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Convergence rate in structural equation models – analysis of estimation methods and implications in the number of observations

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ABSTRACT. Structural Equation Modeling (SEM) is used to analyze the causal relationships between observable and unobservable variables. Among the assumptions considered, but not essential, for the application of the SEM are the presence of multivariate normality between the data, and the need for a large number of observations, in order to obtain the variances and covariances between the variables. It is not always possible to have access to a sufficiently large number of observations to enable the calculation of parameters, and the convergence of the iterative algorithm is one of the problems in obtaining the results. This work investigates the convergence of iterative algorithms, which minimize the variation of parameters, through a stipulated convergence rate, using the Maximum Likelihood (ML) and Generalized Least Squares (GLS) estimation methods on structural equation models using confirmatory factor analysis (CFA) and regression models. Convergences were evaluated in relation to the number of observations, in order to obtain a minimum quantity sufficient for a convergence rate above 50%. The calculations were performed in the statistical environment R® version 3.4.4, and the results obtained showed a convergence rate above 50% for models estimated by GLS, even with the data showing lack of multivariate normality, kurtosis and accentuated asymmetry. Thus, it was possible to define a minimum number of observations necessary for an adequate convergence of the iterative algorithms in obtaining the necessary parameters.

Keywords: modeling of structural equations; convergence rate; estimation methods.

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Introduction

Structure Covariance Analysis or Structural Equations Modeling - SEM combines multivariate statistical methods to describe the causal relationships between observable and unobservable variables. Assuming that the parameters of the model are identified, these relationships are represented by regression coefficients, variances and covariances between exogenous variables, variances and covariances of disturbance terms and indicate the magnitude of the effect that variables have on each other (Kaplan, 2009).

For the application of SEM some assumptions must be considered. One of these concerns the adequate number of observations relative to the number of variables, parameters to be determined, and the complexity of the model. Another point in question, before estimation, is the verification of the model's identifiability, because when the number of parameters to be estimated is greater than the number of data, the model is undetermined.

There are many attempts to determine minimum and/or maximum quantities of observations for an adequate parameter estimation.

One of the attempts is from Monte Carlo simulations made by Boomsma (Westland, 2010) that, considering a ratio r obtained from the number of manifest (or observed) items or variables (p) and latent variables (or factors; f) of the model of the shape $r = p / f$, adjusted a curve to the data obtained, and Westland (2010) proposed a formula to determine the appropriate size (n) for a sample defined by

$$n \geq 50r^2 - 450r + 1100, \quad r = p / f \qquad (1)$$

Bentler and Chou (1987) observed that the sample size must be considered related to the number of parameters to be estimated. However, the number of observations depends on other conditions that include similarity and number of indicators per factor. In summary, the sample size recommendations required in the SEM literature are simply guesswork.

But it is worth remembering that, for structural equation models, the data are not the individual observations of each subject in each variable, but the variances and covariances between the manifest variables (Marôco, 2014). The sample size requirement is not equivalent to the data array size. But we must remember that, in order to estimate the model parameters, iterative algorithms must show convergence, that is, they minimize a function of the adjustment errors estimated by the difference between the covariances observed in the sample and the covariance matrix generated by the theoretical model with parameters.

Statistics show that the problem of the estimation is summarized in tune with the matrix, the covariance-based estimates of $\Sigma(\hat{\theta})$ is the matrix of covariance observed in the sample $S = (s_{ij})$ of order $p \times p$, where the algorithms are iterative successive approximations, we obtain the estimates of the parameters that minimizes a function of the difference between the matrix $\Sigma(\hat{\theta})$ and S of the type $F(S, \Sigma(\hat{\theta}))$, with $F \geqslant 0$, then the function call to the discrepancy (distance) between $\Sigma(\hat{\theta})$ e S. The matrix $E = S - \Sigma(\hat{\theta})$ is called the residual matrix (Marôco, 2014). If the structural equation model is 'correct', the data 'generated' by the model is sufficiently close to the observed data, and the model error will be minimal.

