

# CONSTRUCTION OF COVARIANCE MATRICES WITH A SPECIFIED DISCREPANCY FUNCTION MINIMIZER, WITH APPLICATION TO FACTOR ANALYSIS

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**Abstract.** The main goal of this paper is to develop a numerical procedure for construction of covariance matrices such that for a given covariance structural model and a discrepancy function the corresponding minimizer of the discrepancy function has a specified value. Often construction of such matrices is a first step in Monte Carlo studies of statistical inferences of misspecified models. We analyze theoretical aspects of the problem, and suggest a numerical procedure based on semi-definite programming techniques. As an example, we discuss in details the factor analysis model.

**Key words.** Model misspecification, covariance structure analysis, maximum likelihood, generalized least squares, discrepancy function, factor analysis, semi-definite programming.

**AMS subject classifications.** 62H25, 90C26

**1. Introduction.** Covariance structure analysis, and its structural equation modeling extensions, had become one of the widely used methodologies in the social sciences such as psychology, education, economics, and sociology (e.g., [1]). An important issue in such analysis is to assess the goodness-of-fit of a considered model. For this purpose various test statistics were suggested and their behavior have been studied in numerous publications (see, e.g., [2], [5], [11]). It is well understood that in real applications no model fits data exactly and at best a good model can be considered as an approximation of reality (see, e.g., [3]). This raises the question of properties of the respective test statistics for misspecified models. This, in turn, brings the need for constructing covariance matrices with specified discrepancy values for their consequent use in Monte Carlo experiments. A procedure for such construction was developed in Cudeck and Browne [4].

The main goal of this paper is to extend the Cudeck - Browne approach by constructing such covariance matrices in a systematic way aiming at achieving a *largest* possible *range* of attainable discrepancies, with the considered model, while retaining the same minimizer of the discrepancy function. More specifically, consider a covariance structure model defined by functional relation  $\Sigma = \Sigma(\theta)$ . Here  $\theta = (\theta_1, \dots, \theta_q)$  is the parameter vector varying in a parameter space  $\Theta \subset \mathbb{R}^q$ , and  $\theta \mapsto \Sigma(\theta)$  is a mapping from  $\Theta$  into the space of positive definite  $p \times p$  symmetric matrices. We denote by  $\mathcal{S}^{p \times p}$  the (linear) space of  $p \times p$  symmetric matrices. Also  $\mathcal{S}_+^{p \times p} = \{A \in \mathcal{S}^{p \times p} : A \succeq 0\}$  denotes the space (cone) of positive semidefinite matrices, and  $\mathcal{S}_{++}^{p \times p} = \{A \in \mathcal{S}^{p \times p} : A \succ 0\}$  denotes the space (cone) of positive definite matrices, where  $A \succeq 0$  ( $A \succ 0$ ) means that matrix  $A$  is positive semidefinite (positive definite).

Let  $F(S, \Sigma)$  be a real valued function measuring a discrepancy between two matrices  $S, \Sigma \in \mathcal{S}_{++}^{p \times p}$ . For a specified value  $\theta_0 \in \Theta$  of the parameter vector, and (positive definite) matrix  $\Sigma_0 = \Sigma(\theta_0)$ , we want to construct a covariance matrix  $S = \Sigma_0 + X$ , for some  $X \in \mathcal{S}^{p \times p}$ , such that

$$\theta_0 = \arg \min_{\theta \in \Theta} F(\Sigma_0 + X, \Sigma(\theta)). \quad (1.1)$$

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That is, we want that the minimum discrepancy function estimator, corresponding to the matrix  $S$ , will have the specified value  $\theta_0$ . Consequently, in Monte Carlo experiments, one would like to have at a disposal such covariance matrices  $S$  yielding different discrepancy values  $\delta = F(S, \Sigma(\theta_0))$ . Moreover, it could be desirable to have a large range of the discrepancy values  $\delta$  while maintaining property (1.1). We approach this goal by solving a certain optimization problem aimed at a construction of a largest discrepancy value subject to the constraint (1.1). Once such a covariance matrix  $S = \Sigma_0 + \bar{X}$  is computed, one can construct smaller discrepancy values by rescaling, i.e., by taking  $S = \Sigma_0 + t\bar{X}$  for different values of the scaling parameter  $t \in [0, 1]$ . Numerical experiments indicate that the developed approach often gives a significant improvement of the Cudeck - Browne procedure in terms of the magnitude of attained discrepancy values, and can be considered as an alternative to the Cudeck - Browne method.

We discuss in details the following discrepancy functions which are of practical interest: the Maximum Likelihood (*ML*) discrepancy function

$$F_{ML}(S, \Sigma) = \ln |\Sigma| - \ln |S| + \text{Tr} [S\Sigma^{-1}] - p, \quad (1.2)$$

and the Generalized Least Squares (*GLS*) discrepancy function

$$F_{GLS}(S, \Sigma) = \frac{1}{2} \text{Tr} \{[(S - \Sigma)W]^2\}, \quad (1.3)$$

where  $W \in \mathcal{S}_{++}^{p \times p}$  is either a fixed (independent of  $S$  and  $\Sigma$ ) matrix or  $W = S^{-1}$ . Note that in both cases the corresponding discrepancy function has the properties: (i)  $F(S, \Sigma) \geq 0$  for any  $S, \Sigma \in \mathcal{S}_{++}^{p \times p}$ , and (ii)  $F(S, \Sigma) = 0$  iff  $S = \Sigma$ . Subsequently, while talking about a discrepancy function  $F(S, \Sigma)$  we assume, unless stated otherwise, that it is either *ML* or *GLS* discrepancy function.

We assume that  $\theta_0$  is an *interior* point of the parameter space  $\Theta$  and that mapping  $\Sigma(\theta)$ , defining the considered covariance structure, is smooth in the sense that it is twice continuously differentiable. It is said that the covariance structure is *linear* if it can be represented in the form  $\Sigma(\theta) = G_0 + \theta_1 G_1 + \dots + \theta_q G_q$ , where  $G_i \in \mathcal{S}^{p \times p}$ ,  $i = 0, \dots, q$ , are given matrices and  $\Theta = \{\theta \in \mathbb{R}^q : \Sigma(\theta) \succ 0\}$ . An example of linear covariance structure is  $\Sigma(\theta) = \text{diag}(\theta_1, \dots, \theta_p)$ , i.e.,  $\Sigma(\theta) = \sum_{i=1}^p \theta_i D_i$ , where  $D_i$  denotes  $p \times p$  diagonal matrix with all entries equal 0 except the  $i$ -th diagonal entry equal 1. An important example of a nonlinear covariance structure is the factor analysis model

$$\Sigma(\Lambda, \Psi) = \Lambda\Lambda^T + \Psi. \quad (1.4)$$

Here the parameter vector is formed from the components, counted in some specified order, of the  $p \times k$  matrix  $\Lambda$  and the diagonal elements of the  $p \times p$  positive semidefinite diagonal matrix  $\Psi$ .

