GENERALISED BAYESIAN STRUCTURAL EQUATION MODELLING

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ABSTRACT
We propose a generalised framework for Bayesian Structural Equation Modelling (SEM) that can be applied to a variety of data types. The introduced framework focuses on the approximate zero approach, according to which parameters that would before set to zero (e.g. factor loadings) are now formulated to be approximate zero. It extends previously suggested models by Muthén and Asparouhov (2012) and can handle continuous, binary, and ordinal data. Moreover, we propose a novel model assessment paradigm aiming to address shortcomings of posterior predictive $p$-values, which provide the default metric of fit for Bayesian SEM. The introduced model assessment procedure monitors the out-of-sample predictive performance of the fitted model, and together with a list of guidelines we provide, one can investigate whether the hypothesised model is supported by the data. We incorporate scoring rules and cross-validation to supplement existing model assessment metrics for Bayesian SEM. We study the performance of the proposed methodology via simulations. The model for continuous and binary data is fitted to data on the ‘Big-5’ personality scale and the Fagerstrom test for nicotine dependence respectively.

Keywords Factor analysis · Cross-validation · Bayesian model assessment · posterior predictive $p$-values · scoring rules

1 Introduction

Structural Equation Modelling (SEM) is a general framework for testing research hypotheses arising in psychology and social sciences in general. It is used to model directional (regression coefficients) and non-directional (correlations) relationships among latent variables (structural model) which are identified by observed variables (measurement model) (Bollen, 1989). Initial inference methods for SEM have mostly been frequentist, but recently their Bayesian counterpart has gained popularity (see e.g. Scheines et al., 1999; Dunson et al., 2005; Kaplan, 2014; Merkle and Rosseel, 2015; Van De Schoot et al., 2017). Bayesian SEM offers several potential advantages. It has been shown to perform well with small sample sizes (Depaoli and Clifton, 2015) or small number of groups in hierarchical modelling (Hox et al., 2012), and can help resolve issues of inadmissible estimates (Can et al., 2015). Moreover, it provides computationally efficient schemes for models with large numbers of latent variables (Lüdtke et al., 2013; Oravecz et al., 2011), and can quantify uncertainty via credible intervals of quantities that are functions of parameters such as reliability (Geldhof et al., 2014) or indirect effects (Yuan and MacKinnon, 2009). It can also provide a unified framework for handling missing data (Lee and Xia, 2008) and semi-parametric models (e.g. Yang and Dunson, 2010; Song et al., 2013).

In this paper, we focus on the Bayesian SEM framework introduced by Muthén and Asparouhov (2012). Structural equation models impose some kind of restrictions on the number of parameters to be estimated. Usually, some parameters are set to zero and thus not estimated at all (e.g. cross-loadings, error correlations, regression coefficients). Muthén and Asparouhov (2012) suggested treating such parameters as approximate rather than exact zero, by assigning informative priors on them that place a large mass around zero; we will refer to this approach as the approximate
zero framework. The introduction of such informative priors is convenient in situations where there are concerns regarding the fit of the exact zero model. More specifically, it allows using the model as an exploratory tool to identify the source of model misfit. An alternative option for such a task is the use of modification indices (e.g., MacCallum et al., 1992). However, the approximate zero framework offers several advantages, see for example the discussion in Stromeyer et al. (2015), and its implementation is possible for the case of continuous and normally distributed data in the Mplus package (Muthén and Muthén, 2017). More specifically, a modification index measures the improvement in model fit that would result if a previously omitted parameter were to be freely estimated. This can often lead to a model unsupported by the hypothesised substantive theory. Moreover, the greedy nature of the procedure does not guarantee convergence to an optimal model (Muthén and Asparouhov, 2012; Asparouhov, Muthén, and Morin, 2015). On the other hand, the approximate zero approach provides information on model modification in one go, while the hypothesised theory is reflected clearly via the priors on the loadings. To our knowledge, the approximate zero approach offers the only Bayesian alternative to the modification indices. In theory, one can approach the same problem via Bayesian model searching using e.g. spike and slab priors and stochastic search variable selection but this is a substantially more challenging approach; see for example Lu et al. (2016).

In this paper, we aim to improve upon two aspects of the approximate zero framework. First, the existing framework covers models for continuous data and relies on the normality assumption. Here, we propose a generalised approximate zero framework that can accommodate more distributions, such as the logistic which is commonly employed in item response theory (IRT). This is achieved by introducing in the measurement model item-individual random effects. The model by Muthén and Asparouhov (2012) becomes then a special case of the proposed framework.

Second, we focus on the task of assessing model fit under the approximate zero framework (Garnier-Villarreal and Jorgensen, 2020; Asparouhov and Muthén, 2020). Several approaches exist in the literature, with posterior predictive p-values (PPP) (Meng, 1994) being the most widely used. However, concerns have been raised regarding their suitability in this framework (see e.g. Stromeyer et al., 2015; Hoijtink and van de Schoot, 2018). Special consideration has to be given to the choice of prior distributions for the model parameters, which can potentially affect the PPP performance (MacCallum et al., 2012; Van Erp et al., 2018; Liang, 2020). Perhaps a more fundamental question is whether priors should be set on the basis of fit indices, rather than formal Bayesian model choice quantities, such as the Bayes factor. Nevertheless, the Bayes factor requires calculating the model evidence, or else marginal likelihood (Gelman et al., 2017), which can be quite a challenging task especially in models with latent variables (e.g., Lopes and West, 2004; Vitoratou et al., 2014). Moreover, the Bayes factor is a relative measure and therefore does not directly address the question of whether a model fits the data well. Asparouhov et al. (2015) suggest avoiding the use of the approximate zero model to reach binary decisions on goodness of fit, but instead use it as an exploratory tool leaving the choice up to the subject matter experts.

Our approach aims towards reaching a middle ground between exploring lack of fit and assessing its severity. This is done by developing a decision framework that monitors the out-of-sample predictive performance to explore model misfit (i.e. validity of the hypothesised theory). Our proposed decision framework uses collectively fit indices and scoring rules via cross-validation to examine whether the approximate zero parameters are picking up random noise rather than systematic patterns in the data. From a machine learning viewpoint, cross-validation is one of the standard tools to guard against overfit, while at the same time ensuring a good fit. The advantages of using cross-validation to measure model performance have been noted in the SEM context; see, for example, MacCallum et al. (1992), Browne (2000) and recommendation 4 of Stromeyer et al. (2015). An intuitive argument in favour of cross-validation is that if a measurement scale does not generalise well in parts of the existing data it is highly unlikely that it will in future data. Merkle et al. (2019) use the DIC and WAIC indices that can be viewed as approximate versions of cross-validation (Gelman et al., 2014), although their resulting approximation is not always satisfactory; see for example Plummer (2008). From a Bayesian viewpoint, cross-validation, when combined with the log posterior predictive scoring rule, has tight connections with the model evidence and is less sensitive to priors (Fong and Holmes, 2020). Our proposed framework is developed by combining fit and out of sample predictive performance indices from different models.

The paper is structured as follows. In Section 2, we define the proposed generalised Bayesian SEM framework, illustrate how existing Bayesian SEM formulations are special cases, and provide examples of new models. Section 3 introduces the framework for assessing Bayesian SEM models. In Section 4, we illustrate and assess our methodology through several simulation experiments. Section 5 presents the analyses of two real applications: the first is a standard example on examining the ‘Big 5’ personality factors on data from the 2005-06 British Household Panel Survey (BHPS), whereas the second example is on the Fagerstrom Test for Nicotine Dependence (FTND). Finally, Section 6 concludes with some relevant discussion and extensions. The code for this work is available in the accompanying repository ‘bayes-sem’ hosted on github.\(^1\)

\(^1\)https://github.com/bayesways/bayes-sem/
2 Generalised framework for Bayesian SEM

2.1 Model specification

We use a unified Bayesian framework that encompasses models for categorical and continuous responses. Suppose there are $p$ observed variables (items) denoted by $y = (y_1, \ldots, y_p)$ and that their associations are explained by $k$ continuous latent variables (factors) denoted by $z = (z_1, \ldots, z_k)$. Categorical variables (binary and ordinal) can be accommodated in the same framework as for continuous data by assuming that the categorical responses are manifestations of underlying (latent) continuous variables denoted by $y^* = (y^*_1, \ldots, y^*_p)$. When continuous variables are analysed, $y_j = y^*_j$, $(j = 1, \ldots, p)$. The classical linear factor analysis model (measurement model) is:

$$y^*_i = \alpha + \Lambda z_i + \epsilon_i, \quad i = 1, \ldots, n$$  \hspace{1cm} (1)

where $\alpha$ is a $p \times 1$ vector of intercept parameters, $\Lambda$ is a $p \times k$ matrix of factor loadings and $n$ is the sample size. The vector of latent variables $z_i$ has a Normal distribution, $z_i \sim N_k(0, \Phi)$, where the covariance matrix $\Phi$ is either unstructured or defined by a parametric model that relates latent variables with each other and observed covariates (structural model). The $\epsilon_i$s are error terms assumed to be independent from each other and from the $z_i$s.