Taking an initial estimate for the parameters denoted $\hat{\theta}^1$ and successively generating new estimates denoted $\hat{\theta}^2$, $\hat{\theta}^3$, ... within the allowed parametric space such that $F(\hat{\theta}| \quad |n+1) < F(\hat{\theta}| \quad |n)$. This process continues until convergence is achieved. The lower the value of F the better the adjustment of the theoric model to the observed data. The perfect fit occurs when the value of $F\left(S, \Sigma(\hat{\theta})\right) = 0$. The classic adjustment methods vary according to the software used and the assumptions about the data and distribution of variables, with the Generalized Least Square - GLS and Maximum Likelihood - ML methods being the most used.

If the observation vector has a multivariate normal distribution and the sample size is large enough, the GLS and ML methods will produce unbiased and consistent estimates for the parameters. The adjustment per ML estimates the parameters that maximize the likelihood of observing the sample covariance matrix.

The method produces estimates of the centered and consistent parameters as the sample size increases, approaching the true value of the parameter, with normal distribution. The GLS method has the same asymptotic properties, the maximum likelihood method, consistency and efficiency, but can be used with less restrictive assumptions about the normality of the data (Marôco, 2014). For both methods, the sample size determines the best estimate of the parameters with minimal errors in the residual matrix. It is clear that the greater the amount of data observed, the smaller the value of the discrepancy function and, consequently, the better the fit of the model.

However, until minimum amount of data can be assured, it is necessary an adequate adjustment and essentially, and the convergence of the iterative approximation algorithm, in order to obtain model parameters with satisfactory fit quality. Small amounts of data can lead to problems in estimates and in the estimation and adjustment models, and the alternatives would be to obtain more data, which in some cases may be impossible or expensive, or, increase the value of the discrepancy function, which could lead to large differences between the covariance matrix observed in the sample in relation to the real values. In this work it will be analyzed the determination of a minimum number of observations, in which an adequate convergence can be obtained without changes in the discrepancy function of the estimation models, from a small study of simulations generated on data from structural equation models, and analysis of the stipulated convergence rate obtained for the ML and GLS models. The results obtained with the number of varied observations and limited values of variables are neither statistically justified nor generalizable to general conditions (Yang, Jiang, & Yuan, 2018), but they can add one more factor in determining a minimum amount possible to lead to satisfactory results in SEM.

Material and methods

For the verification of the convergence of SEM models with respect to the estimation method and the number of observations, 5 models of structural equations with their respective database will be used. The models have the following characteristics:

Model 1: 1st order factorial analysis model with 17 observable variables, 3 factors, 116 degrees of freedom and 199 observations;

Model 2: model of 2nd order factorial analysis, with 13 observable variables, 3 First-order factors, 1 latent second-order factor, having 51 degrees of freedom and 296 observations;

Model 3: structural model of regression with 9 observable variables, 3 factors, 23 degrees of freedom and 352 observations;

Model 4: structural model of regression with 13 observable variables, 4 factors, 59 degrees of freedom and 485 observations;

Model 5: model of regression structure with 23 observable variables, 8 factors, 222 degrees of freedom and 512 observations.

The models described above were used with the permission of the authors and chosen because they present the respective databases with an adequate number of observations for the proposed work. The necessary calculations will be performed in the software environment R® version 3.4.4, and written algorithms, functions and packages will be used for the language.

Initially, the data will be evaluated in relation to multivariate normality through the Monte Carlo Test of Multivariate Normality Based on Distances (*Teste Monte Carlo de Normalidade Multivariada Baseado em Distâncias* – TMCNMD), proposed by Biase and Ferreira (2012) and, regarding kurtosis and asymmetry by the Mardia Test. In the multivariate case, the Shapiro-Wilks test presents an inferior performance compared to normality tests based on skewness and kurtosis deviations (Cantelmo & Ferreira, 2007), whereas in relation to multivariate skewness and kurtosis, Mardia's indices are more widely used. For both tests, the normality hypothesis is rejected if the p-value is less than the generally adopted significance level of 5%.

