It's time! 10 + 1 reasons we should start replicating simulation studies

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Abstract

The quantitative analysis of research data is a core element of empirical research. The performance of statistical methods that are used for analyzing empirical data can be evaluated and compared with computer simulations. A single simulation study can determine the analyses of thousands of empirical studies to follow. With great power comes great responsibility. Here, we argue that this responsibility includes replication of simulation studies to ensure a sound foundation for data analytical decisions. Furthermore, being designed, run and reported by humans, simulation studies face challenges similar to other experimental empirical research and hence should not be exempt from replication attempts. We highlight that the potential replicability of simulation studies is an opportunity and a luxury that quantitative methodology as a field should proudly embrace and use as a chance to lead by example.

Keywords: simulation studies, replication, data analysis, research statistics, reproduction

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Statistical simulation studies are computer experiments, in which data are generated using computer algorithms (Burton et al., 2006; Morris et al., 2019). They are an important tool for investigating the properties of data analysis methods and often inform choices about how empirical data will be analyzed (Boulesteix et al., 2017).

Replicability has been a prominent issue in the social and biomedical sciences over the past decade, yet simulation studies have until recently been largely exempt from replication attempts or demands. It is easy to see why: artificial data generated by a computer and analyzed without human input might appear to be the epitome of reproducibility. The researcher who is performing a statistical simulation study can set every parameter at will and knows the data generating mechanism (or algorithm) that was used. The apparent lack of human manipulation in simulation studies lends them an air of infallibility and some therefore regard simulation studies as equivalent to analytical derivations, carved in stone (Gray & Marwick, 2019).

We argue, however, that simulation studies have more in common with empirical research than might meet the eye. The replication of a published simulation study, i.e. writing and running new code based on the description provided in the original publication (Rougier et al., 2017), might produce incompatible results for many of the same reasons seen in the social and biomedical sciences. These reasons include human error, design choices, suboptimal execution as well as reporting of simulation studies, and may jeopardize their theoretically perfect replicability. Figure 1 and table 1 summarizes 10 issues regarding replicability that we have identified. In the remainder of the article we discuss each of these issues in more detail.

1) Simulation studies can have a major impact

Methodological decisions for the choice of a certain method, the use of a specific cut-off or rule of thumb can quickly become mainstream, particularly if the method is convenient. A simulation study that inspired a given recommendation often reaches seminal status and

thousands of citations. Famous examples are Hu and Bentler (1999) whose simulation study of cut-off values for fit indices in structural equation models was cited over 70,000 times or Peduzzi and colleagues (1996) whose simulation study promoting the 1 in 10 rule for the events-per-variable in logistic regression has accumulated over 6,000 citations by May 2021. After a data analytical recommendation has reached the state of common practice, these citation counts are likely an underestimation. The impact of simulation research investigating the performance of statistical methods furthermore crosses discipline boarders. Whenever the method under investigation is of broad application in various fields so might be a simulation study investigating its properties.

2) Authors of simulation studies are not immune to conflicts of interest

Most researchers are genuinely interested in the progress of science and happy to understand the limitations of their theories, hypotheses or methods in order to refine and evolve them (see White and Higgins for such a commendable example (Higgins et al., 2012; Turner et al., 2021)). Yet the feeling of ownership and pride in the context of ones own scientific contributions make us prone to engaging in questionable research practices like HARKING, cherry picking or p-hacking. We have no reason to believe that quantitative methodologists are an exception. They also find themselves in the very same academic rat race and may be biased towards their own methods just as empirical researchers are biased towards their theories. Even the slightest perceived threat of reputation or citation loss might make authors of simulation studies conflicted when deciding (1) which methods to compare, (2) which scenarios to study, and (3) which performance measures to compare them on, as well as (4) how to present and interpret the results (Boulesteix et al., 2017). Confirmation bias makes it furthermore less likely for errors to be detected whenever the simulation code yielded a ‘favorable’ result.

