
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 in iterative imputation algorithms. Our study found that—in the cases considered—inferential validity was achieved after five to ten iterations, much earlier than indicated by diagnostic methods. We conclude that it never hurts to iterate longer, but such calculations hardly bring added value.

1. Iterative Imputation

To draw inference from incomplete data, most imputation software packages use iterative imputation procedures. With iterative imputation, the validity of the inference depends on the state-space of the algorithm at the final iteration. This introduces a potential threat to the validity of the imputations: What if the algorithm has not converged? Are the imputations then to be trusted? And can we rely on the inference obtained on the completed data?

These remain open questions since the convergence properties of iterative imputation algorithms have not been systematically studied (Van Buuren, 2018, § 6.5.2). While there is no scientific consensus on how to evaluate the convergence of imputation algorithms (Zhu & Raghunathan, 2015; Takahashi, 2017), the current practice is to visually inspect imputations for

signs of non-convergence. This approach may be undesirable for several reasons: 1) it may be challenging to the untrained eye, 2) only severely pathological cases of non-convergence may be diagnosed, and 3) there is not an objective measure that quantifies convergence (Van Buuren, 2018, § 6.5.2). Therefore, a quantitative, diagnostic method to identify non-convergence would be preferred.

2. Identifying Non-Convergence

In our study, we consider two non-convergence identifiers:¹ autocorrelation (conform Lynch, 2007, p. 147) and potential scale reduction factor \hat{R} (conform Vehtari et al., 2019, p. 5). Aside from the usual parameters to monitor—chain means and chain variances—we also investigate convergence of the multivariate state-space of the algorithm.

We implement (Van Buuren, 2018)’s recommendation to track the parameter of scientific interest, and henceforth propose a novel parameter: the first eigenvalue of the variance-covariance matrix that is obtained after imputing the missing data. This novel parameter has the appealing quality that it is not dependent on the model of scientific interest. With that, it suits one of the main advantages of imputation techniques—solving the missing data problem and the substantive scientific problem separately.

We evaluate the performance and plausibility of these diagnostic methods through model-based simulation in R (R Core Team, 2020). For reasons of brevity, we only focus on the iterative imputation algorithm implemented in the popular `mice` package in R (Van Buuren & Groothuis-Oudshoorn, 2011).

3. Simulation Study

The aim of the simulation study is to determine the impact of non-convergence on the validity of statistical inferences, and to assess whether non-convergence may be detected using several diagnostic methods. Inferential validity is reached when estimates are both

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¹(as recommended by e.g. Cowles & Carlin, 1996)

unbiased and have nominal coverage across simulation repetitions ($n_{\text{sim}} = 1000$).

We induce non-convergence in the imputation algorithm with two sets of simulation conditions: early stopping and missingness severity. Early stopping implies that we vary the number of iterations before terminating the imputation algorithm (between 1 and 100 iterations). And the missingness severity is determined by the proportion of incomplete cases (between 5 and 95%)². The simulation set-up is summarized in pseudo-code (see Algorithm 1). The complete script and technical details are available from github.com/hanneoberman/MissingThePoint.

Algorithm 1 Simulation set-up

```

Simulate data
repeat
  for all missingness conditions do
    Create missingness
    for all early stopping conditions do
      Impute missingness
      Perform analysis of scientific interest
      Compute non-convergence diagnostics
      Pool results across imputations
      Compute performance measures
    end for
  end for
  Combine outcomes of all conditions
until all simulation repetitions are completed
Aggregate outcomes across simulation runs

```

4. Results

Our results demonstrate that inferential validity is achieved after five to ten iterations—even in the worst missingness conditions (i.e., up-to 95% of cases having missing values). Conditions with a lower proportion of incomplete cases yield valid inferences almost instantly (after just two iterations). This is in grave contrast to the non-convergence identified by the diagnostic methods. Autocorrelation- and \hat{R} -values still indicate improving convergence after 20 to 30 iterations.

For example, in Figure 1 we see that... The novel parameter has equal performance to the quantity of scientific interest as parameter ($r = .975$), while having the advantage of being model-independent.

²We only consider a ‘missing completely at random’ missingness mechanism (Rubin, 1976).

5. Discussion

With this study, we show that iterative imputation algorithms can yield correct outcomes, even when a converged state has not yet formally been reached. Any further iterations would then burn computational resources without improving the statistical inferences. Our study found that—in the cases considered—inferential validity was achieved after five to ten iterations, much earlier than indicated by the autocorrelation and \hat{R} diagnostics. Of course, it never hurts to iterate longer, but such calculations hardly bring added value.

