Using Computer Algebra Systems together with lavaan to generate symbolic model-implied covariance matrices in SEM

Henrik Kenneth Andersen

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This article is meant as (*brief, introductory*) guide to using computer algebra systems to work out analytical model-implied covariance matrices for structural equation models. To my knowledge there is no pre-packaged software available for this task. The article is meant primarily for those with experience with structural equation modeling as well as `lavaan` and ideally R in general.

Any questions or comments can be sent to henrik.andersen@soziologie.tu-chemnitz.de.

Introduction

A careful inspection of the model-implied covariance matrix should be considered an essential step in any SEM-based regression model. Software **default settings**, cluttered or **inaccurate path diagrams** as well as an over reliance on **modification indices** often hide important aspects of SEM-based regression models. In complex models, researchers may not even be aware of the underlying algebra that is responsible for the reported parameter estimates.

This brief article demonstrates the use of Computer Algebra Systems (CAS) such as `Ryacas` (Andersen et al. 2019), an R interface with the software `Yacas` (“Yet Another Computer Algebra System”), along with the popular Structural Equation Modeling (SEM) package `lavaan` (Rosseel 2012) to generate symbolic representations of model-implied covariance matrices.

The model-implied covariance matrix can be derived using traditional methods such as the **tracing rule**, or with **covariance algebra**. However, these methods are a) tedious, b) prone to errors, c) must be done by hand and entered into the software of choice later. The method outlined here involves entering the model matrices into `Ryacas` and letting the software come up with the entire symbolic covariance matrix in one go. It saves time, is less error prone and can reveal details that may not be obvious (especially with more complex models or ones with latent variables, e.g. fixed-effects regression in SEM).

The article is outlined as follows: first I simulate a simple mediation model with manifest indicators to be used as the dataset in the later demonstration. Then I outline the model matrices used in popular SEM software like `lavaan` and `Mplus` and derive the equation for the model-implied covariance matrix. I then run the model as outlined in the simulation in `lavaan` and show how to double-check the model matrices. Before demonstrating the CAS-based approach, I give an example of generating the model-implied covariance between just two model variables algebraically. After doing so, I then introduce the CAS-based approach. This involves introducing the model elements as symbols into `Ryacas` and entering in the model matrices. Then I generate the entire symbolic model-implied covariance matrix and show that the procedure does in fact give the proper results. Lastly, I show just one example of how a close inspection of the model-implied covariance matrix can help researchers gain a better understanding of their SEM models. This applies regardless of the method of generating the model-implied covariance matrix. The CAS-based approach can be seen as another available tool towards this goal.

Set-up

The only packages needed are `lavaan` and `Ryacas`.

```
install.packages( "lavaan")
install.packages( "Ryacas")
library( "lavaan")
library( "Ryacas")
```

Let us simulate a simple model using tools available in base R (R Core Team 2017) to use as our dataset. That way, the ‘true’ parameter values are known so that it will be possible to later double-check the work.

```
x1 <- rnorm( 10000, 0, 1)
x2 <- 0.1*x1 + rnorm( 10000, 0, 1)
z1 <- 0.3*x1 + 0.15*x2 + rnorm( 10000, 0, 1)
y1 <- 0.2*z1 + 0.05*x1 + 0.0*x2 + rnorm( 10000, 0, 1)
df <- data.frame( x1, x2, z1, y1)
```

I chose a sample size of $n = 10,000$ in order to minimize but not eliminate sampling error, and each of the exogenous (independent) variables in the model (x_1 , δ_2 , v_1 and ε_1) are $N \sim (0, 1)$.

The empirical covariance matrix can be viewed with

```
cov( df)

##           x1           x2           z1           y1
## x1 0.98880443 0.09639345 0.3002384 0.10500371
## x2 0.09639345 0.99990831 0.1850999 0.03891528
## z1 0.30023840 0.18509987 1.1147841 0.24146647
## y1 0.10500371 0.03891528 0.2414665 1.07471688
```

We can write equations for each of the model variables

$$\begin{aligned}x_1 &= \delta_1 \\x_2 &= \varphi_1 x_1 + \delta_2 \\z_1 &= \gamma_1 x_1 + \gamma_2 x_2 + v_1 \\y_1 &= \beta_1 x_1 + \beta_2 z_1 + \varepsilon_1\end{aligned}$$

where, from the code above, we know $\varphi_1 = 0.1$, $\gamma_1 = 0.3$, $\gamma_2 = 0.15$, $\beta_1 = 0.05$, $\beta_2 = 0.2$. Notice we have also written an equation for the only observed exogenous variable, $x_1 = \delta_1$, which basically states that the entire variance is due to influences not contained in the model. This will be important to note below when we specify the model matrices. The path diagram of our model is shown in Figure 1.