For binary data, the connection between the observed binary variable $y_j$ and the underlying variable $y^*_j$ is $y_j = I(y^*_j > 0)$. Similarly, for an ordinal variable with $m_j$ categories, $y_j = a$ if $\tau^{(j)}_a < y^*_j \leq \tau^{(j)}_a$, $a = 1, \ldots, m_j$ where $\tau^{(j)}_0 = -\infty, \tau^{(j)}_1 < \tau^{(j)}_2 < \ldots < \tau^{(j)}_{m_j - 1}, \tau^{(j)}_{m_j} = +\infty$. More specifically, for a binary item $j$ and individual $i$, the probability of success (positive) response is given by:

$$P(y_{ij} = 1 \mid z_i) = P(y^*_i > 0 \mid z_i) = P(\alpha_j + \Lambda_j z_i + \epsilon_{ij} > 0 \mid z_i) = P(\epsilon_{ij} < \alpha_j + \Lambda_j z_i \mid z_i) = F(\alpha_j + \Lambda_j z_i),$$

where $F$ stands for the cumulative distribution function (CDF) of $\epsilon_{ij}$. Finally, the model becomes:

$$F^{-1}\{P(y_{ij} = 1)\} = \alpha_j + \Lambda_j z_i,$$

where $F^{-1}$ is the inverse of the CDF also known as the link between the probability of success and the linear predictor. Specific choices for the distribution of the error term $\epsilon_i$ lead to the following well known models:

$$\epsilon_i \sim \begin{cases} N(0_p, \Psi), & \Psi = \text{diag}(\psi_1^2, \ldots, \psi_p^2), \text{ if } y_i \text{ is continuous} \backslash N(0_p, \Psi), & \Psi = I_p, \quad \text{ if } y_i \text{ is binary \& } F^{-1} \text{ is the inverse CDF of the normal} \backslash \prod_{j=1}^J \text{Logistic}(0, \pi^2/3), \quad \text{ if } y_i \text{ is binary \& } F^{-1} \text{ is the inverse CDF of the logistic}, \end{cases}$$  \hspace{1cm} (2)

where $0_p$ is a $p$-dimensional vector of zeros and $I_p$ denotes the identity matrix of dimension $p$. The inverse CDF of the normal and the logistic distributions are known as the probit and logit links respectively. In case of continuous or categorical items with the probit link, the marginal distribution of $y^*_i$ is:

$$y^*_i \sim N(\alpha, \Lambda \Phi \Lambda^T + \Psi).$$  \hspace{1cm} (3)

However, such an expression is not available for the logit model.

The model defined in (1) and (2) applies to confirmatory factor analysis (CFA) and exploratory factor analysis (EFA), and the differences between them are expressed in terms of restrictions on the parameters $\Lambda$ and $\Phi$. CFA is a method used to verify the factor structure of a set of observed variables. This is achieved by setting several elements of $\Lambda$ to zero that are referred to as cross-loadings. EFA, on the other hand, uses a much more flexible $\Lambda$ by only placing identifiability restrictions on it, and sets $\Phi = I_k$. An assumption, which is common to both approaches, is the conditional independence of the variables given the factors. This is equivalent to setting the off-diagonal terms in the covariance of the $\epsilon$, also known as error correlations, to zero.

2.2 Generalised Bayesian model framework

The Bayesian SEM approach introduced in Muthén and Asparouhov (2012) (approximate zero framework), mostly covers continuous items, and it can potentially be extended to binary and ordinal data under the probit specification. We propose here a more general specification that includes the logistic model for categorical data and for which the model by Muthén and Asparouhov (2012) is a special case.

Model (1) is extended by adding an item-individual specific random effect $u_{ij}$ giving:

$$y^*_i = \alpha + \Lambda z_i + u_i + \epsilon_i,$$  \hspace{1cm} (4)
where $\epsilon_i$ in (1) is split into $u_i$, a $p$-dimensional vector of random effects with a non-diagonal covariance matrix $\Omega$, and $e_i$, an error term with a diagonal covariance matrix $\Psi^*$. The $u_i$ terms aim to capture associations among the items beyond those explained by the vector of latent variables $z_i$. Those associations can be due to question wording, method effect, etc. Furthermore, the item-individual specific random effects $u_{ij}$ can be seen as an additional residual term that provides model diagnostics information for the detection of two-way outliers (e.g. leaked items and cheating behaviour in educational testing or secondary response strategies employed by some of the respondents to some of the items). Moreover, we note that now, contrary to equations (1) and (2), the cross loadings $\Lambda$ in (4) and (5) are non-zero parameters that are assigned informative priors centred around zero, e.g. $N(0, 0.01)$.

For continuous normally distributed data, Model (4) becomes the model proposed in Muthén and Asparouhov (2012) written as

$$y_i^* \sim N(\alpha, \Lambda \Phi \Lambda^T + \Omega + \Psi^*), \quad i = 1, \ldots, n,$$

(5)

where $u_i \sim N(0, \Omega)$, $z_i \sim N(0, \Phi)$ and $e_i \sim N(0, \Psi^*)$.

As it will be discussed in Section 2.3, it is essential to assign an informative prior on $\Omega$. A reasonable choice that favours diagonal matrices is the Inverse Wishart, which is also used in Muthén and Asparouhov (2012). This choice of prior can be thought of as controlling the magnitude of model flexibility the researcher is willing to allow for capturing the effects of external factors on measurement, such as question wording. Hence, it is important when setting this prior to ensure that the $u_i$s are of lower magnitude than the $e_i$s.

The generalised framework of (4) provides several extensions. It is now possible to define the approximate zero model for logistic models by assuming $e_{ij} \sim \text{Logistic}(0, \pi^2/3)$ (see Section 2.2.2 for details). Other distributions (e.g. $t$-distribution, non-Normal) can also be assumed for $e_i$ and $u_i$s. Setting $\Phi = I_k$ in (4) leads to the EFA model, nevertheless fitting such a model with MCMC may challenging as we discuss later on; see also (Lopes and West, 2004; Erosheva and Curtis, 2017; Frühwirth-Schnatter and Lopes, 2018; Conti, Frühwirth-Schnatter, Heckman, and Piatek, 2014) for some relevant Bayesian EFA schemes.

Inference is carried by adopting a fully Bayesian framework. This requires assigning priors on all the model parameters $\theta$, denoted by $\pi(\theta)$, and proceeding based on their posterior given the data $Y = \{y_i\}_{i=1}^n$, denoted by $\pi(\theta | Y^*)$, obtained via the Bayes theorem. A key feature of the approximate zero framework is that the priors on the cross loadings given in $\Lambda$ and the error covariances of $\Omega$ are informative and point towards zero. Next, we discuss in detail the model and prior specifications for continuous and categorical data.

### 2.2.1 Model and priors for continuous normally distributed data

The model in (4) originates from the specification below:

$$\begin{align*}
\begin{cases}
y_i &= \alpha + \Lambda z_i + u_i + e_i \\
z_i &\sim N(0, \Phi) \\
e_i &\sim N(0, \Psi^*) \\
u_i &\sim N(0, \Omega)
\end{cases}
\end{align*}$$

Nevertheless, as mentioned earlier, non-Normal distributions can be assigned on $e_i$s, $u_i$s and even $z_i$. In the case where all these are assumed to be Normal, the following augmentation is also equivalent:

$$\begin{align*}
\begin{cases}
y_i | u_i &\sim N(\alpha + u_i, \Lambda \Phi \Lambda^T + \Psi^*) \\
u_i &\sim N(0, \Omega)
\end{cases}
\end{align*}$$

Regarding priors, we begin with $\Omega$, the non-diagonal covariance matrix that introduces the error correlations. As mentioned earlier, it is essential that the overall amount of error correlations is not substantial and this can be achieved by ensuring that the impact of $\Omega$ is low compared to $\Psi^*$. One approach to make this more specific is to use an estimate of diagonal matrix $\Psi$ under the same model without error correlations, and then set the prior of $\Omega$ to favour low values for its diagonal elements compared to the estimate. For example, in the applications considered in this paper, the elements of the $\Psi$ matrix were all estimated to be relatively closed to one. The Inverse Wishart distribution with identity scale matrix and $p + 6$ degrees, also used in (Muthén and Asparouhov, 2012), may therefore provide a reasonable choice. Under this prior, the diagonal elements of $\Omega$ have mean 0.2 and standard deviation 0.163 (see appendix A for explicit formulae for the prior mean and variance and note that $p$ cancels out), hence the prior probability mass is concentrated well below the $\Psi$ estimates.