We use the following notation and terminology throughout the paper. For a  $p \times p$  matrix  $A$  we denote by  $\text{Tr}(A)$  and  $|A|$  its trace and determinant, respectively. By  $A^T$  we denote the transpose of matrix  $A$ , and by  $A \otimes B$  the Kronecker product of two matrices. By  $e_i$  we denote the  $i$ -th coordinate vector,  $e_i = (0, \dots, 1, \dots, 0)^T$ , with all its components equal zero except the  $i$ -th component equal 1, and by  $D_i = \text{diag}(0, \dots, 1, \dots, 0)$  the  $i$ -th diagonal matrix.

This paper is organized as follows. A review of the model and theoretical background is given in Section 2. We study the optimality conditions of the problem and develop a numerical solution in terms of semidefinite programming. Section 3 presents

simulation studies to illustrate the developed procedure and to compare the suggested method to other method. Section 4 gives some remarks and future directions of this research.

**2. Theoretical Analysis.** In this section we give a theoretical analysis of the problem of constructing covariance matrices  $S = \Sigma_0 + X$  satisfying (1.1) and having a specified discrepancy value with respect to the considered model. This involves the following conditions which should be maintained:

(C1) The minimizer of  $F(S, \Sigma(\theta))$ , over  $\theta \in \Theta$ , should be the specified value  $\theta_0$ .

(C2) The covariance matrix  $S = \Sigma_0 + X$  should be positive definite.

We denote by  $\mathfrak{M}(\theta_0)$  the set of matrices  $X \in \mathcal{S}^{p \times p}$  satisfying the above condition (C1) and such that  $\Sigma_0 + X \succeq 0$ . This set is slightly bigger than what is required by condition (C2) since it imposes on  $\Sigma_0 + X$  to be positive semidefinite rather than positive definite matrix. Note that the set  $\mathfrak{M}(\theta_0)$  is closed (see Proposition 2.3 below), while the set of matrices  $X$  satisfying conditions (C1) and (C2) is not necessarily close. We will show that for many covariance structure models, the set  $\mathfrak{M}(\theta_0)$  is bounded, and hence the corresponding discrepancy value  $\delta = F(S, \Sigma(\theta_0))$  cannot be made arbitrarily large. Therefore we would like to evaluate the largest discrepancy value while maintaining the above conditions (C1) and (C2). It is worthwhile to remark that condition (1.1) holds if and only if (iff)

$$\Sigma_0 = \arg \min_{\Sigma \in \mathfrak{S}} F(\Sigma_0 + X, \Sigma), \quad (2.1)$$

where  $\Sigma_0 = \Sigma(\theta_0)$  and

$$\mathfrak{S} = \{\Sigma \in \mathcal{S}^{p \times p} : \Sigma = \Sigma(\theta), \theta \in \Theta\}. \quad (2.2)$$

With matrices  $S, \Sigma, X \in \mathcal{S}^{p \times p}$  we associate corresponding vectors  $s = \text{vec}(S)$ ,  $\sigma = \text{vec}(\Sigma)$  and  $x = \text{vec}(X)$ , where  $\text{vec}(S)$  operator transforms matrix  $S$  into  $p^2 \times 1$  vector by stacking columns of  $S$ . Note that since the matrices  $S, \Sigma, X$  are symmetric, the corresponding  $p^2 \times 1$  vectors will have duplicated elements; this should be remembered, in particular, in the equations (2.5) below. Interchangeably we may write the model  $\sigma = \sigma(\theta)$  and the discrepancy function  $F(s, \sigma)$  in terms of the corresponding vectors rather than matrices. We have that

$$\frac{\partial F(\sigma_0 + x, \sigma(\theta_0))}{\partial \theta} = \Delta^T \mathbf{g}(x), \quad (2.3)$$

where

$$\Delta = \partial \sigma(\theta_0) / \partial \theta \quad \text{and} \quad \mathbf{g}(x) = \partial F(\sigma_0 + x, \sigma_0) / \partial \sigma \quad (2.4)$$

are the respective  $p^2 \times q$  Jacobian matrix and  $p^2 \times 1$  gradient vector.

Since it is assumed that  $\theta_0$  is an interior point of  $\Theta$ , the (first order) necessary optimality conditions for  $\theta_0$  to be the respective minimizer, i.e., (1.1) to hold, are  $\partial F(\sigma_0 + x, \sigma(\theta_0)) / \partial \theta = 0$ . In view of (2.3) this can be written as equations  $\Delta^T \mathbf{g}(x) = 0$ . For the *ML* and *GLS* discrepancy functions we have that  $\mathbf{g}(x) = -Qx$ , where  $Q = \Sigma_0^{-1} \otimes \Sigma_0^{-1}$  for the *ML* discrepancy function and  $Q = W \otimes W$  for the *GLS* discrepancy function. Consequently, in both cases, we can write the first order necessary conditions as equations (cf., Cudeck and Browne [4]):

$$\Delta^T Qx = 0. \quad (2.5)$$

Note that for the *ML* and *GLS* discrepancy functions the corresponding matrix  $Q$  is independent of  $x$ , provided that in the *GLS* case the weight matrix  $W$  is fixed (independent of  $S$ ). In these cases the first order necessary conditions (2.5) are linear in  $x$  equations. For  $W = S^{-1}$  the situation is more involved, we will discuss this later.

The function  $F_{GLS}(S, \Sigma)$  is convex in  $\Sigma$ , and hence if the covariance structure is *linear*, then  $F_{GLS}(S, \Sigma(\theta))$  is convex in  $\theta$ . Therefore, in that case, the first order necessary conditions are also sufficient for optimality of  $\theta_0$ . Similarly in the *ML* case the first order conditions are sufficient if  $\Sigma^{-1}(\theta)$  is linear in  $\theta$ . For nonlinear covariance structures we can only assert such result locally for  $x$  sufficiently close to 0. Recall that it is said that the model  $\Sigma(\theta)$  is *identified* (respectively, *locally identified*) at  $\theta_0$  if  $\Sigma(\theta^*) = \Sigma_0$ ,  $\theta^* \in \Theta$ , (respectively,  $\theta^* \in \Theta \cap \mathcal{V}$  for some neighborhood  $\mathcal{V}$  of  $\theta_0$ ) implies that  $\theta^* = \theta_0$ . A sufficient, and ‘‘almost necessary’’, condition for the local identifiability is for the Jacobian matrix  $\Delta$  to have full column rank  $q$  (cf., [10]).

Recall  $F(S, \Sigma)$  is nonnegative and equals zero iff  $S = \Sigma$ . Therefore, if  $S = \Sigma_0$ , then  $\theta_0$  is always a minimizer of  $F(\Sigma_0, \Sigma(\theta))$ , and if, moreover, the model is identified at  $\theta_0$ , then the minimizer  $\theta_0$  is unique. Under mild additional regularity conditions we have the following *consistency* property:

- (♣) For all  $S$  sufficiently close to  $\Sigma_0$  the function  $F(S, \Sigma(\theta))$  possesses a minimizer  $\hat{\theta} = \hat{\theta}(S)$ , over  $\theta \in \Theta$ , and any such minimizer converges to  $\theta_0$  as  $S$  tends to  $\Sigma_0$ .

