Gramian Matrices in Covariance Structure Models

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Covariance structure models frequently contain out-of-range estimates that make no sense from either substantive or statistical points of view. Negative variance estimates are the most well-known of these improper solutions, but correlations that are out of range also occur. Methods to minimize improper estimates have been accomplished by reparameterization and estimation under simple inequality constraints; but these solutions, discussed previously in this journal (Marsh, 1989), do not guarantee that the covariance matrices involved represent variances and covariances of real numbers, as required. A general approach to avoiding improper solutions in structural equation models is proposed. Although this approach does not resolve inadequacies in the data or theoretical model that may generate an improper solution, it solves the long-standing problem of obtaining proper estimates. *Index terms: confirmatory factor analysis, EQS, Gramian matrices, Heywood cases, improper solutions, LISREL, structural equation models, underidentification.*

One of the oldest, and most widely recognized, problems in the application of covariance structure analysis or structural equation models is the frequent occurrence of negative variance estimates, especially for unique (error) factors. For example, Bollen (1987) estimated a one-factor factor analysis model for three variables. Two of the unique variances were estimated as positive, but one was negative. Such estimates, often called Heywood cases (after Heywood, 1931), present serious problems, because the variances being estimated are supposed to represent the variances of persons' scores on real and not imaginary variables. Because real random variables must have non-negative variances, a negative variance estimate has no meaning, that is, it is inadmissible or improper. Yet, such variance estimates occur frequently in covariance structure analysis, especially when the sample size is small and a model has an insufficient number of indicators having high loadings on each factor (e.g., Anderson & Gerbing, 1984; Boomsma, 1985). Bollen's (1987) improper estimate was eliminated when outlier cases were deleted.

A recent discussion of this problem, and an evaluation of some suggested solutions, can be found in Dillon, Kumar, & Mulani (1987). Their discussion, however, was incomplete. It did not deal with various other ways that "offending estimates" can occur in covariance structure analysis. Rindskopf (1984) discussed several sources of this problem; Marsh (1989) also addressed the issue. Since this paper was completed, an excellent review of the topic was provided by Wothke (1993). The purpose of the present paper is to summarize the issues, and then to provide a solution to the fundamental problem that Wothke believes still remains: "There is a definite need for the development and teaching of a more general statistical solution to the estimation problems discussed here" (p. 288).

Although negative variance estimates are the most widely known inadmissible estimates, correlations that are out of range occur frequently as well. Marsh (1989) reported a number of confirmatory multitrait-multimethod models that had factor correlations outside the −1 to +1 range. Because factor correlations are intended to represent the correlations between persons' scores on real and not imaginary factors, to be meaningful such correlations should not exceed 1.0 in absolute value. Although

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improper values of correlations are not reported as frequently as negative variance estimates, it is suspected that such estimates often are not recognized. For example, many reported models contain so-called correlated errors. Covariances between a variable that has an estimated zero or negative variance and any other variable will be improper, but covariances can be out of range even when the variances are admissible. LISREL (Jöreskog & Sörbom, 1988) provides a valuable admissibility test that evaluates whether or not its estimated covariance matrices are positive definite, but "the computer program does not in general constrain the solution to be admissible" (p. 24). EQS (Bentler, 1992) also has no provision to assure proper estimates, but EQS can constrain correlations to the -1 to +1 range (Bentler, 1992; Bentler & Wu, 1993).

A number of reasons for the occurrence of these improper estimates have been advanced, including inappropriateness or misspecification of the model, theoretical and/or empirical underidentification of the parameters, population parameters close to the boundary of admissible values, too many parameters or factors, too many highly correlated factors, sampling fluctuations and small sample size, inappropriate handling of missing data or use of improper sample covariance matrices in estimation, and outlier or non-normal observations (see Bollen, 1989; Fuller, 1987; Van Driel, 1978). Wothke (1993) provided an excellent summary.

Clearly, the data and the model should be reevaluated if an improper estimate is obtained, because either the model is incorrect or the data provide too little information about the model's parameters. To avoid these problems, correctly specified and identified models, latent variables with many high-loading indicators, large sample sizes, and data that meet the relevant statistical assumptions of the methods such as independence of observations and, depending on the estimation method, perhaps multivariate normality are needed. In practice, the ideal situation may not be achievable, especially because the problem may stem from population models or parameters that are near a boundary condition or nearly underidentified. The more limited goal of obtaining meaningful estimates that lie within an appropriately defined parameter space thus must be addressed. Although this approach does not cure inadequacies in the data or theoretical model that may generate an improper solution, it solves the long-standing problem of obtaining proper estimates. To date, this problem has been only partially addressed.

Most attention has been given to negative variance and out-of-range correlation estimates, but the problem of improper estimates is not limited to these type of inadmissible values. Situations can occur in which every parameter estimate is inside its appropriate boundary, but the solution as a whole nonetheless is inadmissible. Existing procedures do not adequately diagnose or prevent this from happening. An illustrative example is given by the following matrix, which represents a factor correlation matrix obtained from a confirmatory factor analysis:

$$\begin{bmatrix} 1 & .945 & .840 & .735 \\ .945 & 1 & .720 & .630 \\ .840 & .720 & 1 & -.360 \\ .735 & .630 & -.360 & 1 \end{bmatrix} . \qquad (1)$$

The matrix appears to be ordinary. All numbers are in the expected range. Nonetheless, the matrix cannot represent the correlations among real numbers as will be discussed below and as LISREL's admissibility test would show. In this paper, a computational method to avoid improper solutions is provided. Existing computational approaches to avoid improper estimates generally involve the use of artificial boundaries, reparameterization, or constrained estimation (e.g., Bentler, 1992; Dillon et al., 1987; Marsh, 1989; Rindskopf, 1983; Wothke, 1993). These procedures are partially success-

ful in avoiding negative variance estimates and out-of-range correlations, but they are not general enough to cover the entire spectrum of improper solutions.

