

# Maximum Likelihood Dynamic Factor Modeling for Arbitrary $N$ and $T$ Using SEM

Manuel C. Voelkle

*Max Planck Institute for Human Development*

Johan H. L. Oud

*Radboud University*

Timo von Oertzen and Ulman Lindenberger

*Max Planck Institute for Human Development*

This article has 3 objectives that build on each other. First, we demonstrate how to obtain maximum likelihood estimates for dynamic factor models (the direct autoregressive factor score model) with arbitrary  $T$  and  $N$  by means of structural equation modeling (SEM) and compare the approach to existing methods. Second, we go beyond standard time series analysis ( $T$  large and  $N = 1$ ) and conventional SEM ( $N$  large and  $T = 1$  or small) by integrating both approaches. The resulting combined model offers a variety of new modeling options including a direct test of the ergodicity hypothesis, according to which the factorial structure of an individual observed at many time points is identical to the factorial structure of a group of individuals observed at a single point in time. Third, we illustrate the flexibility of SEM time series modeling by extending the approach to account for complex error structures. We end with a discussion of current limitations and future applications of SEM-based time series modeling for arbitrary  $T$  and  $N$ .

*Keywords:* dynamic factor analysis, factorial invariance, maximum likelihood estimation, time series analysis

Structural equation models have a long history in the social sciences and related disciplines and are well established in present-day research. Since their earliest use almost a century ago (Wright, 1920), structural equation modeling (SEM) has been extended in various ways, making it a powerful and highly general data analytic approach (cf. Muthén, 2002). The vast majority of research using SEM has focused on the variation among individuals. This applies equally to cross-sectional studies (e.g., confirmatory factor analysis) and longitudinal studies (e.g., latent growth curve models). A typical example of such a between-person structural equation model for  $N$  independent individuals with  $p = 2$  orthogonal factors and  $q = 6$  indicators, along with

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Correspondence should be addressed to Manuel C. Voelkle, Max Planck Institute for Human Development, Lentzeallee 94, 14195 Berlin, Germany. E-mail: voelkle@mpib-berlin.mpg.de

an illustration of its raw data structure, is provided in the left part of Figure 1. We return to Figure 1 later on.

However, some researchers have also used SEM to study variation within a single individual (cf. Molenaar, 2004; Molenaar & Campbell, 2009). P-technique factor analysis was one of the earliest attempts to apply factor analysis to the repeated measurements of a single case (Cattell, Cattell, & Rhymer, 1947; Cattell, 1963). Molenaar and Nesselroade (2009), Luborsky and Mintz (1972), Nesselroade and Ford (1985b), and Jones and Nesselroade (1990) provide overviews of P-technique and its contributions to the advancement of the study of intraindividual variability. Despite its popularity, P-technique has been criticized early on, primarily because it fails to account for lagged relationships among the components of a multivariate time series (Anderson, 1963; Cattell, 1963; Molenaar, 1985). As a solution to this problem a number of procedures, generically referred to as dynamic factor analysis (DFA), have been proposed (Molenaar, 1985; Molenaar & Nesselroade, 2009). In contrast to P-technique, these procedures explicitly model lagged relations between factors, observed variables, or both. An example of a dynamic factor model for a single individual ( $N = 1$ ), along with an illustration of its raw data structure is shown in the right part of Figure 1.

Although most dynamic factor models can be expressed as special variants of the more general class of state-space models (e.g., Durbin & Koopman, 2001), different variants of DFA models are referred to by different names in the literature. Most important, Nesselroade, McArdle, Aggen, and Meyers (2002) distinguished between the *direct autoregressive factor score model* (Engle & Watson, 1981) and the *white noise factor score model* (Geweke & Singleton, 1981; see also Browne & Nesselroade, 2005; Molenaar, 1985). The exact definition of the direct autoregressive factor score model, which is used in this article, is provided later.

Along with alternative versions of dynamic factor models, a number of different estimation methods have been proposed. Most important, these are (a) the Kalman filter based on the state-space representation, (b) Bayesian approaches, and (c) approaches based on the block-Toeplitz covariance matrix, which is computed in a first step, before parameter estimates are obtained in a second step (e.g., via least squares, asymptotically distribution free, or “pseudo” maximum likelihood estimation; see Molenaar & Nesselroade, 1998; Zhang, Hamaker, & Nesselroade, 2008). In particular, block-Toeplitz matrices have been commonly used to fit SEM models to single time series. Unfortunately, however, this approach is associated with a number of difficulties (e.g., Hershberger, Molenaar, & Corneal, 1996). Most important, SEM assumes that the sample covariance matrix is computed from independent rows, an assumption that is violated in P-technique as well as in the construction of the block-Toeplitz covariance matrix for DFA. As a consequence, parameter estimates are no maximum likelihood (ML) estimates and their inferential properties (i.e., standard errors and likelihood) are unknown (cf. Oud, 2004). In contrast, the Kalman filter does not suffer from these problems and provides ML estimates. However, the Kalman filter does not operate in an SEM framework, which has certain advantages—but also disadvantages—as discussed later. For a recent comparison of SEM and state-space modeling techniques see Chow, Ho, Hamaker, and Dolan (2010; see also Oud & Singer, 2008). It has been shown that ML estimates can be obtained for individual autoregressive moving average (ARMA) models using SEM (Hamaker, Dolan, & Molenaar, 2003; Singer, 2010). However, so far SEM has not been used to obtain ML estimates for dynamic factor models with  $N = 1$ .

These observations lead to the first major objective of this article: to demonstrate how to obtain ML estimates for the direct autoregressive factor score model by means of SEM. We eval-