In particular, the consistency property (♣) holds if the model is identified at  $\theta_0$  and the set  $\Theta$  is compact (see, e.g., [7, 9] for a discussion of consistency in the analysis of covariance structures).

**PROPOSITION 2.1.** *Suppose that the consistency property (♣) holds and the Jacobian matrix  $\Delta$  has full column rank  $q$ . Then there exists a neighborhood  $\mathcal{U}$  of  $0 \in \mathcal{S}^{p \times p}$  such that for  $X \in \mathcal{U}$  satisfying the first order optimality conditions  $\Delta^T \mathbf{g}(x) = 0$ , it holds that  $\theta_0$  is the unique minimizer of  $F(\Sigma_0 + X, \Sigma(\theta))$  over  $\theta \in \Theta$ .*

*Proof.* Consider Hessian matrix  $V = \frac{\partial^2 F(s, \sigma)}{\partial \sigma \partial \sigma^T} \Big|_{s=\sigma_0, \sigma=\sigma_0}$ . For the *ML* and *GLS* discrepancy functions this matrix is equal to  $\Sigma_0^{-1} \otimes \Sigma_0^{-1}$  and  $W \otimes W$ , respectively, and hence is positive definite. Moreover,

$$\frac{\partial^2 F(\sigma_0, \sigma(\theta))}{\partial \theta \partial \theta^T} \Big|_{\theta=\theta_0} = \Delta^T V \Delta, \quad (2.6)$$

and since  $\Delta$  has full column rank, it follows that matrix  $\Delta^T V \Delta$  is also positive definite.

We argue now by a contradiction. Suppose that the assertion is false. That is, there exists a sequence  $x_k$  converging to 0, such that  $\Delta^T \mathbf{g}(x_k) = 0$  and  $\theta_0$  is not a minimizer of  $F(\sigma_0 + x_k, \sigma(\theta))$  over  $\theta \in \Theta$ . By the consistency property (♣) we have that for all  $k$  large enough there is a minimizer  $\theta_k = \hat{\theta}(\sigma_0 + x_k)$ , such that  $\theta_k$  tends to  $\theta_0$  as  $k \rightarrow \infty$ . Since  $\theta_k \neq \theta_0$ , we also have that

$$F(\sigma_0 + x_k, \sigma(\theta_k)) < F(\sigma_0 + x_k, \sigma(\theta_0)). \quad (2.7)$$

By continuity arguments, the Hessian matrix  $\partial^2 F(\sigma_0 + x_k, \sigma(\theta_0)) / \partial \theta \partial \theta^T$  is positive definite for  $k$  large enough. It follows that first order necessary and second order sufficient conditions hold at point  $\theta_0$  and hence  $\theta_0$  is a strict local minimizer of  $F(\sigma_0 + x_k, \sigma(\theta))$ , i.e., there is a neighborhood  $\mathcal{V}$  of  $\theta_0$  such that for  $k$  large enough,

$$F(\sigma_0 + x_k, \sigma(\theta_0)) < F(\sigma_0 + x_k, \sigma(\theta)), \quad \forall \theta \in \mathcal{V} \setminus \{\theta_0\}. \quad (2.8)$$

Note that here the neighborhood  $\mathcal{V}$  can be taken to be independent of  $k$ . Now since  $\theta_k \rightarrow \theta_0$ , we have that  $\theta_k \in \mathcal{V}$  for  $k$  large enough. This gives a contradiction between (2.7) and (2.8), and hence the proof is complete.  $\square$

Assuming that the consistency property holds, and in particular that the model is identified at  $\theta_0$ , we have by the above theorem that for any “sufficiently small” solution  $x$  of equations (2.5), the matrix  $S = \Sigma_0 + X$  satisfies condition (C1). Since the matrix  $\Sigma_0$  is positive definite, the matrix  $S = \Sigma_0 + X$  is also positive definite for “sufficiently small”  $x$ . Therefore for any “sufficiently small” solution  $x$  of equations (2.5) we have that  $X \in \mathfrak{M}(\theta_0)$ . Next we address the question of whether the discrepancy  $\delta = F(\Sigma_0 + X, \Sigma_0)$  can be made arbitrarily large for  $X \in \mathfrak{M}(\theta_0)$ . Recall that  $\mathbf{g}(x) = -Qx$  with  $Q = A \otimes A$ , where  $A = \Sigma_0^{-1}$  for the *ML* discrepancy function and  $A = W$  for the *GLS* discrepancy function.

PROPOSITION 2.2. *Consider the set*

$$\mathfrak{F}(\Sigma_0) = \{X \in \mathcal{S}^{p \times p} : \Delta^T Qx = 0, \Sigma_0 + X \succeq 0\}, \quad (2.9)$$

where  $Q = A \otimes A$  with  $A$  being  $p \times p$  positive definite matrix. We have that: (i) The set  $\mathfrak{F}(\Sigma_0)$  is unbounded if and only if there exists a positive semidefinite matrix  $X \neq 0$  such that  $\Delta^T Qx = 0$ . (ii) Suppose, further, that the image set  $\mathfrak{S}$ , defined in (2.2), contains matrices of the form  $\Sigma_0 + \Psi$ , where  $\Psi$  can be any diagonal matrix sufficiently close to  $0 \in \mathcal{S}^{p \times p}$ . Then the set  $\mathfrak{F}(\Sigma_0)$  is bounded.

*Proof.* Since the set  $\mathfrak{F}(\Sigma_0)$  is given by the intersection of the linear space with the convex set  $\{X \in \mathcal{S}^{p \times p} : \Sigma_0 + X \succeq 0\}$ , it is a convex set. Consequently the set  $\mathfrak{F}(\Sigma_0)$  is unbounded iff it has a nonzero recession direction, i.e., iff there exists  $X \in \mathcal{S}^{p \times p}$ ,  $X \neq 0$ , such that  $\Delta^T Qx = 0$  and  $\Sigma_0 + tX \succeq 0$  for all  $t \geq 0$ . We also have that the property “ $\Sigma_0 + tX \succeq 0$  for all  $t \geq 0$ ” holds iff the matrix  $X$  is positive semidefinite. This proves (i).

