

The compatibility of theoretical frameworks with machine learning analyses in psychological research[☆]

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Supervised machine learning has been increasingly used in psychology and psychiatry research. Machine learning offers an important advantage over traditional statistical analyses: statistical model training in example data to enhance predictions in external test data. Additional advantages include advanced, improved statistical algorithms, and empirical methods to select a smaller set of predictor variables. Yet machine learning researchers often use large numbers of predictor variables, without using theory to guide variable selection. Such approach leads to Type I error, spurious findings, and decreased generalizability. We discuss the importance of theory to the psychology field. We offer suggestions for using theory to drive variable selection and data analyses using machine learning in psychological research, including an example from the cyberpsychology field.

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Current Opinion in Psychology 2020, **36**:83–88

This review comes from a themed issue on **Cyberpsychology**

Edited by **Jon D Elhai** and **Dmitri Rozgonjuk**

For a complete overview see the [Issue](#) and the [Editorial](#)

Available online 25th May 2020

<https://doi.org/10.1016/j.copsyc.2020.05.002>

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Introduction

Machine learning has been increasingly used in psychology and psychiatry research in recent years [1[•],2^{••}]. Machine learning analyses are typically conducted in an exploratory and atheoretical manner, analyzing many predictor variables (often called ‘features’) for associations with a dependent variable [3[•],4]. We focus on the

field of psychology, where in recent years numerous subfields have become quite theory-driven in the conduct of data analysis [5,6]. Machine learning’s exploratory approach seems at odds with psychology’s theory-driven analytic approach. We focus in this paper on possible compatibility between machine learning’s exploratory approach and psychology’s theory-driven approach to data modeling.

Review

Machine learning within cyberpsychology

Elsewhere in this special issue on cyberpsychology, we discuss that one of the main branches of the cyberpsychology field involves using computer technology to solve psychology-related challenges [7]. Thus, using machine learning to answer psychological research questions represents an example of this branch of cyberpsychology — briefly discussed in this special issue on using artificial intelligence in studying mental health [8]. For just a few examples, machine learning has been used to examine anxiety levels extracted from social media [9], relations between public mood and financial stock prices [10], suicide risk detection [11], and antidepressant treatment response [12]. In all of these examples, the authors used ‘supervised machine learning,’ which we define next.

Supervised machine learning and its advantages

Supervised machine learning is the most common type of machine learning approach. Supervised machine learning uses computational statistical methods to analyze examples of data in order to detect patterns, extrapolate and test these patterns in a new, external test dataset (often called the ‘hold-out’ dataset) in solving a specific problem [13,14]. Supervised machine learning is different from unsupervised machine learning. Unsupervised machine learning uses computational methods with ‘unlabeled’ (i.e. non-grouped) data, to empirically place the unlabeled data into groups based on empirical similarity, using cluster or latent class analysis. However, in contrast to supervised machine learning, unsupervised learning does not use example data before data analysis. We will focus in this paper on supervised machine learning.

For instance, perhaps a psychological researcher intends to model the influence of 20 baseline psychopathology features (predictor variables) on a treatment response dependent variable, using a multiple regression-based

[☆] Reprints from this paper can be requested from Jon Elhai through his website: www.jon-elhai.com