3) Selective reporting is the norm rather than the exception in simulation studies

Simulation studies frequently compare multiple statistical methods on multiple performance measures. Furthermore, full-factorial designs, i.e. the crossing of all experimental conditions, are often regarded as the gold-standard. The potential number of scenarios that might be included in any given simulation study is ever increasing due to the evolution of computing capacities of modern computers and the growing availability of high performance clusters and cloud computing. As a result, authors of simulation studies are faced with the challenging task of taming an overwhelming number of results. Elaborate accounts are limited by the restrictions of scientific journals and author guidelines on the number of figures and/or tables. Rigorous researchers might make use of online supplements. However, these are less frequently subjected to peer-review, often formatted by the authors and sometimes hard to access. Less rigorous researchers might fall prey to temptations of a clean story and aesthetic standards (Giner-Sorolla, 2012) and omit ‘less informative’ configurations of the data-generating mechanism (Morris et al., 2019). It is arguably fair that authors wish to focus on when methods perform particularly badly or well, but unless readers are fully aware of all the data-generating scenarios actually explored and the entailing adequacy of methods for unreported configurations, this may give a false impression; this is particularly important for the next point.

4) Simulation studies serve two masters

In addition to the overwhelming quantity of data that a simulation study author has to make digestible for readers, the readership they have to serve can be divided into two broad groups – albeit caricatured – with different needs and preferences. On the one hand, simulation studies are typically written and reviewed by methodologists, and thus the writing will suit a methodological audience. Fellow methodologists are interested in the broad picture. They would like to learn about general properties of a given statistical

method: when it performs well, when it performs poorly, and why. On the other hand, simulation studies provide guidance for applied researchers. The applied researcher might be interested in a more specific use case, i.e. a single combination of simulation factors. They would like to know which of the compared methods is most suitable for the analysis of their own particular research data. Their choice of method should be informed by simulation results more relevant to their study, for example in terms of design, sample size and expected structure of the data. A method that works well for a randomized trial but poorly in non-randomized settings will not concern the applied researcher if they are analyzing a randomized trial, but should do if they are not (White & Thompson, 2005). Providing a broad narrative about a simulation studies' results in addition to results for specific scenarios requires care in the analysis, presentation and interpretation of results, akin to challenges faced by other empirical researchers. A replicator might have a different perspective and might try to please one master more than the other. This might lead to different choices in data analysis, presentation and (in particular) interpretation, potentially altering some conclusions or providing different insights.

5) Simulation studies might be run by computers but the code is written by humans

Questioning the replicability of simulation studies might seem absurd. After all they are merely the result of computer code that can be rerun at will. There are three problems with this notion. First, rerunning computer code requires the availability of computer code. As Morris and colleagues found in a recent review, this is unfortunately almost never the case (Morris et al., 2019). Second, the computer code has to be error free. Mistakes can happen in any human endeavor, with computer code being no exception. Third, the computer code has to match the intended simulation design. The authors' methodological intentions have to be correctly translated into computer code. Code including a design-implementation-gap is reproducible in the sense that rerunning the code would

produce the same results. However, it is not replicable. A replicator trying to accurately translate the intended design into code would likely get diverging results. Such a gap can be of a more systemic nature and affect multiple simulation studies implementing similar concept (see Astivia and Zumbo, 2017 for an example) or can closely resemble coding errors. The latter was the case in the study by Schönbrodt and Perugini who published a corrigendum for their popular Monte Carlo simulation investigating the sample size at which correlations stabilize. It had been brought to the researchers' attention that the description provided in the paper did not match the accompanying code. While fortunately not altering the main conclusions the authors took the corrigendum as an opportunity to highlight the necessity of open reproducible code. (Schönbrodt & Perugini, 2018)

A different source of coding errors might be the software implementation of a given method (e.g. in a package used in the simulation code). This may lead to a given method appearing to perform poorly, while, in fact, the method is fine and merely the specific software implementation faulty. Naturally, authors will take more care to check the implementation of their own method than competing methods.

6) We cannot simulate every possible scenario

In statistical simulation studies, synthetic data sets are usually generated according to one or more specific conditions (often termed *scenarios*). Different data analysis strategies are then applied to each of the resulting data sets. For promising methods, generalizability of results is a primary concern, since the parameter space that can be covered by a single simulation study is, by definition, finite. Conclusions about the performance of a given method therefore hold as long as those specific conditions under which it was studied are met and do not necessarily extend to other conditions or settings. For the applied researcher faced with a data set (see point 4), it would be very unusual to know which specific scenarios are most relevant to the study at hand. As obvious as this may sound, it is hard to say how broadly the results of a simulation study may apply. While it is possible

to model the results of simulation studies, this typically involves extrapolation. Instead of speculating about the generalizability of the results of simulation studies, replication for these further scenarios provides a means of direct investigation.