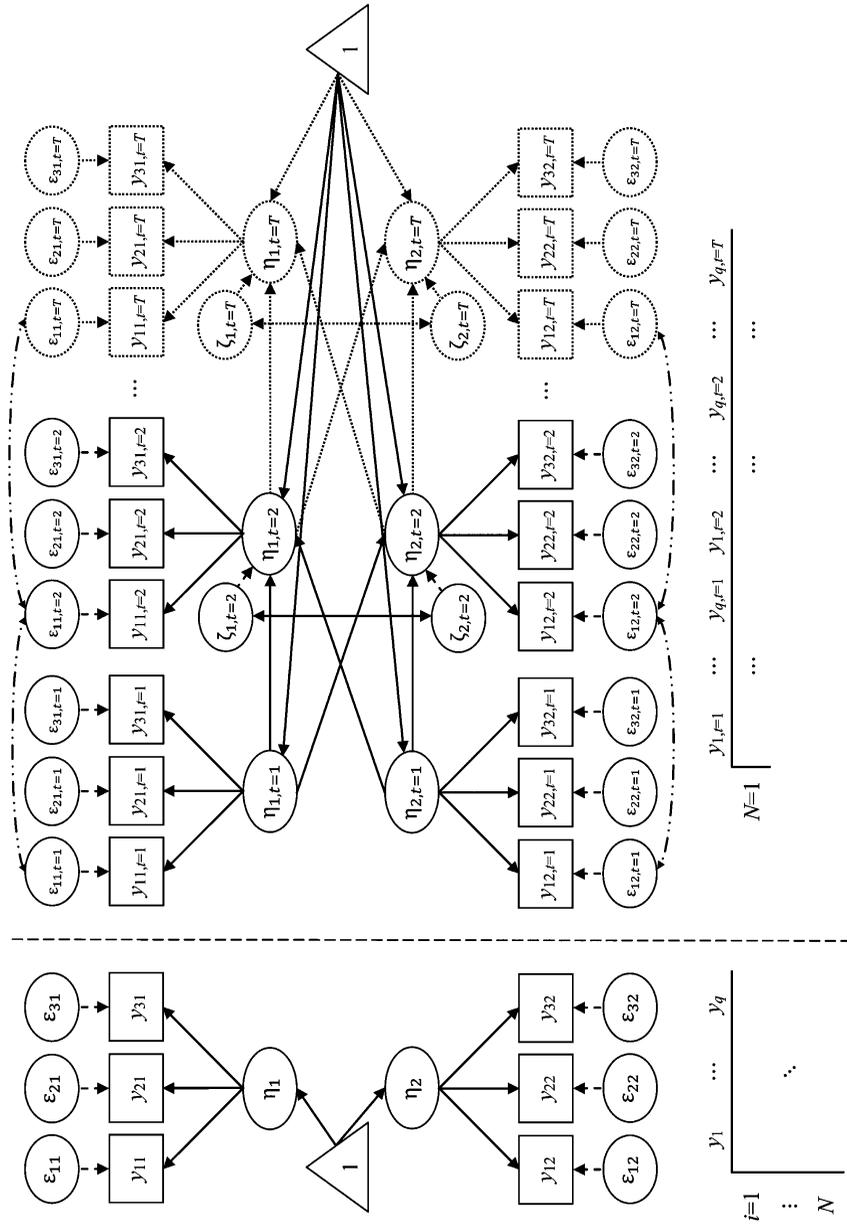


FIGURE 1 The left part shows an orthogonal two-factor model at a single point in time for  $N$  independent individuals. The right part shows a dynamic two-factor model for a single individual ( $N = 1$ ). The corresponding raw data structures are illustrated in the lower part. Both models can be estimated separately or jointly via maximum likelihood structural equation modeling. By constraining the parameters of the left model to equality with all relevant parameters of the right model, a direct likelihood ratio test can be carried out to test whether the factorial structure of an individual observed at many time points is identical to the factorial structure of a group of individuals observed at a single point in time. The four dash-pointed double-headed arrows illustrate the two measurement error covariances over time introduced in the last Monte Carlo simulation.

uate the performance of this new approach by comparing it to four estimation methods investigated by Zhang et al. (2008) in a recent simulation study. Apart from being yet another approach to estimate dynamic factor models, one advantage of this method is that it generalizes readily to any arbitrary sample size; that is, it allows a continuous shift from idiographic to nomothetic analysis. Furthermore, we demonstrate how multiple group analysis can be used to integrate individual time series analysis and conventional SEM based on between-subject variation. The combined model offers a variety of new modeling options, including a direct test of whether the factorial structure of an individual observed at many time points is identical to the factorial structure of a group of individuals observed at a single point in time. Another advantage of the new approach to time series modeling—referred to as ML-SEM in the following—is that it generalizes readily to account for complex error structures. This is illustrated by fitting a dynamic factor model to an individual time series with measurement errors that are correlated over time.

### MAXIMUM LIKELIHOOD STRUCTURAL EQUATION MODELING WITH ARBITRARY $T$ AND $N$

Different approaches to formulating structural equation models exist. Here, we make use of the RAM notation (McArdle, 2005; McArdle & McDonald, 1984). In contrast to other approaches (e.g., LISREL; Jöreskog, 1973), RAM makes use of the observation that three matrices are sufficient to completely define any structural equation model: one matrix  $\mathbf{A} \in \mathbf{R}^{(p+q) \times (p+q)}$  that contains all asymmetric (i.e., directional) effects, one matrix  $\mathbf{S} \in \mathbf{R}^{(p+q) \times (p+q)}$  that contains all symmetric relationships (i.e., variances and covariances) and one filter matrix  $\mathbf{F}$ , which is a fixed known matrix of order  $q \times (p + q)$  with prescribed unity and zero constants to filter out the manifest variables (i.e., separate observed from latent variables). As defined earlier,  $p$  represents the number of latent factors and  $q$  the number of observed variables.

For example, the correlated two-factor model with three indicators per factor as depicted on the left side of Figure 1 corresponds to

$$\mathbf{F} = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \lambda_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \lambda_{21} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \lambda_{31} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_{32} & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathbf{S} = \begin{bmatrix} \sigma_{\eta_1}^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sigma_{\eta_2}^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sigma_{\varepsilon_{11}}^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_{\varepsilon_{21}}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sigma_{\varepsilon_{31}}^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sigma_{\varepsilon_{12}}^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{\varepsilon_{22}}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma_{\varepsilon_{32}}^2 \end{bmatrix},$$

with  $\lambda$  representing the factor loadings,  $\sigma_{\varepsilon}^2$  the residual variances, and  $\sigma_{\eta}^2$  the variances of the latent factors  $\eta$ . To be identified, we need to fix the variances of the two factors to a prechosen value (here  $\sigma_{\eta_1}^2 = \sigma_{\eta_2}^2 = 1$ ) or constrain one of the factor loadings of each factor.

Having defined the three matrices  $\mathbf{F}$ ,  $\mathbf{A}$ , and  $\mathbf{S}$ , the  $q \times q$  model-implied covariance matrix  $\Sigma$  is generated by

$$\Sigma = \mathbf{F}(\mathbf{I} - \mathbf{A})^{-1}\mathbf{S}(\mathbf{I} - \mathbf{A})^{-1'}\mathbf{F}', \quad (1)$$

with  $\mathbf{I}$  being a  $(p + q) \times (p + q)$  identity matrix. To model means and intercepts, an additional vector  $\mathbf{M} \in \mathbf{R}^{(p+q) \times 1}$  is necessary that contains possible “effects” on any of the  $p + q$  variables in the model. In our example in Figure 1,  $\mathbf{M}' = [\mu_{\eta_1} \ \mu_{\eta_2} \ \mu_1 \ \cdots \ \mu_6] = [\mu_{\eta_1} \ \mu_{\eta_2} \ 0 \ \cdots \ 0]$ , with  $\mu$  representing the means, respectively intercepts. The according  $q \times 1$  model-implied mean vector  $\boldsymbol{\mu}$  is generated by

$$\boldsymbol{\mu} = \mathbf{F}(\mathbf{I} - \mathbf{A})^{-1}\mathbf{M}. \quad (2)$$

Let  $\mathbf{S}$  denote the  $q \times q$  observed covariance matrix and  $\mathbf{m}$  the  $q \times 1$  observed mean vector. Under the assumption of multivariate normality, a function of the likelihood of the data under the model is given in Equation 3. ML estimates are obtained by minimizing this function:

$$F_{ML} = \frac{1}{2}[\log |\Sigma| + \text{tr}(\mathbf{S}\Sigma^{-1}) - \log |\mathbf{S}| - q] + \frac{1}{2}[(\mathbf{m} - \boldsymbol{\mu})' \Sigma^{-1}(\mathbf{m} - \boldsymbol{\mu})]. \quad (3)$$