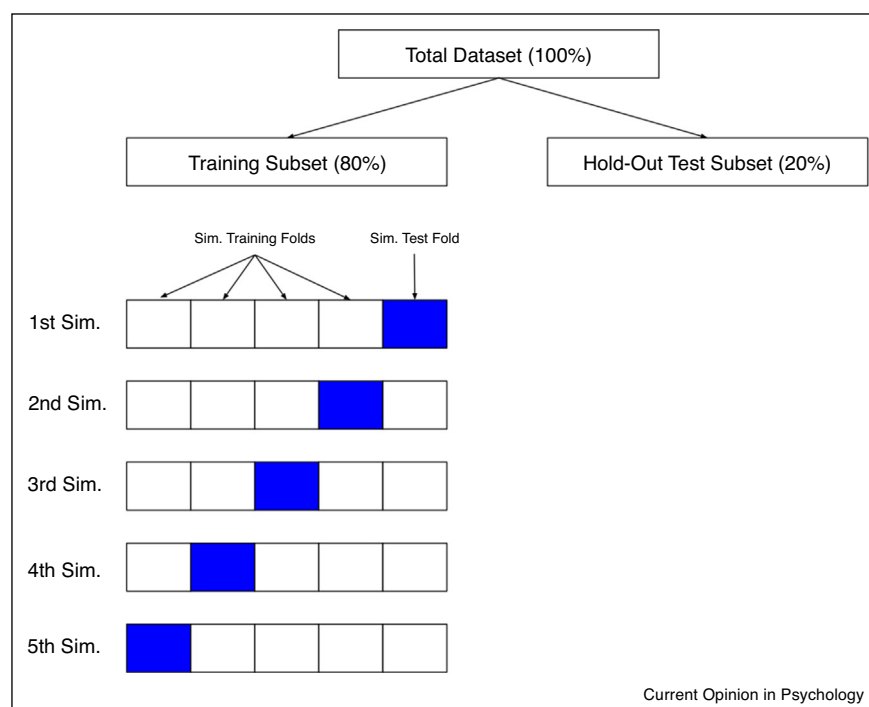
statistical model with 1000 research participants. The dependent variable could be a measurement of whether participants improved or did not improve from psychological treatment (a categorical variable), or alternatively could be a symptom improvement score (a continuous variable). The researcher could use supervised machine learning to analyze and train the 20-feature statistical model in modeling the dependent variable using a subset of (for example) 800 participants as the training data subset. Subsequently, the researcher can apply the trained statistical model (incorporating its parameter estimates) to the remaining 200 participants as the test data subset. In fact, training:test subset size ratios quite often range from 70%:30% to 90%:10% [13,14]; our example of 80%:20% thus falls in the middle of this range. Starting with pattern detection and training using the example data before applying to the external test data can yield better predictive ability compared to implementing the traditional analytic approach of only using the test dataset or complete dataset [3*].

Analyzing training data before application to external test data is a hallmark element of supervised machine learning. In addition, machine learning studies typically conduct repeated simulated cross-validations of their statistical model in the training dataset for further

validation, beyond solely using a single external test dataset [15]. Most commonly, researchers use k -folds repeated cross-validation, where a training dataset is first randomly split into an equal number of k subsets (folds); often, 5–10 folds are used [13,14]. Next, the statistical model is computed and trained on all but one of the folds, with the remaining fold serving as a simulated test fold; this process is conducted so that each fold serves as the simulated test fold once (for a total of k simulations), further repeating the entire process across numerous iterations and aggregating the final results before applying to the external test dataset [15]. Figure 1 shows a depiction of splitting a dataset into training and test subsets, and subsequently using the training subset for five-fold cross-validation (without repeated iterations beyond the first five simulations, for visual simplicity). See Marengo and Settanni for a discussion of various cross-validation methods within the cyberpsychology context [16]. We also discuss two other aspects commonly (but not always) used in supervised machine learning that offer substantial advantages over traditional data analyses: a) advanced statistical algorithms, and b) feature selection.

Machine learning studies quite often include advanced statistical algorithms from the computer science literature that are not yet well known in the psychology field. In fact,

Figure 1



Assigning a dataset to training and hold-out test subsets, and conducting five-fold cross-validation on the training subset. In this example, the total dataset was divided into a training subset (80% of participants), and a hold-out test subset (20% of participants). Subsequently, the training subset was divided into five equally sized folds. In each simulation, a different fold (the shaded one) served as the simulated test fold.