Let us prove (ii). The property that  $\mathfrak{S}$  contains matrices of the form  $\Sigma_0 + \Psi$ , where  $\Psi$  can be any diagonal matrix sufficiently close to  $0$ , implies that the linear space generated by the Jacobian matrix  $\Delta$  contains vectors  $\text{vec}(D_i)$ ,  $i = 1, \dots, p$ . Consequently it follows from the condition  $\Delta^T (A \otimes A)x = 0$  that  $\text{Tr}(D_i A X A) = 0$ ,  $i = 1, \dots, p$ . This implies that all diagonal elements of matrix  $A X A$  are zeros. In turn this implies that the matrix  $X$  cannot be positive semidefinite unless  $X = 0$ . Indeed, if  $X \neq 0$  and  $X \succeq 0$ , then  $\text{Tr}[A X A] = \text{Tr}[X A^2] > 0$ , which is a contradiction with  $A X A$  having all diagonal entries equal zero. By the assertion (i) this completes the proof of (ii).  $\square$

Subsequently, when talking about the set  $\mathfrak{F}(\Sigma_0)$ , we assume that the matrix  $A$  is either  $A = \Sigma_0^{-1}$  for the *ML* discrepancy function or  $A = W$  for the *GLS* discrepancy function. Since (2.5) is a necessary optimality condition, we have that the set  $\mathfrak{M}(\theta_0)$  is included in the set  $\mathfrak{F}(\Sigma_0)$ , and hence if the set  $\mathfrak{F}(\Sigma_0)$  is bounded, then the set  $\mathfrak{M}(\theta_0)$  is also bounded. Of course, if  $\mathfrak{M}(\theta_0)$  is bounded, then the corresponding set of discrepancy values is also bounded. The condition “the image set  $\mathfrak{S}$  contains matrices of the form  $\Sigma_0 + \Psi$ , where  $\Psi$  can be any diagonal matrix sufficiently close to  $0$ ” holds if the model is invariant with respect to adding a sufficiently small diagonal matrix. Many covariance structure models, in particular the factor analysis model, satisfy this property. Note that the notion of “sufficiently small” (“sufficiently close to  $0$ ”) is essential there, since for example in the factor analysis model (1.4) the diagonal matrix  $\Psi$  should be positive semidefinite and hence cannot be an arbitrary diagonal matrix.

The first order optimality conditions (2.5) consist of  $q$  equations and  $p(p+1)/2$  unknowns formed by nonduplicated components of vector  $x = \text{vec}(X)$ . Typically  $q$  is

smaller than  $p(p+1)/2$ , and hence we have  $p(p+1)/2 - q$  “degrees of freedom” in choosing a solution of (2.5). It makes sense to improve the quality of the perturbation  $X$  by enforcing second order optimality conditions. That is, in addition to the first order optimality conditions we would like to ensure that the Hessian matrix

$$H(x) = \frac{\partial^2 F(\sigma_0 + x, \sigma(\theta))}{\partial \theta \partial \theta^T} \Big|_{\theta=\theta_0} \quad (2.10)$$

is positive definite (semidefinite). This leads to the following optimization problem

$$\begin{aligned} \text{Max}_{X \in \mathcal{S}^{p \times p}} \quad & F(\Sigma_0 + X, \Sigma_0) \\ \text{s.t.} \quad & \Delta^T Q x = 0, \quad H(x) \succeq 0, \quad \Sigma_0 + X \succeq 0. \end{aligned} \quad (2.11)$$

Note that for  $x = 0$  the Hessian matrix  $H(0)$  is always positive semidefinite, and hence  $x = 0$  is a feasible point of the above problem (2.11). Note also that it is possible to enforce positive definiteness (rather than positive semidefiniteness) of  $H(x)$  by replacing the constraint  $H(x) \succeq 0$  with constraint  $H(x) \succeq \varepsilon I$  for some small number  $\varepsilon > 0$ . This, however, makes a small difference in practice.

An optimal solution  $\bar{X}$  of the problem (2.11) gives a direction for constructing discrepancy values of the form  $F(\Sigma_0 + t\bar{X}, \Sigma_0)$  for  $t > 0$ . Of course, since conditions  $\Delta^T Q x = 0$  and  $H(x) \succ 0$  ensure only *local* optimality of  $\theta_0$ , there is no guarantee that  $\bar{X} \in \mathfrak{M}(\theta_0)$ . Nevertheless, we may try to find a largest  $\bar{t} > 0$  such that  $\Sigma_0 + \bar{t}\bar{X} \in \mathfrak{M}(\theta_0)$ . A natural question is whether for any  $t \in [0, \bar{t}]$  we will have then that  $\Sigma_0 + t\bar{X} \in \mathfrak{M}(\theta_0)$ . In that respect we have the following useful result.

**PROPOSITION 2.3.** *For the ML and GLS discrepancy functions, with fixed weight matrix  $W$  in the GLS case, the set  $\mathfrak{M}(\theta_0)$  is convex and closed.*

*Proof.* By the definition and because of (2.1), the set  $\mathfrak{M}(\theta_0)$  is given by the intersection of the set  $\{X : \Sigma_0 + X \succeq 0\}$  and the set  $\bigcap_{\Sigma \in \mathfrak{S}} \mathfrak{X}_\Sigma$ , where

$$\mathfrak{X}_\Sigma = \{X : F(\Sigma_0 + X, \Sigma_0) \leq F(\Sigma_0 + X, \Sigma)\}. \quad (2.12)$$

The set  $\{X : \Sigma_0 + X \succeq 0\}$  is convex and closed, so we only need to verify convexity and closedness of the set  $\mathfrak{X}_\Sigma$  for every  $\Sigma \in \mathfrak{S}$ . For the *ML* discrepancy function the set  $\mathfrak{X}_\Sigma$  is given by matrices  $X \in \mathcal{S}^{p \times p}$  satisfying

$$\ln |\Sigma_0| - \ln |\Sigma_0 + X| + \text{Tr}[(\Sigma_0 + X)\Sigma_0^{-1}] \leq \ln |\Sigma| - \ln |\Sigma_0 + X| + \text{Tr}[(\Sigma_0 + X)\Sigma^{-1}]. \quad (2.13)$$

The inequality (2.13) can be written in the following equivalent form

$$\text{Tr}[(\Sigma_0 + X)(\Sigma_0^{-1} - \Sigma^{-1})] \leq \ln |\Sigma| - \ln |\Sigma_0|. \quad (2.14)$$

The above inequality (2.14) defines a convex closed set (half space) in the space of symmetric matrices  $X$ . The intersection of these half spaces is also a convex closed set. This shows that for the *ML* discrepancy function the set  $\mathfrak{M}(\theta_0)$  is convex and closed.

Similar arguments can be applied to the *GLS* discrepancy function with fixed weight matrix, by noting that in this case the corresponding set defined in (2.12) is given by the half space

$$\text{Tr}[X(W\Sigma W - W\Sigma_0 W)] \leq \frac{1}{2} \text{Tr}[(\Sigma W)^2 - (\Sigma_0 W)^2]. \quad (2.15)$$

This completes the proof.  $\square$

Clearly the null matrix belongs to the set  $\mathfrak{M}(\theta_0)$ , and hence by the above proposition we have the following.

