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TITLE: "Getting a Step Ahead: Using the Regularized Horseshoe Prior to Select Cross-Loadings in Bayesian CFA"
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Abstract

This is the first study to compare the Regularized Horseshoe Prior (RHSP) to the Small Variance Normal Prior (SVNP) in their performance in regularizing cross-loadings in Bayesian CFA. The SVNP can be used to shrink cross-loadings in CFA to(wards) zero to identify models. This often results in biased model estimates, as not only small, irrelevant, but also large cross-loadings are shrunken substantially. The RHSP was expected to regularize cross-loadings more efficiently, avoiding the bias of the SVNP, by allowing large cross-loadings to escape shrinkage within a single estimation step. It was found that indeed the SVNP had overall higher levels of bias than the RHSP with large cross-loadings. Hereby, the RHSP was robust across sample sizes, and different hyper-parameter settings, although under some convergence failed. Regarding the Power and Type-I-Error rate in selecting cross-loadings as non-zero, both priors performed poorly, which is partially explained by the low sample sizes considered.

Keywords

Regularization, *Regularized SEM*, *Bayesian CFA*, *Small Variance Normal Prior*, *Regularized Horseshoe Prior*.

Introduction

The art of statistical modeling revolves around coming up with an appropriate simplification, a *model*, of a true *data-generating process*. Hereby, a fundamental trade-off between model simplicity and model complexity arises, that is mostly known as *bias-variance trade-off*. Simple models with few parameters have high bias, meaning that they deviate substantially from the true data-generating process, and low variance, such that they generalize well to other datasets from the same population. Complex models with large numbers of parameters tend to have low bias and high variance. They are thus prone to over-fitting, i.e. picking up patterns that are only relevant in the dataset at hand, but do not generalize well to other datasets. Moreover, complex models can be cumbersome to interpret and often a large number of observations is required to estimate them (Cox, 2006; James, Witten, Hastie, & Tibshirani, 2021).

In confirmatory factor analysis (CFA, Bollen, 1989) it is common practice to deal with the bias-variance trade-off in a brute-force manner, by imposing a so-called simple structure. Here, cross-loadings, factor loadings that relate items to factors that they theoretically do not belong to, are fixed to zero to yield an identified and easy-to-interpret model. This often leads to poor model fit, which forces researchers to free some cross-loadings after the fact based on empirical grounds (modification indices) to improve fit. This procedure is flawed, as it risks capitalization on chance and thereby over-fitting (MacCallum, Roznowski, & Necowitz, 1992).

As a Bayesian solution to this issue Muthén and Asparouhov (2012) proposed identifying CFA models, by setting the so-called *Small Variance Normal Prior* (SVNP) for cross-loadings, which is a normal distribution with mean zero and a very small variance (e.g. $\sigma^2 = 0.01$). This prior attaches large prior mass to cross-loadings of or near zero, while attaching almost no prior mass to cross-loadings further from zero, such that all cross-loadings in the model are shrunken. However, shrinking also the cross-loadings that

are further from zero introduces substantial bias to the model (Lu, Chow, & Loken, 2016). Consequently, Bayesian CFA requires a two-step approach. First, the model is estimated with the SVNP set for the cross-loadings and cross-loadings are selected as non-zero when their 95% credible intervals do not contain zero (Muthén & Asparouhov, 2012). The model is then re-estimated, where cross-loadings that have been selected to be non-zero are freely estimated without shrinkage, and the remaining cross-loadings are fixed to zero, avoiding the bias in the model of the previous step. Correctly selecting cross-loadings as non-zero can pose a challenge in practice, as the performance of different selection criteria depends on a broad set of conditions, making it difficult to formulate general recommendations for researchers (Zhang, Pan, & Ip, 2021). This calls for shrinkage priors that allow us to 'get a step ahead', by regularizing CFA models without causing substantial bias within a single estimation step.

One promising regularization prior that can be expected to allow estimating CFA models with less bias within a single step is the so-called Regularized Horseshoe Prior (RHSP), which is designed to let large parameters escape shrinkage. While the Regularized Horseshoe Prior has been shown to perform excellently in the selection of relevant predictors in regression (Piironen & Vehtari, 2017b; Van Erp, Oberski, & Mulder, 2019), no previous research has validated its performance in regularizing cross-loadings in CFA. We therefore aim to compare the RHSP to the SVNP in their performance in regularizing cross-loadings in Bayesian Regularized SEM.

In the remainder of this article we will first introduce regularization, whereby we will discuss the advantages of Bayesian over frequentist regularization. We will then outline Bayesian applications of regularized SEM. Here we will explain different shrinkage priors in detail, in particular the SVNP and the RHSP. Next, a simulation study is reported that assesses the performance of the RHSP vs. the SVNP in selecting cross-loadings in a simple CFA model. We conclude by proposing directions for future research in further establishing

the usefulness of the RHSP in Bayesian regularized SEM.

Theoretical Background

Regularization

A classic method of trying to find a balance between model complexity and model simplicity is *regularization* (Hastie, Tibshirani, & Wainwright, 2015). Regularization entails adding some bias to a model on purpose to reduce its variance. This helps to make models easier to interpret and more generalizable. In a frequentist context, regularization is achieved by adding a so-called penalty term to the cost function of a model. This ensures that model parameters that are irrelevant, e.g. small regression coefficients in a regression model with a large number of predictors, are shrunken to (or towards) zero. For a regression model, where we predict the scores of i, ..., N individuals on an outcome y_i based on scores on a vector of predictors x_i, the vector of regression coefficients β, and a random error term e_i:

$$y_i = \beta x_i + e_i, \text{ where}$$

$$e_i \sim \mathcal{N}(0, \sigma^2),$$

the Ordinary Least Squared Residuals estimates of β are obtained by minimizing the sum of squared residuals:

$$\hat{\beta} = \underset{\beta}{argmin}\{\Sigma_{i=1}^{N}(y_i - \beta x_i)^2\}.$$

Penalized regression adds a a penalty term to this cost function, which is generally denoted as $||\beta||_L$:

$$\hat{\beta} = \underset{\beta}{argmin}\{\Sigma_{i=1}^{N}(y_i - \beta x_i)^2 + \lambda||\beta||_L\}.$$

When L = 1, we speak of the so-called L-1 norm. In this case the penalty is: $||\beta||_1 = \Sigma_{j=1}^{p}|\beta_j|$. This is the well-known LASSO (Least Absolute Shrinkage and Selection Operator) penalty (Tibshirani, 1996, 2011). Here, the absolute values of the regression coefficients are added up, multiplied by λ, and then added to the sum of the squared errors

within the model's cost-function. The basic intuition is as follows. Just as minimizing the sum of the (squared) residuals leads to estimates of the model parameters with minimally small residuals, minimizing the (absolute) sum of the regression coefficients results in smaller values of the regression coefficients. The larger λ, the more weight the penalty has, and thereby the higher the amount of shrinkage to(wards) zero. In practice the hyper-parameter λ is often determined by means of cross-validation. When L = 2 (the so-called L2-norm) $||\beta||_2 = \sqrt{\Sigma_{j=1}^{p}\beta_j^2}$. This is the famous ridge penalty (Hoerl & Kennard, 2000). Here, the same general principle is followed. This time not the absolute sum, but the square root of the sum of squares of the regression coefficients is minimized. In practice, one key difference between the LASSO and the ridge penalty is that the former shrinks some coefficient entirely to zero (thereby actively selecting predictors), whereas in ridge regression coefficients are only shrunken approximately but never entirely to zero.

Regularization can also be applied in more complex models, which is illustrated by the body of literature applying regularization in Structural Equation Modeling. Regularized SEM entails adding penalties to the cost function of SEM models (typically a variant of the maximum likelihood cost function, F_{ML}) to reach sparser models. Now, for any given set of model parameters θ, we can add a penalty function $P(\theta)$ to the cost function of the model:

$$F_{ML,\ penalized} = F_{ML} \ + \lambda P(\theta).$$

Again the penalty function can take on different forms, such as the ridge (the square root of the sum of squares of the parameters) or the LASSO (summing the absolute values of every parameters), and λ is again a hyper-parameter that determines the amount of shrinkage. Regularized SEM has successfully been applied in selecting cross-loadings and residual covariances in CFA, especially under favorable conditions such as large sample sizes (Jacobucci, Grimm, & McArdle, 2016). Also structural model parameters, such as regression coefficients in MIMIC models (Jacobucci, Brandmaier, & Kievit, 2019; Jacobucci

et al., 2016), or indirect effects in mediation models with continuous (Serang, Jacobucci, Brimhall, & Grimm, 2017) or dichotomous outcomes (Serang & Jacobucci, 2020), have successfully been regularized through the usage of penalties such as the LASSO or ridge penalty.

The key disadvantage of the frequentist regularization approach is that it depends on optimization. With more complicated penalties, and in particular for complex models, it can be hard to derive optimizable cost functions in practice. Also the derivation of unbiased standard errors is often challenging under such circumstances, which hinders reliable inference (Jacobucci & Grimm, 2018; Jacobucci et al., 2016). Bayesian approaches to regularization overcome these obstacles (Jacobucci & Grimm, 2018). In Bayesian model estimation, the so-called Joint Posterior Distribution of the model parameters given the data is a combination of the data given the model parameters (the likelihood) and the prior distribution of the model parameters, i.e.,

$$P(\theta|data) \sim P(data|\theta)P(\theta).$$

Priors can therefore be used to shrink model-parameter estimates to(wards) zero. Such priors are called a shrinkage prior. In the most simple case one can simply set a normal prior for parameters that is centered around zero (as the SVNP mentioned above), which resembles the ridge penalty (Hsiang, 1975). The LASSO penalty can be mimicked by setting a Laplace- (double exponential) prior for parameters (Hans, 2009; Park & Casella, 2008; see Van Erp et al., 2019 for the Bayesian equivalents of other relevant penalties). The fact that in Bayesian inference the whole joint posterior distribution of the model parameters can be sampled by means of Markov chain Monte Carlo (MCMC) methods poses a central advantage. This renders it unnecessary to derive standard errors, as the variance of the posterior distribution of model parameters is directly available. Also complex shrinkage priors with unique desired properties can be implemented without having to yield an optimizable cost-function, making Bayesian regularization a very flexible

approach.