Model matrices

The SEM-matrix notation I use most closely mimics the one used in popular SEM software like **lavaan** and **Mplus**. It has been outlined by (Bollen 1989; Graff 1979) The basic model is

$$\begin{aligned}\boldsymbol{\eta} &= \mathbf{B}\boldsymbol{\eta} + \boldsymbol{\zeta} \\ \mathbf{y} &= \mathbf{A}\boldsymbol{\eta}.\end{aligned}$$

If m stands for the number of independent latent variables, n is the number of dependent latent variables, p is the number of independent observed (manifest) variables and q is the number of dependent observed variables, then the $(m + n + p + q \times 1)$ vector $\boldsymbol{\eta}$ holds the observed and latent variables, $\boldsymbol{\zeta}$ is also $(m + n + p + q \times 1)$

Figure 1: Path diagram

and holds any latent variables and the errors of the manifest variables and $\mathbf{y}$ is $(p + q \times 1)$ and holds only the observed variables. The matrix $\mathbf{\Lambda}$ is $(p + q \times m + n + p + q)$ and has only ones and zeros as elements and selects the observed variables from $\boldsymbol{\eta}$. The $\mathbf{\Psi}$ matrix (introduced below) is $(m + n + p + q \times m + n + p + q)$ and specifies the (co-)variances of the variables in $\boldsymbol{\zeta}$. Finally, the $\mathbf{B}$ matrix is also $(m + n + p + q \times m + n + p + q)$ and holds the model coefficients.

For this example model, we have: $\boldsymbol{\eta}' = (x_1, x_2, z_1, y_1)$, $\boldsymbol{\zeta}' = (\delta_1, \delta_2, v_1, \varepsilon_1)$ and $\mathbf{y}' = (x_1, x_2, z_1, y_1)$. Because there are no latent variables in this example, $\boldsymbol{\eta}$ is identical to $\mathbf{y}$ and the matrix $\mathbf{\Lambda}$ is an identity matrix

$$\mathbf{\Lambda} = \begin{matrix} & \begin{matrix} x_1 & x_2 & z_1 & y_1 \end{matrix} \\ \begin{matrix} x_1 \\ x_2 \\ z_1 \\ y_1 \end{matrix} & \begin{bmatrix} 1.0 & 0 & 0 & 0 \\ 0 & 1.0 & 0 & 0 \\ 0 & 0 & 1.0 & 0 \\ 0 & 0 & 0 & 1.0 \end{bmatrix} \end{matrix},$$

and $\mathbf{B}$ will be

$$\mathbf{B} = \begin{matrix} & \begin{matrix} x_1 & x_2 & z_1 & y_1 \end{matrix} \\ \begin{matrix} x_1 \\ x_2 \\ z_1 \\ y_1 \end{matrix} & \begin{bmatrix} 0 & 0 & 0 & 0 \\ \varphi_1 & 0 & 0 & 0 \\ \gamma_1 & \gamma_2 & 0 & 0 \\ \beta_1 & 0 & \beta_2 & 0 \end{bmatrix} \end{matrix}.$$

The $\mathbf{\Psi}$ matrix is important as it specifies the covariances of the independent variables (including the errors), essentially laying out all the model assumptions. Before showing the $\mathbf{\Psi}$ matrix we must first derive the the $\boldsymbol{\Sigma}(\boldsymbol{\theta})$ **model-implied covariance matrix** of the observed variables analytically. To do so, we first put $\boldsymbol{\eta}$ in reduced form

$$\begin{aligned} \boldsymbol{\eta} &= \mathbf{B}\boldsymbol{\eta} + \boldsymbol{\zeta} \\ &= (\mathbf{I} - \mathbf{B})^{-1}\boldsymbol{\zeta} \end{aligned}$$

and find the expected value of $\mathbf{y}\mathbf{y}'$

$$\begin{aligned}
yy' &= (\Lambda\eta)(\Lambda\eta)' \\
&= (\Lambda(I - B)^{-1}\zeta)(\Lambda(I - B)^{-1}\zeta)' \\
&= (\Lambda(I - B)^{-1}\zeta)(\zeta'(I - B)^{-1'}\Lambda') \\
&= \Lambda(I - B)^{-1}\zeta\zeta'(I - B)^{-1'}\Lambda' \\
E[yy'] &= \Lambda(I - B)^{-1}E[\zeta\zeta'](I - B)^{-1'}\Lambda' \\
\Sigma(\theta) &= \Lambda(I - B)^{-1}\Psi(I - B)^{-1'}\Lambda'.
\end{aligned}$$