Regarding $\Lambda$ and $\Phi$ there are generally two parametrisations to ensure identifiability. Under the first one, $\Phi$ is a full covariance matrix and the leading loadings in $\Lambda$ for each factor are set to one. In this case, an Inverse Wishart prior with relatively low amount of information, compared to the prior of $\Omega$, is sought for $\Phi$, e.g. the Inverse Wishart with
the identity as the scale matrix and $p + 4$ degrees of freedom or lower. Under the second formulation, the leading loadings in $\Lambda$ for each factor are just constrained to be positive and $\Phi$ is a correlation matrix. It is also possible to remove these positivity constraints and therefore assign Normal priors to all of the elements of $\Lambda$; this formulation may be viewed as a special case of the parameter expansion suggested in Ghosh and Dunson (2009) for EFA. To ensure identifiability under this formulation, post-processing should be applied on the MCMC output. More specifically, the posterior samples of the columns corresponding to each factor should be multiplied by $-1$ if the relevant leading loading is negative, otherwise they are left as they are. In our experience, this option results in more efficient MCMC performance, in terms of mixing and convergence, when running the model in Stan. Regarding the correlation matrix $\Phi$, the LKJ prior, introduced in Lewandowski et al. (2009), can be used.

The variances of the Normal priors assigned on the elements of $\Lambda$ depend on whether these are regarded as cross-loadings or free parameters according to the hypothesised model. The cross loadings are assigned Normal distributions with zero mean and a variance of $0.01$ as in Muthén and Asparouhov (2012), whereas the remaining parameters of $\Lambda$ require some extra attention. A frequently used option is to assign large variance Normal priors, but this can lead to issues such as Lindley’s paradox (Lindley, 1957). One way to guard against such problems is to use unit information priors (Kass and Wasserman, 1996). The main idea behind unit information priors is to avoid the very large prior variances causing the paradox, by setting them so that they correspond to information from a single observation point. Lopes and West (2004) and Ghosh and Dunson (2009), in the context of EFA, recommend the following unit information priors:

$$
\Lambda_{ij} \sim N(0, \psi^2_j)
$$

where $\psi^2_j$ are the idiosyncratic variances of the diagonal matrix $\Psi$ that are treated as unknown parameters. Note, however, that the above priors may cause problems in cases where the $\psi^2_j$s are quite small as it is essential to differentiate from the prior variance of $0.01$ used for the cross loadings. For this reason, a fixed value may be used instead for the prior variance of the free elements of $\Lambda$, based on preliminary estimates of them, or even the value of one if the items are on similar scales.

Regarding the diagonal matrix $\Psi$, independent Inverse Gamma priors, introduced in Frühwirth-Schnatter and Lopes (2018) and used in Conti et al. (2014), can be assigned on each $\psi_j^2$. The hyper-parameters of these Inverse Gamma priors are set in a way so that Heywood cases are given very small prior weight. More specifically, the prior given to the idiosyncratic variance is

$$
\psi^2_j \sim \text{InvGamma}(c_0, (c_0 - 1)/(S_{yy}^{-1})_{jj})
$$

where $S_y$ is the empirical covariance matrix and $c_0$ is a constant that the researcher can choose in order to limit the probability of running into Heywood issues that arise when

$$
1/\psi^2_j \geq (S_{y}^{-1})_{jj}.
$$

Following Frühwirth-Schnatter and Lopes (2018); Conti et al. (2014), the constant $c_0$ can be chosen such that the prior probability of the event above is quite small. In the data considered in this paper, the value of $c_0 = 2.5$ was chosen on that basis. This is a data-dependent prior but the impact incorporates a minimal amount of information and it also helps avoid identification and MCMC convergence issues that are associated with Heywood problems. To back this up we also conducted a sensitivity analysis that is presented in appendix A.2. The results using the chosen data-dependent prior were practically identical with those obtained using several data-independent priors.

Finally, large variance Normal priors are assigned on the $\alpha$ parameters. In every analysis that follows we use the following wide prior Normal, $\alpha \sim N(0, 10^2)$.

### 2.2.2 Model and priors for binary and ordinal data

The model for binary data using the underlying variables $y_{ij}^*$, ($j = 1 \ldots, p$) can be written as

$$
y_{ij} = \mathcal{I}(y_{ij}^* > 0),
y_{i}^* = \alpha + \Lambda z_i + u_i + e_i, 
\quad e_i \sim \prod_{j=1}^{p} \text{Logistic}(0, \pi^2/3) \quad \text{or} \quad \prod_{j=1}^{p} N(0, 1)
\quad z_i \sim N(0, \Phi)
\quad u_i \sim N(0, \Omega).
$$

In the above models the $e_{ij}$s correspond to the logistic and probit specifications that are the most frequently used models, although other choices of distributions are also possible. The above expressions may be simplified by integrating
out the $e_{i,s}$ and obtain

$$
\begin{align*}
y_i & \sim \prod_{j=1}^{p} \text{Bernoulli}(\pi_{ij}(\eta_{ij})) \\
\pi_{ij}(\eta_{ij}) & = \sigma(\eta_{ij}) \text{ or } \pi_{ij}(\eta_{ij}) = \Phi(\eta_{ij}), \quad \eta_{ij} = [\eta_{ij}]_j \\
\eta_i & := \alpha + \Lambda z_i + u_i, \\
z_i & \sim N(0, \Phi) \\
u_i & \sim N(0, \Omega)
\end{align*}
$$

(6)

where $\sigma(\cdot)$ denotes the sigmoid function and leads to the logit model, whereas $\Phi(\cdot)$ denotes the cumulative density function of the standard Normal distribution and leads to the probit model. Note that the distribution of $u_i$s, and even $z_i$s, need not be Normal under the framework, this was only done for exposition purposes. In the cases where $u_i$s are indeed assumed to be Normal, the amount of data augmentation can be reduced further by the following equivalent formulation

$$
\begin{align*}
y_i & \sim \prod_{j=1}^{p} \text{Bernoulli}(\pi_{ij}(\eta_{ij})) \\
\pi_{ij}(\eta_{ij}) & = \sigma(\eta_{ij}) \text{ or } \pi_{ij}(\eta_{ij}) = \Phi(\eta_{ij}) \\
\eta_i & \sim N(\alpha, \Lambda \Phi \Lambda^T + \Omega).
\end{align*}
$$

(7)

In the simulation experiment and real-world examples the formulations of (6) and (7) were used as they are more convenient in the context of MCMC for models based on the logit link.

In terms of interpretation, it is interesting to note that the proposed model extends the two-parameter logistic IRT model by allowing for an item-individual random effect in addition to the standard individual latent variable $z_i$. The probability of a correct response to item $j$ by individual $i$ can be written as

$$
\frac{1}{1 + \exp \left(-[\alpha + \Lambda z_i]_j - u_{ij}\right)}.
$$

Similarly to the binary case, to model an ordinal observed variable $y_{ij}$ with $m_j$ categories, we assume the existence of an underlying continuous variable $y^*_j$ so that $y_{ij} = a$ if $\tau_{a-1}^{(j)} < y_j^* \leq \tau_a^{(j)}$, $a = 1, \ldots, m_j$.

The multinomial model is assumed to be:

$$
y_{ij,s} \sim \prod_{s=1}^{m_j} \pi_{j,s}(\eta_{ij})
$$

where $y_{ij,s} = 1$ if the response $y_{ij}$ is in category $s$ and 0 otherwise, $\pi_{j,s}(\eta_{ij}) = (\gamma_{ij,s}(\eta_{ij}) - \gamma_{ij,s-1}(\eta_{ij}))$ and $\gamma_{ij,s}(\eta_{ij})$ is a cumulative probability of a response in category $s$ or lower to item $y_j$. Furthermore,

$$
\begin{align*}
y_i \mid \eta_i & \sim \prod_{j=1}^{p} \text{Multinomial}(\pi_{ij}(\eta_{ij})) \\
\gamma_{ij}(\eta_{ij}) & = \sigma(\eta_{ij}) \text{ or } \gamma_{ij}(\eta_{ij}) = \Phi(\eta_{ij}) \\
\eta_i & = \tau + \Lambda z_i + u_i, \\
z_i & \sim N(0, \Phi) \\
u_i & \sim N(0, \Omega).
\end{align*}
$$

The parameters $\tau$ are unknown parameters also referred to as ‘cut-points’ on the logistic, probit or other scale, where $\tau_0^{(j)} = \infty, \tau_1^{(j)} < \tau_2^{(j)} < \ldots < \tau_{m_j-1}^{(j)}, \tau_{m_j}^{(j)} = +\infty$.

Similar priors can be assigned as in the case of continuous data. Regarding the elements of the $\Lambda$ matrix that are not approximate zero, unit information priors can be used. In the case of the 2PL IRT model this translates to a $N(0, 4)$ prior (Vitoratou et al., 2014).

### 2.3 Overview of the models and their estimation procedure

In this Section, we highlight some models, within the framework defined so far, that are essential for the methodology developed in this paper. We then provide details and discussion regarding their implementation. These models are defined below:

- The exact zero (EZ) model. This is the standard structural equation model and provides the starting point in the analysis considered here. It is defined by equations (1) and (2) with the cross-loadings in $\Lambda$ being fixed to zero.
• The approximate zero (AZ) model. This is the model first introduced in Muthén and Asparouhov (2012) and generalised in this paper. In its general form it is defined in equation (4). In the case of normally distributed $u_i s$, $e_i s$ and $z_i s$, is simplified to (5). An important feature is that the cross-loadings in $\Lambda$ are no longer being fixed to zero. It is a model to be used only in the Bayesian sense, as the informative priors on the $\Omega$ and on the cross-loadings in $\Lambda$ are essential.