Bayesian CFA and The Small Variance Normal Prior (SVNP)

Confirmatory Factor Analysis (CFA, Bollen, 1989) is an essential tool for modeling measurement structures, falling under the class of Structural Equation Models (SEM). For every individual i, the scores on a vector of p observed indicators y_i:

$$y_i = \mu + \Lambda\eta_i + e_i,$$

where y_i is a $p \times 1$ vector of observed indicators, μ is a $p \times 1$ vector of intercepts, Λ is a $p \times q$ matrix of factor loadings, η_i is a $q \times 1$ vector of scores on the q latent factors, and e_i is a $p \times 1$ is a random vector of random (measurement) error terms. Here, Λ is thus the part of the equation that relates the latent variables to the observed scores on the items.

We can differentiate between so-called main-loadings, and cross-loadings. The former are factor loadings that relate factor and items to one another that are theoretically expected to have a relationship. Cross-loadings are factor loadings that relate factors to items between which, theoretically, no relationship should exist. One key property of CFA is that a clear expectation on the factor structure, i.e. which factor loads on which items, is assumed. This allows to formulate clear expectations on which items can be viewed as cross-loadings. Consequently, a natural way of identifying CFA (on top of other relevant identification constraints, such as scaling the factors) is to fix all cross-loadings to zero. Not only does that identify models, but it also ensures that the measurement structure is easy to interpret. However, in practice, fixing all cross-loadings to zero often results in poor model fit. So-called modification indices can be derived, which indicate how much model-fit improves when adding or removing a certain parameter (for instance, a cross-loading) to the model. Based on modification indices, researchers often re-add some cross-loadings to the model, until a desired level of fit is reached. However, a core property of modification indices is that they are only based on the dataset at hand, and may therefore only pick up

noise that is not relevant in the underlying population. Identifying cross-loadings based on modification indices thus risks capitalization on chance. Consequently, measurement structures may be selected that do not generalize well to other datasets from the same population, hence over-fitting may occur (MacCallum et al., 1992).

As solution to this issue, Muthén and Asparouhov (2012), proposed a Bayesian way of identifying CFA models. They argued that fixing cross-loadings of factor j on item k $\lambda_{c,jk}$ to zero can be interpreted as setting a normal prior with both a mean and a variance of zero on them:

$$\lambda_{c,jk} \sim \mathcal{N}(0,\ 0).$$

Now, since usually most cross-loadings are indeed zero, but there are some that are a bit larger (in absolute terms) than zero, and few that are substantially larger, they argue that a more realistic prior would be a normal distribution that is still centered around zero, but does have a small variance, e.g.

$$\lambda_{c,jk} \sim \mathcal{N}(0,\ 0.01).$$

The intuition of setting such a prior, which we refer to as Small Variance Normal Prior (SVNP), becomes clear when looking at Figure 1. In Bayesian model estimation the prior of a parameter directly influences the final posterior parameter estimate. By assuming that most cross-loadings are zero, most posteriors of cross-loadings will be centered around zero. At the same time, the prior allows for some deviations from zero, as there is also some prior mass for cross-loadings that are marginally larger or smaller than zero. Of course, applying the SVNP as prior for cross-loadings is thus nothing but a Bayesian variant of Regularized SEM, which strongly resembles the frequentist ridge penalty that was for instance applied by Jacobucci et al. (2016).

In practice an issue arises with the Bayesian CFA method, once substantially large cross-loadings enter the picture. The estimates of truly large cross-loadings should be large,

as otherwise the (co-)variance structure of the data is not explained properly. With the SVNP, however, the estimates of large cross-loadings are also shrunken substantially to(wards) zero, as the prior with its thin tails attaches no prior mass to them. This causes bias. First, bias naturally occurs in the large cross-loadings itself. However, also in other parameters, such as factor-correlations or main-loadings, substantial bias can arise, as they are estimated conditionally on the cross-loadings. To overcome this, the method is presented as a 2 step-approach (Muthén & Asparouhov, 2012). First, the model is estimated with the shrinkage prior set for the cross-loadings. Cross-loadings are then selected as non-zero if their 95% credible interval does non contain zero. Then the model is re-estimated. The as non-zero selected cross-loadings are estimated freely without shrinkage, avoiding the bias in their estimates of the previous step. The as zero selected cross-loadings are fixed to zero.

Alternative Shrinkage Priors

One alternative to the SVNP is the Bayesian LASSO, which has successfully been applied in regularized SEM previously (Chen, Guo, Zhihan, Zhang, Lijin, & Pan, Junhao, 2021; Zhang et al., 2021). In general, its performance is similar to that of the SVNP. While a core difference between the ridge- and the LASSO penalty is that the LASSO penalty automatically shrinks some parameters to zero, the Bayesian equivalent of the LASSO also requires manual selection. This is because Bayesian model estimates, posterior means, will never be entirely zero (Zhang et al., 2021). As the SVNP, the Laplace prior of the Bayesian LASSO has thin tails, though slightly thicker than those of the SVNP, attaching only little prior mass to large cross-loadings. Consequently, as with the SVNP, a two-step approach is required to estimate parameters without bias. Zhang et al. (2021) pointed out that it is difficult to formulate general recommendations on how to best select cross-loadings as non-zero when applying the Bayesian LASSO. It is thus desirable to find regularization priors that can be applied in Bayesian CFA that allow for estimating model parameters

without bias within a single step, to overcome the dependence on correctly selecting cross-loadings.

One suitable alternative regularization prior for the purpose of selecting cross-loadings in regularized Bayesian SEM is the so-called Spike-and-Slab Prior (George & McCulloch, 1993; Ishwaran & Rao, 2005; Mitchell & Beauchamp, 1988). This prior is a discrete mixture of an extremely peaked prior around zero (the spike), and a very flat prior for larger parameters (the slab). Formally, and applied to the cross-loadings in CFA, for every Cross-loading of factor j on item k, the Spike-and-Slab Prior can be specified as (Lu et al., 2016):

$$\lambda_{c,jk}|r_{jk} \sim (1 \ - \ r_{jk})\delta_0 + r_{jk}\mathcal{N}(0, c_{jk}^2), \text{ with}$$

$$r_{jk} \sim \mathcal{B}ernoulli(p_{jk}).$$

The basic intuition is as follows. When $r_{jk} = 1$, $\lambda_{c,jk} \sim \mathcal{N}(0, c_{jk}^2)$, hence $\lambda_{c,jk}$ is assigned to the slab. When $r_{jk} = 0$, $\lambda_{c,jk} \sim \delta_0$. In this case, the cross-loading is thus assigned to a point-mass at zero, i.e. it is assigned to the spike. This ensures that large cross-loadings, that are relevant are not shrunken while small, negligible cross-loadings are shrunken to zero. Lu et al. (2016) found that this prior performs well in shrinking truly zero cross-loadings to zero, while not shrinking (relevant) large cross-loadings to avoid bias, especially under favorable conditions with large sample sizes and cross-loadings. The prior is thus in general more suited to estimate CFA models without substantial bias within a single estimation step, due to its refined nature in differentiating between large and small cross-loadings. However, the Spike-and-Slab Prior cannot be implemented in STAN, one of the most popular software package for MCMC-sampling, as STAN does not allow for discrete mixture priors (Betancourt, 2018; Stan Development Team, 2021). This calls for a *non-discrete* alternative shrinkage prior that also outperforms the SVNP within a single estimation step.

The Regularized Horseshoe Prior (RHSP)

A fully continuous alternative to the Spike-and-Slab Prior that is implementable in STAN is the so-called *Regularized Horseshoe Prior* (RHSP, Piironen & Vehtari, 2017a, 2017b). This prior is an extension of the Horseshoe Prior (Carvalho, Polson, & Scott, 2010). The main idea of the original Horseshoe Prior is that there is a *global shrinkage parameter* τ, shrinking all cross-loadings to zero. Next to this, there is a *local shrinkage parameter* $\bar{\omega}_{jk}$[1] that allows truly large cross-loadings to escape the shrinkage, by setting thick Cauchy tails for the local scales ω_{jk} (Polson & Scott, 2010). Formally, the Horseshoe prior for every cross-loading of factor j on item k is specified as follows:

$$\lambda_{c,jk}|\omega_{jk}, \tau, c \sim \mathcal{N}(0,\ \omega_{jk}^2\tau^2),\ \text{where}$$

$$\omega_{jk} \sim \mathcal{C}^+(0,1).$$

The name-giving intuition behind the horseshoe prior becomes clear when considering the finding that a so-called shrinkage factor k_{jk} can be derived for the individual cross-loadings (Carvalho et al., 2010; Piironen & Vehtari, 2017b). This shrinkage factor ranges from zero to one, with zero meaning no, and one meaning a lot of shrinkage. When plotting the density of k_{jk} there is a very high peak at low values and a very high peak at high values, resulting in a plot that resembles a horseshoe, illustrating that the Horseshoe Prior has the desired property of either shrinking parameters very little, or very much, with very few parameters that are shrunken in a non-extreme fashion.

