Covariance Matrix is Not Positive Definite Error Message

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There can be a number of possible reasons for an error message regarding "covariance matrix is not positive definite" -- so the solution may not always be straight forward and, therefore, may require some “tinkering” in order to fix the problem.

In general, a covariance matrix being not positive definite refers to a problem that can occur where there is some sort of problem in inverting the matrix to perform multiplication. A simple case is where there is where the determinant of the matrix is almost zero (indicating vary little generalized variance in the matrix). When this is near zero when the matrix is inverted it will be like multiplying by zero. If the determinant of the matrix is exactly zero, then the matrix is referred to as "singular" (see also Rigdon, 1997; Wothke, 1993). This is a situation where there is a perfect (or near perfect) linear dependency of one variable with another (i.e., one variable can be expressed as a linear combination of the others. This often occurs in a situation where there is multicollinearity (high correlations) between two or more variables in the model. Singularity can also occur when the number of observations is less than the number of variables.

A covariance matrix should always be positive semi-definite, which means that the matrix has no negative eigenvalues, and it will be positive definite, unless it has one variable that is an exact linear combination of the others. If you have a negative eigenvalue, it means there is a negative variance somewhere in the model. We cannot have negative variances in the estimated covariance matrix (i.e., by definition, only a positive-semidefinite matrix can be a covariance matrix). A matrix with negative eigenvalues is not positive semidefinite, but note it can be definite (no zero eigenvalues) or singular (with at least one zero eigenvalue). When a matrix has positive and negative eigenvalues we refer to it as indefinite.

Here are several reasons why not positive definite covariance matrices can occur with data in "real data" settings.

1. Small sample sizes (like at your level 2) may result in the sample covariance or correlation matrix being not positive definite, which can just be due to sampling fluctuation. This can result from an improper solution where one or more variances is estimated as zero or estimated as negative. This might be the case in a variance decomposition analysis where there is not enough variance at level 2 for the program to provide an accurate estimate. Measurement inconsistency can also provide problems in estimation.

The appearance of a negative variance can also mean the model is not specified correctly. For example, often with small sample sizes it may be more difficult to estimate a random slope at level 2, since they often will not be as reliably estimated since the slope may depend on relationships between other variables within the unit. We can usually estimate random intercepts pretty accurately even in a small sample size, since we only need the mean for each unit (and not
a slope). So one "fix" is to not estimate a random slope at level 2. It may be there is one "offending" parameter that is making estimation not proceed normally. Related to this might be the type of covariance matrix the analyst may be trying to estimate at level 1 (e.g., if one had a longitudinal model, there are several types of covariance matrices that can be chosen and one or more different types might not fit the data very well).

2. Another possible cause is "too much" missing data. If one is using a certain data replacement technique (e.g., listwise or pairwise deletion), this may result in an inaccurate matrix being produced. Depending on how you deal with missing values, sample covariance matrices may or may not be positive semi-definite. If pairwise deletion is used, for example, then there's no guarantee of positive semi-definiteness.

3. A third possible cause is a variable that has "constant variance" --that is, it essentially has zero variance so it is a constant. As noted previously, this will create a matrix that is not positive definite.

Here are some possible ways to fix the problem--

1) Small level-2 sample size (e.g., N = 20) is causing a random parameter not be estimated properly. This will go away often if you fix the random parameter (generally a slope) within level-1 units. If the intercept is not being estimated (or shows a variance near 0) it may be an indication that the data will not support a multilevel outcome (at least for that particular outcome variable).

2) Multicollinearity between two variables or too much missing data, which leads back to a matrix that is not being properly estimated. One can often look at the correlation matrix and find if there are two variables that are too highly correlated (even the total correlation matrix for the sample would likely show this problem).

Where there is a linear dependency, the fix involves finding the situation and removing one of the two variables from the covariance matrix. To check for this, you can add variables one by one to the model until one creates a singularity. If it does, drop it, and go on to the next variable.

3) Wrong type of covariance matrix specified at either level 1 or level 2 (which can yield this message if there really is not variance present or the program cannot accurately estimate it). The matrix being not positive definite can result from a random parameter, or a covariance between two variables, a residual error term etc. This is often a matter of finding the parameter that is causing the message. It generally reflects that a variance is zero or slightly negative -- something like that where the program cannot perform a needed operation to find a solution.

4) With small sample sizes, level-2 estimates may be harder to obtain, especially with several random parameters. With multilevel generalized linear models in SPSS (GENLINMIXED), I have found it is much harder to estimate parameters. Multilevel models with categorical outcomes generally require "more data" than models with continuous outcomes in order to produce reasonable estimates. Since the expected values of the outcomes result from other
sampling distributions than the normal distribution and require link functions, some software programs such as Mplus require numerical integration to estimate model parameters with full maximum likelihood, while SPSS uses a type of quasi-likelihood estimation (so caution must be used in comparing multilevel categorical models). Estimating categorical outcomes, for example, takes more computing time than estimating continuous outcomes (especially as the number of random parameters in the model increases) and, in SPSS, this sometimes results in "estimation" stopping for various reasons -- including small sample sizes which don't really facilitate using ML type of estimation. Smaller sample sizes often use restricted ML (which I believe is the only estimation available in the SPSS multilevel categorical platform currently).

5) Check for parameters in the model that do not “make sense” (negative error variances, model fit indices that indicate a poor fit of the model to the data, large residuals for one more parameters in the model).

6) In SEM analyses, we may fix a parameter to some value (e.g., set better starting values, constrain a covariance between factors to some value, fix a negative error variance to be positive, fix an error variance to be zero). It is often useful to examine the model modification indices for indications that the model is misspecified in some way. You can try building the model up in smaller steps so you can isolate the problem more readily.

References