It should be clear from this that the model is specified primarily according to the assumptions we place on B and Ψ .¹ In B we are deciding how the variables are related to one another and in Ψ we are (often implicitly) stating our further model assumptions. In this example, we are assuming that the model errors are uncorrelated with the exogenous variable x_1 and with each other (see the path diagram in Figure 1). Therefore, Ψ has the variances of the exogenous variables on the diagonal and zeros everywhere else

$$\Psi = \begin{matrix} & \begin{matrix} x_1 & x_2 & z_1 & y_1 \end{matrix} \\ \begin{matrix} x_1 \\ x_2 \\ z_1 \\ y_1 \end{matrix} & \begin{bmatrix} \sigma_{\delta_1}^2 & 0 & 0 & 0 \\ 0 & \sigma_{\delta_2}^2 & 0 & 0 \\ 0 & 0 & \sigma_{v_1}^2 & 0 \\ 0 & 0 & 0 & \sigma_{\varepsilon_1}^2 \end{bmatrix} \end{matrix},$$

(keeping in mind that x_1 is exogenous, so $x_1 = \delta_1$).

Running the model in lavaan

Having now reached our model specification, we can compare the matrices outlined above to the ones that `lavaan` used to come to the estimates. First though, the model is run to check the estimates. I use labels, e.g. `x2 ~ p1*x1`, to help remind me later that the coefficient for the regression of x_2 on x_1 was called “phi one”.

```

m1 <- '
x1 ~ 1*x1 # Simply to preserve order of variables as they appear in the output
x2 ~ p1*x1
z1 ~ g1*x1 + g2*x2
y1 ~ b1*x1 + b2*z1
'

summary(m1.fit <- sem(m1, data = df))

## lavaan 0.6-3 ended normally after 16 iterations
##
## Optimization method          NLMINB
## Number of free parameters      9
##
## Number of observations        10000
##
## Estimator                      ML
## Model Fit Test Statistic      0.106
## Degrees of freedom            1
## P-value (Chi-square)          0.745
##

```

¹The only choices we make regarding the vectors η , ζ and y are which variables to include in the model in the first place.

```
## Parameter Estimates:
##
##      Information                               Expected
##      Information saturated (h1) model          Structured
##      Standard Errors                           Standard
##
## Regressions:
##      Estimate Std.Err z-value P(>|z|)
##      x1 ~
##      x1      1.000
##      x2 ~
##      x1      (p1) 0.097 0.010 9.740 0.000
##      z1 ~
##      x1      (g1) 0.288 0.010 28.546 0.000
##      x2      (g2) 0.157 0.010 15.665 0.000
##      y1 ~
##      x1      (b1) 0.044 0.011 4.152 0.000
##      z1      (b2) 0.205 0.010 20.504 0.000
##
## Variances:
##      Estimate Std.Err z-value P(>|z|)
##      .x1      0.989 0.014 70.711 0.000
##      .x2      0.990 0.014 70.711 0.000
##      .z1      0.999 0.014 70.711 0.000
##      .y1      1.021 0.014 70.711 0.000
```

Because of the large sample size, the estimated parameters are very close to the ones we used to generate the data. This should come as no surprise because we simply copied the data-generating process into our code and let the software come up with the estimates. Now, we can inspect the model matrices using the `inspect()` function in `lavaan`, where `'est'` returns a list of the model matrices

```
inspect( m1.fit, 'est')

## $lambda
##      x1 x2 z1 y1
## x1  1  0  0  0
## x2  0  1  0  0
## z1  0  0  1  0
## y1  0  0  0  1
##
## $theta
##      x1 x2 z1 y1
## x1  0
## x2  0  0
## z1  0  0  0
## y1  0  0  0  0
##
## $psi
##      x1      x2      z1      y1
## x1 0.989
## x2 0.000 0.990
## z1 0.000 0.000 0.999
## y1 0.000 0.000 0.000 1.021
##
```

```
## $beta
##      x1      x2      z1 y1
## x1 1.000 0.000 0.000 0
## x2 0.097 0.000 0.000 0
## z1 0.288 0.157 0.000 0
## y1 0.044 0.000 0.205 0
```

Here we see the matrices used to estimate the model are, in fact, the exact same ones we outlined above. The only difference is that here the estimated coefficients have been substituted in already.