The Horseshoe Prior was found consistently to possess the theoretical properties of not shrinking large parameters while shrinking small parameters substantially to zero in practice (Carvalho et al., 2010; Datta & Ghosh, 2013; Polson & Scott, 2010; Van Der Pas, Kleijn, & Van Der Vaart, 2014). However, due to its heavy Cauchy tails it suffers from the

[1] We deviate from the common notation of the local shrinkage parameter as $\bar{\lambda}$, as this letter is commonly used to denote factor loadings in CFA.

same issues as a Cauchy prior. Specifically, not shrinking large parameters at all can lead to estimation issues, especially when parameters are weakly identified. This happens for instance in logistic regression with separable data, where a flat likelihood and thereby a weakly identified model arises (Ghosh, Li, & Mitra, 2018). The RHSP prevents such issues by shrinking also large parameters a little bit. The RHSP is specified as follows. For every cross-loading of factor j on item k:

$$\lambda_{c,jk}|\bar{\omega}_{jk}, \tau, c \sim \mathcal{N}(0,\ \bar{\omega}_{jk}^2\tau^2),\ \text{with}\ \bar{\omega}_{jk}^2 = \frac{c^2\omega_{jk}^2}{c^2 + \tau^2\omega_{jk}^2},$$

$$\tau|df_{global}, s_{global} \sim half - t_{df_{global}}(0,\ s_{global}^2),\ \text{with}\ s_{global} = \frac{p_0}{p - p_0}\frac{\sigma}{\sqrt{N}},$$

$$\omega_{jk}|df_{local}, s_{local} \sim half - t_{df_{local}}(0,\ s_{local}^2),$$

$$c^2|df_{slab}, s_{slab} \sim \mathcal{IG}(\frac{df_{slab}}{2},\ df_{slab} \times \frac{s_{slab}^2}{2}),$$

where p_0 represents a prior guess of the number of relevant cross-loadings. Allowing to incorporate prior expectations on the expected number of non-zero parameters is another core advantage of the RHSP over the original Horseshoe Prior. However, it is not necessary to use p_0. One can simply set s_{global} manually, whereby it is worth to consider that a s_{global} created based on a p_0 will typically be much lower than 1 (Piironen & Vehtari, 2017b). Note that we specify the RHSP in its most general form. Setting the degrees of freedoms of the half-t-distributions to 1 results in half-Cauchy distributions. Strictly speaking, the prior is only a Regularized *Horseshoe* Prior when this is the case. In the current study we vary the degrees of freedoms of all scale parameters to assess the extent to which the sparcifying properties as well as the convergence of the RHSP are influenced by this.

The intuition of how the RHSP shrinks large parameters a little bit is best illustrated by assuming that c is a given constant. Now, when $\tau^2\omega_{jk}^2 < c^2$, $\bar{\omega}_{jk}^2 \rightarrow \omega_{jk}^2$. Hence, in this case the RHSP approaches the original Horseshoe Prior, with equally pronounced shrinkage to zero. However, when τ is far from zero, hence under large true cross-loadings, $\tau^2\omega_{jk}^2 > c^2$, and $\bar{\omega}_{jk}^2 \rightarrow \frac{c^2}{\tau^2}$. Then, the prior of $\lambda_{c,jk}$ approaches a slab $\mathcal{N}(0, c^2)$. Under the

above specification, when c is no constant but a parameter for which an Inverse-Gamma hyper-prior is set, the slab becomes a t-distribution with df_{slab} degrees of freedom, a mean of zero and a scale of s^2_{slab} (Piironen & Vehtari, 2017b).

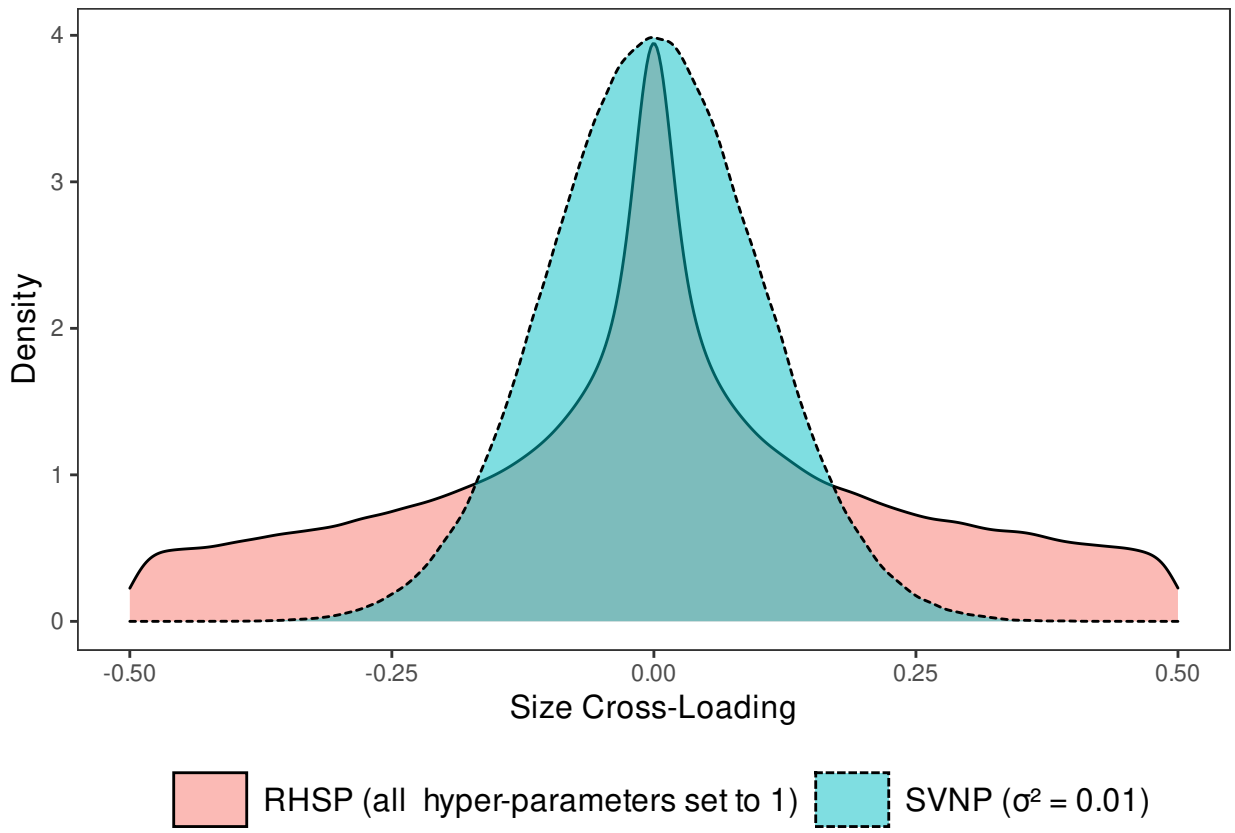

Figure 1. Density Plots of the Regularization Priors of Interest.

Figure 1 compares the two shrinkage priors that are the focus of our study. Both priors share a large peak at zero, which ensures that cross-loadings are shrunken to(wards) zero. However, the RHSP has much thicker tails. Here, for larger cross-loadings, there is thus much more prior mass than with the SVNP. This ensures large cross-loadings (and consequently other model parameters) can be estimated without bias within a single estimation step.

The current study

Study Procedure and Parameters

A Monte Carlo simulation study was conducted using STAN (Stan Development Team, 2021) and R (R Core Team, 2021). We used `cmdstandr` to interface STAN with R (Gabry & Češnovar, 2022), while also heavily relying on `rstan` (Stan Development Team, 2022) and `bayesplot` (Gabry & Mahr, 2022) for the post-processing of the posterior samples. Results were further post-processed using `tidyr` (Wickham & Girlich, 2022) & `dplyr` (Wickham, François, & Müller, 2022). All plots were made using `ggplot2` (Wickham, 2016). We ran up to 46 replications in parallel using the `parallel` package (R Core Team, 2022). This manuscript was written using R Markdown and the `papaja` package (Aust & Barth, 2022). All code that was used to run the simulations can be openly accessed on the author's **github**[2]. The models were sampled using the No-U-Turn-Sampler (Homan & Gelman, 2014), with two chains, a burnin-period of 2000 and a chain-length of 4000. These sampling parameters were identified in pilot runs to be required for the RHSP to reach convergence, and were therefore also used for the SVNP in order to ensure a fair comparison.

Conditions

Population Conditions. The datasets were simulated based on a true 2-factor model, with three items per factor, and a factor correlation of 0.5. The true model is summarized below, both in equations (Appendix A) and graphically (Figure 2).[3] The

[2] Specifically, the R-scripts needed to run the simulation can be found on https://github.com/JMBKoch/1vs2StepBayesianRegSEM/tree/main/R. `parameters.R` can be adjusted to adjust study parameters, and `main.R` is used to run the main simulation. Required packages are listed at the top of `parameters.R`.

[3] The STAN code of the model can be found on https://github.com/JMBKoch/1vs2StepBayesianRegSEM/blob/main/stan/

factors were scaled by fixing their means to zero and their variances to 1. All main-loadings were set to 0.75, and all residual variances to 0.3, to ensure that the largest proportion of variance in the items would be explained by their corresponding factor. We varied the size of the two truly non-zero cross-loadings λ_{c1} and λ_{c6} between 0.2, a negligible magnitude such that shrinkage to zero is desired, and 0.5, a size for which shrinkage towards zero should be avoided. We varied the sample sizes of the simulated datasets between 100 and 200. Larger sample sizes of for instance 500 were not included despite being common place in previous simulation studies, because adding them would have rendered the run-time of the simulations for the RHSP unfeasible. This is appropriate because for simple factor models applied researchers are unlikely to collect such larger sample sizes in practice, such that our findings still generalize to real-life settings.

For all parameters except the cross-loadings, non-informative priors were set: for the main-loadings a normal prior with mean of zero and a variance of 25, for the residual variances a half-Cauchy-prior with a location-parameter of 0 and a scale of 5, and for the factor-correlation STAN's default uniform prior.

SVNP: Prior Conditions. We varied the hyper-parameter of the SVNP, σ^2, between 0.001, 0.01 and 0.1, based on Muthén and Asparouhov (2012). For the SVNP this left us with a total number of 2 (size cross-loading) x 2 (N) x 3 (hyper-parameter σ^2) = 12 individual conditions. Per condition, 200 replications were run, yielding a total of 2400 replications for this prior.