Note: Sim. = Simulation. Simulated training folds are displayed transparently, while simulated test folds are displayed with color shading.

such analyses offer major improvements over the more traditionally used general linear model and logistic regression algorithms [13,14], often used in psychological research [17]. For instance, shrinkage algorithms (e.g. lasso, ridge, and elastic net) can alleviate collinearity limitations from traditional statistical algorithms by imposing a penalty on large regression coefficients [18,19]. Additionally, support vector machine algorithms model feature-outcome relationships in three-dimensional space, optimizing linear boundaries between values of the dependent variable, and work well even for non-linear relationships [20]. And ensemble models (e.g. random forest, and boosted regression) use many iterations based on weaker learners (testing many smaller subsets of features and/or participants) in building a strong final model [13]. In fact, a commonly used method for conducting supervised machine learning is to use the R software [21], with the *caret* package [22]. *Caret* currently provides access to 238 machine learning algorithms from which to choose, including the examples mentioned above, as well as neural networks, Bayesian classifiers, multivariate adaptive regression splines, multi-layer perceptrons, and many others [23].

The other often-used advantageous element of supervised machine learning that we discuss is feature selection. Feature selection empirically reduces the number of features in a statistical model, eliminating features that are redundant or relatively unimportant in the final model [24]. This approach is important, because as we detail below, machine learning often starts with a very large number of features. Most often in machine learning, wrapper, filter, or embedded methods are used, which represent slightly different methods for conducting feature selection [25]. Using such feature selection methods, the researcher trains the statistical model (using simulated cross-validation, mentioned above), and conducts feature selection simultaneously. These methods minimize Type I error observed in other approaches such as stepwise regression which uses a greedy algorithm to repeatedly test hypotheses using prior iterations, adding and/or removing variables at each iteration automatically [26]. Stepwise regression is still sometimes used in psychology [27], but has been on the decline [17]. Because of its advantages, using feature selection in machine learning produces more generalizable results [26].

Finally, we should comment on the feasibility of conducting machine learning analyses. In our experience, researchers unfamiliar with machine learning hold mistaken beliefs that special equipment or very powerful computers are needed in conducting machine learning. However, this is not the case. Typically, all that is necessary is a contemporary personal computer and statistical software that can conduct machine learning analyses — most commonly, R, Python or Matlab. Some of the machine learning algorithms discussed above are computationally intensive and require time to process.

Ensemble models such as random forests are particularly intensive, and may take several hours to compute if analyzing many features; though Kuhn and Johnson discuss the use of parallel computer processing to substantially reduce computation time [26].

Machine learning usually includes a large number of features

Most typical in supervised machine learning studies, the researcher uses a statistical model of many (perhaps dozens of) features in predicting a dependent variable [3^{*}]. And often, the researcher empirically selects a subset of the many features using feature selection procedures. We provide several fairly representative examples of supervised machine learning from the psychology and psychiatry areas. For example, Delgadillo *et al.* [28] used 15 socio-demographic and mental health features to model depression treatment response in a sample of 1435 patients. Leightley *et al.* [29] used 22 sociodemographic and psychological features to model posttraumatic stress disorder as the dependent variable in 13,690 military personnel. Auer and Griffiths tested 33 player behavior features to model changes in online gambling among 70,789 participants [30]. And Grassi *et al.* [31] included 36 sociodemographic, health and mental health features to model development of Alzheimer's disease in 123 participants.

Yet there are many examples of substantially greater numbers of features sometimes used. For example, Walsh *et al.* [32] used more than 600 features to model adolescent suicide attempts, with 476 adolescents, and control groups of 7059 participants with a depression history, and 25,081 randomly selected hospital patients. Finally, Jing *et al.* [33] used about 1000 features to model substance use disorder in 700 participants. Prior work shows that at least several hundred participants are needed for accurate machine learning results [34]. However, including only a few hundred participants should yield accurate results if only analyzing a small number of features; including increasingly large numbers of features requires larger samples in order to reach accurate results [35].