Model-implied covariance matrix

Typical approaches

If we are interested in looking at how the parameter estimates were found, we need to look closer at the model-implied covariances.

It is of course possible to use the tracing rule (Kenny 1979) to come up with the underlying model-implied covariances but this is inefficient, tedious and it must be done by hand. Another option is to find the algebraic equation per covariance which is straightforward, but also tedious. For example, if we want to know how the effect $x_1 \xrightarrow{\beta_1} y_1$ was estimated, then we need to look at $Cov(y_1, x_1)^2$

$$\begin{aligned}
Cov(y_1, x_1) &= E[y_1 x_1] \\
&= E[(\beta_1 x_1 + \beta_2 z_1 + \varepsilon_1)(x_1)] \\
&= E[\beta_1 x_1^2 + \beta_2 z_1 x_1 + \varepsilon_1 x_1] \\
&= \beta_1 Var(x_1) + \beta_2 E[z_1 x_1] \\
&= \beta_1 Var(x_1) + \beta_2 E[(\gamma_1 x_1 + \gamma_2 x_2 + v_1)(x_1)] \\
&= \beta_1 Var(x_1) + \beta_2 E[\gamma_1 x_1^2 + \gamma_2 x_2 x_1 + v_1 x_1] \\
&= \beta_1 Var(x_1) + \beta_2 \gamma_1 Var(x_1) + \beta_2 \gamma_2 E[x_2 x_1] \\
&= \beta_1 Var(x_1) + \beta_2 \gamma_1 Var(x_1) + \beta_2 \gamma_2 E[(\varphi_1 x_1 + \delta_2)(x_1)] \\
&= \beta_1 Var(x_1) + \beta_2 \gamma_1 Var(x_1) + \beta_2 \gamma_2 E[\varphi_1 x_1^2 + \delta_2 x_1] \\
&= \beta_1 Var(x_1) + \beta_2 \gamma_1 Var(x_1) + \beta_2 \gamma_2 \varphi_1 Var(x_1) \\
\hat{\beta}_1 &= \frac{Cov(y_1, x_1) - \beta_2 \gamma_1 Var(x_1) - \beta_2 \gamma_2 \varphi_1 Var(x_1)}{Var(x_1)}
\end{aligned}$$

which we can double-check by substituting in the model estimates (the option 'list' gives the parameter table in the form of a matrix that can easily be accessed and worked with)

```
# The square brackets are used to access elements of the matrix
# E.g. the parameter estimate for beta1 is found in row 5, column 14
b1 <- inspect( m1.fit, 'list')[ 5, 14] # beta1
b2 <- inspect( m1.fit, 'list')[ 6, 14] # beta2
g1 <- inspect( m1.fit, 'list')[ 3, 14] # gamma1
g2 <- inspect( m1.fit, 'list')[ 4, 14] # gamma2
p1 <- inspect( m1.fit, 'list')[ 2, 14] # phi1

# Cov(y1, x1)      - b2*g1*Var(x1)      - b2*g2*p1*Var(x1)      /Var(x1)
( cov( df)[ 4, 1] - b2*g1*cov( df)[ 1, 1] - b2*g2*p1*cov( df)[ 1, 1])/cov( df)[ 1, 1]

## [1] 0.04402362
```

²Here the covariance algebra is simplified because the variables are all centered with mean zero.

```
# Compare with the lavaan estimate of beta1
inspect( m1.fit, 'list')[ 5, 14]
```

```
## [1] 0.04402362
```

The equation for $\hat{\beta}_1$ tells us that it is the result of the covariance of y_1 and x_1 *minus* the weighted (by $\hat{\beta}_2$) covariance of z_1 and x_1 , divided by the variance of x_1 .

However, as I stated earlier, this procedure is tedious if one wants to inspect the model-implied covariances of each of the elements in the covariance matrix. And the more complex the model in terms of the number of variables and the number of relationships between the variables, the more tedious the procedure becomes.