• The exploratory factor analysis model (EFA). It is the standard EFA model, defined here by equations (1) and (2) where low informative priors are assigned to all the components of $\Lambda$ and $\Phi = I$.

• The EFA model with item-individual random effects (EFA-C). It is defined as the EFA model but with equation (4) instead of (2). This approach to EFA allows for a small amount of item dependencies conditional on the extracted independent factors. That model specification might result in greater amount of dimension reduction than EFA, since the stricter assumption of conditional independence could require a model with additional factors.

In terms of implementation, it is generally possible to use MCMC and several schemes can be used, (see e.g. Edwards, 2010). In cases where the $e_i s$, $u_i s$ and $z_i s$ are all assumed to be Normal, Gibbs samplers may be formed, (see e.g. Geweke and Zhou, 1996; Chib and Greenberg, 1998), and the model may also be fitted with standard software such as MPlus. Nevertheless, if any of these are assumed to be non-Normal, e.g. logistic models, different software and MCMC algorithms are needed. In this paper, we recommend the use of Hamiltonian Monte Carlo (HMC) (Neal, 2011), as it covers all cases. HMC is a Markov Chain Monte Carlo (MCMC) technique for Bayesian inference that updates the parameters simultaneously. It utilises information from the gradient of the log-posterior via the Hamiltonian equations in order to provide an efficient Markov chain with good mixing and convergence properties. The user is referred to Neal (2011) for more details. HMC can be implemented with the help of programming frameworks such as Stan (Carpenter et al., 2017). It is supported by high-level software packages such as ‘blavaan’ (Merkle and Rosseel, 2015), PyStan or RStan which are the Python and R language interfaces of the Stan language respectively. In this work, we chose to implement all model inference using HMC and the Stan language to take advantage of the generality of the HMC methodology and the software ecosystem built around the Stan language. For a complete repository of the code and further implementation details we refer the interested reader to the code repository for this work hosted on github at ‘bayes-sem’.

Fitting the EZ model in Stan is generally straightforward although we note that it may be useful to consider different parametrisations to improve MCMC performance and stability. For example, one may set the leading loadings in $\Lambda$ to one and consider a full covariance matrix $\Phi$ or just restrict the leading cross loadings to be positive and consider a correlation matrix for $\Phi$.

While the EZ model is identifiable both under the frequentist and Bayesian framework, this is not the case for the AZ model that, as mentioned earlier is to be approached in a Bayesian manner. The AZ model was introduced in Muthén and Asparouhov (2012) to relax the exact zero conditions so that it better reflects a hypothesised substantive theory and better serves the goal of confirming it. The cross-loadings or error correlations that would be constrained to zero under the EZ model, become free parameters in the AZ model but with highly informative priors centred at zero. Usually, there is information in the data to identify some of those parameters but not all of them. Hence, if all those parameters were freed and a frequentist model was adopted one would run into identifiability issues. As we typically do not know which of these parameters to free, an alternative is to adopt the AZ model, where identifiability is less of a concern given the informative priors that are concentrated around zero. Hence, AZ models essentially satisfy two goals: i.) the model stays close to the substantive hypothesis, only replacing the exact zero assumptions, used in traditional SEM modelling, with approximate zero, and ii.) it protects against any identifiability issues since the prior contains enough information to guide the inference algorithm to completion.

In cases where the EZ model does not perform well it is essential to find an appropriate benchmark to assess the performance of the AZ model. As discussed in more detail in the next section, such benchmarks can be provided by the EFA and EFA-C models. In general, fitting EFA models using MCMC can be a challenging task, due to issues such as rotational indeterminacy. The problem lies in the fact that the likelihood is specified in terms of $\Lambda \Lambda^T$ but often interest lies instead on $\Lambda$. The lower triangular set of restrictions (see e.g. Geweke and Zhou, 1996) ensures the mapping between those matrices is well defined, but introduces order dependence among the observed variables. The choice of the first $k$ variables, which is an important modelling decision (Carvalho, Chang, Lucas, Nevin, Wang, and West, 2008), thus becomes influential. The schemes of Conti et al. (2014); Frühwirth-Schnatter and Lopes (2018); Bhattacharya and Dunson (2011) provide an alternative to setting these restrictions and can also be used to identify the
number of factors in a single MCMC run. However, as also noted in Bhattacharya and Dunson (2011), for a number of tasks such as choosing the number of factors or assessing the predictive performance, there is no need to focus on \( \Lambda \), but on \( \Lambda \Lambda^T \) instead which is free of rotational issues. In such cases, the restrictions on \( \Lambda \) can be omitted as long as there are no MCMC convergence and mixing issues on the \( \Lambda \Lambda^T \) elements. As described in the next section, EFA and EFA-C models are only used in this paper to establish a benchmark for their predictive performance, hence focusing on \( \Lambda \Lambda^T \) is sufficient. It is important to note here that this does not apply for the SEM driven EZ and AZ models, where we are also interested on the \( \Lambda \) elements and the fit of the model. But for these models, the restrictions implied by the hypothesised SEM ensure that the elements of \( \Lambda \) are free of rotational issues. The number of factors of the EFA and EFA-C models can either be matched to that of the EZ model or, alternatively, models with different number of factors can be fit separately and compared. The comparison can be done by standard indices, such as the model evidence, BIC, etc., or via the model assessment framework introduced in this paper and presented in the next section. Drawing inference on \( \Lambda \) in the EFA context, in addition to \( \Lambda \Lambda^T \), remains an interesting and challenging problem, especially in the case of binary data and the presence of item-individual random effects. But, as it is beyond the scope of the paper, it is left for future research.

3 Model assessment

In this section, we introduce a model assessment framework that collectively uses fit indices and cross-validation to detect overfit. The aim is to complement PPP values, or other similar indices, with scoring rules to evaluate the prediction extracted from the model. The aim is to achieve a good fit and avoid overfit. The suggested procedure involves calculating these metrics for the EZ and AZ models as well as the EFA and EFA-C models with the same number of factors. We begin by presenting the proposed indices in detail, and finally provide our suggested procedure along with some guidelines and recommendations.

3.1 Assessing goodness of fit with PPP values

PPP values are perhaps the most frequently used method to assess model fit in the Bayesian SEM framework. Posterior predictive checking relies on a discrepancy function denoted by \( D(Y, \theta) \) that quantifies how far the fitted model is from the data. For continuous data, the discrepancy function used here is the likelihood ratio test (LRT) function (see e.g. Scheines et al., 1999) comparing the estimated model (\( H_0 \) hypothesis), and the unconstrained variance-covariance matrix model (\( H_1 \) hypothesis). The unconstrained model is also known as the saturated model (perfect fit). \( D(Y, \theta) \) is given by:

\[
LR[S, \Sigma(\theta)] = (n - 1) \left\{ \log |\Sigma(\theta)| + \text{tr} \left[ \Sigma^{-1}(\theta) \right] - \log |S| - p \right\},
\]

where \( S \) and \( \Sigma(\theta) \) are the sample and model implied variance-covariance matrix respectively. Furthermore, \(|\cdot|\), \(\text{tr}(\cdot)\) denote the determinant and trace of a matrix respectively. For example, if the maximum likelihood estimate (MLE) of \( \theta \), is plugged in (8), then \( LR[\cdot] \) is a statistic, but if \( \theta \) is unknown then \( LR[\cdot] \) may be viewed as a metric. Given the discrepancy function \( D(Y, \theta_m) \) defined in (8), a suitable MCMC algorithm and \( M \) posterior draws, the PPP value is computed as follows:

1. At each (or some) of the MCMC samples \( \theta_m, m = 1, \ldots, M \), do the following:
   
   (a) Compute \( D(Y, \theta_m) \).
   
   (b) Draw \( \tilde{Y} \) having the same size as \( Y \), from the likelihood function \( f(Y|\theta_m) \) of the implied model in Equation (3) or (5) and using the current value \( \theta_m \).
   
   (c) Calculate \( D(\tilde{Y}, \theta_m) \) and \( d_m = \mathcal{I}[D(Y, \theta_m) < D(\tilde{Y}, \theta_m)] \), where \( \mathcal{I}[\cdot] \) is an indicator function.

2. Return \( \text{PPP} = \frac{1}{M} \sum_{m=1}^{M} d_m \).

In the case of binary and ordinal data, the model is written as the probability of a response pattern. For \( p \) binary items, there are \( 2^p \) possible response patterns, denoted by \( \{y_j\}_{j=1}^R \), with corresponding observed frequencies denoted by \( O_r \), where \( r = 1, \ldots, R \). The probability of a response pattern, based on the logistic model with a parameter vector \( \theta \), and the assumption of conditional independence given \( z \) and \( u \) is:

\[
\pi_r(\theta) = \int \prod_{j=1}^{p} \text{Bernoulli} \left\{ y_j | \sigma(\eta_j) \right\} f(z)f(u)dzdu,
\]

where \( \text{Bernoulli}(y|\pi) \) denotes the Bernoulli probability mass function for a binary observation \( y \) and probability of success \( \pi \). \( \eta \) is as defined in Section 2.2.2, i.e. \( \eta = \alpha + \Lambda z + u \), and \( z \) and \( u \) are the latent components in the implied
model. The integral in (9) can be approximated using Monte Carlo. Similar expressions can also be obtained for the probit specification.