Thus, machine learning is often used atheoretically to empirically select features in an exploratory manner, without using prior theory to inform feature selection. This approach has led to criticism of machine learning as being a 'black box' approach, where it is not possible to discern the logic behind what the algorithm learns, thus limiting interpretability [36]. Also, ethical issues may arise if machine learning results are adversely used, such as learning to detect sexual orientation [37] which could be used for discrimination purposes.

The emphasis of theory in psychology

With such large numbers of features commonly analyzed in machine learning studies (mentioned above), it should not be surprising that most machine learning studies

(even in psychology) have not used theory to guide their selection of features. After all, theoretical frameworks in psychology often include only a handful of constructs.

In fact, numerous subfields and specialty areas within psychology have become quite theory-driven over the years [5,6]. In modern times, psychological researchers (depending on the discipline) often use theoretical frameworks to drive their model selection. Specifically, rather than conducting exploratory analyses on relations between numerous features and a dependent variable, many psychological researchers instead use a smaller number of precisely chosen features to test, drawn from theory [5,6]. Additionally, psychological researchers often use statistical mediation and moderation [38,39] in order to examine specific psychological mechanisms that may account for relationships between a pair of variables. One particular reason why emphasis on theory has recently increased in psychology may be because the prior common practice of exploratory modeling in psychology drew negative attention [40].

In fact, the long-term practice of p-hacking has been identified as a major problem in psychological science [41]. p-hacking involves exploratory modeling and cherry-picking only statistically significant variables and findings to present in a published paper. This strategy can result in spurious findings, as analyzing large numbers of variables will result in numerous significant associations by chance alone, inflating Type I error [40,42]. Among other factors, p-hacking likely contributed to the replication crisis in psychology, resulting in the inability to reproduce many historically important psychological research findings [43,44].

Relying on theory to guide feature selection, and preregistration of the resulting hypothesis on platforms such as the Open Science Framework, is one of the effective ways to guard against unreliable results from p-hacking [6]; though other suggestions have been offered as well [44]. Yet as we discussed above, machine learning (including in psychology) is often used in an exploratory manner, choosing dozens (or hundreds) of features, without being guided by theory. We next offer some suggestions regarding the infusion of theory into machine learning analyses in psychology.

Infusing theory into machine learning in psychology and cyberpsychology

One way in which psychological theory can be integrated into machine learning is by informing the researcher on which features to include in a statistical model. Rather than selecting dozens of features that the researcher has available in his/her dataset, the researcher could instead use theory to select a smaller number of features that fit well within the chosen theoretical framework. With this approach, the researcher has the advantage of using a theory-driven statistical model, while also capitalizing on

the statistical advantages of machine learning discussed above. Some theoretical frameworks in psychology (and cyberpsychology) stipulate specific categories or types of variables that are important to the framework, but there may be many possible examples of such variables within the framework that the researcher could include as features. The researcher could use psychological theory to select a manageable set of numerous features that are subsequently reduced to an even smaller set of features using feature selection in machine learning.

For example, we recently used cyberpsychology theory to guide our machine learning analyses. We used the Interaction of Person-Affect-Cognition-Execution (I-PACE) theoretical framework of problematic internet use [45,46] to select a small set of features in modeling severity of problematic smartphone use (PSU) [47^{**}]. The I-PACE model proposes that predispositional/personal background characteristics ('P-variables'), affective/cognitive responses ('A-variables' and 'C-variables'), and executive control ('E-variables') contribute to the use and problematic use of internet communications [45]. Yet I-PACE includes numerous categories of background variables (e.g. psychopathology, personality) and response variables (e.g. coping styles, internet-related cognitive bias). And within these categories, many specific constructs could be included within each category (e.g. within psychopathology: depression, social anxiety, psychosis, etc.).