Note that Equation 3 assumes that  $\mathbf{S}$  and  $\Sigma$  are both positive-definite matrices. This assumption would be violated, for example, if one would try to compute the “covariance” matrix for observations obtained from a single individual by taking the outer product of the observed  $1 \times qT$  data vector to fit an individual time series of length  $T$ . Because the rank of the resulting  $qT \times qT$  matrix  $\mathbf{S}$  equals 1, it is singular and  $\log |\mathbf{S}|$  does not exist.<sup>1</sup> However, closer inspection of Equation 3 reveals that it is only a convenient, but common, simplification of the log-likelihood ( $LL$ ) function for a sample of  $i = 1, \dots, N$  independent individual observations on each of the  $q$  variables (see Bollen, 1989, pp. 133–134):

$$LL = \frac{-Nq}{2} \log(2\pi) - \frac{N}{2} \log |\Sigma| - \frac{1}{2} \sum_{i=1}^N (\mathbf{y}_i - \boldsymbol{\mu})' \Sigma^{-1} (\mathbf{y}_i - \boldsymbol{\mu}). \quad (4)$$

Allowing the number of variables to differ across individuals (i.e., allowing for missing data), the so-called *raw data maximum likelihood (RML) function* (or *full information maximum likelihood [FIML] function*) given in Equation 5 is a natural extension of Equation 4 (Hamaker et al., 2003; cf. Lange, Westlake, & Spence, 1976). Here the number of observed variables  $q_i$  can differ from person to person, resulting in a person-specific mean vector ( $\boldsymbol{\mu}_i$ ) and a

<sup>1</sup>More generally speaking,  $\mathbf{S}$  is singular; that is,  $\log |\mathbf{S}|$  cannot be computed, as long as the number of independent cases is smaller than the number of time points multiplied by the number of observed variables (i.e.,  $N < Tq$ ).

person-specific covariance matrix ( $\Sigma_i$ ):

$$RML = \sum_{i=1}^N [constant_i + \log |\Sigma_i| + (\mathbf{y}_i - \boldsymbol{\mu}_i)' \Sigma_i^{-1} (\mathbf{y}_i - \boldsymbol{\mu}_i)]. \quad (5)$$

This is the likelihood function employed by many SEM programs, including Mx (Neale, Boker, Xie, & Maes, 2003) and OpenMx (Boker, Neale, Maes, & Wilde, 2010), which is used for the analyses in this article. Note that instead of maximizing the *LL* as in Equation 4, the fitting functions in Equations 3 and 5 are minimized.

In contrast to Equation 3, however, Equations 4 and 5 no longer contain the log of the determinant of the sample covariance matrix  $\mathbf{S}$ . For a given sample,  $\log |\mathbf{S}|$  is a constant term and thus irrelevant for parameter estimation. It can therefore be dropped from the estimation function, as is done in Equations 4 and 5. Likewise, the first term in Equation 4 also represents just a constant and is therefore irrelevant for parameter estimation, as parameter estimates are independent of whether a constant is added or subtracted from the likelihood function. Given suitable identification, it now becomes possible to obtain ML estimates by using SEM for any arbitrary number of observations including  $N = 1$  (Hamaker et al., 2003; Singer, 2010). As a matter of fact, as demonstrated by Hamaker et al. (2003), the likelihood function is equivalent to the likelihood function used to estimate ARMA models as implemented, for example, in SPSS. The fact that there is no need for computing  $\log |\mathbf{S}|$ , however, is not widely acknowledged in the literature and is probably one of the main reasons why essentially no research exists on ML-SEM with  $N = 1$ .

Finally, multiple groups of cases can be estimated by maximizing (Equation 4)—or minimizing (Equations 3 and 5)—the sum of the weighted likelihood function over  $g = 1, \dots, G$  independent groups. As discussed in more detail later on, this permits users to impose parameter constraints within and across groups of individuals and conduct explicit tests of their plausibility.

#### MODELING THE INDIVIDUAL ( $N = 1$ ): AN ML-SEM APPROACH TO DYNAMIC FACTOR ANALYSIS

Suppose now we are interested in the factor structure of a single individual observed at  $t = 1, \dots, T$  time points as illustrated in the right part of Figure 1. The traditional approach (P-technique; Cattell et al., 1947) would be to transform the data set from a person-level format, where each of the  $q$  observed indicators is represented by  $T$  separate variables, into a person-period format with  $q$  columns and  $T$  rows, and apply the same analysis as in the between-person case with  $N$  rows and  $q$  columns. As described earlier, however, in this case the rows are no longer independent because of their relation in time. As a consequence, parameter estimates are not strict ML estimates, and their properties are unknown. In principle, the same argument applies to the use of block-Toeplitz covariance matrices for fitting dynamic factor models. Although the serial dependency is taken into better account, the resulting parameter estimates are not strict ML estimates (Molenaar & Nesselroade [1998] speak of pseudo, or p-ML, estimation). In contrast, raw ML of a full structural equation model does not suffer from these problems (cf. Hamaker et al., 2003, for ARMA models; Singer, 2010). Thus, we

conjectured that it is also possible to obtain ML-SEM estimates for dynamic factor models, like the direct autoregressive factor score model (Nesselroade et al., 2002). For this purpose we define the dynamic factor model as

$$\mathbf{A} = \begin{bmatrix} \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{B}_{t=1} & & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & & \mathbf{0} \\ & \ddots & & & & & & \vdots \\ \mathbf{0} & & \mathbf{B}_{t=T-1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & & \mathbf{0} \\ \mathbf{\Lambda}_{t=1} & & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & & \mathbf{0} \\ & \ddots & & & & & & \vdots \\ \mathbf{0} & & \mathbf{\Lambda}_{t=T-1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{\Lambda}_{t=T} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \end{bmatrix},$$

$$\mathbf{S} = \begin{bmatrix} \Phi_{t=1} & \mathbf{0} & & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \Psi_{t=2} & & \mathbf{0} & \mathbf{0} & & \mathbf{0} \\ & & \ddots & & & & \vdots \\ \mathbf{0} & \mathbf{0} & & \Psi_{t=T} & \mathbf{0} & & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & & \mathbf{0} & \Theta_{t=1} & & \mathbf{0} \\ \vdots & & & & & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & & \mathbf{0} & \mathbf{0} & & \Theta_{t=T} \end{bmatrix},$$

$$\mathbf{M}' = [\boldsymbol{\mu}'_{\eta,t=1} \quad \cdots \quad \boldsymbol{\mu}'_{\eta,t=T} \quad \boldsymbol{\mu}'_{y,t=1} \quad \cdots \quad \boldsymbol{\mu}'_{y,t=T}].$$

For a  $p$ -factor model with a total of  $q$  indicators observed at  $T$  time points, the  $\mathbf{A}$  matrix is now of the order  $(pT + qT) \times (pT + qT)$ , with the autoregressive coefficients contained in the upper left part, the factor loadings in the lower left part, and zeros everywhere else. The  $\mathbf{S}$  matrix is of the same order as the  $\mathbf{A}$  matrix. As shown earlier, the first  $p \times p$  elements of  $\mathbf{S}$  contain the initial covariances of the  $p$  factors ( $\Phi_{t=1}$ ), followed by the covariance matrices of the latent residuals ( $\Psi_t$ ) and the measurement error covariances ( $\Theta_t$ ) on the main diagonal. Assuming stationarity, the factor variances, or residual variances, are typically constrained to equality over time. Finally, the  $\mathbf{M}$  matrix is of the order  $(pT + qT) \times 1$ , with the first element  $\boldsymbol{\mu}'_{\eta,t=1}$  representing the means of the factors at time point  $t = 1$ , followed by the intercept vectors of the latent factors at  $t = 2, \dots, T$  and the  $qT$  intercept vectors of the indicators ( $\boldsymbol{\mu}'_y$ ). The latter two are usually constrained to equality over time. Choosing an appropriate mean vector of the factors at the first time point is of crucial importance for initializing the time series. The  $\mathbf{F}$  matrix is a selection matrix of the order  $qT \times (pT + qT)$  as defined before.