An equivalent model can now be defined for the observed frequencies \((O_1, \ldots, O_R)\) given the model-based \(\pi_r(\theta)\)'s via the Multinomial distribution

\[
(O_1, \ldots, O_R) \sim \text{Multinomial } [n, \pi_1(\theta), \ldots, \pi_R(\theta)] .
\]  

(10)

In the context of PPP values, a frequently used discrepancy measure, (see e.g. Sinharay, 2005), is the \(G^2\) statistic given by

\[
D(Y, \theta) = \sum_{r=1}^{R} O_r \log \left( \frac{O_r}{n \pi_r(\theta)} \right). 
\]  

(11)

For a given \(\theta\), e.g. a sample draw from the posterior, (11) can be derived from the likelihood ratio between the model in (10) and the saturated version of it where each \(\pi_r(\theta)\) is replaced by \(O_r/n\). Given \(M\) MCMC samples from the posterior, the PPP value is then calculated following the steps given above for continuous data. PPP values are not \(p\)-values and therefore are not necessarily connected with the relevant type I error argument. Instead, they are regarded merely as fit indices. In terms of criteria on the PPP values, we follow the relevant discussion in Muthén and Asparouhov (2012). As such, the fit of a model with a PPP value around 0.5 is regarded as excellent. It is generally not clear how low a PPP value should be to warrant poor fit but usually this threshold is set to 0.1 or 0.05.

The discrepancy function used here checks the overall fit of the model. Other discrepancy functions can be used that check the fit on lower order margins. In the case of categorical data, one can compute chi-square type residuals (see e.g. Jöreskog and Moustaki, 2001) on the univariate, bivariate and trivariate margins as well as utilise the work on check the fit on lower order margins. In the case of categorical data, one can compute chi-square type residuals (see e.g. Sinharay, 2005), is the \(G^2\) statistic given by

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The above may be viewed as the likelihood ratio test statistic based on point parameter estimates from the training data $Y^{tr}$, but evaluated on the unseen test data $Y^{te}$.

Note that in (13), the predictive distributions do not account for the uncertainty in the parameter estimates, which can be substantial for small training sample sizes. The Bayesian framework accounts for this source of uncertainty in a natural way via the posterior predictive distribution (12). Computing some scoring rules, such as the log score require access to the predictive distribution. However, this predictive distribution may be intractable and only samples from it are available, for example via MCMC. When predicting one dimensional data, one can use posterior draws to estimate the distribution using techniques involving kernel densities or the mixture of parameters approach (Krüger et al., 2020; Jordan et al., 2019). But in the SEM context, such techniques cannot be applied since the forecasts for the continuous data case are multivariate. It is possible, however, to use other scoring rules such as the energy score (Gneiting and Raftery, 2007) and the variogram score (Scheuerer and Hamill, 2015). These scores, which are presented in Section 3.3, can be computed using posterior draws and do not require access to the exact distribution. For the categorical data case, as we illustrate in Section 3.4, the log score can actually be calculated by reformulating the model in terms of the response pattern frequencies.

So far we have assumed a single split between the training and test data, but this may not provide representative results in cases where there are too many peculiar data points in the training or the test data. To limit the effect of such unfortunate splits, cross validation may be used. The procedure can be described as follows:

1. Split the data randomly into $K$ parts.
2. For each of the $K$ parts repeat the following steps:
   (a) Designate the selected group as the test data set and use the other $K - 1$ groups together as the training data set.
   (b) Fit the model in the training data set and draw samples from its posterior and its posterior predictive distribution to predict the data in the test set.
   (c) Evaluate the predictions via the chosen scoring rule against the test data.
3. Aggregate the values of the scoring rules across all $K$ groups by summing or averaging.

A nice feature of the above procedure is that all data points appear both in the training and test datasets. Regarding the choice of $K$, the aim is to ensure a good balance between having an adequate amount of data points in both training and test samples, so this depends on the sample size. For large enough sample sizes a choice of $K = 3$ often works well. Another option is to use more than one $K$ and average over them as well. For the choice of $K = 3$, the model has to be fitted three times, but in each of these times the sample size is two-thirds the size of the entire sample. The computational time therefore increases with $K$.

It is interesting to note that the calculation of both PPP values and scoring rules are based on the posterior predictive distribution. Nevertheless, there is an essential difference between the two approaches. PPP values are based on the posterior distribution conditional on the entire dataset and the prediction is made again on the entire dataset. In the scoring rules approach the posterior is conditional only on a subset of the data (training sample) and the prediction is made on the complement of that set (test sample).

3.3 Scoring rules for continuous and normally distributed data

In order to assess the predictive performance we need to select a scoring rule. As mentioned in the previous section, the log score is not available in the case of continuous data and the available options are the energy and the variogram scores. To choose between these two, we note that the energy score has been reported to have little sensitivity in detecting misspecifications on correlation matrices (Pinson and Girard, 2012; Scheuerer and Hamill, 2015), which is in line with our empirical findings from our simulation experiments. For this reason, we proceed with the variogram score. To calculate this score for a single data point $y_i = (y_{i1},\ldots,y_{ip})$, we need a set of $M$ samples from the corresponding predictive distribution; let $\tilde{y}_m = (\tilde{y}_{m1},\ldots,\tilde{y}_{mp})$ be the $m$-th sample of a draw and denote all these samples together by $\bar{\tilde{Y}} = \{\tilde{y}_m\}_{m=1}^M$. The variogram score for this point is defined in its general form as

$$V S(y_i, \bar{\tilde{Y}}) = \sum_{j=1}^p \sum_{k=1}^p w_{j,k} \left( |y_{ij} - y_{ik}|^P - \frac{1}{M} \sum_{m=1}^M |\tilde{y}_{mj} - \tilde{y}_{mk}|^P \right)^2$$

(14)

where, in (14), the $j,k$ are just indices to consider all pairs of each data point $y_i$ of dimension $p$, the $w_{j,k}$s are weights and $P$ is the order of the variogram. We follow common practice by setting all weights to one, and $P$ at its default value of 0.5. In the context of cross-validation, for each split between training ($Y^{tr}$) and test data ($Y^{te}$), the variogram score
can be computed by obtaining samples from the posterior based on $Y^{tr}$, and using them to draw samples $\{\tilde{Y}_m\}_{m=1}^M$ from the posterior predictive distribution (12). The samples can then be inserted in (14) together for each of the data points in the test set $Y^{te}$ in place of $y_i$. The scores are then added over all points in the test set, to calculate the score corresponding to this train-test split for the model considered. In the case of 3-fold cross-validation, this procedure is repeated for all 3 train-test splits and aggregated by summing or averaging.

3.4 Scoring rules for binary and ordinal data

It is possible to compute the log score in the case of binary or ordinal data via the alternative formulation based on frequency patterns, hence we focus on this scoring rule. Note that the posterior predictive density is given by Equations (10) and (9) where the integral in the latter is with respect to the posterior based on the training data. We can therefore write the log scoring rule for a set of observed frequencies in the test data $O^{te} = (O^{te}_1, \ldots, O^{te}_R)$ based on probabilities $\pi^{tr} = (\pi_1(\theta)^{tr}, \ldots, \pi_R(\theta)^{tr})$, obtained based on the posterior from the training data, as

$$LS(O^{te}, \pi^{tr}) = -\log f(O^{te} | \pi^{tr}) = -\log \left[ c \prod_{r=1}^R [\pi_r(\theta)^{tr}]^{O^{te}_r} \right] = -\sum_{r=1}^R O^{te}_r \log \pi_r(\theta)^{tr} + c,$$

where $c$ represents a constant. Note that the log score only differs as a metric to $G^2$ by a constant, which essentially confirms the argument made earlier in Equation (13), about the connection of the likelihood ratio test and the log score, and makes it more specific to categorical data.

3.5 Model assessment with fit and predictive performance indices

Our procedure contains two main elements: assessing goodness of fit, as done routinely under current practice, but also assessing out-of-sample predictive performance. For goodness of fit, the governing well-known procedure is to check if the fit of the hypothesised model, the EZ model in our framework, is no worse than that of the unconstrained model (also known as the saturated model). As described earlier this can be checked by looking at the PPP values of the EZ model. In case of satisfactory PPP value, our recommendation is no different than the standard course of action, to support the hypothesised model, and there is no need to look further.

Now let us consider a situation where the EZ model does not fit the data well, in terms of a PPP value, but the AZ model does. One of the main arguments of this paper is that the researcher should not rush to support the hypothesised model as the satisfactory PPP value may as well be due to the AZ model overfitting the data. Our definition of ‘overfit’, specifically to the SEM context is the following: If the AZ model is better than its EZ counterpart in terms of goodness of fit but also worse in terms of out-of-sample predictive performance, then it overfits the data. In other words, if the gains in goodness of fit of the AZ model, over the corresponding EZ model, are not based on systematic patterns of the data, then these gains would be of no help when predicting unseen data. Moreover the slightly increased model complexity of the AZ model may have an adverse effect in terms of prediction over the corresponding EZ model. In other words, we are seeking parsimony in addition to goodness of fit. Hence, according to our suggested framework, if the AZ model is worse than the EZ model in terms of the relevant scoring rule, then there is little support in the data for the hypothesised model.