Ryacas model-implied covariance matrix

The more efficient option I will present converts the model matrices specified above into the entire symbolic model-implied covariance matrix. This method is efficient because it uses only the matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{\Psi}$ and an $(m + n + p + q)^2$ identity matrix. The matrices will get larger the more complex the model, but they will not become more numerous.

The first step is to introduce all the model variables (including the errors) and coefficients as symbols using the `Sym( 'variable' )` function in `Ryacas`.

```
# Symbols for variables (including errors)
x1 <- Sym( 'x1' )
x2 <- Sym( 'x2' )
z1 <- Sym( 'z1' )
y1 <- Sym( 'y1' )
d1 <- Sym( 'd1' ) # Delta1
d2 <- Sym( 'd2' ) # Delta2
u1 <- Sym( 'u1' ) # Upsilon1
e1 <- Sym( 'e1' ) # Epsilon1

# Symbols for coefficients
p1 <- Sym( 'p1' ) # Phi1
g1 <- Sym( 'g1' ) # Gamma1
g2 <- Sym( 'g2' ) # Gamma2
b1 <- Sym( 'b1' ) # Beta1
b2 <- Sym( 'b2' ) # Beta2
```

Second, one specifies the model matrices as they were shown above. In `Ryacas`, vectors are inputted as row vectors using `vector := {a, b, c}` while for matrices, one uses double curly braces: `matrix := {{a, b, c}, {d, e, f}}`. Matrices are entered row-wise, so element `d`, for example, is found in the second row, first column. Besides defining the symbolic variables, to use `Ryacas` one must enclose the code in `yacas( "" )`.

```
# Lambda
yacas( "L := {{1, 0, 0, 0},
              {0, 1, 0, 0},
              {0, 0, 1, 0},
              {0, 0, 0, 1}}")

# Psi
yacas( "P := {{x1^2, 0, 0, 0},
              {0, d2^2, 0, 0},
              {0, 0, u1^2, 0},
              {0, 0, 0, e1^2}}")
```

```

# Beta
yacas( "B := {{0, 0, 0, 0},
             {p1, 0, 0, 0},
             {g1, g2, 0, 0},
             {b1, 0, b2, 0}}")

# Identity matrix -
# "I" is reserved, must use "Id" or something else
yacas( "Id := {{1, 0, 0, 0},
              {0, 1, 0, 0},
              {0, 0, 1, 0},
              {0, 0, 0, 1}}")

```

After inputting the model matrices, the equation for $\Sigma(\theta)$ can be derived straightforwardly. Note that matrix multiplication works with `Dot( matrix1, matrix2)`, and that the functions in `Ryacas` are case sensitive. The transpose and inverse of a matrix works with `Transpose( matrix)` and `Inverse( matrix)`, respectively. Remember, the equation for the model-implied covariance matrix was $\Lambda(I - B)^{-1}\Psi(I - B)^{-1'}\Lambda'$

```

# First make the (I-B)^(-1) matrix
yacas( "IdmB := Id - B")
yacas( "iIdmB := Inverse( IdmB)") # iIdmB stands for "inverse of Identity minus B"

# Then use matrix multiplication to arrive at model-implied covariance matrix
yacas( "LB := Dot( L, iIdmB)")
yacas( "LBP := Dot( LB, P)")
yacas( "LBPB := Dot( LBP, Transpose( iIdmB))")
yacas( "LBPBL := Dot( LBPB, Transpose( L))")

```

Doing so results in the symbolic model-implied matrix.

```

## Yacas matrix:
##      [,1]
## [1,] x1^2
## [2,] p1 * x1^2
## [3,] (g1 + g2 * p1) * x1^2
## [4,] (b1 + b2 * (g1 + g2 * p1)) * x1^2
##      [,2]
## [1,] x1^2 * p1
## [2,] x1^2 * p1^2 + d2^2
## [3,] (g1 + g2 * p1) * x1^2 * p1 + g2 * d2^2
## [4,] (b1 + b2 * (g1 + g2 * p1)) * x1^2 * p1 + b2 * g2 * d2^2
##      [,3]
## [1,] x1^2 * (g1 + g2 * p1)
## [2,] p1 * x1^2 * (g1 + g2 * p1) + d2^2 * g2
## [3,] x1^2 * (g1 + g2 * p1)^2 + d2^2 * g2^2 + u1^2
## [4,] (b1 + b2 * (g1 + g2 * p1)) * x1^2 * (g1 + g2 * p1) + b2 * g2 * d2^2 * g2 + b2 * u1^2
##      [,4]
## [1,] x1^2 * (b1 + b2 * (g1 + g2 * p1))
## [2,] p1 * x1^2 * (b1 + b2 * (g1 + g2 * p1)) + d2^2 * (b2 * g2)
## [3,] (g1 + g2 * p1) * x1^2 * (b1 + b2 * (g1 + g2 * p1)) + g2 * d2^2 * (b2 * g2) + u1^2 * b2
## [4,] x1^2 * (b1 + b2 * (g1 + g2 * p1))^2 + d2^2 * (b2 * g2)^2 + u1^2 * b2^2 + e1^2

