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A problem with discretizing Vale-Maurelli in simulation studies

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Abstract

Previous influential simulation studies investigate the effect of underlying non-normality in ordinal data using the Vale-Maurelli (VM) simulation method. We show that discretized data stemming from the VM method with a prescribed target covariance matrix are usually numerically equal to data stemming from discretizing a multivariate normal vector. This normal vector has however a different covariance matrix than the target. It follows that these simulation studies have in fact studied data stemming from normal data with a possibly misspecified covariance structure. This observation affects the interpretation of previous simulation studies.

Keywords: polychoric correlation, Vale-Maurelli, non-normal data, structural equation modeling

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Introduction

In the social and behavioral sciences we often work with variables that are ordinal or dichotomous rather than continuous. In psychology, for instance, Likert scales are ubiquitous. In structural equation modeling (SEM) it was originally assumed that the indicator variables were continuous, but during the last decades ordered categorical variables have been incorporated into SEM through the intermediate step of estimating polychoric correlations (e.g., Muthén, 1984; Jöreskog & Moustaki, 2001). Then the matrix of polychoric correlations is used as input to estimate the model, and the resulting parameter estimates and fit information are interpreted as referring to the underlying vector of continuous variables.

The polychoric correlation is the correlation between two hypothesized continuous variables, each of which underlies an ordinal/dichotomous variable, and was introduced already by Pearson (1901). In order to identify the polychoric correlation a bivariate distribution must be assumed for the underlying continuous variables. The natural candidate for such a distribution is the bivariate normal, for which Olsson (1979) deduced a two-step maximum-likelihood estimator which has been implemented in most SEM software packages. It is therefore of practical importance to evaluate by Monte Carlo simulation the extent to which this estimator is robust to deviations from normality. An often used simulation method is to discretize a continuos non-normal random vector generated by the Vale-Maurelli (VM) method (Vale & Maurelli, 1983).

The present article notes a suprising problem with simulating ordinal data by discretizing a VM vector that originates from identifiability considerations. Namely, we show that using the VM method for ordinal data simulation is in most cases equivalent to discretizing normal data. Therefore this method is unsuitable for studying consequences of deviations from underlying normality. However, many studies have employed discretizing a VM vector for robustness investigations (e.g. Flora & Curran, 2004; Rhemtulla, Brosseau-Liard, & Savalei, 2012; Nestler, 2013; Moshagen & Musch, 2014; Yang & Green, 2015; Natesan, 2015; Li, 2016; Jin, Luo, & Yang-Wallentin, 2016; Monroe, 2018; Wang, Su, & Weiss, 2018). Especially influential has been the work of Flora and Curran (2004), which reported that methodology based on polychoric estimation was quite robust to modest violation of the underlying normality assumption. This claim has since been re-iterated in the SEM literature, see, e.g., the textbook by Bollen and Curran (2006, p. 233) and the chapter on SEM in the handbook of psychology by Ullman and Bentler (2012, p. 679). Also, the highly cited study by Rhemtulla et al. (2012) used a discretized VM approach in ordinal data simulation to compare normal-theory based maximum likelihood estimation for continuous variables with estimation based on the polychoric correlations. They found that the latter estimation method was "more sensitive than robust ML parameter estimates to violations of the assumption of normality of underlying continuous variables". This conclusion may be explained by our finding that the employed simulation technique amounts to discretizing a normal random vector with a possibly misspecified covariance matrix.

In the present article we first briefly discuss ordinal data simulation through discretizing continuous vectors and also give a description of the VM method. Next we demonstrate that, surprisingly, using the VM method for ordinal data simulation is in most cases equivalent to normal data simulation. The covariance matrix of this normal vector is found analytically. Implications of our finding are then discussed, and illustrated with a detailed analysis of two representative studies that discretized VM. For transparency, complete R code underlying our analysis is available as supplementary material. We also illustrate our results with a small simulation study. Implications of our findings for the evaluation of robustness are briefly discussed in the concluding section.

Simulating ordinal variables using the VM method

A general technique for simulating ordinal data is to simulate a continuous vector and then discretize each variable according to given thresholds. In the following we outline this technique in its generality, before turning into the specifics when the continuous vector stems from the VM simulation method.