RHSP: Prior Conditions. The RHSP has six hyper-parameters in the specification that we apply. We varied the scales of the global shrinkage parameter τ, s_{global} between, 0.1 and 1. Here 1, is a natural maximum given that the scale generally does not become larger than 1 when applying a prior guess p_0 (Piironen & Vehtari, 2017b), and 0.1 a logical minimum given the (standardized) scale of the model. Also the scale of the local shrinkage parameter ω_{jk} was varied between, 0.1 and 1. The degrees of freedoms of these two parameters, df_{local} and df_{global} were varied between 1 and 3. Larger degrees

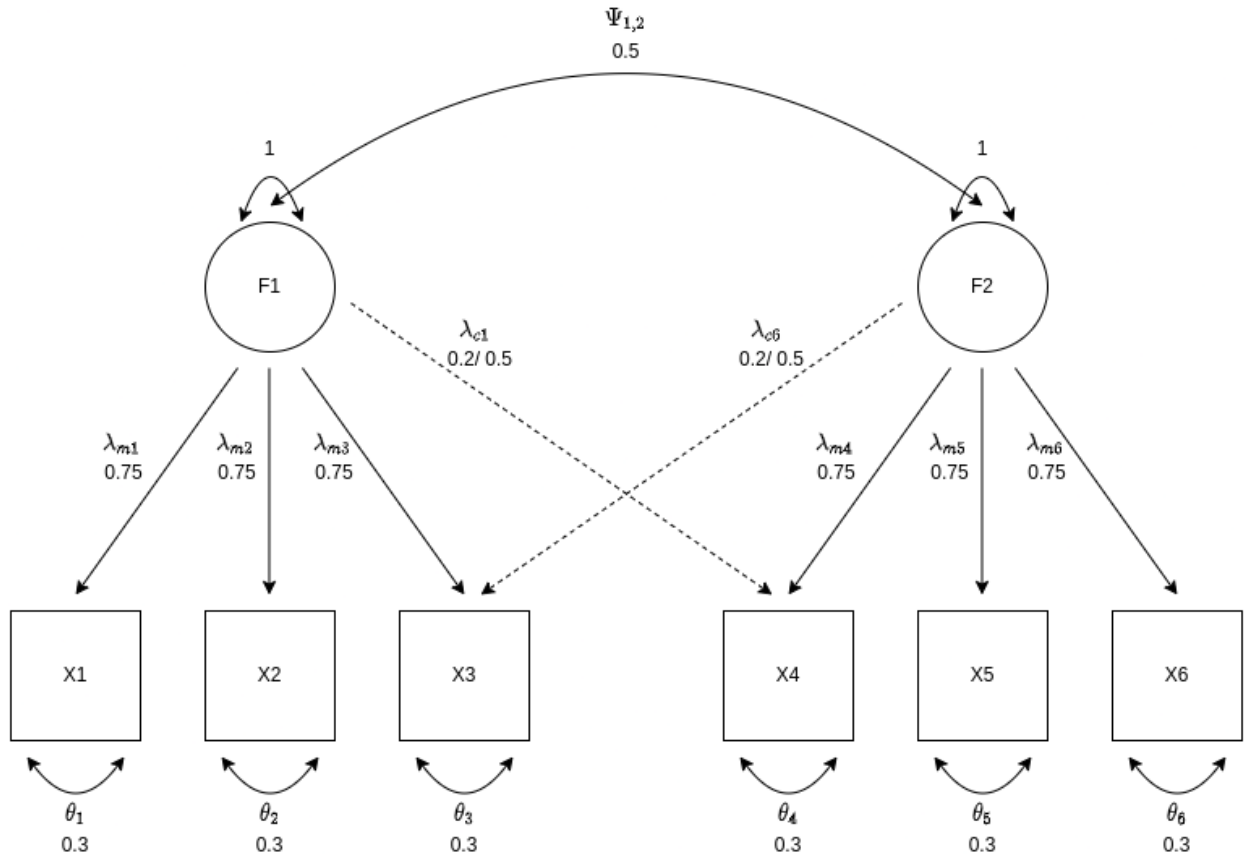

Figure 2. Graphical Representation of the True Model.

of freedoms may help to overcome sampling issues that can arise when the df's are set to one. Finally, for the scale of the distribution of c^2, s_{slab} was varied between 0.1, 1 and 5, and df_{slab} between 1 and 3. We decided to include a broader range of scales for the slab, as the slab is crucial in determining the shrinkage of large cross-loadings. We were thus left with 2 $(s_{global}) \times 2$ $(df_{global}) \times$ 2 $(s_{local}) \times 2$ $(df_{local}) \times 3$ $(s_{slab}) \times 2$ $(df_{slab}) = 96$ hyper-parameter conditions for the RHSP. In combination with the 2×2 population conditions this yielded 384 individual conditions for this prior. In total there were thus $384 \times 200 = 76800$ replications run for the RHSP. Table 1 summarizes all conditions.

Table 1

Overview study conditions.

Condition	Levels	Values
Population		
Sample size (N)	2	100, 200
Size cross-loading $\lambda_{c1,6}$	2	0.2, 0.5
SVNP		
σ^2	3	0.1, 0.01, 0.001
RHSP		
s_{global}	2	0.1, 1
df_{global}	2	1, 3
s_{local}	2	0.1, 1
df_{local}	2	1, 3
s_{slab}	3	0.1, 1, 5
df_{slab}	2	1, 3

Note. SVNP = Small Variance Normal Prior. RHSP = Regularized Horseshoe Prior. There was a total number of 396 conditions for both priors combined. All conditions were replicated 200 times.

Outcomes

All outcomes[4] were computed based on both mean and median posterior estimates of the model parameters. We only present the results of the mean estimates, but those concerning the median estimates (which do not differ relevantly from those of the mean estimates) can be accessed on github[5].

Mean Absolute Bias. For every model parameter θ and for every condition that has been sampled for N_{rep} replications, we computed the Mean Absolute Bias:

$$\bar{Bias}_{\bar{\theta}} = \frac{1}{N_{rep}} \Sigma_{i=1}^{N_{rep}} |\bar{\theta}_i - \theta_{true}|.$$

Given that the core issue of the SVNP is biased model estimates, this outcome naturally plays a central role in our study.

Relative Bias. The Relative Bias was computed per model parameter estimate and set of conditions by dividing the estimates of the Mean Absolute Bias by the true value of the parameter:

$$\bar{Bias}_{rel,\ \bar{\theta}} = \frac{\bar{Bias}_{\bar{\theta}}}{\theta_{true}}.$$

This outcome gives an indication of the magnitude of the bias by expressing it relative to the parameter's true value. However, given the standardized scale of the true model, the Mean Absolute Bias is a quantity that can be interpreted rather intuitively in the context of this study and conlusions do not differ based on the relative bias. We therefore do not discuss these results in detail, and refer the interested reader to the study repository on github[6].

[4] Summaries of all outcomes can be found on https://github.com/JMBKoch/1vs2StepBayesianRegSEM/tree/main/Rmd/analyses.

[5] see TBA LINK for the SVNP and TBA LINK for the RHSP

[6] see https://github.com/JMBKoch/1vs2StepBayesianRegSEM/blob/main/Rmd/analyses/SVNP/plotsRelBiasSVNP.html for the relative bias of the SVNP and TBA LINK for the relative bias of the RHSP

Mean Squared Error: The Mean Squared Error (MSE) was computed per model parameter and set of conditions as:

$$MSE_{\bar{\theta}} = \frac{1}{N_{rep}} \Sigma_{i=1}^{N_{rep}} (\bar{\theta}_i - \theta_{true})^2.$$

Another way to express the MSE is as the sum of the bias and the variance of a model parameter, which explains its added value over the Mean Absolute Bias alone. As with the Relative Bias we refrain from presenting results here as they do not add to the conclusions based on the Mean Absolute Bias[7].

Power and Type-I-Error Rate. Per set of conditions, we computed the Power (true positive rate) in selecting truly non-zero cross-loadings as non-zero by calculating the proportion of replications where they were selected as non-zero. The Type-I-Error (false positive) rate in selecting truly zero cross-loadings as non-zero was computed per set of conditions as the proportion of replications where the truly non-zero cross-loadings were selected as non-zero.

For both of these outcomes, we applied a variety of selection criteria for selecting cross-loadings as non-zero, based on earlier research (Zhang et al., 2021). First, we used a variety of thresholding rules, where a cross-loading is selected as non-zero when the absolute value of its estimate exceeds a specific threshold: $0, 0.05, 0.1, 0.15$. Next, we considered four credible intervals (50%, 80%, 90%, 95%), where cross-loadings are selected as non-zero when the interval does not contain zero.

Results

Convergence

Criteria. We removed replications for which at least one parameter did not converge. Convergence was determined based on two criteria. A parameter was viewed as

[7] MSE estimates and plots can be found on TBA Link for the SVNP and TBA LINK for the RHSP

having reached convergence when its value of the effective sample size N_{Eff} exceeded 10% of the chain-length and its value of $\hat{R}$ did not exceed 1.05. Moreover, we looked into the number and proportion of divergent transitions. Divergent transitions can be thought of as values of the Hamiltonian Monte Carlo Markov chain that diverge so much from their previous value that they cannot be trusted (see Betancourt, 2018 for details).

SVNP. The SVNP showed excellent performance in terms of convergence. Not a single replication had to be removed for not fulfilling the criteria outlined above. Moreover, across all runs there was not a single divergent transition. All 2400 replications were therefore included in the results.

RHSP. The RHSP showed weaker performance in terms of convergence than the SVNP. In total 742 replications were removed for not reaching convergence.

A total of 156 replications failed entirely, in terms of not yielding any output at all, This happened in one specific condition:
$N = 100,\ size\ \lambda_{c1,6} = 0.2,\ s_{global} = s_{local} = s_{slab} = 0.1,\ df_{global} = df_{local} = df_{slab} = 1.$
We removed the remaining 44 replications of this set of conditions, as there were too little left to give a reliable picture.