If the data do not present multivariate normality, data with multivariate normality will be generated from the original data. The original data of each model will be considered in the form of an *r x c* matrix, where each column (*c*) represents an observed variable, and each row (*r*) a single observation. To obtain data, obtained randomly with multivariate normality, the mean of each observed variable and the original data covariance matrix is calculated. Using the 'rmvnorm' function of the R® software an *r x c* matrix of normal data is obtained. It is important to consider the analysis for normal and non-normal data for two reasons, the data collected in problems involving SEM may not present multivariate normality and, based on the presence or absence of multivariate normality, it is possible to determine the best estimation method to be used, and the ML method is more restricted as to use on non-normal data.

Subsequently, the multivariate normality analysis is carried out and, using formula (1), the minimum number of observations to be considered for each model is determined, with 150 observations being the smallest of the quantities calculated among the five models. Using the original data available, initially, 150 observations from the database of a model are randomly chosen and a simulation is carried out. The simulation is repeated 100 times, and those that show convergence to the iterative algorithm are counted. The same procedure is performed on all evaluated models.

The entire procedure above is repeated for a small number of observations, with each group of simulations being reduced by 10 observations, until there is no convergence for any of the models in all simulations. If the data do not show multivariate normality, all simulations will be repeated using normal data, obtained from the original data, according to the procedure described above. Simulations that showed convergence are counted and this value is used to calculate the convergence rate of the models in relation to the number of observations considered, per model used. This convergence rate (*CR*) is determined by:

$$CR = \left(\frac{numberofsuccessfuladjustments}{totalattempts}.100\right)\%, \quad (2)$$

where the number of successful fits is equal to the fits that showed convergence.

The convergence rate will be calculated for simulations made with the original data and, in case they do not present multivariate normality, for the data generated from the original data with multivariate normality, and for the ML and GLS estimation methods.

As described, there may be four distinct scenarios, where you can have data without multivariate normality being estimated by ML or GLS and data with multivariate normality being estimated by ML and GLS.

Results and discussion

First, the multivariate normality of the available data should be assessed in order to evaluate the behavior of the estimation methods regarding the presence or non-presence of multivariate normality. The TMCNMD and Mardia test results applied on the data for each model are described in Table 1, noting that in both tests the hypothesis of normality is rejected if the p value is lower than the level of significance α (5%).

Table 1. Results of the TMCNMD test and Mardia's test to verify the multivariate normality of the data from the evaluated models.

	TMCNMD		Mardia test				Result
	R^2	p-value	Skewness	p-value (Skewness)	Kurtosis	p-value (Kurtosis)	
Model 1	0.9720818	0.005997001	2976.6037	1.3789 e-202	33.6492	0	NO
Model 2	0.94255918	0.0004997501	1184.8849	19334 e-66	13.2254	0	NO
Model 3	0.9122142	0.00149925	1111.5849	4.8087 e-140	19.2766	0	NO
Model 4	0.9122142	0.0004997501	1735.4559	1.5613 e-148	33.3922	0	NO
Model 5	0.8216363	0.0004997501	17669.6776	0	172.4151	0	NO

Source: Authors.

A strong multivariate asymmetry is observed in the results obtained from the Mardia test, mainly for models 1 and 5, with very high values compared to the other models. There is no consensus among researchers about the threshold value of kurtosis and multivariate asymmetry, obtained by specific tests, for the application of the maximum likelihood estimation technique in non-normal data. There is no generally accepted cut value of multivariate kurtosis which indicates non-normality (Finney & DiStefano, 2013). The application of the maximum likelihood estimation method may be compromised by the marked asymmetry verified. The non-normality of the data does not prevent the application of the Maximum Likelihood (ML) estimation technique, but because we have models with marked multivariate abnormality, the application of the Generalized Least Squares (GLS) estimation technique is more appropriate.