We wish to simulate a *d*-dimensional ordinal random vector $X = (X_1, X_2, \ldots, X_d)'$ whose coordinates takes on the K > 1 possible values x_1, x_2, \ldots, x_K . A standard method to achieve this is to first simulate a *d*-dimensional continuous random vector ξ and then discretize it. In the following we refer to ξ as the *discretized variable*. This means that for $i = 1, 2, \ldots, d$ we let

$$X_{i} = \begin{cases} x_{1}, & \text{if } \tau_{i,0} < \xi_{i} \leq \tau_{i,1} \\ x_{2}, & \text{if } \tau_{i,1} < \xi_{i} \leq \tau_{i,2} \\ \vdots \\ x_{K}, & \text{if } \tau_{i,K-1} < \xi_{i} \leq \tau_{i,K} \end{cases}$$

where $\tau_{i,0} = -\infty < \tau_{i,1} \le \tau_{i,2} \le \cdots \le \tau_{i,K-1} \le \tau_{i,K} = \infty$. A compact representation of X is given by

$$X_{i} = \sum_{j=1}^{K} x_{j} I\{\tau_{i,j-1} < \xi_{i} \le \tau_{i,j}\}$$
(1)

where $I\{A\}$ is the indicator function of A, i.e., it is one if A is true and zero otherwise. The distribution of X is a function of the distribution of ξ and the thresholds $\tau_{i,1}, \ldots, \tau_{i,K-1}$ for $i = 1, 2, \ldots, d$, which are chosen to get desired properties of X.

The simulation technique of Vale and Maurelli (1983) is a popular method to simulate d-dimensional non-normal continuous random vectors ξ with prescribed covariance matrix Σ (which we will call the *target* covariance matrix) and univariate skewness and kurtosis. The method simulates first a multivariate normal random vector $\zeta = (\zeta_1, \zeta_2, \dots, \zeta_d)' \sim N(0, \Sigma_{\zeta})$ called the *generator variable*. The generator variable is then transformed using d third degree polynomials $p_1(\cdot), p_2(\cdot), \dots, p_d(\cdot)$, and the non-normal variable ξ is produced using the formula

$$\xi = \begin{pmatrix} p_1(\zeta_1) \\ p_2(\zeta_2) \\ \vdots \\ p_d(\zeta_d) \end{pmatrix}.$$
(2)

The covariance matrix and marginal skewness and kurtosis of ξ are functions of Σ_{ζ} and the coefficients of the polynomials $p_1(\cdot), p_2(\cdot), \ldots, p_d(\cdot)$. These are selected through a numerical optimization procedure to reach the target covariance matrix Σ and the desired marginal skewness and kurtosis.

The equivalence of discretizing a VM vector and a normal vector in the monotonous case

We assume that the polynomials $p_1(\cdot), \ldots, p_d(\cdot)$ are *monotonous*. This case is often encountered in practice. For instance, monotonous polynomials exist in three of the four conditions studied by Flora and Curran (2004) and in the single condition employed by Rhemtulla et al. (2012).

The general case of non-monotonous polynomials may be analyzed with the techniques used by Foldnes and Grønneberg (2015), who derived the distribution of VM random vectors. However, this comes at the cost of greatly increased notational complexity. Also, the common case of monotonicity is sufficient to demontrate the problems inherent in discretizing VM random vectors for robustness studies. The case of non-monotonicity still leads to the discretization of a multivariate normal vector, with the added complication of random thresholds.

We assume that ξ is generated according to eq. (2) with generator variable ζ , and that X is generated according to eq. (1). We further assume that the VM method is set up such that X has target covariance matrix Σ . Let $1 \leq i \leq d$. We have

$$X_{i} = \sum_{j=1}^{K} x_{j} I\{\tau_{i,j-1} < p_{i}(\zeta_{i}) \le \tau_{i,j}\}.$$
(3)