7) The devil is in the detail

Peer-review is an important element in ensuring the quality and integrity of research. One aspect that is consistently overestimated is a peer-reviewer's ability to detect errors or hidden assumptions. Verification reports and red teams provide an insight into the effort that is required to spot inconsistencies and question decisions that might seem self-evident when presented in the coherent story line of a published manuscript (Chambers, 2020; Lakens, 2020). Only when getting our hands dirty, diving deep into the details and actually retracing each step via replication can less obvious threats to validity be uncovered. An example for such an influential detail is the simulation study by van Smeden and colleagues investigating the 1 variable per 10 events criterion for binary logistic regression (van Smeden et al., 2016). The authors showed that simulation results are highly dependent on the existence of artificial data sets where the outcome can be perfectly predicted by the covariates ('separation').

8) Replication is a chance to learn both as individuals and as a field

The replication crisis has brought about a substantive change to how science is conducted. It initiated reflections on common practices such as reporting guidelines, the role of peer-review and publication formats. Reporting guidelines have for decades been lamenting the poor design and reporting practices of simulation based research (Burton et al., 2006; Hauck & Anderson, 1984; Hoaglin & Andrews, 1975; Maldonado & Greenland, 1997; Morris et al., 2019). Embracing replication and the subsequent change of perspective, from telling your own story to understanding and recreating others' research, might facilitate the long-overdue adoption of some best practices such as open code, code review and pre-registration. In addition to recognizing the merit of the best-practice recommendations

that emerged from the replication crisis in psychology and learning how they might serve us in the context of simulation studies, we might learn our very own lessons and derive reforms specific to simulation studies.

9) Research for research should lead by example

The study of research methodology is inherently prescriptive. Already in 1975, Hoaglin and Andrews pointed out the hypocrisy of methodologists not adhering to their own advice when it comes to simulation studies. The very people who often provide statistical advice to applied researchers and lament the brevity of method sections or lack of rigorous reporting fall prey to the same trappings. Wouldn't it be nice if simulation studies contained not only guidance for data analysis and study design but were additionally exemplary in transparency, data and code sharing (Boulesteix et al., 2020)?

10) Because we can

Large swathes of empirical research are inherently unreplicable. Financial, logistical, historical or ethical reasons can prohibit the direct replication of published research. None of these constraints apply to simulation studies. Generating artificial participants does not require ethical review board approval; we do not need to concern ourselves with participant burden, the costs of large trials, or the inability to recreate the effects of unique historical events. Neither do we face struggles to recruit participants from a small population or have to wait a decade for the long term effects of interventions to manifest. We are free to openly share our code and artificial data without any concerns for privacy. While exact replication is never possible in empirical research, it is possible in simulation studies due to knowledge of all components involved. This allows examination of the root of any discrepancies that might arise in replication attempts. We can improve the research quality of an entire field from the comfort of our desk at the minimal cost of computational time and power. Given the lack of obstacles and costs, combined with the potential benefit, we shouldn't think twice about replicating simulation based research.

Discussion

We have presented a multitude of reasons to argue that simulation studies are subject to the same human error, researcher degrees of freedom, conflicts of interest, questionable research practices, human bias and fallibility as any other empirical research. Their analysis and interpretation is neither neutral nor self-evidently correct. Therefore, just like empirical research, simulation studies warrant replication.

Repetition, Reproduction or Replication - which do we want?