### Simulation 1: Comparing the ML-SEM Dynamic Factor Model to Existing Approaches

To evaluate the ML-SEM-based approach to dynamic factor modeling, in this section we compare the approach to the results of a recent Monte Carlo simulation by Zhang et al. (2008). In that study, the authors compared four different methods for estimating a dynamic factor

model, including (a) the Kalman filter based on the state-space representation, (b) a Bayesian approach using Gibbs sampling, (c) a least-squares approach, and (d) a pseudo-ML approach. In the latter two approaches, a block-Toeplitz covariance matrix was constructed in a first step, which was then analyzed via SEM (cf. Hershberger et al., 1996; Molenaar, 1985). Essentially, the authors arrived at the conclusion that “all 4 methods reach appropriate parameter estimates with comparable precision” (Zhang et al., 2008, p. 377) for the conditions under investigation. This applies in particular to the conditions investigated here, so we only reiterate some selected results for the Kalman filter. For a comparison of our results to the other three estimators, we refer the reader to the additional tables reported by Zhang et al. (2008).

**Method**

To maximize comparability, we employed the same method for data generation as Zhang (2006; Zhang et al., 2008). Also in line with Zhang et al. (2008), we assumed all variables to be in deviation form (i.e., means are zero). Note, however, that this assumption is neither necessary, nor is it always reasonable. The factor and error structure at a given time point  $t$  in the direct autoregressive factor score model used in the Monte Carlo simulation are

$$\Lambda_t = \begin{bmatrix} \lambda_{11_t} & 0 \\ \lambda_{21_t} & 0 \\ \lambda_{31_t} & 0 \\ 0 & \lambda_{12_t} \\ 0 & \lambda_{22_t} \\ 0 & \lambda_{32_t} \end{bmatrix} \Theta_t = \begin{bmatrix} \sigma_{\epsilon_{11_t}}^2 & & & & & & \\ 0 & \sigma_{\epsilon_{21_t}}^2 & & & & & \\ 0 & 0 & \sigma_{\epsilon_{31_t}}^2 & & & & \\ 0 & 0 & 0 & \sigma_{\epsilon_{12_t}}^2 & & & \\ 0 & 0 & 0 & 0 & \sigma_{\epsilon_{22_t}}^2 & & \\ 0 & 0 & 0 & 0 & 0 & \sigma_{\epsilon_{32_t}}^2 & \end{bmatrix},$$

with population parameters  $\lambda_{11_t} = \lambda_{21_t} = \lambda_{31_t} = \lambda_{12_t} = \lambda_{22_t} = \lambda_{32_t} = 1$ , and  $\sigma_{\epsilon_{11_t}}^2 = \sigma_{\epsilon_{21_t}}^2 = \sigma_{\epsilon_{31_t}}^2 = \sigma_{\epsilon_{12_t}}^2 = \sigma_{\epsilon_{22_t}}^2 = \sigma_{\epsilon_{32_t}}^2 = .5$  versus  $.3$  for all variables and all time points. Also in line with Zhang et al. (2008), we assumed orthogonal factors with a fixed error variance of  $\sigma_{\eta_{1,t}}^2 = \sigma_{\eta_{2,t}}^2 = 1 - \beta^2$  at  $t \geq 2$ , and allowed the variances and covariance of the random shocks to be freely estimated:

$$\Phi_{t=1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \Psi_t \text{ with } t > 1 = \begin{bmatrix} \sigma_{\eta_{1,t}}^2 & \\ \sigma_{\eta_{1,t}\eta_{2,t}}^2 & \sigma_{\eta_{2,t}}^2 \end{bmatrix},$$

with  $\sigma_{\eta_{1,t}\eta_{2,t}}^2 = .18$ . Finally, we assumed an autoregressive structure, with

$$\mathbf{B}_t = \begin{bmatrix} \beta_{11,t} & \beta_{12,t} \\ \beta_{21,t} & \beta_{22,t} \end{bmatrix} = \begin{bmatrix} 0.8 & 0 \\ 0 & 0.8 \end{bmatrix}.$$

Under the assumption of a multivariate normal distribution, R version 2.10.1 (R Development Core Team, 2009) was used for data generation and OpenMx 1.0.1 (Boker et al., 2010) for ML-SEM parameter estimation. The simulated conditions were two time series of different length ( $T = 50$  vs.  $T = 100$ ), and two different measurement error variances ( $.3$  vs.  $.5$ ), with a total of 150 replications in each condition.

TABLE 1  
Structural Equation Modeling Parameter Estimates Using Maximum Likelihood Estimation in OpenMx

Labels of Model Parameters	True Population Parameter Value	Amount of Measurement Error				Selected Results From Zhang et al. (2008, Table 1) <sup>a</sup> Using Kalman Filtering <sup>b</sup>	
		0.5		0.3		$T = 50$ & $\sigma_{\epsilon}^2 = 0.5^b$	$T = 100$ & $\sigma_{\epsilon}^2 = 0.5^c$
		Time Series Length		Time Series Length			
		$T = 50$	$T = 100$	$T = 50$	$T = 100$		
$\lambda_{11}$	1	0.99	0.98	0.98	0.98	0.94	0.96
$\lambda_{21}$	1	0.98	0.98	0.98	0.97	0.95	0.97
$\lambda_{31}$	1	0.99	0.98	0.98	0.97	0.93	0.97
$\lambda_{12}$	1	0.98	1.02	0.98	0.98	0.93	0.97
$\lambda_{22}$	1	0.97	1.02	0.98	0.97	0.94	0.98
$\lambda_{32}$	1	0.96	1.01	0.98	0.98	0.91	0.96
$\sigma_{\epsilon_{11}}^2$	0.5 // 0.3	0.47	0.50	0.29	0.30	0.50	0.50
$\sigma_{\epsilon_{21}}^2$	0.5 // 0.3	0.49	0.50	0.29	0.30	0.47	0.49
$\sigma_{\epsilon_{31}}^2$	0.5 // 0.3	0.48	0.49	0.29	0.30	0.49	0.50
$\sigma_{\epsilon_{12}}^2$	0.5 // 0.3	0.47	0.49	0.30	0.30	0.48	0.49
$\sigma_{\epsilon_{22}}^2$	0.5 // 0.3	0.49	0.50	0.29	0.30	0.49	0.51
$\sigma_{\epsilon_{32}}^2$	0.5 // 0.3	0.48	0.49	0.30	0.30	0.53	0.51
$\beta_{11}$	0.8	0.73	0.77	0.75	0.77	0.74	0.78
$\beta_{12}$	0	0.01	0.00	0.01	-0.00	-0.01	-0.01
$\beta_{21}$	0	0.02	0.00	-0.02	-0.00	0.02	0.01
$\beta_{22}$	0.8	0.74	0.76	0.75	0.77	0.72	0.75
$\sigma_{\eta_1, \eta_2}^2$	0.18	0.17	0.18	0.18	0.18	0.16	0.17
$-2LL$		747.2	1,520	630.6	1,277	NA	NA

Note. For purpose of comparison, some selected results of the simulation study by Zhang et al. (2008) are reported in the last two columns. Parameter estimates are based on 150 valid replications. Zhang et al. (2008) used mkfm6 (Dolan, 2010) for estimation.