Next, we removed 542 replications for not fulfilling the criteria outlined above. The maximum number of removed replications for a given set of conditions was 37, which corresponds to 18.5% of the replications under these conditions. Below in Table 2 we present all combinations of conditions under which more than 5% of the replications had to be removed. The conditions had in common that they had an N of 100, true cross-loadings of 0.50, and a s_{global} and s_{local} of 0.1.

Table 3 presents the mean and maximum proportion of divergent transitions per condition, for all conditions under which there were, on average, at least 5% divergent transitions per chain. Again, these were the conditions that also suffered from convergence issues based on N_{Eff} and $\hat{R}$: N = 100, size cross-loadings = 0.50, $s_{global} = s_{local} = 0.1$.

Table 2

Conditions of the RHSP under which more than 5% of replications were removed for not having reached convergence (N = 542).

s_{global}	df_{global}	s_{local}	df_{local}	s_{slab}	df_{slab}	N	Size $\lambda_{c1,6}$	N removed Rep.
0.10	3	0.10	1	0.10	1	100	0.50	10
0.10	3	0.10	1	1.00	3	100	0.50	11
0.10	1	0.10	1	5.00	3	100	0.50	12
0.10	3	0.10	1	5.00	1	100	0.50	12
0.10	3	0.10	1	1.00	1	100	0.50	13
0.10	3	0.10	3	0.10	3	100	0.50	13
0.10	1	0.10	1	5.00	1	100	0.50	15
0.10	3	0.10	1	5.00	3	100	0.50	15
0.10	1	0.10	3	0.10	1	100	0.50	20
0.10	1	0.10	3	1.00	1	100	0.50	24
0.10	1	0.10	3	1.00	3	100	0.50	24
0.10	1	0.10	3	5.00	3	100	0.50	27
0.10	1	0.10	3	5.00	1	100	0.50	30
0.10	3	0.10	3	0.10	1	100	0.50	33
0.10	3	0.10	3	1.00	1	100	0.50	34
0.10	3	0.10	3	5.00	1	100	0.50	34
0.10	3	0.10	3	1.00	3	100	0.50	37
0.10	3	0.10	3	5.00	3	100	0.50	37

Note. Replications were removed for having an $\hat{R} >= 1.05$ or an N_{eff} smaller that 10% of the chain-length, for any of the model parameters.

We decided not to remove these replications, as this would have removed a substantial number of 2770 replications. In general, it is advised not to include any divergent transitions, since they introduce bias. Given the complex nature of the RHSP, which in practice usually leads to some divergent transitions, it is hard to follow this advise in practice. However, it needs to be taken into account in the interpretation of the findings that the divergent transitions may have added bias to the model estimates of the RHSP.

Main Results

Mean Absolute Bias. The Mean Absolute Bias of the SVNP and the RHSP for all parameters is summarized in Figure 3. For parameter estimates that show an identical pattern ($\bar{\lambda}_{c2-5}$, $\bar{\lambda}_{c1,6}$, $\bar{\lambda}_{m1,2,5,6}$, $\bar{\lambda}_{m3-4}$, and $\bar{\theta}_{1-6}$), the first respecting estimate is presented representative for all, both in Figure 3 and in the numbers presented below. As results are almost identical for the two sample sizes, we focus on presenting the findings for N = 100, to not distract from our main conclusions.[8] We extensively compared the Mean Absolute Bias of the RHSP between different hyper-parameter settings and sample sizes.[9] Differences were so little that we do not present them here, to not distract from our main comparison to the SVNP. We decided to present the findings with all hyper-parameters set to one, as this is a logical default hyper-parameter configuration under the scale of a standardized CFA model. The replications under these conditions showed good convergence, such that only a single replication had to be removed.

The truly zero cross-loadings ($\bar{\lambda}_{c2-5}$) had overall little levels of bias, across priors and

[8] The Mean Absolute Bias visualized for the different sample sizes separately can be found on https://github.com/JMBKoch/1vs2StepBayesianRegSEM/blob/main/Rmd/analyses/plotsBiasSVNP.html and https://github.com/JMBKoch/1vs2StepBayesianRegSEM/blob/main/Rmd/analyses/RHSP/plotsBiasRHSPSelection.html.

[9] see https://github.com/JMBKoch/1vs2StepBayesianRegSEM/blob/main/Rmd/analyses/RHSP/plotsBiasRHSP.html

Table 3

Mean and Maximum proportion of divergent transitions per iteration for conditions of the RHSP with on average more than 5% divergent transitions.

s_{global}	df_{global}	s_{local}	df_{local}	s_{slab}	df_{slab}	N	Size $\lambda_{c1,6}$	Mean	Max
0.10	1	0.10	3	0.10	1	100	0.50	0.06	0.56
0.10	1	0.10	3	5.00	1	100	0.50	0.06	0.71
0.10	1	0.10	3	5.00	3	100	0.50	0.06	0.75
0.10	3	0.10	1	0.10	1	100	0.50	0.07	0.66
0.10	3	0.10	1	5.00	1	100	0.50	0.06	0.58
0.10	3	0.10	3	0.10	1	100	0.50	0.07	0.54
0.10	3	0.10	3	1.00	1	100	0.50	0.07	0.65
0.10	3	0.10	3	5.00	1	100	0.50	0.07	0.83
0.10	3	0.10	3	5.00	3	100	0.50	0.08	0.69

Note. Mean = Mean proportion of divergent transitions, Max = maximum proportion of divergent transitions. There was a total of 2770 replications where the divergent transitions exceeded 5% of the chain-length. There were 14373 replications with more than 1% of divergent transitions. There were 1247 replications with more than 10% of divergent transitions. There were 46 replications with more than 50% of divergent transitions.

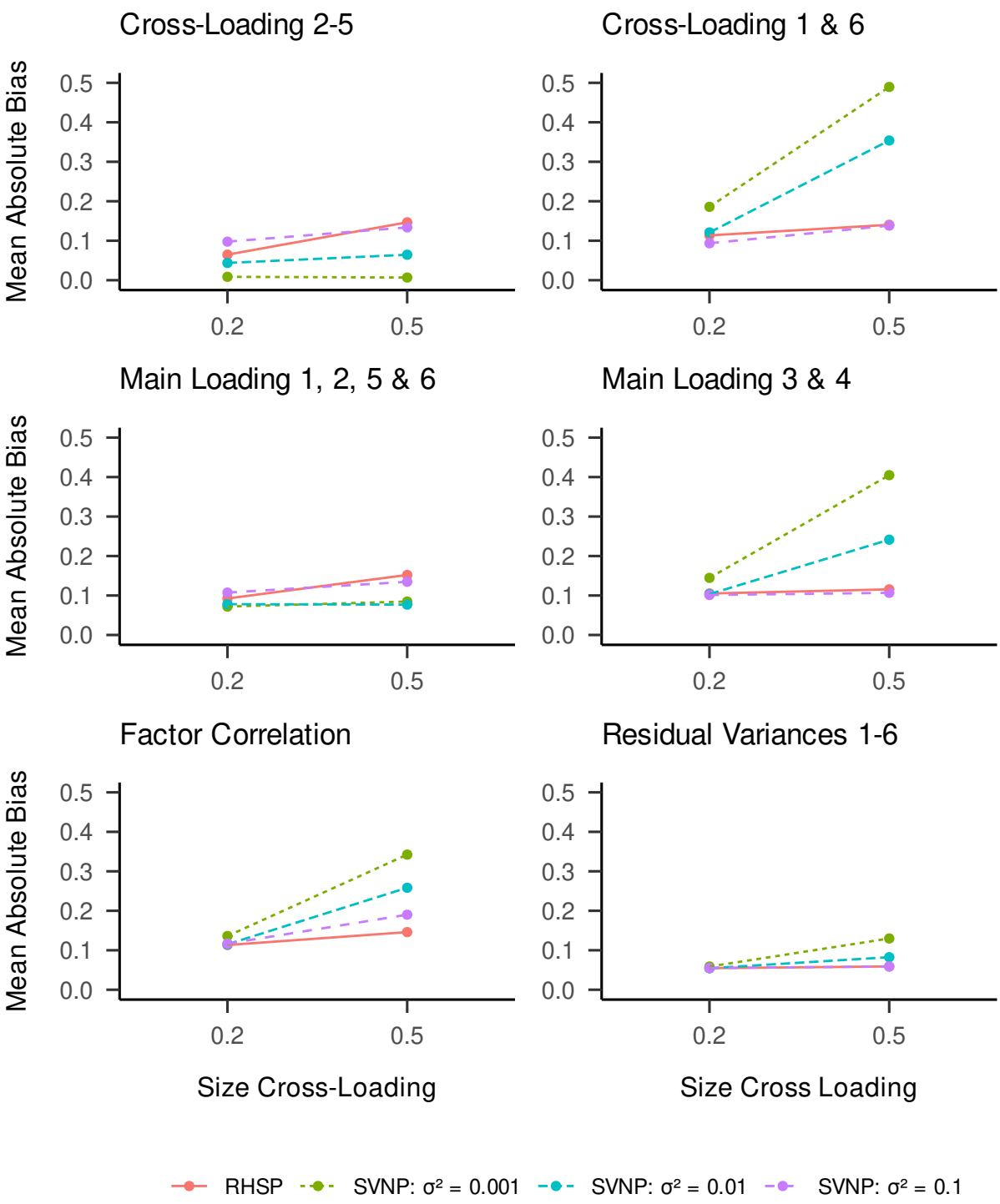

Figure 3. Mean Absolute Bias in the Model Parameters (N = 100). Per set of parameters that showed an identical pattern, the first parameter was used to represent all other parameters, e.g. cross-loading 2 was plotted representative for cross-loading 3-5. All hyperparameters of the RHSP are set to 1 in the results presented here.

hyper-parameter settings. The patterns in the bias of the RHSP was almost identical to that of the SVNP with $\sigma^2 = 0.1$. Note that for both priors the bias in these cross-loadings comes from these cross-loading being under-estimated (i.e., estimated as smaller than zero).