As all models presented data without multivariate normality, samples with multivariate normality will be generated to continue the work from the original data. In order to continue with the procedures described in the methodology, the codes presented in the Figure 1 of this article will be used. The codes were written in R® language.

From the original data, not normally distributed data with multivariate normality are generated and, using codes 2 and 3 in the annex, simulations are carried out to estimate the parameters of the evaluated models, thus verifying the convergence, or not, of the iterative model, in relation to the observations used, mainly in relation to the number of observations.

```
# SEM Function (for original data without multivariate normality)
sem_smry <- function(data, cfa, pp){
# pp defines the number of observations considered
inx <- sample(nrow(data), pp, replace= FALSE
data_p <- data[inx, ]
dataCor <- cov(data_p)
cfaOut <- try(sem(cfa, dataCor, N = pp, objective = objectiveGLS))     # objectiveML for Maximum Likelihood
if (any(class(cfaOut)=='try-error'))
return(cfaOut)
return(try(summary(cfaOut, conf.level = 0.95, fit.indices = c("GFI", "RMSEA"",NFI", "CFI")))) }

# SEM Function (For multivariate normality data obtained from the original data)
sem_smry <- function(data, cfa, pp) {
mean_data <-apply(data,2,mean)
Cov_data <- cov(data)
data_normal_p <- rmvnorm(pp,mean_data,Cov_data)
# Function that generates normal data
dataCor <- cov.wt(data_normal_p, cor = TRUE)
dataCor <- as.matrix(dataCor[[1]])
cfaOut <- try(sem(cfa, dataCor, N = pp, objective = objectiveGLS))     # objectiveML for Maximum Likelihood
if (any(class(cfaOut)=='try-error'))
return(cfaOut)
return(try(summary(cfaOut, conf.level = 0.95, fit.indices = c("GFI", "RMSE"A, "NFI", "CFI")))) }
#Looping (to obtain the number of adjustments that did not show convergence)
for (i in 1:L) {     # Number of desired simulations L = 100
n0 <- sem_smry(data, cfa, pp)
if (any(class(n0) == "try-error")) nnc <- nnc + 1}
nnc        # Returns the number of adjustments that did not show convergence of L attempts
```

Figure 1. Codes used to obtain the results presented, in R® language.

From the original data, not normally distributed data with multivariate normality are generated and, using codes 2 and 3 in the annex, simulations are carried out to estimate the parameters of the evaluated models, thus verifying the convergence, or not, of the iterative model, in relation to the observations used, mainly in relation to the number of observations. The results of the convergence rate, calculated using formula (2), can be seen in the following tables. Table 2 and 3 present the convergence rates calculated for the ML and GLS estimation models on the original data, without multivariate normality, and Table 4 and 5 present the convergence rates calculated on data with multivariate normality, obtained from the normal data, for the ML and GLS estimation models.

From the results, we can describe the following analysis. Of the models used to verify the convergence rate, Model 3 showed the best convergences. The model is the simplest of all those evaluated, containing only 3 factors and 9 well-adjusted variables. The low number of degrees of freedom and the low complexity of the model interferes with convergence.

Table 2. Convergence rate by model using original (non-normal) data estimated per ML (in percentages).

	Sample Size													
	20	30	40	50	60	70	80	90	100	110	120	130	140	150
Model 1	51.5	63.9	61.8	57.3	53.5	51.3	51	48.8	48.7	46.9	46.6	40.8	40.3	37.2
Model 2	44.2	59.5	68.1	74.7	78.8	83.5	86.1	88.2	88.7	90	91.8	91.2	92.8	93.8
Model 3	70.5	81.9	88.7	90.6	92	92.4	93.9	93.3	93.5	94	92.8	92.3	90.6	91.3
Model 4	71.6	88.9	94.2	96.4	97.4	99.1	99	99.6	99.6	99.6	99.9	99.9	100	99.9
Model 5	0	23.1	25.3	26.7	29.8	24.1	24.8	23.5	27.9	26.9	26.4	25.5	29	29.6

Table 3. Convergence rate by model using original (non-normal) data estimated per GLS (in percentages).