Marsh (1989) proposed that, in the context of confirmatory factor analysis, parameterizations that fix factor loadings versus those that fix factor variances may be equivalent in well-defined solutions, but that "... fixing the factor variances introduces an implicit inequality constraint that restricts the factor variances to be non-negative. Thus, fixing factor variance estimates may lead to a proper solution when fixing factor loadings does not" (p. 340). Although it is correct to say that this may happen, there is no particular reason to expect that forcing a factor variance to be non-negative will necessarily yield a factor correlation matrix that is proper (as defined explicitly below). In fact, most of Marsh's models with factor correlations exceeding 1.0 were not made proper by fixing factor variances.

An illustrative example is provided in Table 1. This nine-variable, three-factor model was created artificially. The factor loadings, unique variances, and factor variances and covariances are hypothetical. Note that one of the factor variances is negative. As expected, maximum likelihood estimation without restrictions recovered these estimates exactly when the covariance matrix generated from the example was analyzed. Marsh (1989) suggested analyzing the matrix with factor variances fixed; the results of this analysis are shown in Table 2. First, note that although the factor loadings are not remarkable, the factor correlations are now out of range—there are two values greater than 1.0. Thus, the improper aspect of the solution simply transferred from an improper variance to two improper correlations. Second, the solution is now more constrained, as Marsh predicted. The fit of the model is now no longer perfect as measured by the maximum likelihood estimation fit function (see Equation 5 below), and the unique variances are estimated at different values. The procedure proposed here can be used to further restrict the solution so that it is completely proper.

Gramian Matrices and Improper Solutions

The improper solutions mentioned above are found in the parameter matrices in structural equa-

Table 1
Factor Loadings and Factor Variance-Covariance Matrix for the Original Model Using Artificial Data With a Negative Factor Variance

Variable and Factor	Factor I	Factor II	Factor III	Unique Variance
Variable				
1	1	0	0	6.43
2	.57	0	0	6.43
3	.22	0	0	6.43
4	0	1	0	6.43
5	0	.90	0	6.43
6	0	.98	0	6.43
7	0	0	1	6.43
8	0	0	1.06	6.43
9	0	0	.22	6.43
Factor				
I	−1.46			
II	.88	1.48		
III	.96	.94	1.00	
Eigenvalue	2.62	.29	−1.88	

Note. Integer 0 and 1 entries represent fixed parameters.

Table 2
Factor Loadings and Factor Correlation Matrix for the Reparametized Model Using Artificial Data

Variable and Factor	Factor I	Factor II	Factor III	Unique Variance
Variable				
1	.34	0	0	4.86
2	.22	0	0	5.91
3	.09	0	0	6.35
4	0	1.24	0	6.42
5	0	1.12	0	6.42
6	0	1.22	0	6.42
7	0	0	1.05	6.37
8	0	0	1.12	6.36
9	0	0	.22	6.43
Factor				
I	1			
II	2.34	1		
III	2.99	.75	1	
Eigenvalue	5.18	.27	−2.45	

Note. Integer 0 and 1 entries represent fixed parameters.

tion models that deal with the covariances among variables, especially, covariances among common or unique factors. Consider first the factor analytic model in which observed variables x are hypothesized to be generated by common factors ξ and unique factors ϵ according to the model

$$x = \Lambda\xi + \epsilon, \tag{2}$$

where Λ is the common factor pattern or loading matrix. Assuming that common and unique factors are uncorrelated, the covariance structure of the factor analysis model is given by

$$\Sigma = \Lambda\Phi\Lambda' + \Psi, \tag{3}$$

where

Σ is the covariance matrix of the measured variables,

Φ is the covariance or correlation matrix of the common factors (depending on identification conditions), and

Ψ is the covariance matrix of the unique or error factors.

Equation 2 states that Φ and Ψ must represent the covariances among real-valued variates; therefore, they must be Gramian matrices. A Gramian matrix is a matrix that represents the variances and covariances of real numbers; it must be non-negative definite, that is, its eigenvalues must be non-negative.

An eigenvalue λ_i of a $p \times p$ matrix A is defined by $Av_i = \lambda_i v_i$, where v_i is the eigenvector associated with λ_i, which is usually normalized to have unit length. If A is symmetric, the λ_is are real-valued, and there always exists a set of p linearly independent eigenvectors. When all λ_is are positive, A is referred to as positive definite; when they are non-negative, A is called Gramian or positive semi-definite. As noted by Wothke (1993), an eigenvalue of a covariance matrix is typically interpreted as the variance of a linear combination of the original variables, so that a covariance matrix cannot be allowed to have a negative eigenvalue, because "... this would imply that a certain weighted sum of its variables has a negative variance" (p. 290). Jöreskog & Sörbom (1988) considered a covariance matrix to be admissible only if it was both Gramian and full rank. This is a well-accepted require-

ment for data covariance matrices (e.g., Browne, 1982, p. 88; Wothke, 1993). Model covariance matrices are studied here.

In Equation 3, Φ and Ψ each must be Gramian. A Gramian matrix will not exhibit any of the anomalies discussed above. That is, it will not contain negative diagonal entries (negative variances), and the off-diagonals, when expressed as correlations, will be in the −1 to +1 range. Furthermore, there will be nonarbitrary relations between the diagonal and off-diagonal elements of a Gramian matrix. These relations have been studied and are important in many contexts (e.g., Olkin, 1981). In contrast, the 4 × 4 correlation matrix shown in Expression 1 has eigenvalues of 2.90, 1.36, .08, and −.33. The negative eigenvalue makes the matrix improper as a covariance matrix. Similarly, the factor correlation matrix in Table 2 has a negative eigenvalue. For such improper matrices, squared multiple correlations between one variable and all the other variables may not be in the 0–1 range. Thus, Gramian covariance matrices are a minimal requirement for the model in Equation 3.