<sup>a</sup>Reproduced with permission. <sup>b</sup>Results are based on 90 replications. <sup>c</sup>Results are based on 97 replications.

## Results

Results of the Monte Carlo simulation are reported in Table 1. The left part of Table 1 contains the ML-SEM estimates of this simulation, and for the purpose of comparison, the right part shows the corresponding Kalman filter estimates from the simulation study by Zhang et al. (2008, p. 390).<sup>2</sup> As apparent from Table 1, the parameter estimates of the Kalman filter, as implemented in the program mkfm6 (Dolan, 2010), and the ML-SEM estimates were almost identical. Thus, it is possible to estimate dynamic factor models directly via SEM without recurring to block-Toeplitz covariance matrices. In contrast to estimates based on block-Toeplitz matrices, the resulting parameter estimates are true ML estimates and approach those of existing (non-SEM) procedures.

<sup>2</sup>For a comparison to the three other estimation techniques, the reader is referred to Table 2 to Table 4 in Zhang et al. (2008).

## INTEGRATING THE ANALYSIS OF BETWEEN- ( $N > 1$ ) AND WITHIN- ( $N = 1$ ) PERSON STRUCTURES

Traditionally, SEM has been used to fit between-person models; that is, to estimate relationships between variables observed for many individuals (see left part of Figure 1). We have already shown that SEM can also be used to fit individual time series for  $N = 1$  and many time points, without the need for prior data transformation (e.g., the computation of block-Toeplitz matrices; see right part of Figure 1). Obviously, the approach readily generalizes to any other sample size  $N \geq 1$ , thus allowing for a continuous shift between within-person and between-person analyses. Maybe most important, however, via multiple group analysis it opens up the possibility to simultaneously estimate one or more individual time series (within-person model) together with one or more between-person models, with possible constraints between the two (or more) groups. Among many other new modeling options, this provides us with a direct likelihood ratio (*LR*) test of whether the factorial structure between persons is identical with the factorial structure of a single individual; that is, a test of ergodicity at the model level (as compared to the Bartlett-type test of homogeneity of covariances proposed by Nesselroade & Molenaar, 1999; see also Nesselroade, 2007, p. 256; Molenaar, 2004; Molenaar & Campbell, 2009).

### Simulation 2: Testing Invariance of a Between- and Within-Subject Factor Model

To explore this new modeling option and the associated test of factorial invariance between a within-person dynamic factor model and a between-person factor model, we set up a Monte Carlo simulation in which we generated an individual time series as described earlier and a between-person factor model at a single point in time. In one condition the true factorial structure of the two was identical (i.e., the assumption of ergodicity was met), whereas in the other condition the factorial structure differed (i.e., the assumption of ergodicity was not met).

### Method

The within-person dynamic factor model was generated in the same way as in the previous Monte Carlo simulation, with  $N = 1$  and  $T = 100$  ( $T = 50$ , respectively). With  $T = 1$  and  $N = 100$  independent individuals ( $N = 50$ , respectively), the between-person model is based on the same amount of information (i.e., the same number of data points). Because of the single time point, however, there exists no temporal structure in this group (i.e.,  $\mathbf{B} = \mathbf{\Psi} = \mathbf{0}$ ). In one simulation condition the factorial structure of the two groups was set to be same as in the previous simulation, whereas in the other condition the factorial structure differed with

$$\Lambda(\text{between}) = \begin{bmatrix} 0.7 & 0 \\ 0.7 & 0 \\ 0.7 & 0 \\ 0 & 0.4 \\ 0 & 0.4 \\ 0 & 0.4 \end{bmatrix} \quad \text{versus} \quad \Lambda(\text{within}) = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}.$$

In each simulation run, two integrated between–within-person models were fitted. In the first model the six nonzero loadings were constrained to equality across both groups, whereas they were allowed to differ in the second model. The difference between the two  $-2$  times  $LL$ s corresponds to an  $LR$  test with six degrees of freedom ( $LR = -2(LL_{\text{Model1}} - LL_{\text{Model2}})$ ). As before, we used 150 replications per condition.

## Results

Results of the Monte Carlo simulation are reported in Table 2. As expected, the difference between the two  $-2$  times  $LL$ s between the model with constrained and unconstrained factor loadings was statistically nonsignificant, when the loading structures were indeed identical in the population ( $LR = 6.0, df = 6, ns$ , for  $T = 50$ ;  $LR = 9.0, df = 6, ns$ , for  $T = 100$ ), but significant when the loading structures differed ( $LR = 25.0, df = 6, p < .001$ , for  $T = 50$ ;  $LR = 36.0, df = 6, p < .001$ , for  $T = 100$ ). Furthermore, parameter estimates of the between- as well as within-person model converged on the population parameters, when the model was correctly specified (i.e., factor loadings were allowed to differ, when the factor loadings differed in the population). When the model was not correctly specified (i.e., the between- and within-person factor structures were constrained to equality, while the factor loadings differed in the population), particularly the factor loadings, but also the autoregressive and cross-lagged effects, were biased (see lower half of Table 2).

## Exploring the Degree of Factorial Invariance Across Different Levels of Analysis

As pointed out by Molenaar (2004) “only under very strict conditions . . . can a generalization be made from a structure of interindividual variation to the analogous structure of intraindividual variation” (p. 201). Yet, comparisons between inter- and intraindividual structures have been of fundamental interest to psychologists since the very beginning of individual factor analysis, when Cattell et al. (1947) illustrated P-technique by comparing the personality factor structure obtained for a single individual to personality factors as obtained by R-technique. On visual inspection of the results, they concluded that “[the factors obtained via P-technique] are easily recognizable as well-known primary personality factors as obtained by R-technique” (p. 282), but also that “not all R-technique factors appeared” (p. 282). In a more recent study, Brose, Schmiedek, Lövdén, Molenaar, and Lindenberger (2010) examined the equivalence of the within-person and between-person structures in linking motivational variables to working memory. They demonstrated reliable differences in within-person structures across individuals, thus indirectly defying the ergodicity assumption.