	Sample Size													
	20	30	40	50	60	70	80	90	100	110	120	130	140	150
Model 1	41.4	47.6	50.2	59.5	71.4	81.8	90.2	94.5	96.4	98.8	99.8	99.7	100	100
Model 2	48.5	52.8	63.8	72.8	89.4	91.4	95.5	95.3	97.3	98.8	98.3	99.4	99.9	99.8
Model 3	86.1	96.8	99.6	99.8	99.8	99.8	100	100	100	100	100	100	100	100
Model 4	51	64.8	76.1	78.4	84.4	85.8	86.2	87.9	90.6	92.1	91.7	94.1	94.3	95.1
Model 5	0	57.8	58.1	59.2	64.8	70.4	74.3	77.8	82.7	84.3	87.6	90.6	90.9	91.6

Table 4. Convergence rate by model using normal data generated from original data estimated by ML (in percentages).

	Sample Size													
	20	30	40	50	60	70	80	90	100	110	120	130	140	150
Model 1	68.3	67.9	58.8	55.9	54.2	53.8	51.1	50	46	45.6	46	45.5	46.4	43.8
Model 2	45.1	57	65.2	73.6	74.4	77.3	80.8	82.9	85	87.2	87.4	90	92.4	92.8
Model 3	79.3	89.1	90.7	89.8	93.8	92.3	91.6	91.5	91.6	91.7	92.3	91.6	92.2	91.3
Model 4	79.6	92.3	96.6	98.1	99.2	99	99.5	99.6	99.8	99.7	100	99.7	100	100
Model 5	0	22.3	23.2	27	26.9	27.3	30.5	28.5	30.3	30.9	33.5	32	35.1	35.3

Table 5. Convergence rate by model using normal data generated from original data estimated by GLS (in percentages).

	Sample Size													
	20	30	40	50	60	70	80	90	100	110	120	130	140	150
Model 1	49.5	44.4	55.5	68.8	79.4	86.7	92.1	93.3	95.6	95.9	98.1	98.2	99.3	99
Model 2	48.7	62.2	73.9	84.4	86.3	92.1	93.1	95.2	95.5	97.4	96.2	98.2	98.1	97.4
Model 3	89.5	97.8	99.2	99.9	100	100	100	100	100	100	100	100	100	100
Model 4	52.8	67.4	77.7	81.5	84	87.5	90	90.4	91.6	91.8	93.4	94	93.5	94.2
Model 5	0	61.2	59.9	66.9	72.5	78	85.4	86.3	89.8	92	92.8	93.9	95.6	96.3

Therefore, models with this configuration fit well with small amount of observations. Its lowest convergence rate was 70.5% when evaluating the ML estimation method in the original data and 86.1% when using the GLS method, which is less restricted to non-normality.

For the normal data generated from the original data, the convergence rate behavior was equivalent to the non-normal original data. Models 1 and 5 showed, when analyzing their data using the Mardia test, accentuated kurtosis and asymmetry. Furthermore, as in all models, the data did not show multivariate normality. The effects of non-normality on ML-based results depend on its extent, the greater the non-normality, the greater the impact on the results. However, the convergence rate results when using the ML estimation method on normal data also became very low in both models. This is probably due to the process of numerical optimization of the maximum likelihood function that does not allow us to obtain an explicit solution for estimators.

Studies have shown that the ML methodology is not much affected by the lack of multivariate normality, but its values change with the increase of multivariate kurtosis (Brosseau-Liar & Savalei, 2014).

It is also observed that the convergence rate in models 1 and 5 did not show direct proportion to the number of observations considered when the ML method was applied, and model 1 even revealed a decline in values with the increase of observations (Table 4). The complexity of the model, the low amount of data considered and the accentuated kurtosis and multivariate asymmetry interfere with convergence when using the ML estimate.