Suppose first that p_i is monotonously increasing. Then its inverse function p_i^{-1} is also increasing, and applying the inverse on all three parts of the inequality above gives

$$X_{i} = \sum_{j=1}^{K} x_{j} I\{p_{i}^{-1}(\tau_{i,j-1}) < p_{i}^{-1}(p_{i}(\zeta_{i})) \le p_{i}^{-1}(\tau_{i,j})\} = \sum_{j=1}^{K} x_{j} I\{\tilde{\tau}_{i,j-1} < \zeta_{i} \le \tilde{\tau}_{i,j}\}.$$

where $\tilde{\tau}_{i,j} = p_i^{-1}(\tau_j)$. If all polynomials are increasing, the conclusion is therefore that $X = (X_1, X_2, \ldots, X_d)'$ is numerically identical to discretizing the generator variable ζ , which is exactly normally distributed. The only difference between discretizing the potentially highly non-normal ξ compared to the exactly normal ζ is to replace the threshold values $(\tau_{i,j})$ by $(\tilde{\tau}_{i,j})$.

Now consider the case when a polynomial $p_i(\cdot)$ for a $1 \le i \le d$ is instead monotonously decreasing. Then the inverse p_i^{-1} is also monotonically decreasing, and we have

$$\begin{aligned} X_i &= \sum_{j=1}^K x_j I\{\tau_{i,j-1} < p_i(\zeta_i) \le \tau_{i,j}\} = \sum_{j=1}^K x_j I\{p_i^{-1}(\tau_{i,j}) \le p_i^{-1}(p_i(\zeta_i)) < p_i^{-1}(\tau_{i,j-1})\} \\ &= \sum_{j=1}^K x_j I\{p_i^{-1}(\tau_{i,j}) \le \zeta_i < p_i^{-1}(\tau_{i,j-1})\} \\ &= \sum_{j=1}^K x_j I\{\tilde{\tau}_{i,j-1} < -\zeta_i \le \tilde{\tau}_{i,j}\} \end{aligned}$$

where $\tilde{\tau}_{i,j} = -p_i^{-1}(\tau_{i,j})$. We therefore see that for this coordinate of X, it is as if we discretized not ζ_i but $-\zeta_i$.

Let $\tilde{\zeta}$ be ζ with signs reversed for those coordinates whose corresponding polynomials are decreasing. Since ζ is zero mean multivariate normal, so is $\tilde{\zeta}$. The covariance matrix of $\tilde{\zeta}$, which we call $\Sigma_{\tilde{\zeta}}$ is equal to Σ_{ζ} , the covariance matrix of ζ , but with some signs of the covariances possibly reversed.

Since the above argument holds for each coordinate of X, and takes into account both increasing and decreasing polynomials, we see that discretizing the VM simulation approach is numerically equivalent to simulating directly from the multivariate normal vector $\tilde{\zeta}$. That is, X is numerically equal to having simulated from the exactly multivariate normal vector $\tilde{\zeta}$. Again the polynomial transformation is ineffectual, except for changes in the thresholds and possible sign reversals of covariances.

The implications of the equivalence

We have shown that using the discretized VM approach to simulate ordinal data is numerically equivalent to simulating directly from an exactly multivariate normal random vector $\tilde{\zeta}$ with covariance matrix $\Sigma_{\tilde{\zeta}}$. This is the case, even though ξ may be highly non-normal, with a high degree of univariate skewness and kurtosis. Note also that $\Sigma_{\tilde{\zeta}}$ differs from the prescribed target covariance matrix Σ , but often in a relatively minor way, as further discussed at the end of this section.

Since X is numerically equal to a discretized normal vector $\tilde{\zeta}$, all consistent statistical methods based on the normal assumption will estimate features of $\tilde{\zeta}$ and not of the intended vector ξ . For instance, it is important to note that both the one-step simultaneous estimation of thresholds and polychoric correlations and the two-step estimation method for polychoric correlations proposed by Olsson (1979) will reach $\Sigma_{\tilde{\zeta}}$, and not the intended Σ . Many simulation studies have aimed to investigate the robustness of methods based on polychoric correlations to violations of underlying normality in the discretized vector. A large proportion of such studies have relied on the seemingly reasonable choice of generating non-normality with the popular VM transform. In fact, we could only find a few studies employing a different approach than VM, based on discretizing multivariate t distributions (Maydeu-Olivares, García-Forero, Gallardo-Pujol, & Renom, 2009; Maydeu-Olivares, 2006). We have demonstrated that studies using VM discretization could just as well have discretized a multivariate normal vector, whose covariance matrix might be misspecified for the intended model. Hence, the results reported in studies based on discretizing VM will reflect the consequences of a misspecified covariance structure, or a correctly specified covariance structure at slightly different parameter values than posited by the researcher, and not the claimed robustness with

respect to proper deviation of normality in the discretized variable.