The ML-SEM approach introduced in this article permits a direct and unbiased test of the ergodicity hypothesis through joint estimation of individual time series ( $T$  large and  $N = 1$ ) and cross-sectional data ( $N$  large and  $T = 1$ ). It thereby eliminates the need to rely on subjective inspection of the factor-analytic results. Eventually, however, it remains an empirical question for which constellations of psychological constructs and individuals the ergodicity assumption is tenable and for which it is not. As pointed out by Molenaar (2004), it appears unlikely that one would find many empirical constellations where the structures of

TABLE 2  
Structural Equation Modeling Parameter Estimates and -2 Log-Likelihood of an Integrated Time Series (N = 1 and T large) and Cross-Sectional (T = 1 and N large) Model Using Maximum Likelihood Estimation in OpenMx

Equal Factor Loadings in the Population	Labels of Model Parameters	True Parameters (Inter)	True Parameters (Intra)	Factor Loadings Constrained to Equality						
				Yes			No			
				T = 1 & N = 50 (Inter) N = 1 & T = 50 (Intra)	T = 1 & N = 100 (Inter) N = 1 & T = 100 (Intra)	T = 1 & N = 50 (Inter) N = 1 & T = 100 (Intra)	T = 1 & N = 100 (Inter) N = 1 & T = 50 (Intra)	T = 1 & N = 100 (Inter) N = 1 & T = 100 (Intra)	T = 1 & N = 100 (Inter) N = 1 & T = 100 (Intra)	
Yes	$\lambda_{11}$	1	1	0.97	1.01	0.99	0.99	0.95	1.00	0.98
	$\lambda_{21}$	1	1	0.98	1.01	0.99	0.99	0.95	1.01	0.98
	$\lambda_{31}$	1	1	0.99	1.00	1.01	1.01	0.96	1.00	0.98
	$\lambda_{12}$	1	1	0.98	1.01	0.99	0.99	0.96	0.99	1.01
	$\lambda_{22}$	1	1	0.98	1.00	0.98	0.98	0.95	0.99	1.00
	$\lambda_{32}$	1	1	0.99	1.00	0.99	0.99	0.96	1.00	1.00
	$\sigma^2_{\epsilon_{11}}$	0.5	0.5	0.50	0.50	0.49	0.49	0.49	0.50	0.50
	$\sigma^2_{\epsilon_{21}}$	0.5	0.5	0.49	0.50	0.50	0.49	0.48	0.49	0.49
	$\sigma^2_{\epsilon_{31}}$	0.5	0.5	0.50	0.50	0.50	0.48	0.48	0.49	0.49
	$\sigma^2_{\epsilon_{12}}$	0.5	0.5	0.48	0.50	0.50	0.47	0.47	0.49	0.49
	$\sigma^2_{\epsilon_{22}}$	0.5	0.5	0.47	0.50	0.50	0.47	0.47	0.49	0.49
	$\sigma^2_{\epsilon_{32}}$	0.5	0.5	0.49	0.50	0.50	0.48	0.48	0.49	0.49
	$\beta_{11}$	0.8	0.8	0.76	0.77	0.77	0.76	0.76	0.77	0.77
	$\beta_{12}$	0	0	-0.02	0.00	-0.01	-0.01	0.00	0.00	0.00
	$\beta_{21}$	0	0	0.00	0.00	0.00	0.00	0.00	0.01	0.01
	$\beta_{22}$	0.8	0.8	0.74	0.76	0.76	0.76	0.76	0.76	0.76
	$\sigma^2_{\eta_1, \eta_2}$	0.18	0.18	0.17	0.19	0.16	0.16	0.16	0.18	0.18
	-2LL			1,593	3,207	1,587	1,587	1,587	3,198	3,198
	LR (df)			6.0 (df = 6; ns)	9.0 (df = 6; ns)					

(continued)

TABLE 2  
(Continued)

Equal Factor Loadings in the Population	Factor Loadings Constrained to Equality											
	Yes						No					
	Labels of Model Parameters	True Parameters (Inter)	True Parameters (Intra)	T = 1 & N = 50 (Inter) N = 1 & T = 50 (Intra)	T = 1 & N = 100 (Inter) N = 1 & T = 100 (Intra)	T = 1 N = 50 (Inter)	T = 1 N = 100 (Inter)	T = 50 N = 1 (Intra)	T = 50 N = 100 (Inter)	T = 100 N = 1 (Intra)	T = 100 N = 100 (Inter)	
No	$\lambda_{11}$	0.7	1	0.79	0.79	0.70	0.70	0.96	0.70	0.70	0.70	1.00
	$\lambda_{21}$	0.7	1	0.78	0.79	0.71	0.71	0.94	0.71	0.69	0.69	1.00
	$\lambda_{31}$	0.7	1	0.78	0.79	0.71	0.71	0.96	0.71	0.70	0.70	1.00
	$\lambda_{12}$	0.4	1	0.59	0.62	0.37	0.37	0.95	0.37	0.35	0.35	0.99
	$\lambda_{22}$	0.4	1	0.61	0.63	0.39	0.39	0.98	0.39	0.35	0.35	1.00
	$\lambda_{32}$	0.4	1	0.62	0.62	0.37	0.37	0.99	0.37	0.36	0.36	1.00
	$\sigma_{\eta_1}^2$	0.5	0.5	0.50	0.50	0.49	0.49	0.49	0.49	0.49	0.49	0.49
	$\sigma_{\eta_2}^2$	0.5	0.5	0.49	0.50	0.50	0.50	0.48	0.48	0.50	0.50	0.49
	$\sigma_{\eta_3}^2$	0.5	0.5	0.51	0.51	0.51	0.51	0.48	0.48	0.50	0.50	0.49
	$\sigma_{\eta_4}^2$	0.5	0.5	0.51	0.51	0.51	0.51	0.49	0.49	0.49	0.49	0.49
	$\sigma_{\eta_5}^2$	0.5	0.5	0.51	0.53	0.53	0.53	0.47	0.47	0.50	0.50	0.50
	$\sigma_{\eta_6}^2$	0.5	0.5	0.51	0.52	0.52	0.52	0.48	0.48	0.50	0.50	0.50
	$\beta_{11}$	0.8	0.8	0.72	0.81	0.72	0.72	0.72	0.72	0.77	0.77	0.77
	$\beta_{12}$	0	0	0.05	0.15	0.05	0.05	0.02	0.02	0.00	0.00	0.00
	$\beta_{21}$	0	0	-0.08	-0.03	-0.08	-0.08	0.01	0.01	0.00	0.00	0.00
	$\beta_{22}$	0.8	0.8	0.89	0.88	0.89	0.88	0.74	0.74	0.78	0.78	0.78
	$\sigma_{\eta_1, \eta_2}^2$	0.18	0.18	0.16	0.17	0.16	0.17	0.17	0.17	0.18	0.18	0.18
	-2LL			1,521	3,047	1,496	1,496	3,011	3,011	3,011	3,011	3,011
	LR (df)			25.0 (df = 6; p < .001)	36.0 (df = 6; p < .001)	36.0 (df = 6; p < .001)	36.0 (df = 6; p < .001)					

Note. To test whether the factorial structure of an individual observed at many time points is identical to the factorial structure of a group of individuals observed at a single point in time, factor loadings were either freely estimated or constrained to equality across the two groups. Parameter estimates are based on 150 valid replications. LR = likelihood ratio.

inter- and intraindividual variability are the same across all individuals examined. However, even if individuals exhibit heterogeneity in their factor structures, it might still be possible to identify homogeneous subgroups of individuals for whom the intraindividual factor structure is identical to the interindividual factor structure (Nesselroade & Molenaar, 1999). Thus, rather than conceiving of ergodicity as a categorical yes–no question, it might be worth exploring the degree of ergodicity in a given sample.

