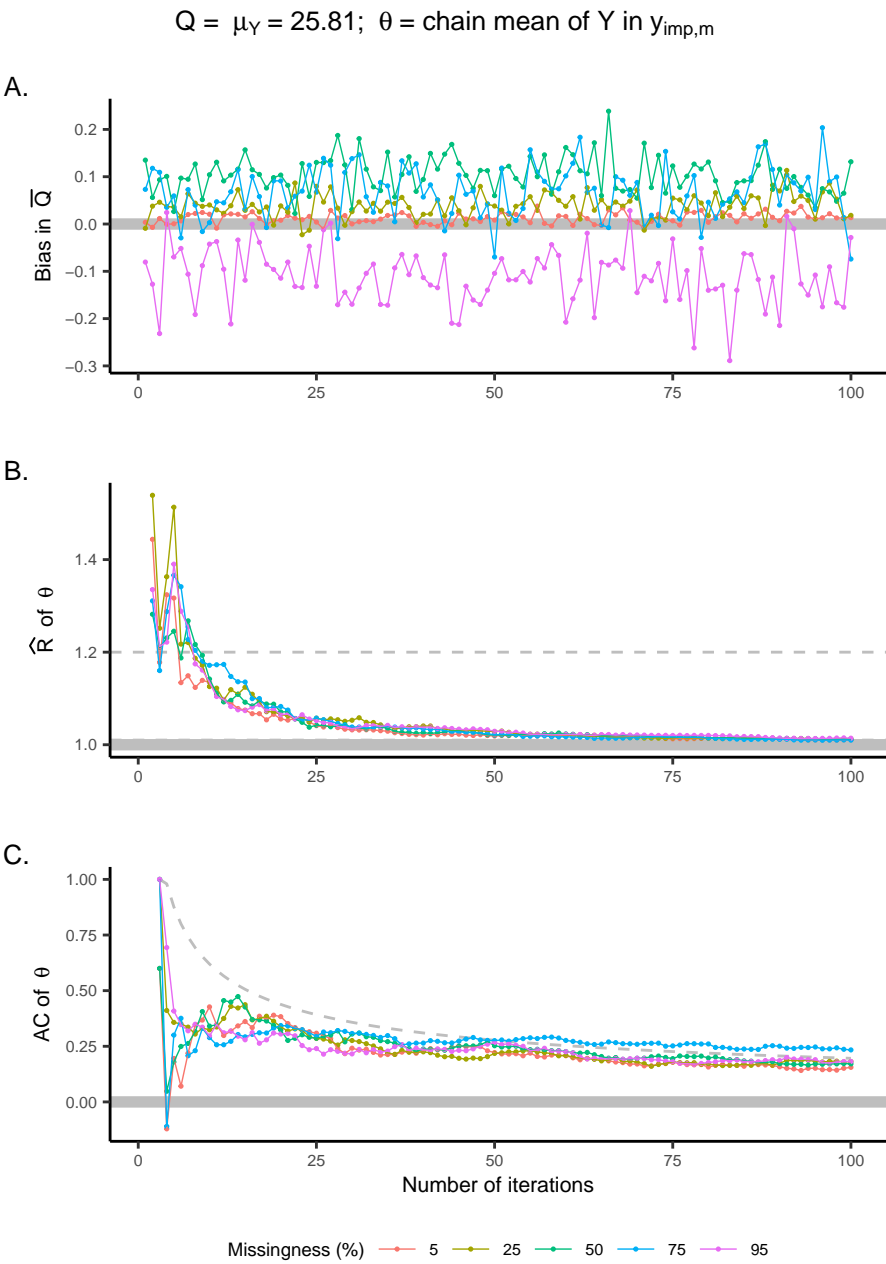
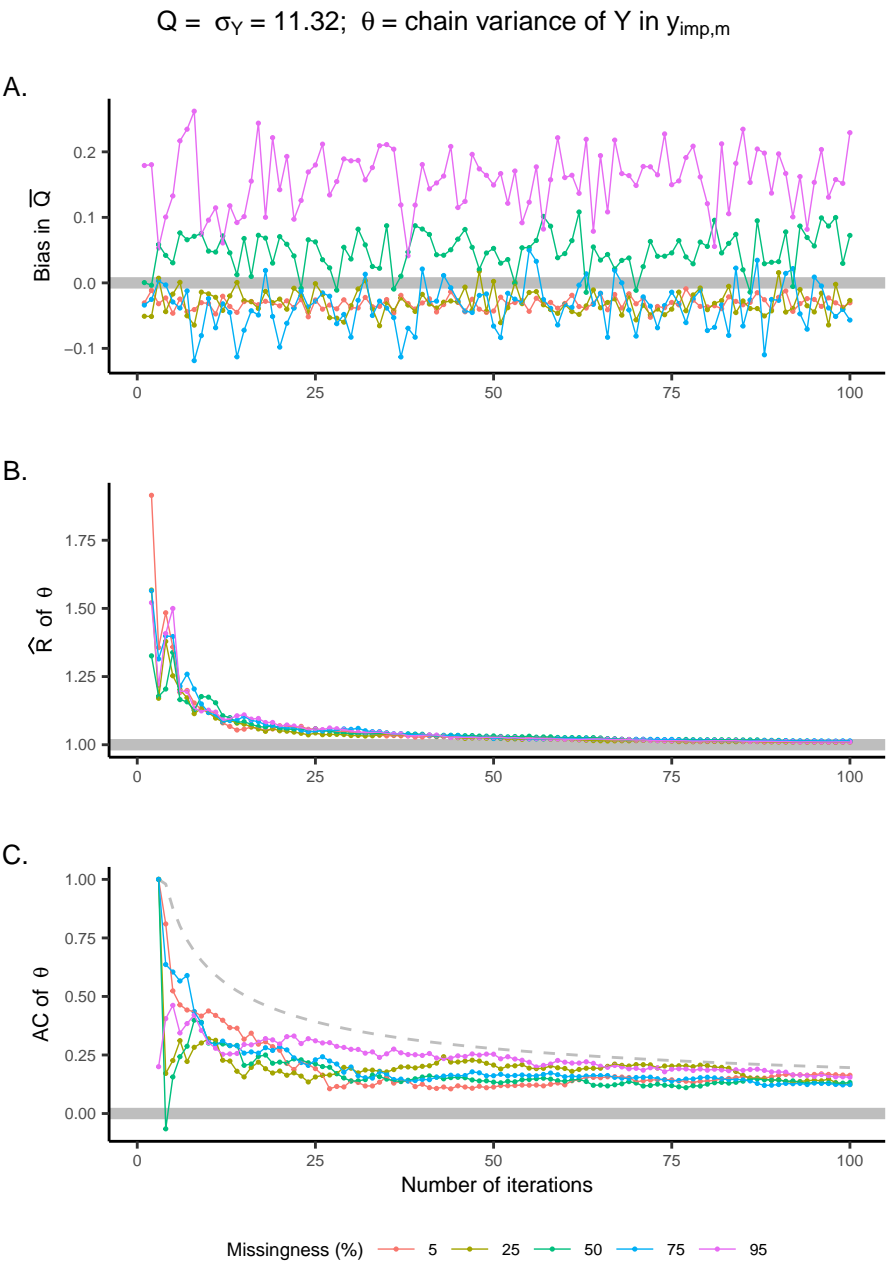
