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Assessing the predictive performance of structural equation model estimators

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ABSTRACT

Structural equation models are traditionally used for theory testing. With the increasing importance of predictive analytics, and the ability of structural equation models to maintain theoretical plausibility in the context of predictive modeling, identifying how best to predict from structural equation models is important. Recent calls for a refocusing of partial least squares path modeling (PLSPM) on predictive applications further increase the need to assess and compare the predictive power of different estimation methods for structural equation models. This paper presents two simulation studies that evaluate the performance of different modes and variations of PLSPM and covariance analysis on prediction from structural equation models. Study 1 examines all-reflective models using blindfolding and the Q^2 statistic. Study 2 examines mixed formative-reflective models using out-of-sample cross-validation and the RMSE statistic. Recommendations to guide researchers in the choice of appropriate prediction method are offered.

1. Introduction

Explanation and prediction are the two main purposes of theories and statistical methods (Gregor, 2006). Explanation is concerned with the identification of causal mechanisms underlying a phenomenon. On the statistical level, explanation is primarily concerned with testing the faithful representation of causal mechanisms by the statistical model and the efficient estimation of unbiased parameter values from samples, that is, making valid inferences to population parameters. In contrast, prediction is the ability to predict values for individual cases based on a statistical model whose parameters have been estimated from a suitable training sample.

Quantitative research in management has been dominated by causal-explanatory statistical modeling at the expense of predictive modeling (Shmueli, 2010; Shmueli & Koppius, 2011). The advent of big data has changed this. Modern organizations, not only analytics leaders such as Facebook, Google, Amazon and Walmart, but also smaller and less prominent businesses, are generating petabytes of data that record billions of digital transactions annually (Davenport, 2006, 2013). Carrying out predictive modeling on such large datasets has the potential to generate fresh insights for business practitioners and drive new theorizing for management researchers (Shmueli, 2010; Shmueli & Koppius, 2011).

Structural equation models represent latent and manifest variables and their relationships in a single statistical model. The estimation of such models has traditionally relied on covariance analysis methods, usually with the maximum likelihood (ML) estimator. However, the use of partial least squares path modeling (PLSPM) to estimate such models is increasing in many management disciplines, for example in strategic management (Hair, Sarstedt, Pieper, & Ringle, 2012; Hulland, 1999), marketing (Hair, Sarstedt, Ringle, & Mena, 2012; Henseler, Ringle, & Sinkovics, 2009), management information systems (Ringle, Sarstedt, & Straub, 2012), operations management (Peng & Lai, 2012) and organizational research (Sosik, Kahai, & Piovoso, 2009).

Covariance analysis estimates a structural equation model by minimizing the difference between the model-implied and the observed covariance matrices. Because covariance analysis offers unbiased estimates and provides tests of model fit (Antonakis, Bendahan, Jacquart, & Lalive, 2010; Rönkkö & Evermann, 2013), covariance analysis is typically associated with explanatory modeling. In contrast, PLSPM treats the latent variables as weighted composites of their manifest indicator variables and estimates the composite model using multiple regression, resulting in biased parameter estimates. Consequently, PLSPM is often recommended for prediction instead (Hair, Ringle, & Sarstedt, 2011; Hair, Sarstedt, Pieper, et al., 2012; Hair, Sarstedt, Ringle, et al., 2012; Henseler et al., 2009; Ringle et al., 2012). Herman Wold, who originally developed PLSPM, positioned PLSPM as a method for prediction (Wold, 1982), de-emphasizing the importance of statistical tests and inference to population parameters. Lohmöller later (1989, p. 72f) writes about PLSPM that "predictor specification is a shortcut term for the type of model building where the investigator starts with the purpose of prediction; sets up a system of relations …where the structure of the relations must be founded in the substance of the matter, and the predictive purpose should not jeopardize a structural causal interpretation of the

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relation; … the contrast between predictive vs. structural/causal is not absolute…For simple models both aspects come at the same time; for complex models there is a parting of the ways."

Most recently, prominent PLSPM researchers have called for a reorientation of PLSPM towards predictive or forecasting applications and its abandonment for explanatory modeling: "We also propose a new 'back-to-basics' research program, moving away from factor analysis models and returning to the original object of constructing indices that extract information from high-dimensional data in a predictive, useful way." (Dijkstra, 2010, p. 23). "PLS path modeling can and should separate itself from factor-based SEM and renounce entirely all mechanisms, frameworks and jargon associated with factor models. … A logical candidate for an alternative measurement framework is one that is based on forecasting." (Rigdon, 2012, p. 348).

Applied research in the management disciplines reflects the emphasis on prediction. Ringle et al. (2012) report that 15% of PLSPM studies in management information systems and almost a quarter of PLSPM studies in other leading management journals claim to focus on prediction. Hair, Sarstedt, Pieper, et al. (2012) report that >30% of PLSPM studies in strategic management appeal to predictive goals. Predictive goals motivate more than one quarter of PLSPM studies in marketing (Hair, Sarstedt, Ringle, et al., 2012).