In order to be meaningful, the parameter estimates of the model in Equation 3 must meet the conditions on the parameters themselves. Factor loading estimates of Λ, $\hat{\Lambda}$, can take on any value, and will thus not be out of range. Negative unique variance estimates refer to negative entries in the diagonal of $\hat{\Psi}$. When Φ is restricted to be a correlation matrix, out-of-range factor correlations refer to improper elements in the offdiagonal of $\hat{\Phi}$. More precisely, $\hat{\Phi}$, $\hat{\Psi}$, and $\hat{\Sigma}$ must be Gramian matrices. Although a Gramian $\hat{\Sigma}$ is typically guaranteed by standard estimation methods (e.g., maximum likelihood), $\hat{\Phi}$ and $\hat{\Psi}$ are not guaranteed to be Gramian.

Although Gramian covariance matrices seem to be a minimal requirement for covariance and correlation estimates, it is possible also to consider stronger requirements that are not an integral part of Equations 2 and 3. In particular, the following conditions also could be required: (1) Λ is of full column rank and has no rows with only zero elements; (2) Φ is positive definite; and (3) Ψ is positive definite. These stronger requirements were suggested by Jöreskog & Sörbom (1988, p. 24), but are not imposed in LISREL. In this paper, Condition 1 above is not addressed. Conditions 2 and 3, while desirable, are not practically achievable without any prior knowledge on the size of the smallest eigenvalue of Φ and Ψ. If a covariance matrix estimate, say $\hat{\Phi}$, is Gramian and has a zero eigenvalue, another solution could be obtained, say $\tilde{\Phi}$, in which the smallest eigenvalue is a small positive number ϵ. Historically, such an approach often was taken to deal with boundary or out-of-range unique variances (e.g., Jöreskog, 1969). This makes sense primarily if there is strong a priori knowledge about the variance involved, but otherwise it is somewhat arbitrary because the size of ϵ depends on subjective judgment.

General structural equation models, such as are estimated by LISREL or EQS, also contain covariance matrices that must be Gramian. In LISREL, four covariance matrices must be considered that represent covariances among exogenous factors (Φ), factor disturbances (Ψ), and correlated errors in variables ($\theta_\delta, \theta_\epsilon$). Each should be Gramian, but no constraints are provided in LISREL to assure that this property will exist in the estimates. In the Bentler-Weeks (Bentler & Weeks, 1980) model used in EQS, there is one matrix to consider. The Bentler-Weeks covariance structure can be written as

$$\Sigma = G(I - B)^{-1}\Gamma\Phi\Gamma'(I - B)^{-1\prime}G' , \tag{4}$$

where

G is a known matrix with 0–1 elements,

B and Γ contain structural regression coefficients that can take on any values, and

Φ is the covariance matrix of all independent variables in the model. In this model, Φ must be Gramian, but EQS does not impose this constraint.

Estimation With Gramian Constraints

Let S represent the usual unbiased estimator based on a sample of size n of a $p \times p$ covariance matrix Σ, in which elements of Σ are functions of a $q \times 1$ parameter vector θ: $\Sigma = \Sigma(\theta)$. Examples of covariance structures were given in Equations 3 and 4 for the factor analysis model and the Bentler-Weeks model, respectively. The q elements of θ are the unknown elements of the matrices in the right-hand side of Equations 3 and 4. A discrepancy function $F = F[S, \Sigma(\theta)]$ is a measure of the discrepancy between S and $\Sigma(\theta)$ evaluated at an estimator $\hat{\theta}$. Many discrepancy functions have been suggested in the literature (e.g., Bentler, 1983; Browne, 1982; Jöreskog, 1969; Kano, Berkane, & Bentler, 1990), and the development here would hold for any of them. The most widely known function, the normal theory maximum-likelihood (ML) discrepancy function, is used here:

$$F = \log|\Sigma| - \log|S| + \mathrm{tr}(S\Sigma^{-1}) - p \ . \tag{5}$$

At the minimum, $\hat{\Sigma} = \Sigma(\hat{\theta})$, and F takes on the value $\hat{F}$. The statistic $T = (n - 1)\hat{F}$ is used as a large-sample χ^2 test with $(p^* - q)$ degrees of freedom, where $p^* = p(p + 1)/2$, to evaluate the null hypothesis $\Sigma = \Sigma(\theta)$.

Consider the confirmatory factor analysis model (Equation 3). In the standard application, Equation 5 is minimized with respect to the unknown elements in Λ, Φ, and Ψ. Since Jöreskog (1969) pointed out the importance of simple constraints on free parameters—for example, the equality constraint $\theta_i = \theta_j$—programs such as EQS and LISREL have incorporated these constraints during the minimization of Equation 5 and adjusted the degrees of freedom for the χ^2 test accordingly. Although more general nonlinear constraints also have been discussed in the literature (e.g., McDonald, 1980; Bentler & Lee, 1983) and their statistical implications developed (e.g., Lee & Bentler, 1980; Satorra, 1989), nothing seems to have been done explicitly on developing a method to assure that the covariance matrices in the models being estimated are Gramian.