**COROLLARY 2.4.** *For the ML and GLS discrepancy functions, with fixed weight matrix  $W$  in the GLS case, the following holds: (i) for any matrix  $X \in \mathcal{S}^{p \times p}$  the set of  $t \geq 0$  such that  $tX \in \mathfrak{M}(\theta_0)$  is a closed convex interval, (ii) if  $\bar{X} \in \mathfrak{M}(\theta_0)$ , then  $t\bar{X} \in \mathfrak{M}(\theta_0)$  for any  $t \in [0, 1]$ .*

For a given matrix  $X \in \mathcal{S}^{p \times p}$ , satisfying the first order necessary conditions, consider the rescaling procedure, i.e., consider the discrepancy value

$$\delta(t) = F(\Sigma_0 + tX, \Sigma_0) \quad (2.16)$$

as a function of the parameter  $t \geq 0$ . For the GLS discrepancy function with fixed weight matrix  $W$  and  $X \neq 0$ , we have that  $\delta(t) = \frac{1}{2}t^2 \text{Tr}[(XW)^2]$  is a monotonically increasing for  $t \geq 0$  quadratic function. For the ML discrepancy function, the function  $\delta(t)$  is also monotonically increasing for  $t \geq 0$ . This follows from the following calculation of its derivative

$$\begin{aligned} \frac{d\delta(t)}{dt} &= \text{Tr} [X(\Sigma_0^{-1} - (\Sigma_0 + tX)^{-1})] \\ &= \text{Tr} [X(\Sigma_0 + tX)^{-1}(\Sigma_0 + tX - \Sigma_0)\Sigma_0^{-1}] \\ &= t \text{Tr} [X\Sigma_0^{-1}X(\Sigma_0 + tX)^{-1}], \end{aligned} \quad (2.17)$$

which is positive as long as matrix  $\Sigma_0 + tX$  is positive definite.

In the following subsections we will discuss in details the optimization problem (2.11) for the GLS and ML discrepancy functions.

**2.1. GLS Discrepancy Function.** Consider the GLS discrepancy function (1.3). We can write

$$F_{GLS}(s, \sigma) = \frac{1}{2}(s - \sigma)^T Q (s - \sigma), \quad (2.18)$$

where  $Q = W \otimes W$ . We discuss first the case when  $W$  is fixed (independent of  $S$ ). The corresponding problem (2.11) takes the form

$$\begin{aligned} \text{Max}_{X \in \mathcal{S}^{p \times p}} \quad & \frac{1}{2} \text{Tr}\{[XW]^2\} \\ \text{s.t.} \quad & \Delta^T Q x = 0, H_{GLS}(x) \succeq 0, \Sigma_0 + X \succeq 0, \end{aligned} \quad (2.19)$$

where

$$H_{GLS}(x) = \frac{\partial^2 F_{GLS}(\sigma_0 + x, \sigma(\theta))}{\partial \theta \partial \theta^T} \Big|_{\theta = \theta_0}.$$

We denote by  $\mathcal{X}$  the feasible set of the above problem (2.19).

Note that  $\mathcal{X}$  is a subset of the set  $\mathfrak{F}(\Sigma_0)$ , defined in (2.9), and hence is bounded, provided that the condition (ii) of Proposition 2.2 holds. Since  $x = 0$  satisfies the constraints of problem (2.19), the feasible set  $\mathcal{X}$  is nonempty. Moreover, for  $x = 0$  the Hessian matrix  $H_{GLS}(0) = \Delta^T Q \Delta$  is positive definite, provided that  $\Delta$  has full column rank  $q$ , and since  $\Sigma_0$  is also positive definite, it follows by continuity arguments that  $H_{GLS}(x) \succeq 0$  and  $\Sigma_0 + X \succeq 0$  for points  $x$  sufficiently close to 0. Consequently, the feasible set  $\mathcal{X}$  contains all points  $x$  sufficiently close to 0 satisfying equations  $\Delta^T Q x = 0$ .

By using the second order Taylor expansion of  $\sigma(\theta)$ , at  $\theta = \theta_0$ , it is not difficult to see that the Hessian matrix  $H_{GLS}(x)$  has the form

$$H_{GLS}(x) = H_{GLS}(0) - \mathcal{A}(X), \quad (2.20)$$

where  $\mathcal{A}$  is a linear operator from  $\mathcal{S}^{p \times p}$  to  $\mathcal{S}^{q \times q}$ . This linear operator depends on  $Q$  and second order partial derivatives of  $\sigma(\theta)$ , at  $\theta_0$ , and can be written in various forms (we will discuss this later). We will discuss below calculation of  $H_{GLS}(x)$  for the factor analysis model. It is worthwhile to note at this point that it follows from (2.20) that  $H_{GLS}(x)$  is an affine function of  $x$ . Therefore, the feasible set  $\mathcal{X}$  is defined by linear equations and two positive semidefinite (psd) affine constraints, and hence is convex. The objective function of problem (2.19) is convex quadratic, and hence (2.19) is a problem of maximization of a convex function over a convex set. Unfortunately, it is difficult to solve such problems to global optimality, we will discuss this later.

*Numerical procedure.* In order to solve optimization problem (2.19) numerically we use the following approach. Consider the objective function  $f(x) = \frac{1}{2} \text{Tr}\{[XW]^2\}$  and the feasible set  $\mathcal{X}$  of this problem. Starting with a feasible point  $x_0 \in \mathcal{X}$ , at a current iteration  $x_k \in \mathcal{X}$  we calculate next iteration  $x_{k+1}$  as the optimal solution of the linearized problem

$$\text{Max}_{x \in \mathcal{X}} g_k^T x \text{ subject to } x \in \mathcal{X}, \quad (2.21)$$

where  $g_k = \partial f(x_k)/\partial x$ . Since function  $f(x)$  is convex, we have that

$$f(x) \geq f(x_k) + g_k^T(x - x_k), \quad \forall x \in \mathcal{X},$$

and hence  $f(x_{k+1}) \geq f(x_k)$ . We continue this process until its convergence, i.e., until the objective value  $f(x_k)$  is stabilized. Generally this procedure converges to a *local* optima of the problem (2.19). Therefore it is an important practical question of how to choose a starting point of this procedure, we will discuss this later.

The linearized problem (2.21) is a (linear) semidefinite programming (SDP) problem and can be solved efficiently. We use here Matlab solver ‘*mincx*’ which handles Linear Matrix Inequality (LMI) optimization problems. This solver implements Nesterov - Nemirovski’s Projective Method [6, 8]. Note that here  $df(x) = \text{Tr}[WXW(dX)]$ , and hence the corresponding linearization is

$$g_k^T x = \text{Tr}[WX_kWX]. \quad (2.22)$$

**Example.** [Factor Analysis] Consider the factor analysis model (1.4). We can write

$$(\Lambda + d\Lambda)(\Lambda + d\Lambda)^T + \Psi + d\Psi = \Lambda\Lambda^T + \Psi + (d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + d\Psi + (d\Lambda)(d\Lambda)^T, \quad (2.23)$$

where  $d\Lambda$  and  $d\Psi$  are “small” perturbations of  $\Lambda$  and  $\Psi$ , respectively. Therefore in the present case the first order necessary optimality conditions take the form (for the sake of notational convenience we omit the subscript in  $\Lambda_0$  and  $\Psi_0$ ):

$$\text{Tr}[WXW(d\Psi)] = 0, \quad \forall d\Psi, \quad (2.24)$$

$$\text{Tr}[(d\Lambda)^T W X W \Lambda] = 0, \quad \forall d\Lambda. \quad (2.25)$$