Next, let’s consider the case where the AZ model has good PPP value, in contrast with the corresponding EZ model, and also better predictive performance as measured by the relevant scoring rule. Our view in this case is to conduct further checks. There is a possibility that AZ model is just improving upon a poorly specified EZ model but there may exist other EZ or AZ models that predict even better. If the poor fit of the EZ model is due to only some small cross loadings or error correlations, then the AZ model that captures these quantities model should perform really well. But if there are also some other systematic patterns missing from the EZ model, the improvement offered by the AZ model would be limited. Ultimately, the question that we want to answer is whether the predictive performance of each one of these models is good enough. Therefore, it is essential to establish a benchmark when comparing predictive performances. In the case of goodness of fit assessment this is done by the performance of the unconstrained saturated model. But this may not be a suitable choice for assessing predictive performance (MacCallum et al., 1992). The problem lies in the fact that the saturated model has substantially higher complexity, or else substantially larger number of parameters, than the hypothesised models. Generally speaking, if two models with different numbers of parameters have similar in-sample performance, then the one with the smaller number of parameters will generally perform better out of sample. An alternative option for a benchmark model, exploited in this paper, is the EFA model with the same number of factors as the hypothesised model. This model has generally fewer parameters than the saturated one and is generally expected to perform well in terms of predictive performance as it is allowed to search for systematic patterns in the data without any restrictions, other than having $k$ factors. This is not the case for the EZ and AZ models, where explicit restrictions are given and it is often hoped that they will not be too far from those indicated from the EFA.
Hence, in order to regard the predictive performance of the hypothesised model as satisfactory, its scoring rule should be comparable with that of the EFA model chosen as the benchmark.

Caution must be exercised over the choice of the benchmark EFA model, as selecting an over-parameterised EFA model will set the bar too low in terms of predictive performance. Therefore it may be more appropriate, in some cases, to check the parsimony of the EFA model selected as the benchmark. This can be done, for example, by considering EFA models with fewer factors, provided that they fit the data well. In line with such considerations, we note that the presence of the small error correlations induced by the $\xi_i$ under the approximate zero framework may offer an advantage to CFA models in terms of prediction as it can be viewed as an additional minor factor. Hence, in order to bring CFA and EFA models onto a level playing field, it may be reasonable to incorporate small error correlations to both of them via the EFA-C model.

Note also that, while the AZ models are more flexible than their EZ counterparts, they can still perform badly in cases of substantial model misspecification. For example, in cases of large enough cross loadings, say more than 0.5, using the Normal$(0, 0.01)$ as prior can still result in poor performance compared to the EFA model. This comparison may thus be exploited to detect misspecified models as we illustrate in Sections 4 and 5.

We summarise below the recommendations of our proposed framework.

1. If the EZ model has satisfactory fit indices such as PPP values, there is strong support towards the hypothesised model.
2. If both EZ and AZ models have poor PPP values then there is little support of the hypothesised model. Perhaps it may be useful to use more vague priors to explore its weaknesses. It would be expected in this case that the EFA models will have better predictive performance otherwise there maybe issues in the fitting algorithms or elsewhere.
3. If the EZ model has poor performance in terms of fit indices, whereas the AZ model is satisfactory, it is essential to check the scoring rules. If the improvement offered by the AZ model is due to overfit, it is expected that the prediction score for the AZ model will be inferior to that of the EZ one. The predictive performance of models that overfit is therefore expected to diminish. On the other hand, a prediction score that still favours the AZ model suggests that overfit is not the case. To check if the predictive performance of the AZ model is good enough, comparisons with EFA type models can be made. In cases of comparable or improved performance there is supporting evidence towards the hypothesised model.

Model fit assessment is by no means an easy task especially in factor analysis modelling where model misfit can be due to various reasons such as misspecification of the latent variable distribution, item dependencies, skewed data and non-linear predictors. In this paper, for the calculation of PPP values we use a discrepancy function that looks at the overall fit of the model both in the case of continuous and categorical data. It is useful to complement those overall goodness of fit tests with other measures of fit such as residuals and limited information test statistics that check the fit on lower order margins and detect item misfit as explained in Section 3.1. It is because of those complexities that our proposed methodology is trying to shed light to model fit challenges using a different set of tools that look at the model’s out of sample prediction performance. This provides new tools within the Bayesian modelling framework in SEM and highlights even further the challenges of fit and problems of PPP values. Furthermore, the new residual term in the linear predictor defined by the item-individual random effects $\xi_i$ plays a key role since it can be used as model diagnostics to detect outliers such as leaked items and cheating behavior in educational testing or secondary response strategies employed by some of the respondents to some of the items.

4 Simulation experiments

4.1 Setup

Simulation experiments were conducted to study the performance of the proposed models and demonstrate the assessment framework for continuous and binary data. We focus on two cases of data generated using Equation (2), i.e. continuous and binary. For each of these two cases, three scenarios were considered when generating simulated data:

- Scenario 1: Data generated from the EZ model.
- Scenario 2: Data generated from the AZ model with small error correlations, introduced by item-individual random effects, and without cross loadings.
- Scenario 3: Data generated from the AZ model with two non-negligible cross loadings and without correlated item-individual random effects.
For both continuous and binary data, we considered $p = 6$ items and $k = 2$ factors. The factor loadings used to generate the data, in each of the three scenarios, are shown in Table 1. Although the data were generated under the

| Scenario 1 | Scenario 2 | Scenario 3 |
|------------|------------|------------|
| $z_1$      | $z_2$      | $z_1$      | $z_2$      | $z_1$      | $z_2$      |
| 1          | 0          | 1          | 0          | 1          |
| .8         | 0          | .8         | 0          | .8         | 0          |
| .8         | 0          | .8         | 0          | .8         | .6         |
| 0          | 1          | 0          | 1          | .6         | 1          |
| 0          | .8         | 0          | .8         | 0          | .8         |
| 0          | .8         | 0          | .8         | 0          | .8         |

Table 1: True factor loadings used in the three simulation scenarios.

three scenarios, in all of them the typical hypothesised model assumes a simple structure in which the first three items load on the first factor whereas the last three load on the second factor. In other words, for the AZ model, the first three elements of the first $\Lambda$ column and the last three of the second $\Lambda$ column are regarded as the major parameters, whereas the other elements of $\Lambda$ are cross-loadings. In all three scenarios, the factor correlation was set to 0.2, and the intercepts $\alpha$ were all zero. The sample sizes were set to $n = 1,000$ in the continuous data and $n = 2,000$ in the binary data. For Scenario 2, equation (5) was used by setting the matrix $\Omega + \Psi^*$ to have ones in the diagonal, and 6 non-zero off-diagonal elements set to 0.2 with the remaining 9 off-diagonal elements set to zero.

For each scenario, the proposed model assessment framework of Section 3 was put into action by computing the PPP values and scoring rules for all the previously mentioned models. After fitting and summarising these models, according to Sections 3.3 and 3.4, we proceeded according to the recommendations of Section 3. The models and priors were specified as outlined in Section 2 and samples from the posterior of each model were obtained using Hamiltonian MCMC programmed using the Stan language. In the case of continuous data, 1,000 iterations were used as the warm-up period and another 2,000 for inference purposes. In the case of binary data, it was 2,000 for warm-up and 2,000 for analysis purposes. The models were run in 4 parallel chains in each case resulting in $4 \times 2,000 = 8,000$ posterior draws. In all cases, we ensured successful convergence of the chains with the help of the automatic metrics implemented in Stan as well as visual inspection of the posterior draws.

In all instances, we applied a 3-fold cross-validation and aggregated the scores by summing. Given that a scoring rule is a comparative index, we reported the difference in scores between each model and the best model. In other words, the best model of each case, or else the one with the smallest score, was given the value of zero.

The next two sections present the results of the simulation experiments for continuous and binary data. The aim of these experiments is to illustrate the performance of the proposed model framework and provide a proof of concept. More detailed simulation experiments will be helpful, as we discuss in the next sections, and are left for future research.

### 4.2 Continuous data

Table 2 gives the variogram score ($VS$) and the PPP values for the three simulation scenarios. We use the variogram score with parameter $P = 0.5$ and weights $w_{ij} = 1$. Starting with Scenario 1, we note that all models fit the data well in terms of the PPP values. In terms of predictive performance, we note that the $EZ$ model performs best, which is not surprising given that the data were generated from it. Note that the $EZ$ model even improves upon the $EFA$ models in terms of predictive performance as it is a more parsimonious model.