Regarding the truly non-zero cross-loadings ($\bar{\lambda}_{c1,6}$) the bias was sometimes very large for the SVNP, particularly with large true cross-loadings of 0.5 and $\sigma^2 = 0.001$ (e.g. $\bar{Bias}_{\bar{\lambda}_{c1}} = 0.49$) since the estimates of the true cross-loadings of 0.5 were shrunken almost entirely to zero (e.g. $\bar{\lambda}_{c1} = 0.01$). Also with $\sigma^2 = 0.01$ (and true cross-loadings of 0.5) substantial bias occured (e.g. $\bar{Bias}_{\bar{\lambda}_{c1}} = 0.35$), as the cross-loadings were still under-estimated considerably ($\bar{\lambda}_{c1} = 0.15$), though not entirely shrunken to zero. With $\sigma^2 = 0.1$ the bias in the estimates of the truly non-zero cross-loadings of 0.5 was less pronounced (e.g. $\bar{Bias}_{\bar{\lambda}_{c1}} = 0.14$). Here σ^2 was large enough to estimate the cross-loadings closer to their true value, $\bar{\lambda}_{c1} = 0.37$. The bias of the RHSP was again almost entirely identical to that of the SVNP with $\sigma^2 = 0.1$.

Also the estimates of the main loadings of factor 1 on item 3 ($\bar{\lambda}_{m3}$) and of factor 2 on item 4 ($\bar{\lambda}_{m4}$) were substantially biased under the SVNP when the true cross-loadings were 0.5 and $\sigma^2 = 0.001$ (e.g. $\bar{Bias}_{\bar{\lambda}_{m3}} = 0.40$). These two loadings showed much higher bias than the other four main-loadings as they loaded on the same two items as the two non-zero cross-loadings ($\bar{\lambda}_{c1}$ and $\bar{\lambda}_{c6}$, see Figure 2). As the cross-loadings were shrunken to zero, these main loadings now also accounted for the variance in the items that was truly explained by the cross-loadings. Consequently, the two main-loadings were over-estimated, e.g. $\bar{\lambda}_{m3} = 1.15$. Both the RHSP and the SVNP with $\sigma^2 = 0.1$ had low levels of bias for the main-loadings both with true cross-loadings of 0.2 and 0.5.

In the factor correlation $\bar{\Psi}_{1,2}$ the bias was al relatively small and approximately the same for the RHSP and the SVNP with different values of σ^2 when the truly non-zero cross-loadings were 0.2. For the SVNP, bias became again much more pronounced with true cross-loadings of 0.5 and small values of σ^2, particularly $\sigma^2 = 0.001$ ($\bar{Bias}_{\bar{\Psi}_{1,2}} = 0.34$).

In this situation the factor correlation was heavily over-estimated ($\bar{\Psi}_{1,2} = 0.84$). This can be explained by the fact that the covariance between item 3 and 4 that arose from the two cross-loadings, was misattributed to the factor-correlation, as the cross-loadings were shrunken to zero. For both the SVNP with $\sigma^2 = 0.1$ and the RHSP, the bias in the factor correlation was much lower, although there was still a noticeable increase between true cross-loadings of 0.2 and 0.5.

For both priors, the bias in the estimates of the residual variances $\bar{\theta}_{1-6}$ was not large across different conditions, although for the SVNP there was a noticeable increase between true cross-loadings of 0.2 and 0.5 when $\sigma^2 = 0.001$.

Power and Type-I-Error Rate. Figure 4 summarizes the Power and the Type-I-Error rate of both priors. Again, the outcomes are presented for the first parameter of an identical set of parameters (e.g., $\lambda_{c,1}$ is presented representative for the two truly non-zero cross-loadings). Moreover, results of the RHSP are again presented with all hyper-parameters set to one. In the plots summarizing the Power the horizontal red dashed line indicates the minimum power of .80 recommended by Muthén and Asparouhov (2012). According to Cham, West, Ma, and Aiken (2012), the maximally acceptable Type-I-Error rate is the upper-bound of a 95% interval of a binomial distribution, in this case $0.05 + 1.96 \times \sqrt{0.05 \times (1 - 0.05)/N_{rep}} = 0.08$. This maximum is visualized by the horizontal red dashed line in the Type-I-Error rate plots. For both priors, with a threshold of 0.00 there is both a Power and Type-I-Error rate of 1. This is logical, since posterior means will never be entirely zero (Zhang et al., 2021). The result thus mostly serves to illustrate this property of Bayesian inference and thereby the need for more complex selection rules in Bayesian regularization, if the goal is variable selection itself, and not only unbiased model parameter estimates. Whether a high Power or a low Type-I-Error rate is prioritized depends on many factors, such as the model at hand and the research goal. In general, one should aim for a balance between both, with high enough levels of Power and low enough Type-I-Error rates co-occuring.

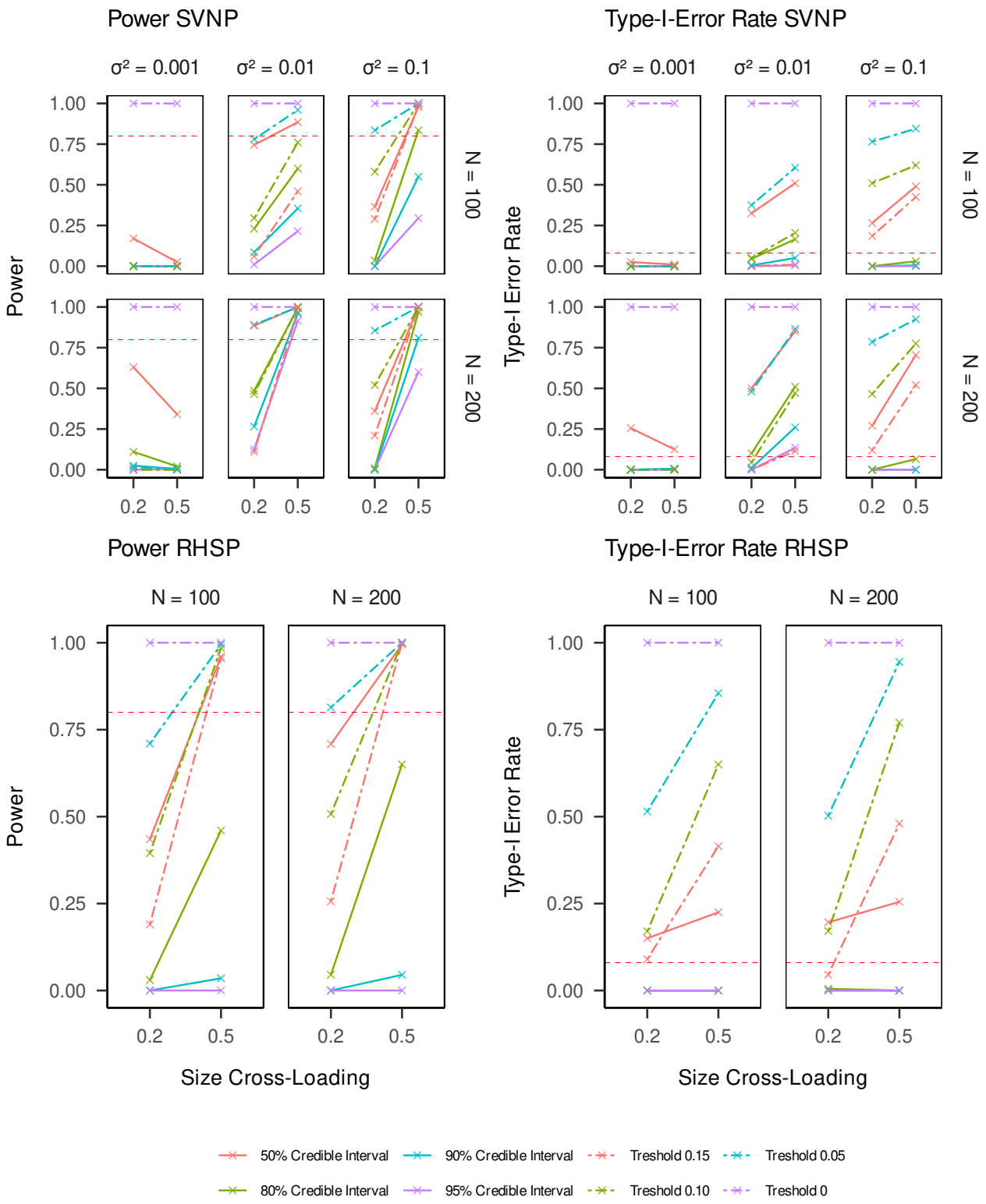

Figure 4. Mean Power and Type-I-Error Rates in Selecting non-zero Crossloadings. All hyper-parameters of the RHSP are set to 1 in the results presented here.

For both priors and across most conditions, the Power fell under the desired threshold of .80. For the SVNP with $\sigma^2 = 0.001$ non-zero cross-loadings were always over-shrunken so much that they were never selected as non-zero. Under $\sigma^2 = 0.01$, the situation improved somewhat, with now cross-loadings of 0.5 being correctly selected as non-zero for all selection rules when N = 200. For N = 100, thresholds of 0.05, and 50% credible intervals also had the desired levels of power, with thresholds of 0.10 also almost reaching a power of .80. The SVNP performed best in terms of power when $\sigma^2 = 0.1$. With N = 200, all selection rules except for the 95% credible intervals reached the desired Power. With N = 100, all selection rules except for the 95% and 90% credible intervals exceeded a power of .80. For the RHSP, in general the Power did also not live up to the standards by Muthén and Asparouhov (2012). The desired power was exclusively reached in selecting cross-loadings that were truly 0.5, when using 50% credible intervals or the three thresholds. Especially the widest (90% and 95%) credible intervals performed very poorly, which is explained by the fact that the lower bounds of these intervals (almost) always exceeded zero.