```

Again, we can double check and see if the proper symbolic model-implied covariance matrix resulted by

Figure 2: Alternative Model Path diagram

looking, for example, at $Cov(y_1, x_1)$ in the fourth row, first column of the results

```
# Remember to save parameter estimates of the lavaan model
# as objects. You may have to clear the symbolic variables
# from memory before you can use the names again as normal
# R objects or use other names, i.e.
# b1 <- Sym( 'b1') # Symbolic variable for Ryacas
# beta1 <- inspect( m1.fit, 'list')[ 5, 14] # Normal R object

# Cov(y1,x1) =
(b1 + b2 * (g1 + g2 * p1)) * var( df$x1)

## [1] 0.1050037
# Compare with the empirical covariance matrix df
cov( df$x1, df$y1)

## [1] 0.1050037
```

Using the analytical model-implied covariance matrix to gain a better understanding of SEM models

Regardless of whether one uses the tracing rule, writes out the covariances algebraically or generates the entire symbolic matrix with the method above, it is important to carefully inspect the model-implied covariance matrix. Doing so can reveal things that are often hidden even in otherwise accurate path diagrams.

For example, suppose we believed the variables x_1 and x_2 in the first model were unrelated. Our path diagram would need to be updated to reflect this, see Figure 2.

The question now is, which of the following two scenarios is true?

$$\begin{aligned} z_1 &= \gamma_1 x_1 + v_{1a} \\ z_1 &= \gamma_2 x_2 + v_{1b} \end{aligned}$$

or

$$z_1 = \gamma_1 x_1 + \gamma_2 x_2 + v_1$$

In other words, are the estimated coefficients γ_1 and γ_2 both total bivariate effects or are they partial coefficients? Could it be that the software is actually basically running two separate bivariate equations for

z_1 ? After all, the covariance between x_1 and x_2 is shown as zero in the model matrix Ψ .³ The answer may be clear to some, but the path diagram does not help us in any way, nor do the typical maximum-likelihood based explanations one often hears along the lines of ‘then the optimal estimates are found in an iterative process’.

One way to approach this problem is to inspect the model-implied covariance matrix and check. We can run a second *lavaan* model, this time without the effect $x_1 \xrightarrow{\varphi_1} x_2$ and again generate the model-implied covariance matrix.

```
m2 <- '
x1 ~ 1*x1 # Simply to preserve order of variables in output
x2 ~ 1*x2 # Here as well
# x2 ~ p1*x1
z1 ~ g1*x1 + g2*x2
y1 ~ b1*x1 + b2*z1
'
summary( m2.fit <- sem( m2, data = df))
```

```
## lavaan 0.6-3 ended normally after 12 iterations
##
## Optimization method          NLMINB
## Number of free parameters    8
##
## Number of observations       10000
##
## Estimator                    ML
## Model Fit Test Statistic     94.528
## Degrees of freedom          2
## P-value (Chi-square)        0.000
##
## Parameter Estimates:
##
## Information                  Expected
## Information saturated (h1) model Structured
## Standard Errors              Standard
##
## Regressions:
##           Estimate Std.Err z-value P(>|z|)
## x1 ~
##   x1           1.000
## x2 ~
##   x2           1.000
## z1 ~
##   x1      (g1)   0.288   0.010  28.681   0.000
##   x2      (g2)   0.157   0.010  15.739   0.000
## y1 ~
##   x1      (b1)   0.044   0.011   4.169   0.000
##   z1      (b2)   0.205   0.010  20.507   0.000
##
## Variances:
##           Estimate Std.Err z-value P(>|z|)
##   .x1           0.989   0.014  70.711   0.000
```

³This example is motivated by a playful argument between myself and thesis advisor concerning whether to explicitly specify covariances between exogenous predictors.

```
##      .x2                1.000    0.014   70.711    0.000
##      .z1                0.999    0.014   70.711    0.000
##      .y1                1.021    0.014   70.711    0.000
```