In simulation Scenario 2, both the $EZ$ and $EFA$ models exhibit poor fit according to their PPP values, which is again not surprising given that these models assume zero error correlations. In contrast, the $AZ$ and $EFA-C$ models that allow for small, yet not exactly, zero error correlations both fit well. At this point, the question is whether the improved fit of the $AZ$ model is due to fitting noise or else overfit as defined in Recommendation 2. But if $AZ$ was overfitting the data, we would not expect to see an improved performance over the $EZ$ model, as we see here. We can expand the investigation of the $AZ$ model further, wondering whether there is another theory that leads to an $AZ$ model with even better predictive performance. Recommendation 3 may shed light on this question when we compare the predictive performance against the $EFA$ models. We see that $AZ$ is quite competitive against those models and, in fact, does better, although their variogram scores are quite close. Hence, according to our proposed framework, there is strong support towards the $AZ$ model and, consequently, the hypothesised model. This appears to be a reasonable conclusion.
in the SEM context given that the poor fit is due to error correlations that are usually linked with observation error rather than factor loading misspecifications. As before, the use of PPP values alone would not have been enough to reach that conclusion.

Finally, let us consider the simulations for Scenario 3, where the EZ model does not have a good fit, as one would expect, but all the other models have PPP values around 0.5. As before, we are interested in whether the AZ model overfits and what conclusions we can draw on the hypothesised model. To answer such questions, we set the benchmark model to be the EFA model with the higher predictive performance; it is the EFA model in this case, as one would expect since the data were simulated without error correlations. The variogram score of the AZ model is again much better than that of the EZ, as it utilises its approximate zero cross loadings to pick up the two cross loadings of 0.6. But it is not better than the EFA model, thus not ruling out the presence of a different hypothesised theory regarding the loading structure of the six items. Indeed, the theory corresponding to factor loadings according to Scenario 3 described in Table 1 provides a better model as the data were simulated from it.

4.3 Binary data

In this section, we summarise the results of the three simulation experiments for the case of binary data. Table 4.3 gives the PPP values and the log scores. The results are very similar to the continuous case. In the case of Scenario 1, all models demonstrate good fit as indicated by the PPP values. Furthermore, the EZ model is the optimal one in terms of predictive performance (Recommendation 2) which is reassuring since data were simulated from the EZ model. In Scenario 2, we see that the EZ model exhibits very poor fit, caused by the additional error correlations in the simulated data, as indicated by the PPP value of 0.02. The rest of the models exhibit a moderately good fit with PPP values above 0.10. Similarly to the continuous case, the AZ model does well in terms of both Recommendation 2 and 3 being the model with the best predictive performance. Finally, in Scenario 3, in terms of model fit the EZ model also fails, due to the presence of non-zero cross loadings. The other models do well, leaving some questions open in terms of the validity of the hypothesised theory. For this reason, Recommendation 3 compares the predictive performance of AZ against the best performing EFA model. In this case, the AZ model is not as good as the EFA.

| Model | Scenario 1 | Scenario 2 | Scenario 3 |
|-------|------------|------------|------------|
| EZ    | 0.52       | 0.00       | 0.02       |
| AZ    | 0.50       | 0.12       | 0.13       |
| EFA   | 0.59       | 0.14       | 0.17       |
| EFA-C | 0.54       | 0.17       | 0.24       |

Table 3: Simulation Results for Binary Data. PPP values and sum of variogram scores of 3-fold cross validation for the relevant models. For each scenario, the best model has log score equal to 0 and the differences from it are reported for the other models.

4.4 Parameter recovery for the AZ model in the binary data case.

To investigate the parameter recovery performance of the AZ model in the binary data case, we performed a simulation experiment where 100 different datasets were simulated and the AZ model was fitted on each one of them to obtain samples from its posterior. More specifically the data were drawn from the EZ model, so that we focus on the main
parameters of interest, namely the factor loadings and the correlation of the factors, each with sample of size 2,000. The factor loadings used to simulate the data are the same as in the Scenario 1 of the simulation experiments of Section 4 and the correlation between the two factors was 0.2. Finally, the intercept parameters used to simulate the data were all set to 0. We used the parameterisation where the loadings are unrestricted and the factors’ variance is fixed to 1 hence their covariance matrix is restricted to be a correlation matrix.

Regarding the prior specification of the AZ model, we assumed that, according to the hypothesised theory, the first factor loads on the first 3 items and the second factor loads on the last 3 items. Hence, the rest of loading parameters were regarded as cross-loadings, and were assigned informative priors around zero. The rest of the priors were assigned as described earlier in the paper.

As informal measures of how well the parameters are recovered, we focused on frequentist properties of some estimators derived from the posterior samples. The estimators consisted of the 95% credible intervals as interval estimators, obtained from the sample 2.5-th and 97.5-th points extracted from the posterior draws, as well as the posterior mean and median as point estimator. We then examined the coverage probability of the former and the bias of the latter. We note that these summaries (95% credible intervals, posterior mean, and posterior median) may not exhibit the desired frequentist performance even in the case the model fits the data well, as they have not been constructed to do so. Nevertheless, if they happen to perform well, it is definitely reassuring.

We examined the main parameters of interest, such as the loadings $\Lambda$ and the factor correlation $\rho$. The results are summarised in Table 4 and they contain coverage probabilities and biases of the previously mentioned posterior summaries. As we can see, the coverage probabilities are reasonably close to 0.95 whereas the biases are not substantial, particularly for the posterior median. We therefore conclude, while noting the informal nature of the experiment, than no substantial concerns regarding parameter recovery are raised.

| Parameter | True Value | Coverage Rate | Bias of Post. Mean | Bias of Post. Median |
|-----------|------------|---------------|--------------------|---------------------|
| $\Lambda_{[1,1]}$ | 1.0 | 0.94 | 0.06 | 0.03 |
| $\Lambda_{[2,1]}$ | 0.8 | 0.96 | 0.05 | 0.03 |
| $\Lambda_{[3,1]}$ | 0.8 | 0.94 | 0.05 | 0.03 |
| $\Lambda_{[4,1]}$ | 0.0 | 1.00 | 0.00 | 0.00 |
| $\Lambda_{[5,1]}$ | 0.0 | 1.00 | 0.00 | 0.00 |
| $\Lambda_{[6,1]}$ | 0.0 | 1.00 | 0.00 | 0.00 |
| $\Lambda_{[1,2]}$ | 0.0 | 1.00 | 0.00 | 0.00 |
| $\Lambda_{[2,2]}$ | 0.0 | 1.00 | -0.01 | -0.01 |
| $\Lambda_{[3,2]}$ | 0.0 | 1.00 | 0.00 | 0.00 |
| $\Lambda_{[4,2]}$ | 0.1 | 0.99 | 0.03 | 0.00 |
| $\Lambda_{[5,2]}$ | 0.8 | 0.95 | 0.06 | 0.04 |
| $\Lambda_{[6,2]}$ | 0.8 | 0.99 | 0.03 | 0.02 |
| $\rho$ | 0.2 | 1.00 | -0.01 | -0.01 |

Table 4: True values, 95% coverage success rate and bias of point estimators out of 100 replications, AZ model for binary data.

5 Real-world data examples

In this section, we demonstrate our proposed model assessment framework with two real datasets. The first dataset is a popular psychometric test, usually referred to as the ‘Big 5 Personality Test’, that decomposes human personality along 5 main traits using 15 items measured on a 7-point likert scale. The second data set is based on the Fagerstrom Test for Nicotine Dependence (FTND) that consists of six binary variables.

5.1 Example 1: ‘Big 5 Personality Test’

The data were collected as part of the British Household Panel Survey in 2005-06 focusing on female subjects between the ages of 50 and 55; the sample size consists of 589 individuals. The ‘Big 5 Personality Test’, as it is known, is a 15-item questionnaire on topics of social behaviour and emotional state. Participants answer each item on a scale from 1 – 7, 1 being ‘strongly disagree’ and 7 being ‘strongly agree’. Items are treated here as continuous. The test is
designed to measure five major, potentially correlated, personality traits. Each trait corresponds to a factor, and each factor is hypothesised to explain exactly 3 out of 15 items.

The data have been analysed in several papers including Muthén and Asparouhov (2012), Stromeyer et al. (2015), and Asparouhov et al. (2015). In these analyses, an interesting finding was that the exact zero (EZ) model did not exhibit good fit based on several standard indices including the PPP values. The approximate zero (AZ) model gave a good fit in terms of the PPP values, but also had many non-zero error correlations. This raised concerns over whether the flexibility of the AZ model is picking up noise, thus resulting in a misleadingly high PPP value. The validity of the ‘Big 5’ scale on these data remains unclear. In an attempt to shed more light on this question we apply our model assessment framework and summarise the results in Table 5.

| Model | PPP  | CV-V |
|-------|------|------|
| EZ    | 0.0  | 56.43|
| AZ    | 0.23 | 0    |
| EFA   | 0.00 | 94.35|
| EFA-C | 0.38 | 78.47|

Table 5: ‘Big 5’ personality test data, BHPS. PPP values and sum of variogram scores of 3-fold cross validation for the relevant models. For each scenario, the best model has 0 variogram score and the differences from it are reported for the other models.