To further explore this line of reasoning, we rank-ordered all individuals based on the likelihood values of the joint ML-SEM model. This is illustrated in Figure 2, in which we treat the 150 independent replications of the Monte Carlo simulation reported earlier as 150 independent individuals. Under the null hypothesis of ergodicity, this function corresponds to a cumulative chi-square distribution. The observed  $-2LL$  values for equal factor loadings in the population are shown in the upper part of Figure 2 (solid line). Allowing the factor loadings to be freely estimated yields only a slight improvement of the likelihood (dashed line is somewhat lower). The overall difference between the two distributions can be tested via the Kolmogorov–Smirnov test, which is not significant ( $D = 0.09$ ,  $p = .626$ ). Thus, the assumption of ergodicity is met for the entire sample. In contrast, the Kolmogorov–Smirnov test indicates a significant difference between the lower two distributions, which resulted from the

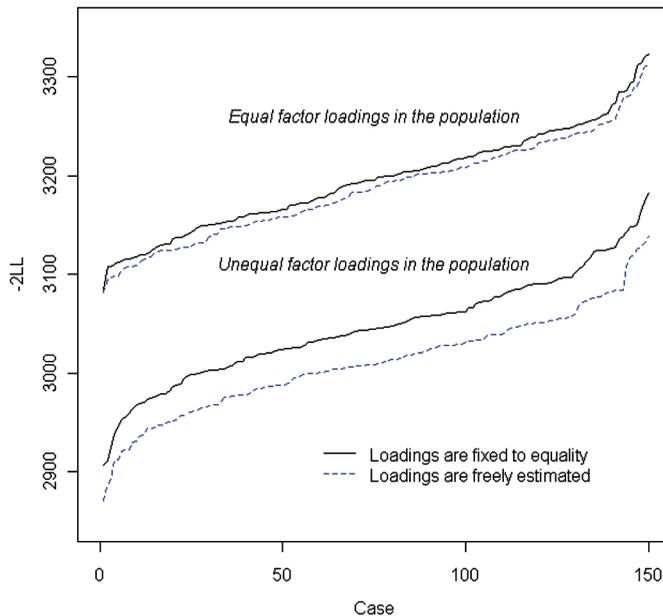


FIGURE 2 One hundred and fifty individuals rank ordered according to their  $-2$  log-likelihood ( $-2LL$ ) values of the joint between–within maximum likelihood structural equation modeling model. The upper two curves correspond to the simulation condition with equal factor loadings in the population, and the lower two curves correspond to the situation with unequal factor loadings in the population. Solid lines indicate equality-constrained and dashed lines freely estimated loadings. (color figure available online)

simulation with unequal factor loadings in the population ( $D = 0.33$ ,  $p < .001$ ). Clearly, the assumption of ergodicity does not hold in this situation. To examine the degree of ergodicity, we plotted the empirical chi-square distributions under the null and alternative hypothesis as shown in Figure 3. From Figure 3 it is also apparent that the empirical distributions clearly approach the theoretical chi-square distributions (solid lines). As expected, if the factorial structure is the same between and within individuals (left part), there are only few cases in which the  $LR$  test turns out significant for  $p < .01$  (i.e., Type I error). In contrast, almost all 150 individual tests turn out significant if the factorial structure indeed differs between and within individuals. Both situations, however, are only examples of the two endpoints of an underlying continuum. What is more likely to happen in applied research is a situation illustrated by the dashed line in Figure 3. Here the factorial structure between and within individuals is the same for about two thirds of the sample, but differs significantly for about one third of the sample. We would like to suggest that psychological constructs like personality or intelligence are likely to vary in relation to the degree of ergodicity they exhibit in a given sample. An important goal of future research in psychology is to explore the mechanisms that influence

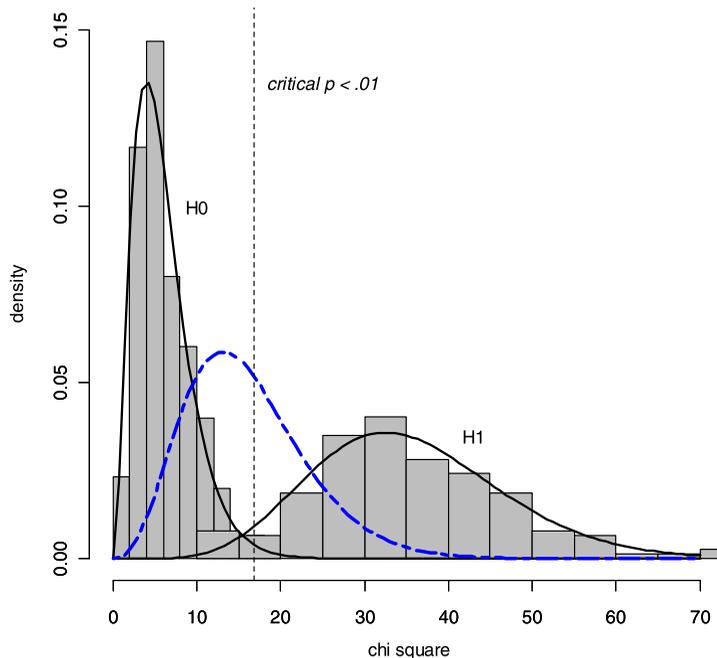


FIGURE 3 Empirical (histogram) and theoretical (solid lines) probability density function of the 150 likelihood ratios ( $\chi^2$  values) under the condition of ergodicity (H0) and the 150 likelihood ratios under the condition of nonergodicity (H1). The vertical line represents the critical  $\chi^2$  value for  $p < .01$  ( $df = 6$ ). The dashed line illustrates a distribution resulting from a hypothetical situation in which about two thirds of a sample exhibits an ergodic factor structure, and the assumption of ergodicity is violated for about one third of the sample. (color figure available online)

the degree of ergodicity. The approach previously introduced offers a statistical tool for this endeavor.

### AN ML-SEM APPROACH TO DYNAMIC FACTOR ANALYSIS WITH COMPLEX ERROR STRUCTURES

The biggest advantage of the ML-SEM approach to DFA introduced here is that it can capitalize on the full potential of general latent variable models (Muthén, 2002). This might involve a number of new modeling options that have not yet been considered but could become important in the future. Notably, given that the estimator makes use of the full matrices **A**, **S**, and **M**, it becomes possible to formulate quite complex models that are specifically tailored to the researchers' needs. For example, in contrast to the use of block-Toeplitz matrices, it is possible to model error variances that are increasing or decreasing over time, or in contrast to the Kalman filter, it is possible to model (undirected) measurement error covariances over time. The latter is demonstrated in the following section.