We next look more closely at select design conditions in two representative and well-cited studies that discretized VM for data generation, with further details provided as supplementary materials to this article. Our aim is to inspect how far the intermediate correlation estimated by the polychoric estimator is from the target correlation. Consider first Model 1 in Flora and Curran (2004), a one-factor model with five indicators. Population values of factor loadings and residual variances are 0.7 and 0.51, respectively, so that the target Σ is a correlation matrix with all off-diagonal elements equal to 0.49. In Flora and Curran (2004) the distributional condition furthest removed from normality has skewness 1.25 and excess kurtosis 3.75, which may be realized by a monotonous Fleishman polynomial $p(\zeta) = -0.161 + 0.819\zeta + 0.161\zeta^2 + 0.049\zeta^3$. With an intermediate correlation between ζ_1 and ζ_2 approximately equal to 0.5084, the correlation between between $p(\zeta_1)$ and $p(\zeta_2)$ will equal the target value of 0.49 (we return to this condition in the next section). In other words, data generation based on VM is here indistinguishable from simulating multivariate normal data whose correlations are all equal to 0.5084. Moreover, Model 1 fits perfectly to such a correlation structure, since all the off-diagonal elements of the polychoric correlation matrix are identical. In fact, estimating the one-factor model to the polychoric correlation matrix results in perfect fit when the factor loading is 0.712, close to the value 0.7 postulated by the authors. The values here calculated for the polychoric correlations and factor loadings are in accordance with the mean values reported in Tables 2 and 8 in Flora and Curran (2004). The conclusion in Flora and Curran (2004) that "... estimation of polychoric correlations is robust to modest violations of underlying normality", may therefore be explained by a data generation procedure indistinguishable from discretizing a multivariate normal vector that fits perfectly to the model, in such a way that the parameter estimates are close to those postulated by the researchers.

In Rhemtulla et al. (2012) the non-normal condition has skewness 2 and excess

kurtosis 7, generated by a monotonous polynomial

 $p(\zeta) = -0.260 + 0.762\zeta + 0.260\zeta^2 + 0.053\zeta^3$. In contrast to Flora and Curran (2004), the population factor loadings are not identical across indicator variables, and hence there are different correlation values contained in Σ . The intermediate correlations in the VM procedure are therefore also not all equal, and the proposed factor model will not fit perfectly to the intermediate correlation matrix (i.e. the population value of the polychoric correlation matrix). However, the intermediate correlations are similar to the corresponding elements in Σ , which means that the model is only mildly misspecified. In fact, for Model 1 the population value of the RMSEA fit index is very low: 0.001. Therefore the reported outcomes, e.g., parameter bias, exhibit mostly acceptable performance under the Cat-LS and ML estimators studied by Rhemtulla et al. (2012).

We conclude that in commonly used conditions of non-normality (i.e. skewness and kurtosis) and target correlation, the intermediate correlation in the VM transform is close to the target correlation. Since the polychoric correlation equals this intermediate correlation, the correlation matrix that is used to fit the model will tend to be only slightly misspecified. In fact, in some conditions the model may be *correctly specified* also for the polychoric correlation matrix (Flora & Curran, 2004). We believe this is the reason why bias in parameter estimation and standard errors, and in the performance of fit statistics, has been repeatedly reported to be overall acceptable in robustness studies that are based on discretizing the VM transform.

Illustration

We illustrate the above deductions for two previously used conditions in the psychometric simulation literature. Code written in R (R Core Team, 2018) that rely on the package lavaaan (Rosseel, 2012) is provided in the supplementary material.

The first condition, C_1 , is a VM bivariate vector whose skewness and excess kurtosis equal 1.25 and 3.75, respectively, in both margins. This condition was used by Flora and

Curran (2004). The second condition, C_2 , involves more severe non-normality in the margins, with skewness and excess kurtosis equal 3 and 21, respectively, and was studied by Curran, West, and Finch (1996). In both conditions the coefficients for a Fleishman polynomial $p(\zeta) = a + b\zeta + c\zeta^2 + d\zeta^3$ are given in Table 1, and yield a monotonously increasing p(z).