The approach presented here involves optimizing Equation 5 under constraints on eigenvalues. This can be illustrated with reference to the covariance matrix Φ of the independent variables in the Bentler-Weeks model (Equation 4), or the factor covariance matrix Φ in the factor analysis model (Equation 3). Let the ith eigenvalue of the matrix Φ in Equations 3 or 4 be denoted as λ_i. The problem to be solved is given as a modification of Equation 5:

$$\min_{\theta} F = \log|\Sigma| - \log|S| + \mathrm{tr}(S\Sigma^{-1}) - p \ , \tag{6}$$

subject to $\lambda_i \geq 0$ $(i = 1, \ldots, p)$.

This is a problem involving nonlinear inequality constraints, because the λ_i are nonlinear functions of the elements in Φ. Although there are many approaches to solving this problem, the theory developed by Jamshidian & Bentler (1993) was used. To solve Equation 6, the gradient and information matrix of F with respect to θ are required. These are well known (see Bentler & Weeks, 1980; Bollen, 1989) and are computed in structural modeling programs. In addition, for the free parameters $\phi_{k\ell}$ the first-order derivatives are needed

$$\frac{\partial \lambda_i}{\partial \phi_{k\ell}} = \begin{cases} v_k^{(i)2} & k = \ell \\ 2v_k^{(i)} v_\ell^{(i)} & k \neq \ell \ , \end{cases} \tag{7}$$

where $v^{(i)}$ is the unit-length eigenvector corresponding to the ith eigenvalue of Φ, and $v_k^{(i)}$ is the kth element of $v^{(i)}$. In the context of the confirmatory factor analysis model (Equation 3), the derivatives $\partial\lambda_i/\partial\Lambda$ and $\partial\lambda_i/\partial\Psi$ are 0.0. These elements, along with Equation 7, make up the constraint

matrix $\partial\lambda/\partial\theta$ needed in the Jamshidian-Bentler algorithm. In the context of the Bentler-Weeks model, the derivatives $\partial\lambda_i/\partial\mathbf{B}$ and $\partial\lambda_i/\partial\mathbf{C}$ are 0.0 and, along with Equation 7, make up the constraint matrix $\partial\lambda/\partial\theta$. Then, the modified Newton method of Jamshidian & Bentler (1993) can be applied. The details of their procedure need not be repeated here, because, in principle, any other method of nonlinear optimization that can solve general nonlinear constrained problems, including eigenvalue constraints, could be used instead (e.g., Browne & Du Toit, 1992; Fletcher, 1985, 1987).

Technically, Equation 7 holds only when the multiplicity of the eigenvalue λ_i is 1 [i.e., there is only one unique (up to a constant multiple) eigenvector associated with λ_i]. If, for example, in the confirmatory factor analysis model the unconstrained solution for $\hat{\Phi}$ has more than one negative eigenvalue, then the restricted solution could have several zero eigenvalues. In this case, the derivative is not defined, and the algorithm theoretically can fail. However, note that computationally the Jamshidian & Bentler (1993) algorithm is still valid because, as noted above, independent eigenvectors still exist, which is a requirement for the algorithm to be computationally feasible. An alternative approach would be to use algorithms that handle nondifferentiable constraints (Fletcher, 1985). Normally, implementation of such algorithms is complicated. To evaluate this situation, the algorithm presented here was tried on many problems in which the unrestricted $\hat{\Phi}$ had more than one negative eigenvalue. It always successfully reached the solution. Examples are given below.

There is one situation in which the procedure described above need not be implemented. This is the case in which the relevant covariance matrix is completely free to be estimated. An example is given by the confirmatory factor analysis model in which the factor covariance matrix is unstructured. In some situations, the model $\Sigma = \mathbf{A}\Phi\mathbf{A}' + \Psi$ could lead to an estimate $\hat{\Phi}$, which is not Gramian. To avoid an improper estimate, the model could be reparameterized. For example, take $\Phi = \mathbf{T}\mathbf{T}'$, where $\mathbf{T}$ is a lower triangular or a symmetric matrix. Then $\Sigma = \mathbf{A}\mathbf{T}\mathbf{T}'\mathbf{A}' + \Psi$, and the model could be estimated with respect to $\mathbf{T}$ rather than Φ. Then the implied matrix $\hat{\Phi} = \hat{\mathbf{T}}\hat{\mathbf{T}}'$ is automatically Gramian (e.g., Jöreskog & Sörbom, 1988, p. 216; Wothke, 1993, p. 283). Some disadvantages of reparameterization include: the reparameterization is not unique, computation of derivatives is somewhat more complicated, and the modified model contains parameters (here, $\mathbf{T}$) that may not have an interesting interpretation. More importantly, this approach does not work when the elements of Φ are set to have fixed values, such as when Φ is restricted to be a correlation matrix.

When the constraints are on the parameters of a large matrix that can be partitioned into blocks containing sets of variables that are mutually uncorrelated, it is not necessary to work with the entire matrix. Computations can be simplified considerably. For example, in the factor analysis model, constraints on Ψ, consistent with the above theory, are easy to impose when Ψ is diagonal, that is, when unique factors are uncorrelated. In that case, the diagonal elements are equivalent to the eigenvalues, and hence methods such as were discussed by Dillon et al. (1987) or the simple inequality constraints provided in EQS (Bentler & Wu, 1993) will be sufficient. When some unique variables are correlated with others, the method of Equation 6 needs to be applied only to the submatrix of Ψ corresponding to the correlated variables. Similarly, in the Bentler-Weeks model the covariance matrix will contain covariances among factors, errors, and other independent variables. Many of these variables may be completely uncorrelated with others (e.g., unique factors in the standard factor model). The eigenvalues corresponding to these diagonal blocks are given by the diagonal entries so that constraints on these entries can be handled by known means. The general eigenvalue constraint discussed above needs to be applied only to those variables that correlate with other variables.