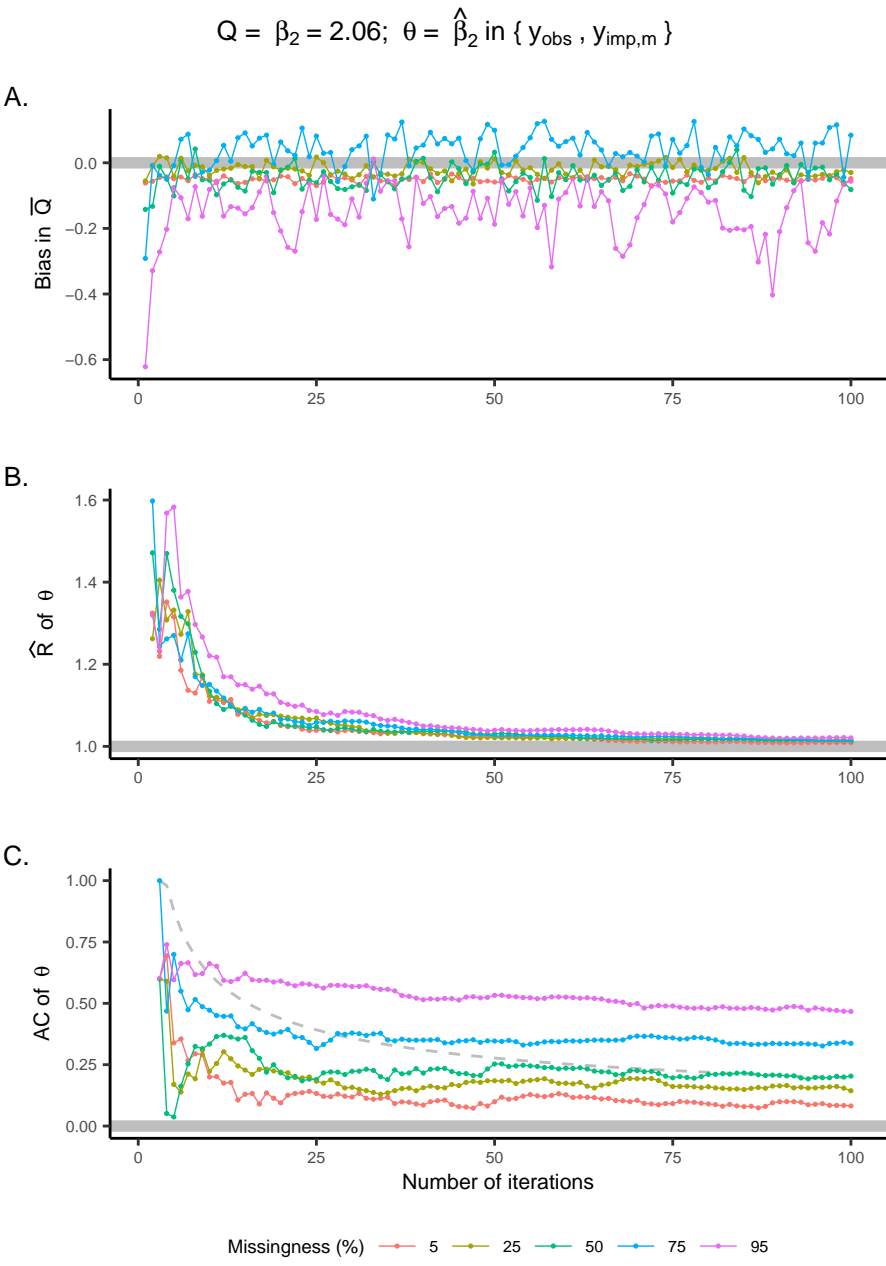