Condition	Skewness	Kurtosis	a	b	С	d
C_1	1.75	3.75	-0.1606	0.8189	0.1606	0.0492
C_2	3	21	-0.2523	0.4186	0.2523	0.1476

Table 1

Two conditions of non-normality, with corresponding coefficients for Fleishman polynomial $p(\zeta) = a + b\zeta + c\zeta^2 + d\zeta^3.$

Following Flora and Curran (2004), we set the target covariance (which is actually a correlation, since the Fleishman polynomials in Table 1 have unit variance) equal to $\phi = 0.49$. The intermediate correlation ϕ_{ζ} for the bivariate normal vector (ζ_1, ζ_2) was then calculated in C_1 and C_2 as suggested by Vale and Maurelli (1983). For C_1 this correlation was equal to $\phi_{\zeta} = 0.5084$, while for C_2 we have $\phi_{\zeta} = 0.5715$. Note that the intermediate correlation ϕ_{ζ} is closer to the target $\phi = 0.49$ in the distribution which is closest to normality, i.e., in C_1 .

To obtain ordinal data we used a five-category condition where the population proportions for increasing levels are 0.05, 0.2, 0.5, 0.2 and 0.05. The corresponding thresholds for a standard normal distribution, and for the Fleishman polynomials in C_1 and C_2 are given in Table 2.

Next, we simulated a large $n = 10^7$ sample from both C_1 and C_2 , and applied the corresponding thresholds in Table 2 to obtained five-category ordinal data. In these ordinal datasets we estimated the thresholds and the polychoric correlation, following the two-step procedure suggested by Olsson (1979). The results are given in table 3. In both conditions

Condition	$ au_1$	$ au_2$	$ au_3$	$ au_4$	
Normal	-1.645	-0.643	0.643	1.645	
C_1	-1.292	-0.634	0.445	1.840	
C_2	-0.915	-0.456	0.160	1.776	

Table 2 $\,$

Thresholds that yield relative frequencies of 0.05, 0.2, 0.5, 0.2 and 0.05.

the estimate of the polychoric correlation misses the target correlation, and is instead close to the intermediate correlation ϕ_{ζ} . This confirms the above deductions. As expected, in both conditions the estimated thresholds are similar and almost identical to the population values given for the normality condition in Table 2.

-	Condition	ϕ	ϕ_{ζ}	$\hat{ ho}$	$\hat{ au}_1$	$\hat{\tau}_2$	$\hat{ au}_3$	$\hat{\tau}_4$
	C_1	0.49	0.5084	0.5087	-1.6454	-0.6433	0.6424	1.6440
	C_2	0.49	0.5715	0.5717	-1.6454	-0.6432	0.6425	1.6438

Table 3

Estimated thresholds $\hat{\tau}_i$ and polychoric correlation $\hat{\rho}$ in a large sample. ϕ : target covariance. ϕ_{ζ} : covariance of generator variables ζ_1 and ζ_2 .

Conclusion

We have demonstrated that simulating ordinal data by the disretization of a VM generated non-normal continuous vector is in many cases equivalent to discretizing a multivariate normal vector. The covariance matrix of this vector is often close to the target covariance matrix of the VM method. This discrepancy between the target covariance matrix for the VM method and the possibly misspecified covariance matrix of the normal vector is therefore hard to separate from small sample variation. We believe that this may explain why the discrepancy has not been discovered before. We may conclude that the use of the VM transform for robustness studies in ordinal SEM is therefore of limited value. The results from such studies may in many cases be interpreted as robustness against very mild model misspecification for an underlying normal vector.

The analysis offered in this paper points to the importance of considering non-identifiability issues arising when ordinal data are treated as discretized continuous data. Starting with the representation in eq. (3), it is clear that we may apply any monotonic transformation to the three parts of the inequality in this equation and thereby transforming the marginals of the discretized variable to any desired distribution. Future simulation studies of robustness to violation of the underlying normality assumption should therefore carefully analyze how the non-identifiability issue may affect the simulation technique.

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