In general, under most conditions the Type-I-Error rate of both the SVNP and the RHSP exceeded the desired maximum. For the SVNP, with $\sigma^2 = 0.001$ and N = 100, the Type-I-Error rate stayed very low for all selection critera (up to the 0.00 threshold), as under this condition all cross-loadings, including the truly zero ones, were always shrunken almost entirely to zero. With N = 200, the 50% credible intervals lead to an undesired large Type-I error rate. With $\sigma^2 = 0.01$ and N = 100, some selection rules (90% & 95% credible intervals, a threshold of 0.15) had an acceptable Type-I-Error rate even with large true cross-loadings of 0.5, but they quickly became unacceptably high with N = 200. With $\sigma^2 = 0.1$, all selection rules except for 90% and 95% credible intervals had unacceptably high Type-I-Error rates for both sizes of non-zero cross-loadings, even though pronounced differences between cross-loadings of 0.2 and 0.5 occured. This was the condition under which the SVNP had the best levels of power, indicating that the good performance in

Power comes with the caveat of a poor Type-I-Error rate. The RHSP performed even worse than the SVNP in terms of its Type-I-Error rate. Only the 90% and 95% credible stayed within the desired boundary, as they always included zero. This, however, is not useful in practice as these intervals were completely unable to identify truly non-zero cross-loadings correctly as non-zero.

Conclusions and Discussion

This was the first study to apply the Regularized Horseshoe Prior (RHSP, Piironen & Vehtari, 2017b) in Bayesian Regularized SEM, by using it to select cross-loadings in CFA. A comparison to the Bayesian CFA approach by Muthén and Asparouhov (2012) was made, where cross-loadings are regularized with the Small Variance Normal Prior (SVNP).

Both the SVNP and the RHSP performed well with small truly non-zero cross-loadings of 0.2, in terms of estimating the model without substantial bias. This can be interpreted as a successful instance of regularization, where an acceptable amount of bias is added to the model by shrinking some parameters to(wards) zero, to reach a sparser solution. However, under some hyper-parameter settings the performance of the SVNP decreased substantially with larger truly non-zero cross-loadings of 0.5. With smaller values of σ^2, particularly with $\sigma^2 = 0.001$, these cross-loadings were still shrunken to zero, even though they were much larger in reality. This caused substantial bias, not only in the estimates of the cross-loadings itself, but also in the estimates of some main-loadings and the factor correlation. In practice, bias in structural parameters is particularly concerning, as it may lead to wrong conclusions in research on structural relationships between latent constructs. With $\sigma^2 = 0.1$, the SVNP was able to estimate the model parameters with little bias. Such relatively large variance still allowed for enough deviations from zero in the cross-loadings to yield relatively accurate estimates of the non-zero cross-loadings itself and, consequently, the other model parameters. The RHSP performed very similar to the SVNP with $\sigma^2 = 0.1$.

While the RHSP and the SVNP were both able to estimate the simple CFA model of this study with little bias, only the RHSP was able to do so consistently across different hyper-parameter settings. This poses a central advantage over the SVNP. Being robust to different hyper-parameter settings, which is achieved though the complex nature of the RHSP that sets hyper-priors on all parameters, may ultimately allow researchers to apply the RHSP without having to worry about choosing optimal values for the hyper-parameters. However, the other side of the coin is that the complex nature of the RHSP makes it sensitive to hyper-parameter settings regarding its performance in terms of convergence, in contrast to the SVNP that had excellent convergence across all conditions. Hereby, a clear pattern arose, with convergence issues arising with large cross-loadings, small sample sizes and small scales for the local and global shrinkage parameter. While this may suggest that one should simply avoid using small values for the scales, using larger scales that shrink parameters less may lead to identification problems in more complex SEM models. Future research is required that incorporates more complex models, in order to assess the performance of the RHSP in terms of convergence in more depth. Ultimately, it is desirable to be able to formulate clear guidelines on which hyper-parameter configurations to use in which situations to avoid convergence issues, to make the RHSP a practical approach.

Particularly under simple models such as the one employed in this study using the less complex SVNP with a relatively large value of σ^2 may thus prove advantageous in practice, to avoid risking bias stemming from non-convergence and divergent transitions. Next to this, the simpler SVNP is easier to implement and takes substantially less time to run. However, simply using larger values of σ^2 with the SVNP is no general solution. In practice, models may include more structural parameters, even more cross-loadings, or a number of residual co-variances. Under these circumstances, large values of σ^2 may lead to identification issues. Moreover, the larger σ^2, the more cross-loadings will be selected as non-zero, which may ultimately lead to over-fitting. Because of this, the RHSP might prove as more advisable for more complex models. While the RHSP, as the SVNP, can be

assumed to run into more and more identification issues with increasing model complexity, its refined nature in giving prior mass only where strictly desired (see Figure 1) might allow for a more efficient identification of complex models than the SVNP. If the RHSP continues to be robust to its hyper-parameter settings in terms of bias when applying it to complex models, using it may thus be the approach of choice in situations where identification is hard to achieve with the SVNP. However, future research comparing the SVNP to the RHSP in regularizing more complex SEM-models is yet to investigate this directly.

Regarding the Power and Type-I-Error rate in selecting cross-loadings as non-zero, both priors performed poorly across a range of selection rules. First of all, this is not surprising, given earlier research which clearly showed that a range of shrinkage priors (SVNP, Bayesian LASSO, Spike-and-Slab Prior, Lu et al., 2016; Zhang et al., 2021) generally need much larger sample sizes than the ones employed in this study to reach desirable levels of Power and Type-I-Error rates (see Jacobucci et al., 2016; Lu et al., 2016, who show that frequentist variable selection methods are sensitive to sample size too). Future research should therefore assess the Power and Type-I-Error rate of the RHSP under larger sample sizes (e.g. N = 500, 1000, 2000) to allow for a more conclusive picture. At the same time, it is an important finding that both priors perform poorly under small sample sizes, as simple CFA models are often fitted with such small sample sizes in practice. Note also that our findings do not imply that the RHSP is useless under low sample sizes. If the goal of regularization is not to select which cross-loadings are zero, but to yield unbiased estimates of the other model parameters, the RHSP still works better than the SVNP under most settings, even with small sample sizes. In practice, researchers often fit SEM-models including a measurement structure to test structural hypotheses. For this purpose, the question of whether or not cross-loadings are zero is not as relevant, as long as the structural model parameters are estimated without substantial bias. Next to this, different selection methods, such as Highest Posterior Density (HPD) intervals (Zhang et al., 2021), or projection predictive inference (Piironen & Vehtari, 2017b) may be more

successful in making a selection that meets the desired balance in Power and Type-I-Error rate.

The large levels of bias found in the SVNP (for the majority of hyper-parameter settings) are not surprising, given the original approach explicitly asking for a second step to circumvent bias (Muthén & Asparouhov, 2012). However, the fact that the SVNP performed so poorly in selecting the cross-loadings across selection rules suggests that in practice the 2-step approach, which heavily relies on a correct selection of cross-loadings as non-zero, is not advisable. This, however, needs to be directly assessed in future research. One approach of doing so would be to first make a selection of cross-loadings and then actively execute the second estimation step using new validation data sets. This would allow to compare the bias of the 2-step SVNP to the (1-step) RHSP directly. While our study formed a valuable first step in establishing the performance of the RHSP in regularized SEM, such a design would allow to more directly answer the question of whether or not the RHSP enables us to 'get a step ahead'.

Next to specific limitations named above, the current study has some general shortcomings, which lead to a number of recommendations for future research. First, we only assessed the performance of the RHSP in regularizing cross-loadings in a very simple CFA model consisting of only two factors. A straightforward way of extending the current study and making its findings more generalizable would be to include factor models with more factors. Within CFA models, another important set of parameters that can be identified through the usage of shrinkage priors are residual co-variances (i.e. the off-diagonal elements of Θ), which are usually fixed to zero in classic CFA (Muthén & Asparouhov, 2012). An important next step is thus to assess the performance of the RHSP in selecting residual co-variances on top of cross-loadings. Hereby, it is advisable to start by regularizing residual co-variances separately rather than on top of cross-loadings, as regularizing both parameters simultaneously can be challenging in practice (Zhang et al.,

2021). Of course, it is also desirable to assess the performance of the RHSP in regularizing model parameters in more complex SEM models, such as structural parameters, e.g. indirect effects in mediation models, or regression coefficients in MIMIC models. Also applying the RHSP in measurement models with non-continuous (i.e., binary, ordinal or nominal) outcomes would be an interesting way of building on the current study. Regarding the SVNP, incorporating extensions of the SVNP where a hyper-prior is set for σ^2 (see for instance Lu et al., 2016) may prove valuable in allowing for a more refined comparison between the SVNP and the RHSP. Note also that in the current study no direct comparison to other relevant shrinkage priors, such as the Bayesian LASSO or the Spike-And-Slab Prior was made. Further down the line the RSHP should be implemented into standard Bayesian SEM software (e.g., by adding it to the BLAVAAN package, Merkle, Fitzsimmons, Uanhoro, & Goodrich, 2020), such that applied researchers can actually take advantage of it in practice.

Despite the limitations named, the current study forms a valuable contribution to the current literature. We set a crucial first step in establishing the usefulness of the RHSP in Bayesian regularized SEM. Our findings show that the RHSP can generally be successfully be applied in Bayesian regularized SEM and point to important directions for future research.

References

Aust, F., & Barth, M. (2022). Papaja: Prepare reproducible APA journal articles with R Markdown. Retrieved from https://github.com/crsh/papaja

Betancourt, M. (2018). A Conceptual Introduction to Hamiltonian Monte Carlo. *arXiv:1701.02434 [Stat]*. Retrieved from http://arxiv.org/abs/1701.02434

Bollen, K. A. (1989). *Structural Equations with Latent Variables*. John Wiley & Sons.