References

- Cowles, M. K. and Carlin, B. P. Markov chain Monte Carlo convergence diagnostics: a comparative review. *Journal of the American Statistical Association*, 91(434):883–904, 1996.
- Lynch, S. M. *Introduction to applied Bayesian statistics and estimation for social scientists*. Springer Science & Business Media, 2007.
- R Core Team. *R: A language and environment for statistical computing*. Vienna, Austria, 2020.
- Rubin, D. B. Inference and Missing Data. *Biometrika*, 63(3):581–592, 1976. doi: 10.2307/2335739.
- Takahashi, M. Statistical Inference in Missing Data by MCMC and Non-MCMC Multiple Imputation Algorithms: Assessing the Effects of Between-Imputation Iterations. *Data Science Journal*, 16:37, July 2017. doi: 10.5334/dsj-2017-037.
- Van Buuren, S. *Flexible imputation of missing data*. Chapman and Hall/CRC, 2018.
- Van Buuren, S. and Groothuis-Oudshoorn, K. mice: Multivariate Imputation by Chained Equations in R. *Journal of Statistical Software*, 45(1):1–67, December 2011. doi: 10.18637/jss.v045.i03.
- Vehtari, A., Gelman, A., Simpson, D., Carpenter, B., and Bürkner, P.-C. Rank-normalization, folding, and localization: An improved \widehat{R} for assessing convergence of MCMC. March 2019. URL <http://arxiv.org/abs/1903.08008>.
- Zhu, J. and Raghunathan, T. E. Convergence Properties of a Sequential Regression Multiple Imputation Algorithm. *Journal of the American Statistical Association*, 110(511):1112–1124, July 2015. doi: 10.1080/01621459.2014.948117.

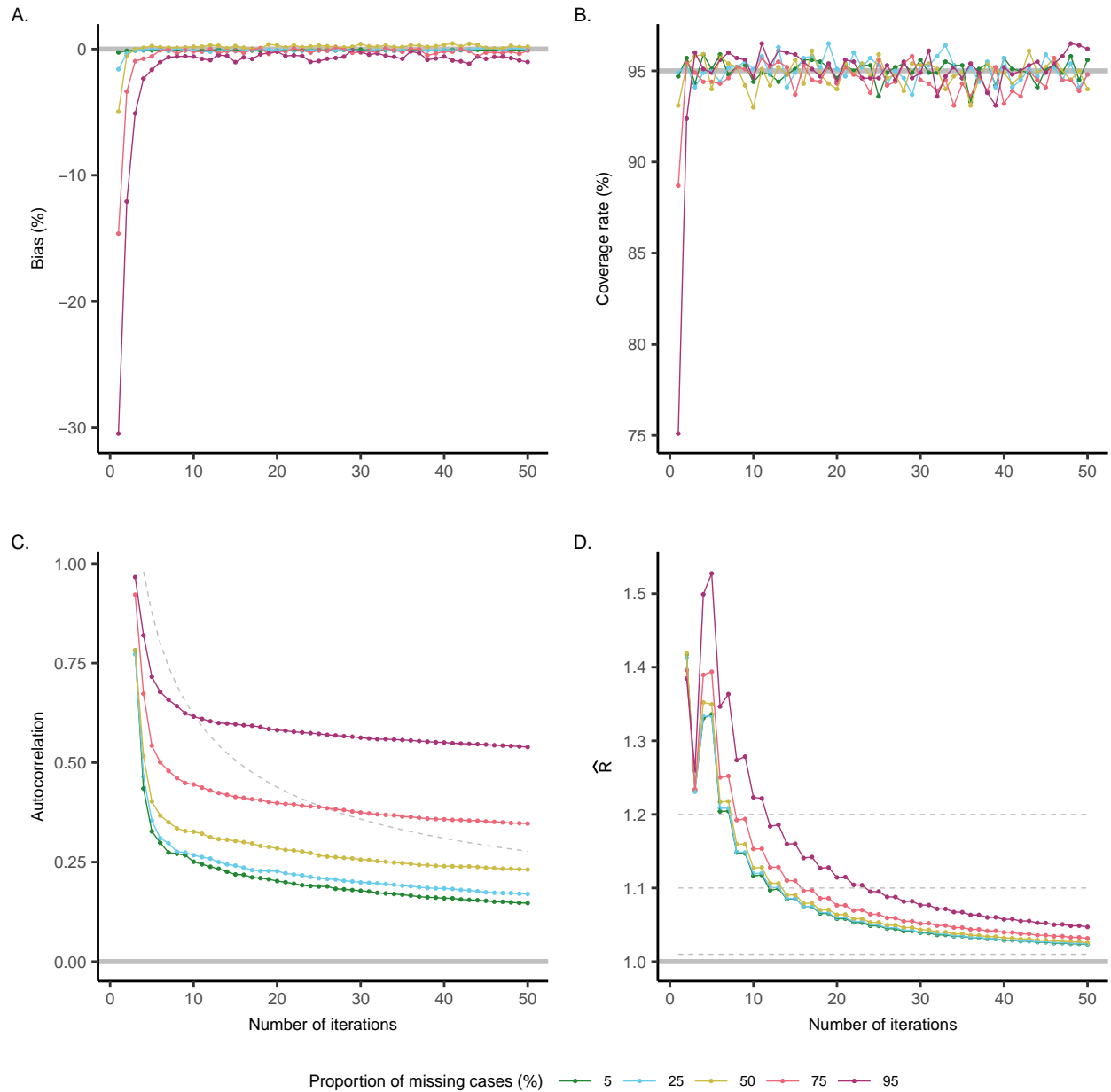


Figure 1. Subset of simulation results (truncated at 50 iterations). Depicted are performance measures bias and coverage rate, and non-convergence identifiers autocorrelation and \hat{R} for the same scientific estimate. The solid gray lines represent inferential validity of the estimate (i.e., unbiasedness and nominal coverage), whereas the dashed gray lines depict the common diagnostic thresholds of the identifiers.