Figure 4. Convergence diagnostics chain mean.

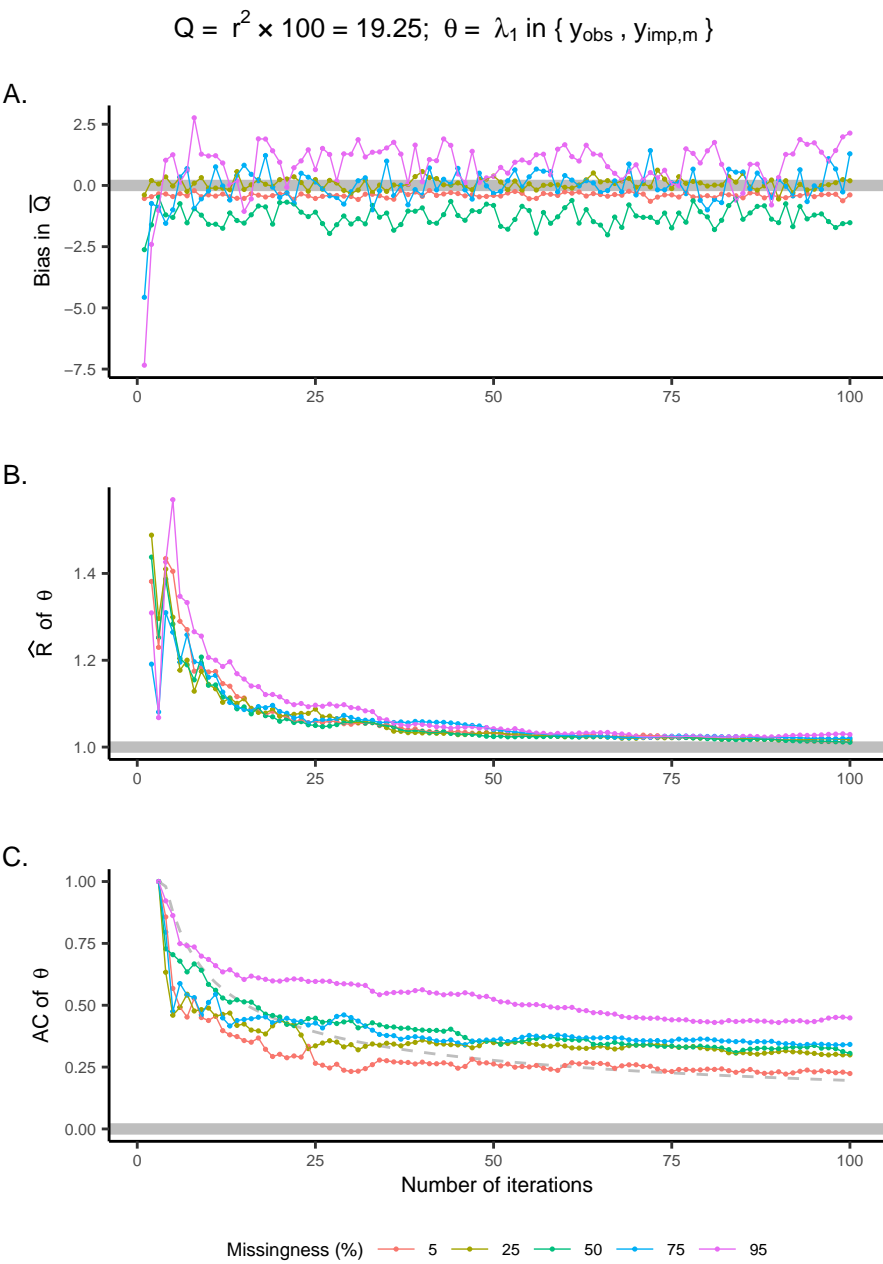


**Figure 5.** Convergence diagnostics chain variance.



**Figure 6.** Convergence diagnostics regression coefficient.





**Figure 7.** Convergence diagnostics regression coefficient.

$T = 3$  and  $T > 6$ . (With the default number of iterations ( $\text{maxit} = 5$ ), this dip in  $\hat{R}$  values would be spotted, so it is no problem.) The point at which an extra iteration does not seem to improve the  $\hat{R}$  value is around  $T = 30$ .

Autocorrelations indicate no sign of trending (**NOT correct anymore, fluke of the stats::acf() function!!**) 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 to the chain means 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

**This is only true for 75% missingness:** 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.

**This is only true for 75% missingness:** 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.

## Discussion

*Proper performance under a ‘missing completely at random’ missingness mechanism is necessary to demonstrate the appropriateness of  $\hat{R}$  and  $AC$  as non-convergence diagnostics. However, results may not be extrapolated to other missingness mechanisms.*

Upon convergence,  $\hat{R} = 1$  and  $AC = 0$ , which are unlikely thresholds for MCMC algorithms, because of its convergence to a distribution. In practice, non-convergence is usually diagnosed when  $\hat{R} > 1.2$  or 1.1 or even 1.01. And a t-test is performed to assess whether  $AC$  is significantly different from zero.

As expected, complete convergence ( $\hat{R} = 1$  and  $AC = 0$ ) is never observed. But what about the thresholds for practice?  $\hat{R} < 1.2$  is not stringent enough, because conditions in which  $\hat{R}$  is smaller than 1.2 do not all yield unbiased estimates of the  $Q$ s. Moreover, there is a dip in the  $\hat{R}$  values, after which  $\hat{R} > 1.2$  again. If the algorithms would be terminated at the iteration where  $\hat{R} < 1.2$  occurs for the first time, the increase in  $\hat{R}$  values might be missed. The threshold  $\hat{R} < 1.1$  is somewhat conservative in comparison with the performance measures. Overall it seems OK.  $\hat{R} < 1.01$  is too stringent compared to the performance measures. And it is not obtained for any number of iterations (**but may be necessary in more complex complete data models???**).

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, the initial dip in  $AC$ -values **(which disappeared!)** 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.

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  $AC = 0$ .

### *Recommendations for empirical researchers*

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 e.g., [GitHub link]). 4) Track your own scalar summary of interest. This is somewhat advanced but explained in Van Buren 2018. Compute  $\hat{R}$  and autocorrelation values for this scalar summary. 5) **Something** about the novel  $\theta$  that is ‘substantive model-independent’.

### *Recommendations for future research*

**Pmm, M(N)AR, Empirical data, Vignette, ShinyMICE, AC across imputations, not iterations (new convergence diagnostic unique for iterative imputation??).**

**If I don’t include it in my study, also: Significance of  $AC$  values.**

## **Grading**

Scientific contribution (clear research question, convincing argumentation that the study adds to the scientific literature)

Theory (use of theory, clear hypotheses, relevant literature)

Method (correct data collection/handling, measures, choice and description of method of analysis)

Results (correct interpretation of findings, clear presentation) Discussion and conclusions (summary, broader implications, limitations, future research)

Written presentation (writing, structure, tables and figures, references)

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