Other factors that can influence the result may be associated with the population, the original data and also the degrees of freedom of the model. Correlations may also occur between the errors of variables and factors that can affect convergence. In these cases, it is recommended to use polychoric correlation as a measure of correlation, but Babakus, Ferguson, and Jöreskog (1987) state that, although polychoric correlation produces better results concerning the precision of parameters and estimates, it produces poor good-fit statistics, which can lead to the rejection of a correctly specified model. Kurtosis and asymmetry, both with steep values, can also affect error estimates and chi-square statistics. The $\chi 2$ test is sensitive to the non-normality of the data, the number of parameters and, especially, the sample size (Hair Jr., Gabriel, & Patel, 2014).

Although model 4 presented kurtosis similar to model 5, it was not associated with high asymmetry, in addition to presented low degrees of freedom. Therefore, these factors, when combined, produce effects on the convergence of the iterative model, especially when the ML estimation method is applied. For the estimates by the GLS method, the convergence rates showed high numbers, even with few observations. It is observed that the accentuated kurtosis and asymmetry in some models, added to the non-normality of the data, did not cause problems in the convergence of the iterative algorithms. The values obtained for the convergence rate increase as the number of observations increases. It can be seen in Tables 3 and 5, reaching values close or equal to 100% in all models. The GLS method has few restrictions and is the best option to estimate model parameters, especially in cases with few observations.

There is no consensus on the number of observations to be applied to SEM problems. The implications for using few observations vary from non-convergence on the model to parameter estimation with excessive bias. The errors result from the lack of sufficient information to compose a matrix that represents the real variances and covariances between the variables involved, generating not very robust measures for small samples. In models with small degrees of freedom and small sample sizes, we may also have model fit problems, often indicated by the RMSEA (Root Mean Square Error of Approximation) adequacy index (Kenny, Kaniskan, & McCoach, 2015). It is also observed that, from 20 observations, model 5 presented a null convergence rate, that is, none of the 100 simulations performed was successful in estimating the parameters.

The small number of observations, the complexity of the model with 23 variables and 222 degrees of freedom and the number of parameters to be determined are factors that can lead to convergence problems. A model cannot do more than what is contained in the data itself. If the data is poor, in the sense of reflecting a substantial lack of reliability in evaluating aspects of a studied phenomenon, the results will be poor, regardless of the particularity of the models used (Raykov & Marcoulides, 2006). Remembering that it is not the individual observations, but the variances and covariances between the manifest variables that are the data for a structural equation model.

The variance and covariance matrix observed for this number of observations does not reproduce the effects and relationships that should be evidenced in the sample. The distribution of data and the randomness of your choice can also be factors that define non-convergence. It is observed that, for the other models, convergence was obtained, with the same number of observations. Even with the possibility of an accentuated bias in the results, it is possible to stipulate quantities of observations from an established convergence rate, having, as a reference, the values obtained with the application of the GLS estimation method, since the ML method presented inconsistency in the models whose data did not show multivariate normality and also with marked kurtosis and marked asymmetry.

Thus, the following values, presented in Table 6, can be proposed.

Table 6. Minimum number of observations per convergence rate, estimated by gls method.

Estimation Method for Generalized Least Squares	Convergence Rate				
	50%	60%	70%	80%	90%
Number of observations - Normal data	40	50	60	80	110
Number of observations - Non-normal data data	40	60	70	100	130

Conclusion

The results obtained in the simulations showed a more satisfactory behavior for the GLS method, both for data with or without multivariate normality. Factors such as model complexity, degrees of freedom, number of indicators, large difference in variance between observable variables, can interfere in the convergence rate of iterative models, when estimated by ML. The kurtosis and marked asymmetry, when associated, also interfered in the convergence in both estimation methods. The results allowed to indicate minimum quantities of observations that can be admitted for each rate of convergence stipulated in the evaluated models, considering possible biases in the results.

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