The development in Equations 5 and 7 based on the ML estimator for the types of structural models shown in Equations 3 and 4 can be modified trivially to apply to other types of models and estimators, such as the model of Jöreskog & Sörbom (1988) and estimators involved in multiple-group

(e.g., Bentler, Lee, & Weng, 1987) and structured means models (e.g., Bentler, 1992, chap. 10).

Examples

Four examples are presented to show how the procedure proposed here diagnoses and prevents improper estimates of factor covariances in the confirmatory factor model. Several specific models were described by Marsh (1989) that yielded improper estimates that could not be cured by existing methods such as reparameterization or estimation under simple inequalities on parameters. Two real and two artificial examples are presented.

Example 1: Ostrom Data

Ostrom (1969) provided data that can be studied by multitrait-multimethod variants of confirmatory factor analysis models. Marsh (1989) studied a number of models for these data, varying trait and method factors as well as the data used. One of these models (1D) that contained no trait factors but several correlated method factors yielded a factor correlation matrix with values that were out of range. The factor loading matrix for the unconstrained solution minimizing Equation 5 that was obtained for the data given by Ostrom (p. 21) is given in Table 3.

The 12 variables are listed with their sequential trait (t_i) and method (m_j) designation. There were three traits and four methods in the data-gathering design; this particular model involved four method factors. In view of the narrow nature of the factors, it might be expected that the model would be misspecified for these data on a priori grounds, and improper solutions would be expected to have a nonzero probability of occurring.

As expected, the factor loading matrix looks ordinary. However, the factor correlation matrix

Table 3
Factor Loadings and Factor Correlation Matrices for the Unconstrained and Constrained Solutions for the Method Factor Model for Ostrom's (1969) Data

Variable and Factor	Unconstrained Solution					Constrained Solution				
	Factor				Unique	Factor				Unique
	I	II	III	IV	Variance	I	II	III	IV	Variance
Variable										
t_1m_1	.80	0	0	0	.37	.80	0	0	0	.37
t_2m_1	.73	0	0	0	.47	.73	0	0	0	.47
t_3m_1	.81	0	0	0	.34	.81	0	0	0	.34
t_1m_2	0	.88	0	0	.23	0	.88	0	0	.23
t_2m_2	0	.90	0	0	.19	0	.90	0	0	.19
t_3m_2	0	.90	0	0	.20	0	.90	0	0	.20
t_1m_3	0	0	.62	0	.62	0	0	.62	0	.61
t_2m_3	0	0	.73	0	.47	0	0	.73	0	.47
t_3m_3	0	0	.77	0	.41	0	0	.78	0	.40
t_1m_4	0	0	0	.93	.13	0	0	0	.93	.13
t_2m_4	0	0	0	.82	.33	0	0	0	.82	.33
t_3m_4	0	0	0	.82	.32	0	0	0	.82	.32
Factor										
I	1					1				
II	.97	1				.97	1			
III	1.01	.99	1			.99	.98	1		
IV	.89	.87	.92	1		.89	.87	.92	1	
Eigenvalue	3.83	.15	.03	−.01		3.82	.32	.15	0.00	

Note. Integer 0 and 1 entries represent fixed parameters.

contains one entry that is out of range. A correlation of 1.01 is obviously inadmissible; however, it is only trivially larger than 1.0. The eigenvalues of the factor correlation matrix diagnosed that the matrix was not Gramian as required under the model. However, the degree of violation was quite small, with the smallest eigenvalue of −.01 being only trivially smaller than 0.0. It was expected that a constrained solution would bring this eigenvalue to 0.0.

The identical model was analyzed using the constrained function given in Equation 6. The results also are given in Table 3. The factor loading and unique variance estimates were virtually identical to those of the unconstrained solution, with only a few estimates differing in the second decimal place. The factor correlations, however, were now all under 1.0. The previous estimate of 1.01 became an estimate of .99. According to the criterion in Equation 6, the optimal solution was not given by taking the offending estimate (1.01) and holding it to the 1.0 boundary. Indeed, none of the correlations was on the boundary in this solution. Nonetheless, one of the eigenvalues of $\hat{\Phi}$ was 0.0 (to seven decimal places). Thus, although there were four factors in this solution, the factor correlation matrix was rank 3, and one of the factors was linearly dependent on the others. Although Factors I and III were not perfectly correlated, the correlation was certainly very close to 1.0.

Example 2: Byrne & Shavelson Data

Byrne & Shavelson (1986) studied three academic self-concept traits measured by three different self-concept instruments. In addition to these nine variables, there were two validity variables in the matrix analyzed by Marsh (1989, p. 348). Marsh analyzed these validity variables as dummy factors, for which the variables had fixed 0.0 unique variances. Following Marsh, the same type of unconstrained analysis was performed here, with three method factors and two dummy factors. The results are given in Table 4. As in Marsh's report, two factor correlations exceeded 1.0 (1.11

Table 4
Factor Loadings and Factor Correlation Matrices for the Unconstrained and Constrained Solutions for the Method Factor Model from Byrne & Shavelson's (1986) Data