Condition (2.24) means that all diagonal elements of matrix  $WXW$  are zeros. Condition (2.25) means that elements of matrix  $WXW\Lambda$  are zeros. This can be written as equations

$$XW\Lambda = 0. \quad (2.26)$$

In order to calculate the corresponding Hessian matrix  $H_{GLS}(x)$  we proceed as follows

$$\begin{aligned}
& F_{GLS}(\Sigma_0 + X, \Sigma_0 + (d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + d\Psi + (d\Lambda)(d\Lambda)^T) = \\
& \frac{1}{2}\text{Tr}\{[(d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + d\Psi + (d\Lambda)(d\Lambda)^T - X]W\}^2 = \\
& \frac{1}{2}\text{Tr}\{[(d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + d\Psi]W\}^2 + \frac{1}{2}\text{Tr}\{[(d\Lambda)(d\Lambda)^T - X]W\}^2 \\
& + \text{Tr}\{[(d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + d\Psi]W[(d\Lambda)(d\Lambda)^T - X]W\} \\
& = F_{GLS}(\Sigma_0 + X, \Sigma_0) - \text{Tr}[(d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + (d\Psi)]W X W \\
& + \frac{1}{2}\text{Tr}\{[(d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + (d\Psi)]W\}^2 - \text{Tr}\{(d\Lambda)(d\Lambda)^T W X W\} \\
& + o(\|(d\Lambda, d\Psi)\|^2).
\end{aligned} \tag{2.27}$$

The term

$$-\text{Tr}[(d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + (d\Psi)]W X W = -\text{Tr}[2(d\Lambda)^T W X W \Lambda + (d\Psi)W X W]$$

is the first order term in the corresponding Taylor expansion. The second order term is

$$\begin{aligned}
& \frac{1}{2}\text{Tr}\{[(d\Lambda)\Lambda^T W + \Lambda(d\Lambda)^T W + (d\Psi)W]^2 - 2(d\Lambda)(d\Lambda)^T W X W\} = \\
& \text{Tr}\{[(d\Lambda)\Lambda^T W(d\Lambda)\Lambda^T W + (d\Lambda)\Lambda^T W \Lambda(d\Lambda)^T W] + \frac{1}{2}(d\Psi)W(d\Psi)W \\
& + 2(d\Lambda)\Lambda^T W(d\Psi)W - (d\Lambda)^T W X W(d\Lambda)\}.
\end{aligned} \tag{2.28}$$

Note that, as it was mentioned before, the Hessian matrix  $H_{GLS}(x)$  is an affine function of  $x$ .

For  $x = 0$  and  $k = 1$  the Hessian matrix  $H_{GLS}(0)$  can be calculated as follows. It is two times the  $2p \times 2p$  block matrix  $\begin{bmatrix} A & B \\ B^T & D \end{bmatrix}$ , with corresponding components

$$\begin{aligned}
a_{ij} &= (\Lambda^T W e_j)(\Lambda^T W e_i) + (\Lambda^T W \Lambda)(e_j^T W e_i), \quad i, j = 1, \dots, p, \\
b_{ij} &= \Lambda^T W D_j W e_i, \quad i, j = 1, \dots, p, \\
d_{ij} &= \frac{1}{2}\text{Tr}\{D_i W D_j W\}, \quad i, j = 1, \dots, p.
\end{aligned} \tag{2.29}$$

Consider the optimization problem (2.19). For  $k = 1$  this problem can be written as

$$\begin{aligned}
& \text{Max}_{X \in \mathcal{S}^{p \times p}} \quad \frac{1}{2}\text{Tr}\{X W X W\} \\
& \text{s.t.} \quad \text{diag}(W X W) = 0, \quad X W \Lambda = 0, \\
& \quad \quad W X W \preceq C, \quad \Sigma_0 + X \succeq 0,
\end{aligned} \tag{2.30}$$

where  $C = A - B D^{-1} B^T$ . Note that  $W X W \preceq C$  is equivalent to  $X \preceq W^{-1} C W^{-1}$ . Note also that constraints  $X \preceq W^{-1} C W^{-1}$  and  $\Sigma_0 + X \succeq 0$  define a convex compact set. Also constraints  $\text{diag}(W X W) = 0$  and  $\Sigma_0 + X \succeq 0$  define a convex compact set (see Proposition 2.2). It follows that problem (2.30) has a nonempty compact (and convex) feasible set, and hence its optimal value is finite and it possesses an optimal solution.

Consider now the case of  $W = S^{-1}$ . In that case the weight matrix is a function of  $S$  and the analysis is more involved. Then problem (2.30) can be written as

$$\begin{aligned}
& \text{Max}_{X \in \mathcal{S}^{p \times p}} \quad \frac{1}{2}\text{Tr}\{X(\Sigma_0 + X)^{-1} X(\Sigma_0 + X)^{-1}\} \\
& \text{s.t.} \quad \text{diag}((\Sigma_0 + X)^{-1} X(\Sigma_0 + X)^{-1}) = 0, \quad X(\Sigma_0 + X)^{-1} \Lambda = 0, \\
& \quad \quad (\Sigma_0 + X)^{-1} X(\Sigma_0 + X)^{-1} \preceq C, \quad \Sigma_0 + X \succ 0.
\end{aligned} \tag{2.31}$$

Note that matrix  $S = \Sigma_0 + X$  should be nonsingular and hence the constraint  $\Sigma_0 + X \succeq 0$  in the above problem is replaced by  $\Sigma_0 + X \succ 0$ . It could be also noted that constraints of the above problem (2.31) are no longer linear in  $X$ . This makes it inconvenient for application of the standard LMI solver. In order to resolve this problem we make the following transformations.

Consider matrices  $Z = \Sigma_0^{-1/2} X \Sigma_0^{-1/2}$  and  $\bar{C} = \Sigma_0^{1/2} C \Sigma_0^{1/2}$ . By substituting  $X = \Sigma_0^{1/2} Z \Sigma_0^{1/2}$  into problem (2.31) we can formulate this problem in terms of  $Z$  as

$$\begin{aligned} \text{Max}_{Z \in \mathcal{S}^{p \times p}} \quad & \frac{1}{2} \text{Tr}\{(I + Z)^{-2} Z^2\} \\ \text{s.t.} \quad & \text{diag}\{\Sigma_0^{-1/2}(I + Z)^{-2} Z \Sigma_0^{-1/2}\} = 0, (I + Z)^{-2} Z \Sigma_0^{-1/2} \Lambda = 0, \\ & (I + Z)^{-2} Z \preceq \bar{C}, I + Z \succ 0. \end{aligned} \quad (2.32)$$

We used here the property that matrices  $Z$  and  $(I + Z)^{-1}$  commute, i.e.,  $Z(I + Z)^{-1} = (I + Z)^{-1}Z$ , which in particular implies that  $(I + Z)^{-2}Z = (I + Z)^{-1}Z(I + Z)^{-1}$  and hence this is a symmetric matrix.