In our paper [47^{**}], we chose not to use a large number of features in modeling PSU severity. Instead, we used a smaller number of features, guided by the I-PACE model. We selected background characteristics from the I-PACE model (depression, anxiety, age and sex; 'P-variables' in I-PACE), as well as affective and cognitive responses (rumination, and the fear of missing out on rewarding experiences, or FOMO; 'A-variables' and 'C-variables') as our features. We conducted supervised machine learning with a training dataset of 768 participants (implementing simulated cross-validation) and a test dataset of 329 participants to model a total of only six features (selected from I-PACE) in predicting PSU severity. Specifically, we used three shrinkage, one support vector machine, and two ensemble machine learning algorithms. We found that FOMO was the most relatively important variable in modeling PSU severity, supporting literature on FOMO's robust association with problematic internet and smartphone use [48]. Our analysis had the benefit of being theory-driven, while also capitalizing on supervised machine learning's statistical advantages. Incidentally, and related to our discussion of computing speed above, all six machine learning algorithms took a combined total of well under 30 min to compute, without implementing parallel processing, using an Intel Core i5 dual-core, 2.3 GHz 2017 Macbook Pro computer with 16 GB of RAM. We also refer the reader to another recent study

using machine learning to model problematic social media use [49].

Machine learning can also be used in psychology and cyberpsychology to test psychological mechanisms, thus serving as a focused mechanistic rather than exploratory test. For example, machine learning models can include interaction terms between features, for testing statistical moderation [e.g. Ref. [50]]. Testing mediation using machine learning is a lesser studied approach, but recent research advances makes this strategy possible [51]. Finally, others have pointed out a drawback of machine learning in its typical use of observed variables with relatively high measurement error [52]. Recent work with structural equation modeling (involving error-free latent variables) has incorporated advanced machine learning algorithms [53]; this advancement is promising, as structural equation modeling is commonly used in psychological research [17].

Conclusion

Machine learning's exploratory analytic focus can be at odds with the theory-driven nature of numerous psychological research subfields and research areas. Supervised machine learning offers statistical advantages that can be useful in psychology and cyberpsychology research, including statistical model training before testing, advanced statistical algorithms, and feature selection procedures. Psychological researchers can use machine learning in a theory-driven manner by using theoretical frameworks to select features for their statistical model, perhaps further empirically reducing the number of features through feature selection. Machine learning can also test moderation and mediation, commonly conducted in psychological research. We hope that our suggestions in this paper will encourage theory-driven psychological researchers to use machine learning in testing their research questions.

Contributors

JE wrote the initial manuscript draft. CM substantially edited and revised the manuscript.

Conflict of interest statement

Jon Elhai (this paper's first author) and Dmitri Rozgonjuk served as co-guest editors for the special issue of this journal in which this article appears. Dmitri Rozgonjuk served as action editor for this article submission. The authors report no conflicts of interest with this paper.

Outside the scope of the present paper, Dr Elhai notes that he receives royalties for several books published on post-traumatic stress disorder (PTSD); is a paid, full-time faculty member at University of Toledo; is a paid, visiting scientist at Tianjin Normal University; occasionally serves as a paid, expert witness on PTSD legal cases; and receives grant research funding from the U.S. National Institutes of Health and Department of Defense.

Dr. Montag mentions that he has received (to Ulm University and earlier University of Bonn) grants from agencies such as the German Research Foundation (DFG). Dr. Montag has performed grant reviews for several agencies; has edited journal sections and articles; has given academic lectures in clinical or scientific venues or companies; and has generated books or book chapters for publishers of mental health texts. For some of these activities he received royalties, but never from the gaming or social media industry. Dr. Montag mentions that he is part of a discussion circle (Digitalität und Verantwortung: <https://about.fb.com/de/news/h/gesprachskreis-digitalitaet-und-verantwortung/>) debating ethical questions linked to social media, digitalization and society/democracy at Facebook. In this context, he receives no salary for his activities. Finally, he mentions that he currently functions as an independent scientist on the scientific advisory board of the Nymphenburg group. This activity is financially compensated.

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