The model matrices can be viewed again using

```
inspect( m2.fit, 'est')
```

```
## $lambda
##      x1 x2 z1 y1
## x1  1  0  0  0
## x2  0  1  0  0
## z1  0  0  1  0
## y1  0  0  0  1
##
## $theta
##      x1 x2 z1 y1
## x1  0
## x2  0  0
## z1  0  0  0
## y1  0  0  0  0
##
## $psi
##      x1      x2      z1      y1
## x1 0.989
## x2 0.000 1.000
## z1 0.000 0.000 0.999
## y1 0.000 0.000 0.000 1.021
##
## $beta
##      x1      x2      z1 y1
## x1 1.000 0.000 0.000  0
## x2 0.000 1.000 0.000  0
## z1 0.288 0.157 0.000  0
## y1 0.044 0.000 0.205  0
```

notice the change to the B matrix. Now modify the `Ryacas` matrix accordingly and generate the symbolic model-implied covariance matrix. All the other matrices stay the same, so as long as they are still in memory one does not need to enter them again.

```
# Beta
yacas( "B := {{0,  0,  0,  0},
              {0,  0,  0,  0},
              {g1, g2, 0,  0},
              {b1, 0,  b2, 0}}")
```

```
# Multiplication
yacas( "IdmB := Id - B")
yacas( "iIdmB := Inverse( IdmB)")

yacas( "LB := Dot( L, iIdmB)")
yacas( "LBP := Dot( LB, P)")
yacas( "LBPB := Dot( LBP, Transpose( iIdmB))")
```

```
yacas( "LBPBL := Dot( LBPB, Transpose( L))")
```

```
## Yacas matrix:
##      [,1]      [,2]
## [1,] x1^2      0
## [2,] 0         d2^2
## [3,] g1 * x1^2  g2 * d2^2
## [4,] (b1 + b2 * g1) * x1^2 b2 * g2 * d2^2
##      [,3]
## [1,] x1^2 * g1
## [2,] d2^2 * g2
## [3,] x1^2 * g1^2 + d2^2 * g2^2 + u1^2
## [4,] (b1 + b2 * g1) * x1^2 * g1 + b2 * g2 * d2^2 * g2 + b2 * u1^2
##      [,4]
## [1,] x1^2 * (b1 + b2 * g1)
## [2,] d2^2 * (b2 * g2)
## [3,] g1 * x1^2 * (b1 + b2 * g1) + g2 * d2^2 * (b2 * g2) + u1^2 * b2
## [4,] x1^2 * (b1 + b2 * g1)^2 + d2^2 * (b2 * g2)^2 + u1^2 * b2^2 + e1^2
```

The resulting matrix seems to support the first scenario, that both regression coefficients are uncontrolled bivariate estimates. However, if we substitute in our estimates and solve for γ_1 (as an example, we could do the same for γ_2), we see that something is not right.

```
# z1*x1 = g1 * x1^2
# g1     = z1*x1/x1^2
cov( df$z1, df$x1)/var( df$x1)
```

```
## [1] 0.3036378
```

```
# Compare with the estimated coefficient
inspect( m2.fit, 'list')[ 3, 14]
```

```
## [1] 0.2883011
```

The analytical equation for the coefficient does not equal the estimate from the `lavaan` model. To check the alternative scenario, that the estimated coefficients are partial coefficients, we can change Ψ to reflect a correlation between x_1 and x_2

```
# Psi
yacas( "P := {{x1^2,  x1*x2, 0,  0},
              {x2*x1, d2^2, 0,  0},
              {0,     0,   u1^2, 0},
              {0,     0,   0,   e1^2}}")
```

