Replicability and Reproducibility for Machine Learning: Applications in Brain Mapping

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Symposium

The brain mapping community is going through a major transformation with increasingly large data sets, an emphasis on open science, and a large diversity of analytic approaches including advanced machine learning approaches. While there have been a number of papers highlighting the importance of replicability and reproducibility, these have largely focused on standard pipeline-based analyses. The use of machine learning approaches, while not new, come with some additional important aspects which have not been broadly appreciated. For example, what are the considerations for ensuring reproducibility when using stochastic solutions that produce slightly different parcellations each time? Algorithmic solutions also come with various properties that can play an important role in their applications such as their uniqueness and identifiability. Bias-variance tradeoffs also play an important role, one which is changing as we enter the era of 'bigger' data in neuroscience. Those attending this symposium will come away with an understanding of these and other terms, their various trade-offs and their application to multimodal brain mapping. We will present the topics in the context of the larger focus on open science and the 5 R's, reproducibility, replicability, reusability, robustness, and reliability/stability. Each speaker will provide a different perspective which will weave together the concepts and provide concrete examples of the issues being discussed.

Objective

• A specific objective of the proposed symposium is providing a bridge between the brain mapping and statistical signal processing/machine learning communities, and to start a much needed effective communication between these communities as data-driven methods have now been widely recognized as having a major role to play in brain mapping. For this reason, the IEEE Signal Processing Society (SPS) is excited about the event, and is likely to provide support for the travel expenses of few attendees for the symposium. The co-organizer, Dr. Adali is currently the Vice-President for Technical Directions for the SPS and her initial request has generated much enthusiasm, and will be an activity of the recently established IEEE SPS Data Science Initiative.
• Our second objective is to highlight the ways in which machine learning approaches have unique challenges related to the replicability and reproducibility and to present those solutions.

• Our third objective is to provide examples from experts in the field, spanning signal processing, statistics, and brain mapping, highlighting both the ways in which lack of attention to the issues discussed can at a minimum add uncertainty to a solution and in the worst case lead to incorrect conclusions.

Target Audience

We are focused on the broader brain mapping community, from novice to expert, including those who are performing analysis of brain imaging data using machine learning tools.

Presentations

Overview, Introduction, and Definitions

After solidifying the concepts of replicability and reproducibility in the context of data-driven methods for brain mapping, we will concentrate on a few key areas of application and highlight the main issues. We will address issues in matrix and tensor factorizations, an area where the discussion on replicability and reproducibility is in its infancy. We will discuss the importance of uniqueness in decompositions, ways to control bias and variance, and the challenges. Another important aspect to address is the use of data-driven atlases in brain mapping. In particular how to address functional and structural variability across different algorithms, algorithm runs within the same approach, within and between sessions and individuals (including anatomical vs dynamic functional connectivity considerations), and across individuals. We will also discuss the impact of blending model-based and data-driven approaches in both unimodal and multimodal data, so-called semi-blind or semi-supervised solutions on robustness, replicability, and biomarker development. We will end with a set of guidelines and recommendations specific to machine learning approaches as applied to brain mapping.

Presenter

Vince Calhoun, Georgia State/Georgia Tech/Emory
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The Role of Replicability and Reproducibility in the Interpretability of Machine Learning Results in Brain Mapping

I will start by describing what is meant by interpretability and the closely linked concept of explainability in the modern machine learning literature (e.g., Hansen & Rieger, 2019). These concepts will be illustrated by contrasting simple statistical tests based on spatially localized brain hypotheses with the challenges of interpretability encountered for multivariate, data-driven, machine learning approaches for brain mapping. In particular, I will describe and use the NPAIRS, split-half subsampling approach to provide concrete examples of these ideas and their links to the following critical concepts: 1) interpretability in the face of correlated input noise (e.g., Haufe et al., 2014); 2) the use of accuracy vs. stability/reproducibility plots and their link to classical bias-variance tradeoffs (e.g., LaConte et al., 2003; Rasmussen et al., 2012), and 3) the link between accuracy vs. stability/reproducibility plots and the interpretability of sparse brain mapping solutions (e.g., Baldassarre et al., 2017). I will close by briefly speculating on the role these ideas may play in the utility of deep neural networks in brain mapping.

Presenter

Stephen Strother, PhD, Rotman Research Institute Toronto, ON
Canada

Reliable and Reproducible Brain Network Estimation

The brain is a complex network that can be conceptualized as patterns of brain regions (or nodes) with inter-related functional or structural properties that define distinct brain networks. Two standard approaches for brain network estimation are iterative data-driven ML approaches (e.g., ICA) and model-based multiple regression. Each approach has distinct strengths for brain network estimation, as well as unique methodological issues that impact reliability and reproducibility of results. In this talk, the following questions will be considered: 1) what are the differences between using an iterative ML approach (like ICA) vs a simpler linear regression approach? 2) to what degree are there unique issues to consider for the ML approach? 3) to what degree does data quality and noise impact each, 4) to what degree should cross-validation play a role in either? 5) to what degree can we incorporate stability measures into these approaches (e.g. for estimating reliable networks), 6) Is this more or less important for ML vs regression-based approaches? Finally, I will briefly highlight some published research investigating the reliability and reproducibility of brain network structure and connectivity.

Presenter

Lisa Nickerson, Harvard Boston, MA
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Beyond reproducibility: reusability and generalizability

Machine learning brings major promises to neuroimaging, to make the most of the increasingly rich datasets. Across stimuli, it decodes neural supports of mental processes. Across individuals, it reveals biomarkers of psychological traits and pathology. Yet, methodological challenges undermine this agenda: published effects are often optimistic and, as a whole, the literature tends to be unreliable. This talk will explain why: Predictive models need large sample sizes that standard statistical approaches to achieve reasonable statistical power. In addition, lacking standard pipelines, the large analytic variability in the literature modulates arbitrarily the conclusions. The talk will also discuss solutions. To fully achieve its scientific promises, machine learning calls for more than archival reproducibility: models extracted should be applied to new data. The talk will detail methodological best practices to establish evidence for prediction. It will also explain why explicit generalization is instrumental to the progress of neurosciences. It will point to software that facilitates such research practices. Woo, C.W., Chang, L.J., Lindquist, M.A. and Wager, T.D., 2017. Building better biomarkers: brain models in translational neuroimaging. Nature neuroscience, 20(3), p.365. Varoquaux, G., 2018. Cross-validation failure: small sample sizes lead to large error bars. Neuroimage, 180, pp.68-77. Poldrack, R.A., Huckins, G. and Varoquaux, G., 2019. Establishment of Best Practices for Evidence for Prediction: A Review. JAMA psychiatry. Yarkoni, T., 2019. The generalizability crisis. psyarxiv.com.

Presenter

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