The context of structural equation models for prediction raises important questions. In general, a statistical model (not limited to structural equation models) that leads to optimal explanation (minimizing bias) does not necessarily also lead to optimal prediction (minimizing bias and estimation error) (Shmueli, 2010). Consequently, the development of predictive models is primarily driven by data, not theory, to the point that modern prediction methods are entirely a-theoretical, eschewing easily interpretable regression models for neural networks, support vector machines, nearest-neighbor methods and others (Hastie, Tibshirani, & Friedman, 2009). These considerations naturally raise the question as to the role of theory, and therefore also structural equation models, in prediction, and the general relationship between theory development and prediction (Shmueli, 2010; Shmueli & Koppius, 2011). For example, is the insistence on a, typically theoretically constrained, structural equation model for prediction, as argued for by Lohmöller (1989) in the above quote, over possibly superior a-theoretical models defensible (Rönkkö, Antonakis, McIntosh, & Edwards 2016)? Should researchers take the risk of compromising both prediction and explanation for the pragmatically important interpretability of theoretically plausible models (Davenport, 2013; Freitas, 2013; Huysmans, Dejaeger, Mues, Vanthienen, & Baesens, 2011)? What role does the predictive power of explanatory models play in theory evaluation, selection, and development (Shmueli, 2010; Shmueli & Koppius, 2011)? Moreover, while Shmueli and Koppius (2011) present six ways in which predictive models can contribute to theoretical development, these ways do not imply that the prediction model coincides with the theoretical model, as is the case for prediction from structural equation models considered here.

A thorough discussion of these issues is beyond the scope of this article, which has a narrower focus. Specifically, in light of the arguments about the suitability of PLSPM for predictive purposes (Hair et al., 2011; Hair, Sarstedt, Pieper, et al., 2012; Hair, Sarstedt, Ringle, et al., 2012; Henseler et al., 2009; Rigdon, 2012; Rigdon, 2014; Ringle et al., 2012) combined with the dearth of supporting empirical evidence, *this paper addresses the choice of optimally predictive estimation methods for structural equation models with a focus on the variants of PLSPM and ML estimation*. Two simulation studies evaluate the performance of different PLSPM variants and compare PLSPM based prediction to ML and other methods. Study 1 examines all-reflective models using blindfolding and the Q^2 statistic, as recommended by Chin (2010). Study 2 examines mixed formative-reflective models using cross-validation and the RMSE statistic that are typically used in predictive analytics evaluation (Hastie et al., 2009).

The remainder of the paper is structured as follows. The next section discusses existing work on prediction from structural equation modeling with a focus on PLSPM. The following section presents challenges for prediction from structural equation models, followed by an introduction of the design factors common to both simulation studies. The subsequent two sections present the study design, results, and recommendations for each simulation study. The paper concludes with an overall discussion.

2. Prior work

Numerous studies in the past have focused on evaluating and comparing covariance analysis (particularly ML estimation) and PLSPM. However, almost all of them have focused on parameter accuracy (bias) and statistical power. These are key issues in inferential applications, but are not as important for predictive modeling (Shmueli, 2010). In contrast, despite the oft-repeated claims about the advantage of PLSPM for predictive modeling (Hair et al., 2011; Hair, Sarstedt, Pieper, et al., 2012; Hair, Sarstedt, Ringle et al., 2012; Henseler et al., 2009; Ringle et al., 2012), few studies have systematically tested these claims.

Evermann and Tate (2012) examine the predictive ability of reflective factor models using both PLSPM and ML estimation. Prediction from PLSPM estimated models, judged by the Q^2 statistic on blindfolded data sets, is superior to estimation from ML estimated models. However, their use of reflective exogenous constructs in the factor models precludes out-of-sample evaluation of prediction performance through cross-validation, the accepted standard in the predictive analytics literature (Hastie et al., 2009). Becker, Rai, and Rigdon (2013) examine the predictive ability of PLSPM estimated models with formative/composite constructs. While Becker et al. (2013) use cross-validation, they do not focus on the recoverability of individual scores, but on the R^2 of the regression of the endogenous formative construct. As noted by Sharma, Sarstedt, Shmueli, and Kim (2015) and Shmueli, Ray, Velasquez Estrada, and Chatla (in press), this statistic is a measure of in-sample explanatory power, not a predictive measure. Moreover, because Becker et al. (2013) use a statistically unidentified model, they cannot compare PLSPM with covariance estimation. Most recently, Evermann and Tate (2014) use a cross-validation approach for mixed formative-reflective models and conclude that PLSPM is superior to ML and linear regression methods in their simulation scenario, where predictive power is assessed as the mean RMSE (root mean square error) across indicators.

An important aspect not examined by previous studies is the performance of different PLSPM estimation methods. Specifically, Evermann and Tate (2012) use only PLSPM mode A estimation, because, as they argue, PLSPM mode A is the accepted way of estimating reflective models in the applied literature. For their later work, Evermann and Tate (2014) use only one combination of mode A and B, again reflecting current practice in the applied literature. Recently, Dijkstra and colleagues (Dijkstra & Schermelleh-Engel, 2013; Dijkstra & Henseler, 2015a, 2015b) have developed a consistent PLS estimator (PLSc) that uses disattenuation by estimated composite reliabilities to correct estimated regression path coefficients, yielding yet another PLSPM variant. Their initial simulation studies focus only on parameter bias and efficiency of estimation, so that the usefulness of PLSc for prediction remains to be explored.

A second aspect that has been neglected is prediction from misspecified models. While one would expect prediction from a model with random misspecifications to be poor, more interesting misspecifications are those that add paths to the model, leading, in the limit, to a fully saturated model. Given the lack of a model fit test for PLSPM (Evermann & Tate, 2010), researchers using PLSPM may be inclined to saturate their model with additional paths. Moreover, because of the different aims of explanatory and predictive models, underspecified models, trading off bias against variance, may be able to predict better than fully specified models (Hastie et al., 2009; Shmueli

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