Carvalho, C. M., Polson, N. G., & Scott, J. G. (2010). The horseshoe estimator for sparse signals. *Biometrika*, *97*(2), 465–480. https://doi.org/10.1093/biomet/asq017

Cham, H., West, S. G., Ma, Y., & Aiken, L. S. (2012). Estimating Latent Variable Interactions With Nonnormal Observed Data: A Comparison of Four Approaches. *Multivariate Behavioral Research*, *47*(6), 840–876. https://doi.org/10.1080/00273171.2012.732901

Chen, J., Guo, Zhihan, Zhang, Lijin, & Pan, Junhao. (2021). A Partially Confirmatory Approach to Scale Development With the Bayesian Lasso. *Psychological Methods*, *26*(2), 210–235. Retrieved from https://oce-ovid-com.proxy.library.uu.nl/article/00060744-202104000-00005/HTML

Cox, D. R. (2006). *Principles of Statistical Inference*. Cambridge University Press.

Datta, J., & Ghosh, J. K. (2013). Asymptotic properties of Bayes risk for the horseshoe prior. *Bayesian Analysis*, *8*(1), 111–132.

Gabry, J., & Češnovar, R. (2022). Cmdstanr. Retrieved from https://mc-stan.org/cmdstanr/

Gabry, J., & Mahr, T. (2022). Bayesplot: Plotting for Bayesian Models. Retrieved from https://mc-stan.org/bayesplot/

George, E. I., & McCulloch, R. E. (1993). Variable Selection Via Gibbs Sampling. *Journal of the American Statistical Association*, *88*(423), 881–889.

https://doi.org/10.2307/2290777

Ghosh, J., Li, Y., & Mitra, R. (2018). On the Use of Cauchy Prior Distributions for Bayesian Logistic Regression. *Bayesian Analysis*, *13*(2), 359–383. https://doi.org/10.1214/17-BA1051

Hans, C. (2009). Bayesian lasso regression. *Biometrika*, *96*(4), 835–845. Retrieved from https://www.jstor.org/stable/27798870

Hastie, T., Tibshirani, R., & Wainwright, M. (2015). Statistical learning with sparsity. *Monographs on Statistics and Applied Probability*, *143*, 143.

Hoerl, A. E., & Kennard, R. W. (2000). Ridge Regression: Biased Estimation for Nonorthogonal Problems. *Technometrics*, *42*(1), 80–86. https://doi.org/10.2307/1271436

Homan, M. D., & Gelman, A. (2014). The No-U-turn sampler: Adaptively setting path lengths in Hamiltonian Monte Carlo. *The Journal of Machine Learning Research*, *15*(1), 1593–1623.

Hsiang, T. C. (1975). A Bayesian View on Ridge Regression. *Journal of the Royal Statistical Society. Series D (The Statistician)*, *24*(4), 267–268. https://doi.org/10.2307/2987923

Ishwaran, H., & Rao, J. S. (2005). Spike and slab variable selection: Frequentist and Bayesian strategies. *The Annals of Statistics*, *33*(2), 730–773. https://doi.org/10.1214/009053604000001147

Jacobucci, R., Brandmaier, A. M., & Kievit, R. A. (2019). A Practical Guide to Variable Selection in Structural Equation Modeling by Using Regularized Multiple-Indicators, Multiple-Causes Models. *Advances in Methods and Practices in Psychological Science*, *2*(1), 55–76. https://doi.org/10.1177/2515245919826527

Jacobucci, R., & Grimm, K. J. (2018). Comparison of Frequentist and Bayesian Regularization in Structural Equation Modeling. *Structural Equation Modeling:*

A Multidisciplinary Journal, *25*(4), 639–649. https://doi.org/10.1080/10705511.2017.1410822

Jacobucci, R., Grimm, K. J., & McArdle, J. J. (2016). Regularized Structural Equation Modeling. *Structural Equation Modeling: A Multidisciplinary Journal*, *23*(4), 555–566. https://doi.org/10.1080/10705511.2016.1154793

James, G., Witten, D., Hastie, T., & Tibshirani, R. (2021). *An Introduction to Statistical Learning: With Applications in R*. New York, NY: Springer US. https://doi.org/10.1007/978-1-0716-1418-1

Lu, Z.-H., Chow, S.-M., & Loken, E. (2016). Bayesian Factor Analysis as a Variable-Selection Problem: Alternative Priors and Consequences. *Multivariate Behavioral Research*, *51*(4), 519–539. https://doi.org/10.1080/00273171.2016.1168279

MacCallum, R. C., Roznowski, M., & Necowitz, L. B. (1992). Model modifications in covariance structure analysis: The problem of capitalization on chance. *Psychological Bulletin*, *111*(3), 490–504. https://doi.org/10.1037/0033-2909.111.3.490

Merkle, E. C., Fitzsimmons, E., Uanhoro, J., & Goodrich, B. (2020). Efficient Bayesian Structural Equation Modeling in Stan. *arXiv:2008.07733 [Stat]*. Retrieved from http://arxiv.org/abs/2008.07733

Mitchell, T. J., & Beauchamp, J. J. (1988). Bayesian Variable Selection in Linear Regression. *Journal of the American Statistical Association*, *83*(404), 1023–1032. https://doi.org/10.2307/2290129

Muthén, B., & Asparouhov, T. (2012). Bayesian SEM: A more flexible representation of substantive theory, 78. https://doi.org/10.1037/a0026802

Park, T., & Casella, G. (2008). The Bayesian Lasso. *Journal of the American Statistical Association*, *103*(482), 681–686. https://doi.org/10.1198/016214508000000337

Piironen, J., & Vehtari, A. (2017a). On the Hyperprior Choice for the Global Shrinkage Parameter in the Horseshoe Prior. In *Proceedings of the 20th International Conference on Artificial Intelligence and Statistics* (pp. 905–913). PMLR. Retrieved from https://proceedings.mlr.press/v54/piironen17a.html

Piironen, J., & Vehtari, A. (2017b). Sparsity information and regularization in the horseshoe and other shrinkage priors. *Electronic Journal of Statistics*, *11*(2), 5018–5051. https://doi.org/10.1214/17-EJS1337SI

Polson, N. G., & Scott, J. G. (2010). Shrink globally, act locally: Sparse Bayesian regularization and prediction. *Bayesian Statistics*, *9*(501-538), 105.

R Core Team. (2021). R: A Language and Environment for Statistical Computing. Retrieved from https://www.R-project.org/

R Core Team. (2022). Package 'parallel'. Retrieved from https://stat.ethz.ch/R-manual/R-devel/library/parallel/doc/parallel.pdf

Serang, S., & Jacobucci, R. (2020). Exploratory Mediation Analysis of Dichotomous Outcomes via Regularization. *Multivariate Behavioral Research*, *55*(1), 69–86. https://doi.org/10.1080/00273171.2019.1608145

Serang, S., Jacobucci, R., Brimhall, K. C., & Grimm, K. J. (2017). Exploratory Mediation Analysis via Regularization. *Structural Equation Modeling: A Multidisciplinary Journal*, *24*(5), 733–744. https://doi.org/10.1080/10705511.2017.1311775

Stan Development Team. (2021). Stan User Guide. Retrieved from https://mc-stan.org/docs/2_27/stan-users-guide-2_27.pdf

Stan Development Team. (2022). Rstan: The R interface to Stan. Retrieved from https://mc-stan.org/

Tibshirani, R. (1996). Regression Shrinkage and Selection Via the Lasso. *Journal of the Royal Statistical Society: Series B (Methodological)*, *58*(1), 267–288. https://doi.org/10.1111/j.2517-6161.1996.tb02080.x

Tibshirani, R. (2011). Regression shrinkage and selection via the lasso: A retrospective. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)*, *73*(3), 273–282. Retrieved from https://www.jstor.org/stable/41262671

Van Der Pas, S. L., Kleijn, B. J., & Van Der Vaart, A. W. (2014). The horseshoe estimator: Posterior concentration around nearly black vectors. *Electronic Journal of Statistics*, *8*(2), 2585–2618.

Van Erp, S., Oberski, D. L., & Mulder, J. (2019). Shrinkage priors for Bayesian penalized regression. *Journal of Mathematical Psychology*, *89*, 31–50. https://doi.org/10.1016/j.jmp.2018.12.004

Wickham, H. (2016). ggplot2: Elegant Graphics for Data Analysis. Retrieved from https://ggplot2.tidyverse.org

Wickham, H., François, R., & Müller, K. (2022). Dplyr: A Grammer of Data Manipulation. Retrieved from https://dplyr.tidyverse.org, https://github.com/tidyverse/dplyr

Wickham, H., & Girlich, M. (2022). Tidyr: Tidy Messy Data. Retrieved from https://tidyr.tidyverse.org, https://github.com/tidyverse/tidyr

Zhang, L., Pan, J., & Ip, E. H. (2021). Criteria for Parameter Identification in Bayesian Lasso Methods for Covariance Analysis: Comparing Rules for Thresholding, p -value, and Credible Interval. *Structural Equation Modeling: A Multidisciplinary Journal*, 1–10. https://doi.org/10.1080/10705511.2021.1945456

Appendix

Appendix A: True Model

For every individual i in i = 1,..., N:

$$Y_i \sim \mathcal{N}(\mathbf{0}, \Sigma),$$

where

$$\Sigma = \Lambda \Psi \Lambda',$$

$$\Lambda = \begin{bmatrix} 0.75 & 0 \\ 0.75 & 0 \\ 0.75 & 0.2/0.5 \\ 0.2/0.5 & 0.75 \\ 0 & 0.75 \\ 0 & 0.75 \end{bmatrix},$$

$$\Psi = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix},$$

and

$$\Theta = diag[0.3, 0.3, 0.3, 0.3, 0.3, 0.3].$$