Variable and Factor	Unconstrained Solution						Constrained Solution					
	Factor					Unique	Factor					Unique
	I	II	III	IV	V	Variance	I	II	III	IV	V	Variance
Variable												
t_1m_1	.52	0	0	0	0	.73	.52	0	0	0	0	.73
t_2m_1	.14	0	0	0	0	.98	.09	0	0	0	0	.99
t_3m_1	.83	0	0	0	0	.31	.90	0	0	0	0	.18
t_1m_2	0	.47	0	0	0	.78	0	.44	0	0	0	.81
t_2m_2	0	.14	0	0	0	.98	0	.14	0	0	0	.98
t_3m_2	0	.92	0	0	0	.16	0	.98	0	0	0	.04
t_1m_3	0	0	.66	0	0	.56	0	0	.64	0	0	.59
t_2m_3	0	0	.21	0	0	.95	0	0	.18	0	0	.97
t_3m_3	0	0	.91	0	0	.17	0	0	.94	0	0	.12
v_1	0	0	0	1	0	0	0	0	0	1	0	0
v_2	0	0	0	0	1	0	0	0	0	0	1	0
Factor												
I	1						1					
II	1.11	1					.98	1				
III	1.05	.95	1				.96	.87	1			
IV	.36	.22	.35	1			.29	.18	.31	1		
V	.66	.54	.70	.52	1		.61	.50	.68	.52	1	
Eigenvalue	3.73	.99	.39	.03	−.14		3.49	1.03	.38	.09	0.00	

Note. Integer 0 and 1 entries represent fixed parameters.

and 1.05. As expected, the factor correlation matrix was not Gramian. Its eigenvalues were not non-negative. Again, $\hat{\Phi}$ cannot be the correlation matrix of real-valued factors.

The constrained solution based on Equation 6 also is presented in Table 4. The factor loadings and unique variances were close to those of the unconstrained solution, but some entries differed by more than .01. The largest difference in factor loading estimates was .07; the largest difference in unique variance estimates was .13. However, the relative magnitudes of small and large values was virtually unchanged, so the interpretations would not differ. As expected, the factor correlation matrix $\hat{\Phi}$ no longer had values that were out of range and, as in Example 1, those correlations that exceeded 1.0 were not simply held to the boundary. Their values were .98 and .96. Although the estimates in $\hat{\Phi}$ showed no perfectly correlated factors, there was a linear dependency among the factors because the rank of $\hat{\Phi}$ was 4. (The 0.0 eigenvalue was 0 to eight decimal places).

Example 3: A Model With Two Negative Eigenvalues

This hypothetical example illustrates the importance of examining and constraining the eigenvalues of variance-covariance matrices. Wothke (1993) noted that "A major purpose for estimating a model under semidefiniteness constraints is to obtain information about what promotes indefinite estimates in an unconstrained parameterization" (p. 285). In this example, the data cannot support as many factors as are requested. Table 5 shows the variance-covariance matrix for an artificial example in which the unconstrained maximum likelihood solution yielded two negative eigenvalues in the covariance matrix $\hat{\Phi}$ of the factors. The unconstrained solution for a four-factor model is presented in Table 6. Although it was not obvious from the matrix itself, the covariance matrix $\hat{\Phi}$ clearly was not the covariance matrix of real factors. The corresponding constrained solution also is given in Table 6. Although the model specified four factors, and the unconstrained solution implied that there were four, two of them were superfluous when considering only factors with non-negative variances. Theoretically, the Jamshidian-Bentler (1993) algorithm could break down when there is more than one zero eigenvalue at the solution. In this example, the two zero eigenvalues were not exactly numerically equal, and hence the algorithm did not break down. The algorithm can be expected to work in most cases in which there are several zero eigenvalues because, due to computer precision, their values will not necessarily be numerically equal.

Table 5
Variance-Covariance Matrix for the Example of Table 6

	Variable											
Variable	1	2	3	4	5	6	7	8	9	10	11	12
1	3.00											
2	.30	1.04										
3	.18	.10	1.75									
4	.36	.20	.12	1.55								
5	.04	.02	.01	.03	2.35							
6	.09	.05	.03	.05	.01	1.84						
7	.42	.23	.14	.67	.08	.16	2.19					
8	.10	.05	.03	.16	.02	.04	.17	1.66				
9	.32	.18	.11	.52	.07	.13	.56	.13	2.36			
10	.91	.49	.30	.68	.08	.16	.77	.18	.60	1.20		
11	.68	.37	.22	.51	.06	.12	.58	.14	.45	.55	2.71	
12	.66	.36	.22	.49	.06	.12	.56	.13	.44	.54	.40	3.33

Table 6
Factor Loadings and Factor Variance-Covariance Matrices for the Unconstrained and Constrained Solutions from the Data of Table 5

Variable and Factor	Unconstrained Solution					Constrained Solution				
	Factor				Unique	Factor				Unique
	I	II	III	IV	Variance	I	II	III	IV	Variance
Variable										
1	1	0	0	0	2.44	1	0	0	0	2.11
2	.54	0	0	0	.88	.53	0	0	0	.79
3	.33	0	0	0	1.69	.32	0	0	0	1.66
4	0	1	0	0	1.33	0	1	0	0	.93
5	0	.12	0	0	2.35	0	.11	0	0	2.34
6	0	.24	0	0	1.83	0	.21	0	0	1.81
7	0	0	1	0	1.47	0	0	1	0	1.42
8	0	0	.24	0	1.62	0	0	.23	0	1.62
9	0	0	.78	0	1.92	0	0	.77	0	1.90
10	0	0	0	1	.46	0	0	0	1	.14
11	0	0	0	.75	2.30	0	0	0	.56	2.37
12	0	0	0	.73	2.94	0	0	0	.55	3.00
Factor										
I	.56					.88				
II	.37	.22				.42	.62			
III	.42	.67	.72			.49	.69	.77		
IV	.91	.68	.77	.74		.90	.68	.77	1.06	
Eigenvalue	2.53	.31	−.38	−.23		2.86	.48	0.00	0.00	

Note. Integer 0 and 1 entries represent fixed parameters.