While we predominantly used the term *replication* in the present article, we also see the need for *repetition* and *reproduction* (Rougier et al., 2017). *Repetition* by the same team using the same setup ensures that the original simulation pipeline is robust. Repetition can reduce or prevent slip-ups, such as accidentally running an old version of the code or including the wrong version of a figure in the manuscript. *Reproduction* involves a different team running the original code, and is a first step towards code-review. Reproducibility checks are already common practice at some research institutes and are increasingly finding their way into the peer review process (e.g. at Behavior Research Methods, Biometrical Journal, Meta-psychology to name but a few). These commendable examples increase the reputation of code as a research product. *Replication* as defined above can be done for the existing body of research, for which code might not be available – or no longer functional due to evolving software environments. This approach is implemented in the RepliSims project (<https://zenodo.org/communities/replisims>): an international interdisciplinary collaboration of quantitative methodologists that aims to replicate influential simulation studies from the biomedical and social sciences and to learn from that endeavor. Nosek and Errington use a broader understanding of *replication* which they define as anything that changes or confirms our conclusion of the research question (Nosek & Errington, 2020). Simulation studies are regularly interpreted as answers to very broad research questions even though they just cover a very specific interpretation of the

problem. Common examples might be the simulation of publication bias or multivariate non-normality (Astivia, 2020) the operationalization of which are highly dependent on subjective beliefs and assumptions of the original author. We argue that the replication of simulation studies should therefore also be extended to *conceptual replications* where the principle that inspired a data generating mechanism might be implemented in alternative ways.

Conclusion

It is time! Time to embrace the methodological knowledge we have as a field and adhere to our own advice. For methodologists, the promotion and adherence to principles that ensure credibility, validity, and generalizability of the results of scientific research should be self-evident and not require a wake up call in the form of a scandal to do what we know to be best practice: clear and extensive description of methodology in the form of a technical simulation protocol, public availability of computer code and mandatory code review are the very first steps towards a firm foundation. We might find that adopting modern publishing formats such as registered reports, verification reports (Chambers, 2020) or interactive visualization tools (Gasparini et al., 2020) are the next steps. Once these practices become the norm we can rise to the ensuing replication related challenges such as independent implementations, long term reproducibility, implementation using open source tools as well as cumulative research by extension of the existing code base. This requires a change that does not only include individual researchers, but also their institutional environment as well as editors, peer-reviewers, funders and publishers. We hope to stimulate methodologists to take replication of simulation studies more seriously and provide a basis for fruitful discussion among all stakeholders. After all, simulation studies that are worth publishing are worth replicating.

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Author Contributions

The authors assumed the following roles according to the Contributor Roles Taxonomy (credit.niso.org):

A. Lohmann: Conceptualization, Writing - original draft, Writing - review & editing.

R.H.H. Groenwold: Conceptualization, Supervision, Writing - review & editing.

T. P. Morris: Investigation, Writing - review & editing.

O.L.O. Astivia: Investigation, Writing - review & editing.

All authors approved the final submitted version of the manuscript.

Conflicts of Interest

The authors declare that there were no conflicts of interest with respect to the authorship or the publication of this article. TPM declares that he consults for Kite Pharma, Inc.

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Table 1

10 + 1 Reasons to replicate simulation studies.

Reasons to replicate simulation studies	Explanation
1) Major impact	<ul style="list-style-type: none"> – Broad reach – Highly cited – Foundation of data analysis
2) Conflicts of interest	<ul style="list-style-type: none"> – Authors invested in certain methods – Proposing novel method improve publication probability – Favoritism can bias design choices
3) Selective reporting of results	<ul style="list-style-type: none"> – Favoritism towards one method can bias focus of reported results – Too many details destroy story line – Journal restrictions demand brevity
4) Competing aims	<ul style="list-style-type: none"> - Two different audiences: – Methodological reader: interested in general properties – Applied researcher: guidance for use case
5) Coding errors	<ul style="list-style-type: none"> - Bugs can happen to anyone – Lack of code review – Design-implementation-gap – Frequent unavailability of simulation code
6) Limited scope	<ul style="list-style-type: none"> – Finite parameter space
7) Importance of details	<ul style="list-style-type: none"> – Insufficiency of reported information not apparent even to dedicated peer-reviewers
8) Insights as individuals and as a field	<ul style="list-style-type: none"> – Replication encourages reflection on reporting standards
9) Lead by example	<ul style="list-style-type: none"> – Methodologists should practice what they preach
10) Because we can	<ul style="list-style-type: none"> – No financial, logistic, historical or ethical constraints to replication. (– But serious time and funding constraints to individuals that produce them!)

10 + 1 Reasons to replicate simulation studies

Figure 1. 10 + 1 Reasons to replicate simulation studies