The picture is very similar to the error correlations scenario in Section 4.2, yet much more pronounced. Our analysis confirms the poor fit of the EZ and the EFA with five factors. Both AZ and EFA-C models have reasonably good PPP values. This implies that error correlations contribute to the lack of fit to a large extent. In order to assess the question of overfit and draw conclusions on the validity of the ‘Big 5’ scale, we calculate the variogram scores for each model. The variogram score of the AZ model clearly dominates all the other models, suggesting that the model is fitting consistent patterns in the data and it clearly outperforms the EFA models. This points to strong support towards the ‘Big 5’ scale, attributing the fit issues of the EZ model to error correlations that could have been caused by the wording and other issues often present in survey data like the BHPS.

5.2 Binary Data: Fagerstrom Test for Nicotine Dependence

In this section we use data on 566 patients available through the National Institute on Drug Abuse (study: IDA-CTN-0051). The Fagerstrom Test for Nicotine Dependence (FTND) (Heatherton et al., 1991) was designed to provide a measure of nicotine dependence related to cigarette smoking. It contains six items that evaluate the quantity of cigarette consumption, the compulsion to use, and dependence. The original scale consists of 4 binary and 2 ordinal items for self-declared smokers:

1. FNFIRST: How soon after you wake up do you smoke your first cigarette? [‘3’=Within 5 minutes, ‘2’=6 - 30 minutes, ‘1’=31 - 60 minutes, ‘0’=After 60 minutes]
2. FNGIVEUP: Which cigarette would you hate most to give up? [‘1’=The first one in the morning, ‘0’=All others]
3. FNFREQ: Do you smoke more frequently during the first hours after waking than during the rest of the day? [‘1’=Yes, ‘0’=No]
4. FNNODAY: How many cigarettes/day do you smoke? [‘0’=10 or less, ‘1’=11-20, ‘2’=21-30, ‘3’=31 or more]
5. FNFORBDN: Do you find it difficult to refrain from smoking in places where it is forbidden (e.g., in church, at the library, in cinema, etc.)? [‘1’=Yes, ‘0’=No]
6. FNSICK: Do you smoke if you are so ill that you are in bed most of the day? [‘1’=Yes, ‘0’=No].

For the purposes of our analysis, item FNFIRST was dichotomised as ‘1’=[3] and ‘0’=[0,1,2] and item FNNODAY as ‘1’=[2,3] and ‘0’=[0,1].

The mapping between the FTND scale and a CFA model is not clear, see e.g. Richardson and Ratner (2005) and references therein. Richardson and Ratner (2005) fitted a single factor, a correlated two factor, and a two factor model with one cross loading. These models were also considered in our analysis and are denoted as 1F, 2F-EZ, and 2F EZ-b respectively. More specifically, under the EZ model items 1, 2 and 3 load on a ‘morning’ smoking factor, whereas items 4, 5 and 6 load on a ‘daytime’ smoking factor. The EZ-b model is specified by letting item ‘FNFIRST’ load
on both factors. In addition to these models, we also considered their approximate zero versions, denoted as 1F-C, 2F-AZ, and 2F-AZ-b respectively, as well as the two-factor EFA models with and without error correlations (2F-EFA and 2F-EFA-C). The results are shown in Table 6.

| Model   | PPP (%) | CV-L |
|---------|---------|------|
| 1F      | 0.01    | 15.98|
| 1F-C    | 0.32    | 6.63 |
| 2F-EZ   | 0.04    | 10.45|
| 2F-AZ   | 0.40    | 6.23 |
| 2F-EZ-b | 0.41    | 0.00 |
| 2F-AZ-b | 0.44    | 2.01 |
| 2F-EFA  | 0.44    | 2.66 |
| 2F-EFA-C| 0.58    | 2.38 |

Table 6: PPP values and sum of log scores of 3-fold cross validation for the relevant models. The models with ‘-b’ refer to the measurement model with the first item loading to both factors. The best model had log score equal to 0 and the differences from it are reported for the other models.

Examination of the PPP values reveals concerns about the fit of the models 1F and 2F-EZ, so these are ruled out of the discussion. This raises several questions: Is the 2F-EZ-b the best model or do any of the AZ model versions, 2F-AZ or 2F-AZ-b, do better? Is the best of these three good enough? Perhaps more importantly, which measurement scale should be used for the FTND test on the basis of this dataset?

We attempt to shed light on these questions with the use of cross-validated log scores. The best model is the 2F-EZ-b correcting the misspecifications of 2F-EZ with a single additional parameter. The fact that the log score of 2F-EZ-b is smaller than that of the EFA models provides support towards the scale with two correlated factors where the item ‘FNFIRST’ loads on both of them.

6 Discussion

In this paper, we generalise the Bayesian SEM framework, introduced in Muthén and Asparouhov (2012), along two directions. First, by expanding the model to allow for other data distributions than the Normal; e.g. logistic often used in IRT models. Second, in terms of model exploration and assessment, by developing a suitable framework that goes beyond goodness of fit and allows us to address questions that naturally arise from the application of Bayesian SEM. This framework incorporates scoring rules combined with cross-validation to the existing fit indices.

As illustrated on simulated data and real-world examples, the use of the scoring rules can prove quite useful in SEM analysis. Nevertheless, as with any index, it would be helpful to explore it further and get a better understanding of the range of values indicating a good model in different settings. This range may depend on the sample size, the number of factors and parameters, the type of the data, the choice of the scoring rules, the number of folds or the form of cross-validation in general, the choice of the benchmark model etc. Another important component, present in any form of Bayesian analysis, is the prior specification. The behaviour of the scoring rules under different priors, e.g. the spike and slab priors, as in Lu et al. (2016), rather than the ridge-type priors, is also an interesting question.

The calculations can be implemented using MCMC through standard user-friendly software like Stan and can be combined with existing packages for SEM. This opens up the possibility of using fast approximate methods such as Variational Bayes (Kucukelbir et al., 2017) that are automated and readily available. This can be particularly useful in categorical data application where the use of MCMC and the presence of high-dimensional latent variables can result in computation times that are larger than the users’ expectations. Moreover, Variational Bayes can be used to improve the efficiency of MCMC samplers.

Further extensions of the generalised family of models can also be explored; for example, non-Normal errors \( e_i \) or random effects \( u_i \). Inspection of the latter may also provide diagnostic information for detecting outliers and removing items to purify the constructs. It would also be interesting to explore the connections with Bayes factors, as they tend to provide parsimonious models that typically do well in terms of cross-validation. Calculating Bayes factors is not always straightforward and they are also more sensitive to the choice of priors. However, such issues can be alleviated by suitable choice of priors, as done in this paper.
Finally, it is important to note that the developed model assessment framework and the CV index can be applied outside the Bayesian SEM context. In fact, it can be useful in situations where we need to assess the fit of a more flexible model, such as semi-parametric or non-parametric formulations (Yang and Dunson, 2010; Song et al., 2013). In such models, attaining a good fit is not always associated with a good systematic part of the model, as the flexibility in its error part can lead to overfitting. Such models arise in many scientific areas and go well beyond the SEM framework.

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A Inverse Wishart

We recall here that the Inverse Wishart distribution $\mathcal{IW}(D_p, d)$ is parameterised by matrix $D_p$ of dimension $p \times p$ and $d$ degrees of freedom where we need $d > p + 1$ for the distribution to be well defined. The higher the value of $d$ the more concentrated the distribution gets around $D_p$. For example, if we choose $D_p = I_p$, the identity matrix of size $p$, then the marginal distribution of the diagonal elements will be distributed with mean $1/(d - p - 1)$ and variance $2/[(d - p - 1)^2(d - p - 3)]$, whereas the off-diagonal elements will be distributed with mean 0 and variance $1/[(d - p)(d - p - 1)^2(d - p - 3)]$. Note that these expressions simplify when, for example, $d$ is set to $p + 6$. We refer the interested reader to the appendix of Muthén and Asparouhov (2012) for more information.

B Sensitivity analysis for data-dependent priors

We performed a sensitivity analysis to examine the effect of the data-dependent priors on the final result. In order to amplify the prior effect we used a relatively small sample size, by simulating 200 data points from a standard two-factor model, according to simulation Scenario 1 in Section 4. We fit the EZ model with the data-dependent prior of Frühwirth-Schnatter and Lopes (2018); Conti et al. (2014) that protects against Heywood cases for the idiosyncratic variances

$$
\psi^2_j \sim \text{InvGamma}(c_0, (c_0 - 1)/(S^j_{y j}))
$$

with $c_0 = 2.5$. Moreover, the following data-independent priors were also used: InvGamma(0.1,0.1), Half-Cauchy(5), and Uniform(0,10). The posterior samples from all four priors were used to produce kernel density plots for the posterior of the free $\Lambda$ elements that are depicted in Figure 1. As we can see, the posterior density plots are almost identical for all these priors. Similar results were also obtained for the remaining parameters. We therefore conclude that the data-dependent prior does not impact the final results, while helping guard against Heywood cases.
Figure 1: Posterior density plots of the loading matrix parameters under 4 different prior choices. The model using a data-dependent prior (red) produces identical posterior density plots as three other models using priors independent of the data.