Example 4: Gramian Factor Correlations and Boundary Error Variances

Using a different artificial example, a different result was obtained than that in Example 3 when two eigenvalues were negative in an unconstrained solution. The variance-covariance matrix for this example is presented in Table 7, and the four-factor solutions are presented in Table 8. In this example, Factors I, II, and III had only two nonzero indicators, and the factor loading of Variable 3 for Factor IV was extremely small (.09). The unconstrained solution showed that some correlations in the factor correlation matrix were substantially larger than 1.0. The correlation matrix had two negative eigenvalues, but the unique variances were all proper.

Table 7
Variance-Covariance Matrix for the Example of Table 8

Variable	Variable								
	1	2	3	4	5	6	7	8	9
1	2.11								
2	.54	4.36							
3	.06	.05	2.68						
4	.90	.65	.08	.78					
5	1.11	.80	.10	.44	2.26				
6	.45	.33	.07	.60	.74	4.22			
7	.62	.45	.06	.58	.72	.41	3.81		
8	.18	.13	.02	.17	.21	.12	.06	2.97	
9	.57	.41	.08	.74	.92	.61	.52	.15	2.17

Table 8
Factor Loadings and Factor Correlation Matrices for the Unconstrained and Constrained Solutions from the Data of Table 7

Variable and Factor	Unconstrained Solution					Constrained Solution				
	Factor Loadings				Unique Variance	Factor Loadings				Unique Variance
	I	II	III	IV		I	II	III	IV	
Variable										
1	.87	0	0	0	1.36	1.45	0	0	0	0.00
2	.62	0	0	0	3.97	.37	0	0	0	4.22
3	0	0	0	.09	2.67	0	0	0	.05	2.67
4	0	.60	0	0	.42	0	.72	0	0	.26
5	0	.74	0	0	1.72	0	.89	0	0	1.46
6	0	0	0	.71	3.72	0	0	0	.41	4.04
7	0	0	.45	0	3.61	0	0	1.95	0	0.00
8	0	0	.13	0	2.95	0	0	.03	0	2.97
9	0	0	0	.86	1.42	0	0	0	1.47	0.00
Factor										
I	1					1				
II	1.74	1				.86	1			
III	1.58	2.16	1			.22	.41	1		
IV	.76	1.43	1.32	1		.27	.70	.18	1	
Eigenvalue	5.59	.27	-.68	-1.18		2.41	.85	.74	0.00	

Note. Integer 0 and 1 entries represent fixed parameters.

The constrained solution also is shown in Table 8. Although two eigenvalues were negative in the unconstrained solution, only one was 0.0 in the constrained solution in which all correlations were in the appropriate range. Simply assuming that a negative eigenvalue was really 0.0 would lead to an incorrect conclusion here. In this example, the estimates were substantially different from the unconstrained estimates. Thus, the correlation of 2.16 between Factors II and III in the unconstrained solution became .41 in the constrained solution. The constrained solution also had three unique variances constrained to 0.0, so that in this example, problem eigenvalues in the factor correlation matrix in the initial solution offset problems with unique variances.

Discussion

An important feature of covariance structure models and related models is that the covariance matrices of implicit variables are intended to represent the correlations and variances of real variables. Thus, only solutions that meet the conditions of the parameter space—here, Gramian covariance matrices—yield appropriate estimators (e.g., maximum likelihood estimators). A solution with improper estimates then might not be regarded as an appropriate ML solution. Fortunately, it is relatively easy to find proper solutions. Implementing an eigenvalue constraint to assure that covariance matrices being estimated in structural equation models are Gramian is in most instances a relatively straightforward matter from a computational point of view. In the examples presented (and others not reported here), the iterations converged rapidly to the desired solution, even when multiple negative eigenvalues were encountered initially. Thus, this constraint does appear to be practical, and not just theoretical.

From a practical point of view, however, it could be argued that in Examples 1 and 2 the unconstrained and constrained solutions did not differ substantially. In several examples in which the correlations were greater than 1.0 in the unconstrained solution, the corresponding constrained

correlations typically were quite close to 1.0. The remainder of the estimates generally changed by only small amounts. Thus, the interpretations would be approximately the same with or without the Gramian constraint, and it might be questioned whether adding the constraint is worth the computational effort. Clearly it is worth the effort if an improper solution becomes proper and unconstrained, that is, if the eigenvalues are all positive at the solution. However, that situation was not encountered in any of the analyses presented here nor was it encountered in any of the literature. It is doubtful that this situation would occur except when the improper solution occurs as a result of convergence to a local minimum in the space that contains improper solutions. Nonetheless, in general there is no way of deciding a priori that in some particular example there might not be a relatively major change in some estimates when the covariance matrices are constrained to be proper. This happened when several eigenvalues of an unconstrained solution were negative and large (see Example 4, Tables 7 and 8). A correlation substantially larger than 1.0 (2.16, Table 8) was estimated finally at .41. Thus, such out-of-range correlations cannot be treated as essentially equal to 1.0. On the other hand, in a solution in which many boundary constraints were active (such as in Table 8), the appropriateness of the entire model specification might be questioned. Note also that these issues equivalently apply to the special case of negative variances, which, as noted above, has received much attention in the literature.

The negative variance case is interesting. Jöreskog & Sörbom (1988) stated that "zero estimates of error variances are as unacceptable as are negative estimates" (p. 215). Although this may be true in the sense that both imply violation of an implicit assumption that the corresponding covariance matrix is positive definite, it is possible to make only the weaker assumption that the covariance matrix should represent covariation among real-valued—not imaginary—variates. Then negative estimates are inadmissible and non-negative estimates are admissible—more generally, a Gramian constraint is appropriate.

Using Gramian covariance matrix constraints to remove improper solutions does not imply that the underlying causes of improper solutions have been eliminated. These causes were mentioned above (Wothke, 1993), and can include eigenvalues of covariance matrices near the boundary of the permissible space. In general, these hypothesized causes of improper solutions imply problems with the model and/or data. Typically, the problems do not disappear with a constrained solution, and hence a careful investigation regarding potential causes of the unconstrained improper solution or a constrained rank-deficient solution is necessary.