and then re-run the matrix multiplication and see what changes

```
# Multiplication
yacas( "IdmB := Id - B")
yacas( "iIdmB := Inverse( IdmB)")

yacas( "LB := Dot( L, iIdmB)")
yacas( "LBP := Dot( LB, P)")
yacas( "LBPB := Dot( LBP, Transpose( iIdmB))")
yacas( "LBPBL := Dot( LBPB, Transpose( L))")
```

```
## Yacas matrix:
##      [,1]
## [1,] x1^2
## [2,] x2 * x1
## [3,] g1 * x1^2 + g2 * (x2 * x1)
## [4,] (b1 + b2 * g1) * x1^2 + b2 * g2 * (x2 * x1)
##      [,2]
## [1,] x1 * x2
## [2,] d2^2
## [3,] g1 * (x1 * x2) + g2 * d2^2
## [4,] (b1 + b2 * g1) * (x1 * x2) + b2 * g2 * d2^2
##      [,3]
## [1,] x1^2 * g1 + x1 * x2 * g2
## [2,] x2 * x1 * g1 + d2^2 * g2
## [3,] (g1 * x1^2 + g2 * (x2 * x1)) * g1 + (g1 * (x1 * x2) + g2 * d2^2) * g2 + u1^2
## [4,] ((b1 + b2 * g1) * x1^2 + b2 * g2 * (x2 * x1)) * g1 + ((b1 + b2 * g1) * (x1 * x2) + b2 * g2 * d2^2) * g2 + b2 * u1^2
##      [,4]
## [1,] x1^2 * (b1 + b2 * g1) + x1 * x2 * (b2 * g2)
## [2,] x2 * x1 * (b1 + b2 * g1) + d2^2 * (b2 * g2)
## [3,] (g1 * x1^2 + g2 * (x2 * x1)) * (b1 + b2 * g1) + (g1 * (x1 * x2) + g2 * d2^2) * (b2 * g2) + u1^2 * b2
## [4,] ((b1 + b2 * g1) * x1^2 + b2 * g2 * (x2 * x1)) * (b1 + b2 * g1) + ((b1 + b2 * g1) * (x1 * x2) + b2 * g2 * d2^2) * (b2 * g2) + u1^2 * b2^2 +
```

(The equation for y_1^2 gets cut off but that doesn't really matter.)

Now we can solve the alternative equation for γ_1 to show that the estimated coefficients are, in fact, partial coefficients.

```
# z1 * x1 = g1 * x1^2 + g2 * (x2 * x1)
# g1      = ( z1*x1 - g2 * (x2 * x1))/x1^2
(cov( df$z1, df$x1) - inspect( m2.fit, 'list')[ 4, 14]*cov( df$x2, df$x1))/var( df$x1)
```

```
## [1] 0.2883011
```

```
# Compare with estimated gamma1
inspect( m2.fit, 'list')[ 3, 14]
```

```
## [1] 0.2883011
```

From this, we can see that the default behaviour in **lavaan** is to implicitly account for covariances between exogenous variables with common ‘children’ to use the language of Judea Pearl (2009). This was not apparent from the path diagram above, nor was it reflected in the **lavaan** model — even the model matrices showed a 0 in Ψ for the correlation between x_1 and x_2 .⁴ However, by taking a closer look at the algebraically derived equation for the parameter of interest and double checking, we were able to conclude that the estimates are in fact partial effects and we learned something about the default behaviour of the software. Upon reflection, it should be clear that this is the only way the model can work but it was not trivial to find conclusive evidence.

Conclusion

Regardless of the method; tracing, algebraic or using the CAS **Ryacas** method outlined here, knowing how to generate and inspect the model-implied covariance matrix can be a useful tool. By running the model, specifying the matrices in **Ryacas** in exactly the same way and deriving the matrix algebra model-implied covariance matrix, we can be sure that no mistakes were made along the way. The tedious algebraic derivation shown above proves that there are many opportunities to make a mistake.

On the other hand, it should be noted that this approaches does not always make sense. For example, the equation for the variance of y_1 in the last output is probably too long to be of much practical use (although it is accurate!). For a more intuitive understanding of what goes into the variance of that variable, it is likely better to work out the algebra by hand. Then one can decide for themselves when it makes sense to stop expanding. In the algebraic equation for $Cov(y_1, x_1)$ above for example, one could have stopped at line 4 and simply plugged in $Cov(z_1, x_1)$ from the empirical covariance matrix instead of expanding even further. But this is something each researcher must decide for themselves on a case by case basis.

⁴It should, however, have been apparent from the fact that the estimates in both of the **lavaan** models were identical.

The goal of this article was to outline an approach that can compliment the tracing rule and covariance algebra by hand. The benefits are that the CAS approach is efficient, less prone to careless mistakes and that the results are available digitally for further use in **R** — results derived by hand need to be entered in to the software manually. In any case, a close inspection of the underlying algebra of the model-implied covariance matrix should be seen as a necessary step in any SEM regression model. It is often difficult to accurately reflect the SEM model in path diagrams alone and there are even situations where software default settings can be misleading as we have seen from the simple example above.

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