Next define  $Y = (I + Z)^{-2}Z$ . As it was mentioned above,  $Y = (I + Z)^{-1}Z(I + Z)^{-1}$  and  $Y$  is a symmetric matrix. Moreover,

$$Z = 2 \left[ I + (I - 4Y)^{1/2} \right]^{-1} - I, \quad (2.33)$$

provided that  $I - 4Y \succeq 0$ . Substituting this into the objective function of problem (2.32) we obtain the following function

$$\frac{1}{2} \text{Tr} \left\{ 2Y \left[ I + (I - 4Y)^{1/2} \right]^{-1} - Y \right\} = \frac{1}{4} \text{Tr} \left\{ I - 2Y - (I - 4Y)^{1/2} \right\},$$

and hence problem (2.32) takes the form (up to the factor 1/4)

$$\begin{aligned} \text{Max}_{Y \in \mathcal{S}^{p \times p}} \quad & \text{Tr} \{ I - 2Y - (I - 4Y)^{1/2} \} \\ \text{s.t.} \quad & \text{diag}(\Sigma_0^{-\frac{1}{2}} Y \Sigma_0^{-\frac{1}{2}}) = 0, Y \Sigma_0^{-\frac{1}{2}} \Lambda = 0, \\ & Y \preceq \bar{C}, Y \preceq \frac{1}{4} I. \end{aligned} \quad (2.34)$$

Note that constraints of problem (2.34) are linear in  $Y$  and the objective function is convex. Linearization of the objective function of the above problem at a current iteration point  $Y_k$  is given by

$$2 \text{Tr} \{ -Y + (I - 4Y_k)^{-1/2} Y \}. \quad (2.35)$$

□

**2.2. ML Discrepancy Function .** Consider the *ML* discrepancy function (1.2). The relevant first and second order differentials here can be written as follows

$$d \ln |\Sigma| = \text{Tr} [\Sigma^{-1} (d\Sigma)] \quad \text{and} \quad d^2 \ln |\Sigma| = -\text{Tr} [\Sigma^{-1} (d\Sigma) \Sigma^{-1} (d\Sigma)],$$

$$d \text{Tr} [S \Sigma^{-1}] = -\text{Tr} [S \Sigma^{-1} (d\Sigma) \Sigma^{-1}] \quad \text{and} \quad d^2 \text{Tr} [S \Sigma^{-1}] = 2 \text{Tr} [\Sigma^{-1} S \Sigma^{-1} (d\Sigma) \Sigma^{-1} (d\Sigma)],$$

and hence

$$dF_{ML}(S, \Sigma) = \text{Tr} [\Sigma^{-1} (\Sigma - S) \Sigma^{-1} (d\Sigma)], \quad (2.36)$$

$$d^2 F_{ML}(S, \Sigma) = \text{Tr}[\Sigma^{-1}(2S - \Sigma)\Sigma^{-1}(d\Sigma)\Sigma^{-1}(d\Sigma)]. \quad (2.37)$$

It follows from (2.36), as it was mentioned before, that the first order necessary optimality conditions here take the form of linear equations  $\Delta^T Qx = 0$ , with  $Q = \Sigma_0^{-1} \otimes \Sigma_0^{-1}$ . These equations are the same as the respective equations for the GLS discrepancy function with  $W = \Sigma_0^{-1}$  (cf., [4, p.359]). In order to calculate the corresponding Hessian matrix  $H_{ML}(x)$  we can employ formulas (2.36) and (2.37). Note that for  $S = \Sigma$  we have that  $dF_{ML}(S, \Sigma) = 0$  and

$$d^2 F_{ML}(S, \Sigma) = \text{Tr}[\Sigma^{-1}(d\Sigma)\Sigma^{-1}(d\Sigma)] = d^2 F_{GLS}(S, \Sigma). \quad (2.38)$$

It follows that  $H_{ML}(0)$  coincides with  $H_{GLS}(0)$  for  $W = \Sigma_0^{-1}$ . For  $x \neq 0$  the Hessian matrices  $H_{ML}(x)$  are  $H_{GLS}(x)$  are different. Let us show how to calculate  $H_{ML}(x)$  at the example of the factor analysis model.

**Example.** [Factor Analysis] Consider the factor analysis model (1.4). Similar to (2.27), in order to calculate  $H_{ML}(x)$  we need to collect second order terms by substituting

$$d\Sigma = (d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + d\Psi + (d\Lambda)(d\Lambda)^T$$

into the expansion

$$\begin{aligned} & \frac{1}{2} \text{Tr} [2\Sigma^{-1}X\Sigma^{-1}(d\Sigma) + \Sigma^{-1}(\Sigma + 2X)\Sigma^{-1}(d\Sigma)\Sigma^{-1}(d\Sigma)] \\ &= \frac{1}{2} \text{Tr} [\Sigma^{-1}(d\Sigma)\Sigma^{-1}(d\Sigma) + 2\Sigma^{-1}X\Sigma^{-1}(d\Sigma) + 2\Sigma^{-1}X\Sigma^{-1}(d\Sigma)\Sigma^{-1}(d\Sigma)] \end{aligned} \quad (2.39)$$

(for the sake of notational convenience we omit the subscript 0 here).

Recall that for  $x = 0$  the Hessian matrix  $H_{ML}(0)$  coincides with the Hessian matrix  $H_{GLS}(0)$  for the GLS discrepancy function with  $W = \Sigma^{-1}$ , and components of  $H_{GLS}(0)$  are given by formulas (2.29). Moreover,  $H_{ML}(x) = H_{ML}(0) + \mathcal{A}(X)$ , where the linear term  $\mathcal{A}(X)$  can be calculate from the expansion

$$\begin{aligned} & \text{Tr} [(d\Lambda)^T \Sigma^{-1} X \Sigma^{-1} (d\Lambda)] + \\ & \text{Tr} [\Sigma^{-1} X \Sigma^{-1} ((d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + d\Psi)\Sigma^{-1} ((d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T + d\Psi)]. \end{aligned} \quad (2.40)$$

For  $k = 1$ , when  $\Lambda$  is  $p \times 1$  column vector, this expansion takes the form

$$\begin{aligned} & (d\Lambda)^T \Sigma^{-1} X \Sigma^{-1} (d\Lambda) \\ & + \Lambda^T \Sigma^{-1} X \Sigma^{-1} (d\Lambda)\Lambda^T \Sigma^{-1} (d\Lambda) + (d\Lambda)^T \Sigma^{-1} X \Sigma^{-1} (d\Lambda)\Lambda^T \Sigma^{-1} \Lambda \\ & + \Lambda^T \Sigma^{-1} X \Sigma^{-1} \Lambda (d\Lambda)^T \Sigma^{-1} (d\Lambda) + (d\Lambda)^T \Sigma^{-1} X \Sigma^{-1} \Lambda (d\Lambda)^T \Sigma^{-1} \Lambda \\ & + 2\text{Tr} [\Sigma^{-1} X \Sigma^{-1} ((d\Lambda)\Lambda^T + \Lambda(d\Lambda)^T)\Sigma^{-1} (d\Psi)] \\ & + \text{Tr} [\Sigma^{-1} X \Sigma^{-1} (d\Psi)\Sigma^{-1} (d\Psi)]. \end{aligned} \quad (2.41)$$