In the examples taken from Marsh (1989), models based on method factors alone (and no trait factors) were clearly inadequate to account for the sample covariances. Thus, key trait factors were obviously missing. In addition, the factor correlation matrix of the method factor model was always rank deficient in the constrained solution, verifying that there were not as many method factors relevant to the data as was hypothesized initially. Nonetheless, results such as were given in Tables 3 and 4 should not be the final basis of any interpretation because the models were so clearly misspecified. A more completely specified model may, in fact, clear up rank deficiencies found in more parsimonious but inadequate models.

As noted before, improper solutions often imply an inadequate model, at least with respect to the given data. Model inadequacy is more obvious when an estimation routine does not find a stable minimum of the fit function, when the residual covariances are extremely large, or when the standard χ^2 goodness-of-fit test is large compared to the degrees of freedom. Although degrees of freedom are not affected, a solution with active Gramian non-negativity constraints will appear to fit even worse than the unconstrained solution because the test statistic will be at least somewhat larger under the constraints (e.g., Wothke, 1993). Unfortunately, the χ^2 test itself may not be a reliable guide

to evaluating whether a model with one or more active nonlinear inequality constraints on parameters (e.g., one or more eigenvalues or variances estimated at 0.0) provides a statistically adequate fit to the data (Dijkstra, 1992). If these population parameters are truly positive and the model is correct, the standard test (described following Equation 5) can be applied with the usual precautions (e.g., Browne & Cudeck, 1993; Hu, Bentler, & Kano, 1992). In this case, a boundary estimate presumably occurs because the parameter is sufficiently small so 0.0 is within the realm of sampling variability. For example, if a population eigenvalue of Φ is .01, indicating that a factor has a very small, but nonzero, variance, it is possible that there are samples in which this factor's variance would be essentially 0.0 (although never negative, which is the point of Gramian constraints).

On the other hand, if a population eigenvalue or variance actually is 0.0, the goodness-of-fit χ^2 test no longer has an asymptotic χ^2 distribution (Shapiro, 1985). Rather, it is a mixture of χ^2 distributions with different degrees of freedom, with a probability value that cannot easily be obtained. No existing computer program has implemented Shapiro's difficult methodology. Unfortunately, even if it were implemented, because the true population model is unknown, it would not be possible to decide whether the usual χ^2 test is appropriate in the given situation or whether Shapiro's method must be used instead. From a model evaluation point of view, this may not matter if the model is clearly inadequate by various standards (Bollen & Long, 1993), because it is suspected that an extremely inadequate model also would fail Shapiro's test. Whether the model fit is marginal or not is an important issue, and it is a worthy topic for further research.

In the present formulation of the Gramian constraint (Equation 6) presented here, the eigenvalues λ_i of Φ were constrained to be non-negative. Therefore, the constrained solution obtained in each example yielded a matrix $\hat{\Phi}$ with estimated smallest eigenvalues $\lambda_p = 0.0$ to computer precision. Jöreskog's (1969, p. 187) approach for residual variances can be adapted equally well, and the constraint in Equation 6 can be set as $\lambda_i \geq \epsilon$, $i = 1, \ldots, p$, for an arbitrarily small positive number ϵ. The computational procedure presented here remains valid under this restriction. As a result, the matrix $\hat{\Phi}$ will be full rank (positive definite). Although a positive definite $\hat{\Phi}$ may be desirable from the point of view of the model (e.g., Equation 3) if the true model is being estimated, in practice it is not known whether the model is true. It seems more defensible to permit factors to be linearly dependent if more factors than the data can support have been specified.

The constrained estimation approach presented here, based on Jamshidian & Bentler's (1993) adaptation of Han's (1977) globally convergent method for nonlinear programming, has worked well in all trials. The approach is general enough to cover the range of modeling constraints typically encountered in practice. For example, fixed constants (e.g., 1s or 0s) in the Φ matrix are handled automatically because the derivatives (Equation 7) are 0.0 for such elements. Linear or nonlinear equality constraints on parameters also can be handled, either by reparameterization or by adding derivatives of these constraints with respect to the parameters of the constraint matrix. Of course, as noted earlier, other nonlinear programming methods in addition to the method presented here can be used as well. Browne & Du Toit (1992) provided another approach to nonlinear optimization that could be extended to handle the Gramian constraint discussed here (see also Browne, 1982, p. 109). These approaches, like those of Jamshidian & Bentler (1993), require specific adaptation to the problem of Gramian constraints, but these adaptations are not discussed in those papers.

Theoretically, the algorithm presented here can be improved. To better handle the case of several 0.0 eigenvalues, for example, the constraints in Equation 6 can be replaced by $\lambda_1 \geq \epsilon_1$, $\lambda_2 \geq \epsilon_2$, $\ldots$, $\lambda_p \geq \epsilon_p$, where $\epsilon_1 < \epsilon_2 < \ldots < \epsilon_p$, and the ϵ_is are fixed positive numbers close to 0.0. Then the Jamshidian-Bentler (1993) algorithm ensures that at the solution there will not be any 0.0 eigenvalues. In the examples, such restrictions were satisfied numerically, and thus they did not have to be

explicitly imposed. Another improvement is that the Jamshidian-Bentler algorithm uses the information matrix at every point. As they note in their paper, their algorithm can be started with the information matrix and the metric can be updated every iteration based on the Han-Powell update (see Luenberger, 1984, pp. 447–448). Based on limited experience, it seems that the latter approach may work better than that of the information matrix without an update for the type of problems considered here.

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