In that case the operator  $\mathcal{A}$  maps  $X \in \mathcal{S}^{p \times p}$  into  $2p \times 2p$  symmetric matrix with blocks

$$\begin{aligned} [\mathcal{A}_{11}(X)]_{ij} &= \Lambda^T \Sigma^{-1} X \Sigma^{-1} e_i \Lambda^T \Sigma^{-1} e_j + e_i^T \Sigma^{-1} X \Sigma^{-1} e_j \Lambda^T \Sigma^{-1} \Lambda \\ & \quad + \Lambda^T \Sigma^{-1} X \Sigma^{-1} \Lambda e_i^T \Sigma^{-1} e_j + e_i^T \Sigma^{-1} X \Sigma^{-1} \Lambda e_j^T \Sigma^{-1} \Lambda \\ & \quad + e_i^T \Sigma^{-1} X \Sigma^{-1} e_j, \quad i, j = 1, \dots, p, \end{aligned} \quad (2.42)$$

$$[\mathcal{A}_{12}(X)]_{ij} = \text{Tr}[\Sigma^{-1} X \Sigma^{-1} (e_i \Lambda^T + \Lambda e_i^T)\Sigma^{-1} D_j], \quad i, j = 1, \dots, p, \quad (2.43)$$

$$[\mathcal{A}_{22}(X)]_{ij} = \text{Tr}[\Sigma^{-1} X \Sigma^{-1} D_i \Sigma^{-1} D_j], \quad i, j = 1, \dots, p. \quad (2.44)$$

□

TABLE 3.1  
Generated Parameters

$\Lambda_0$						
$\lambda_1$	$\lambda_2$	$\lambda_3$	$\lambda_4$	$\lambda_5$	$\lambda_6$	$\lambda_7$
0.6916	1.2404	0.7971	0.9011	0.5761	1.5620	0.8117
$\Psi_0$						
$\psi_1$	$\psi_2$	$\psi_3$	$\psi_4$	$\psi_5$	$\psi_6$	$\psi_7$
0.8727	0.6480	1.0672	1.0614	3.0594	1.8551	1.3567

TABLE 3.2  
Generated covariance matrix  $\Sigma_0$

	$\Sigma_0$						
$X_1$	1.3510						
$X_2$	0.8579	2.1866					
$X_3$	0.5513	0.9887	1.7026				
$X_4$	0.6232	1.1177	0.7183	1.8734			
$X_5$	0.3984	0.7146	0.4592	0.5191	3.3913		
$X_6$	1.0803	1.9375	1.2451	1.4075	0.8999	4.2949	
$X_7$	0.5614	1.0068	0.6470	0.7314	0.4676	1.2679	2.0156

Similar to (2.30), optimization problem for  $k = 1$  can be written as

$$\begin{aligned}
& \max_{X \in \mathcal{S}^{p \times p}} \quad \text{Tr}\{\Sigma_0^{-1}(\Sigma_0 + X)\} - \ln |\Sigma_0 + X| \\
& \text{s.t.} \quad \text{diag}(\Sigma_0^{-1}X\Sigma_0^{-1}) = 0, \quad X\Sigma_0^{-1}\Lambda = 0, \\
& \quad \quad H_{ML}(x) \succeq 0, \quad \Sigma_0 + X \succeq 0.
\end{aligned} \tag{2.45}$$

Note that also here the objective function is convex in  $x$ . Also linearization of the objective function of (2.45) at a current iteration  $X_k$  is given by

$$\text{Tr}\{[\Sigma_0^{-1} - (\Sigma_0 + X_k)^{-1}]X\}. \tag{2.46}$$

**3. Numerical illustrations.** In this section we report results of some numerical experiments with the suggested method, and in particular compare it with the Cudeck - Browne [4] approach. We have considered one-factor analysis model for the simulated covariance matrix. Specified parameters (of vector  $\Lambda_0$  and diagonal elements of matrix  $\Psi_0$ ) are shown in Table 3.1. The corresponding covariance matrix  $\Sigma_0 = \Lambda_0\Lambda_0^T + \Psi_0$  is given in Table 3.2. Experiments are conducted for the *GLS* and *ML* discrepancy functions.

**3.1. GLS Discrepancy Function .** Consider optimization problems (2.30) and (2.34). Let us refer to the respective procedure as 1st and 2nd order method (1st-2nd), and without 2nd order constraints,  $WXW \preceq C$  in (2.30) and  $Y \preceq \bar{C}$  in (2.34), as 1st order method (1st). Also, we refer to the Cudeck - Browne method as the CB procedure. The comparison of numerical results for these three methods is given in Table 3.3. In that table  $\delta$  denotes maximal value of the respective objective function. For the corresponding optimal solution  $\bar{X}$  we apply the rescaling procedure of replacing  $\bar{X}$  with  $t\bar{X}$ ,  $t > 0$ , such that we can recover the specified parameters exactly when factor analysis is applied to the matrix  $S = \Sigma_0 + t\bar{X}$ . The largest discrepancy value, obtained by this rescaling procedure, is denoted by  $\bar{\delta}$ . We tried different starting

TABLE 3.3  
*GLS discrepancy function value comparison*

Method	$W = I$			$W = S^{-1}$		
	1st-2nd	1st	CB	1st-2nd	1st	CB
$\delta$	18.7906	26.7425	0.0331	0.7922	0.7921	0.2354
Rescale factor ( $t$ )	0.9	0.65	5.5	1	1	1
$\bar{\delta}$	15.2200	11.2990	1.0025	0.7921	0.7921	0.2354

TABLE 3.4  
*ML discrepancy function value comparison*

Method	1st-2nd	1st	CB
$\delta$	1.6541	127.4199	3.0709
Rescale factor ( $t$ )	0.9	0.35	0.45
$\bar{\delta}$	1.3601	0.8638	0.3523

points in the iterative procedure of the form (2.21). From numerical experiments it seems that taking  $x_0 = 0$  is a reasonably good choice of the starting point.

The CB procedure was performed 5 times, for randomly generated perturbations satisfying first order optimality conditions, and the obtained largest discrepancy value is reported in the table. As we can see, the discrepancy function values by 1st-2nd and 1st methods are considerably bigger than the ones obtained by the CB procedure. These results illustrate the utility of these methods for constructing a covariance matrix with a large discrepancy function value.

**3.2. ML Discrepancy Function .** Similar experiments are conducted for the ML discrepancy function. Here the 1st and 2nd order method (1st-2nd) is the procedure to solve the problem (2.45). The 1st order method leaves out 2nd order constraint  $H_{ML}(x) \succeq 0$ . Table 3.4 compares discrepancy function values from three methods. Both the 1st-2nd and 1st methods show an improvement in the computed discrepancy values.

**4. Discussion.** A procedure has been developed for generation of a covariance matrix that has a given discrepancy with the hypothesized model. With this method, the population covariance matrix is constructed as the sum of a matrix satisfying the specified model and a perturbation matrix that satisfies the model discrepancy and first and second order optimality conditions. Computational results indicate that the developed method can give a significant improvement in the range of discrepancy values as compared with the Cudeck - Browne procedure. This method can be a useful tool for Monte Carlo studies examining performance under model misspecification when a given structure model does not hold exactly. Also, this may be of some practical assistance to researchers facing the model evaluation and alternative generation problem so that they can derive reasonable inferences. Additional issue, that may well merit further investigation, involves the behavior of estimators relative to the degree of model misspecification and general cut-off value of the test statistics for model evaluation.

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