#### Simulation 3: Modeling Error Covariances Across Time

In this final Monte Carlo simulation, the ML-SEM approach is extended to DFA of the first simulation by allowing two measurement error terms to be correlated over time. This is illustrated by the dash-pointed double-headed arrows in Figure 1. To keep the model simple we decided to include only two error covariances. The approach, however, generalizes readily to more than two covariances across more than two adjacent time points.<sup>3</sup>

#### Method

The Monte Carlo simulation was set up in the same way as the first simulation study, except that the matrix **S** is extended by the  $q \times q$  off-diagonal matrix  $\Theta_{t-1,t} = \Theta_{t,t-1}$  so that

$$\mathbf{S} = \begin{bmatrix}
 \Phi_{t=1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\
 \mathbf{0} & \Psi_{t=1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & & \mathbf{0} \\
 & & \ddots & & & & \vdots \\
 \mathbf{0} & \mathbf{0} & & \Psi_{t=T} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\
 \mathbf{0} & \mathbf{0} & & \mathbf{0} & \Theta_{t=1} & \Theta_{t-1,t=2} & \mathbf{0} \\
 \mathbf{0} & \mathbf{0} & & \mathbf{0} & \Theta_{t=2,t-1} & \Theta_{t=2} & \mathbf{0} \\
 \vdots & & & & & \ddots & \vdots \\
 \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & & \Theta_{T-1} & \Theta_{T-1,T} \\
 \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & & \Theta_{T,T-1} & \Theta_{t=T}
 \end{bmatrix}$$

<sup>3</sup>Of course, the approach also permits covariances among measurement errors within each time point.

with

$$\Theta_{t-1,t} = \begin{bmatrix} \sigma_{\varepsilon_{11(t-1,t)}}^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_{\varepsilon_{12(t-1,t)}}^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

An  $N = 1$  dynamic factor model was generated with two different numbers of occasions ( $T = 50$  vs.  $T = 100$ ) and two different measurement error variances ( $\sigma_{\varepsilon}^2 = .5$  vs.  $\sigma_{\varepsilon}^2 = .3$ ). For  $\sigma_{\varepsilon}^2 = .5$  an error covariance of  $\sigma_{\varepsilon_{11(t-1,t)}}^2 = .25$  was chosen for the first indicators of the first factor, and an error covariance of  $\sigma_{\varepsilon_{12(t-1,t)}}^2 = .20$  was chosen for the first indicators of the second factor. Likewise, for  $\sigma_{\varepsilon}^2 = .3$  an error covariance of  $\sigma_{\varepsilon_{11(t-1,t)}}^2 = .15$  was chosen for the first indicators of the first factor, and an error covariance of  $\sigma_{\varepsilon_{12(t-1,t)}}^2 = .10$  was chosen for the first indicators of the second factor. Again, we used 150 replications per condition.

## Results

The complete results of the Monte Carlo simulation are given in Table 3. Parameter estimates are comparable to the parameter estimates of the first simulation study as well as the simulation study by Zhang et al. (2008). All estimates approached the population parameters as the number of time points increased. This applied equally to the measurement error covariances over time (e.g., for  $T = 100$ :  $\sigma_{\varepsilon_{11(t-1,t)}}^2 = .25$  vs.  $\hat{\sigma}_{\varepsilon_{11(t-1,t)}}^2 = .24$ ;  $\sigma_{\varepsilon_{12(t-1,t)}}^2 = .20$  vs.  $\hat{\sigma}_{\varepsilon_{12(t-1,t)}}^2 = .19$ ). Thus, the ML-SEM approach to DFA works well, even for more complex error structures, which are more difficult—or impossible—to implement in other approaches to time series analysis.

## LIMITATIONS

Despite the advantages, the ML-SEM approach to DFA is also associated with a number of limitations. Like any other method for the analysis of individual time series, the number of time points needs to be sufficiently large to obtain good parameter estimates. As apparent from all three Monte Carlo simulations, for the factor model used in this study,  $T = 100$  time points appears to work reasonably well, but this represents a lower bound. With an increasing number of time points and variables, however,  $\Sigma$  gets extremely large, and the computation of the corresponding matrix inversion ( $\Sigma^{-1}$ ), involved in the fitting function (Equation 5), becomes increasingly demanding. In other words, the flexibility to specify all elements in  $\mathbf{M}$ ,  $\mathbf{A}$ , and  $\mathbf{S}$  according to the researchers' needs comes at the expense of greatly increased computation time. Particularly for simulation studies, this poses a severe problem, but estimating a single model also becomes practically infeasible with much more complicated (i.e., more time points and more indicators) models than the ones used in this study. However, all matrices involved are sparse matrices with a very simple structure. Thus, it should be possible to avoid or modify the computation of the matrix inverse during parameter estimation in a way that capitalizes on the

TABLE 3  
Structural Equation Modeling Parameter Estimates and  $-2$  Log-Likelihood of a Time Series With Two Measurement Error Covariances Across Time Using Maximum Likelihood Estimation in OpenMx ( $N = 1$  and  $T = 50$  vs.  $100$ )

Labels of Model Parameters	True Population Parameter Value	Amount of Measurement Error			
		0.5		0.3	
		Time Series Length		Time Series Length	
		$T = 50$	$T = 100$	$T = 50$	$T = 100$
$\lambda_{11}$	1	0.96	1.00	0.98	0.98
$\lambda_{21}$	1	0.93	0.98	0.97	0.97
$\lambda_{31}$	1	0.95	0.97	0.96	0.98
$\lambda_{12}$	1	0.99	0.99	0.96	0.97
$\lambda_{22}$	1	0.95	0.97	0.94	0.96
$\lambda_{32}$	1	0.93	0.98	0.94	0.96
$\sigma_{\epsilon_{11}}^2$	0.5 // 0.3	0.46	0.47	0.26	0.28
$\sigma_{\epsilon_{21}}^2$	0.5 // 0.3	0.50	0.50	0.30	0.30
$\sigma_{\epsilon_{31}}^2$	0.5 // 0.3	0.48	0.49	0.30	0.31
$\sigma_{\epsilon_{12}}^2$	0.5 // 0.3	0.43	0.47	0.29	0.28
$\sigma_{\epsilon_{22}}^2$	0.5 // 0.3	0.51	0.50	0.30	0.30
$\sigma_{\epsilon_{32}}^2$	0.5 // 0.3	0.50	0.50	0.30	0.30
$\beta_{11}$	0.8	0.75	0.78	0.74	0.78
$\beta_{12}$	0	0.01	0.00	0.03	0.00
$\beta_{21}$	0	0.03	-0.01	-0.03	0.00
$\beta_{22}$	0.8	0.73	0.78	0.78	0.78
$\sigma_{\epsilon_{11(t-1,t)}}$	0.25 // 0.15	0.22	0.24	0.13	0.14
$\sigma_{\epsilon_{12(t-1,t)}}$	0.20 // 0.10	0.15	0.19	0.09	0.09
$\sigma_{\eta_1, \eta_2}^2$	0.18	0.17	0.18	0.18	0.18
$-2LL$		727.8	1,476	614.3	1,244

Note. Parameter estimates are based on 150 valid replications.

simple structure of the matrices. To this end we are currently exploring different alternatives. Using our own optimization routines based on Gaussian elimination, we were able to fit the two-factor and six-indicator model described earlier for up to 1,000 time points within a reasonable amount of time (42 minutes per estimation process) on a 2.94 GHz personal computer. Given that most optimizers implemented in current SEM packages (e.g., NPSOL in OpenMx; see Gill, Murray, Saunders, & Wright, 1998) do not take advantage of sparse or highly patterned matrices, however, at present the approach remains limited to medium-size models as discussed in this article. However, in other disciplines researchers have developed highly efficient ways to deal with much larger matrices, and integrating these procedures into current SEM packages appears to be a promising route for future research.

Finally, we assumed equal intervals between time points. This assumption applies to all currently available approaches to DFA but we are also in the process of extending the ML-SEM approach to continuous time modeling as described by Oud and Jansen (2000). Unfortunately, standard optimizers are not geared toward handling large matrices in combination with com-

plicated matrix exponential constraints involved in continuous time modeling, so that a routine use of single-subject ML-SEM-based continuous time models cannot be recommended at this time.

## SUMMARY AND IMPLICATIONS

In this article we have demonstrated for the first time that (a) it is possible to obtain true ML estimates for dynamic factor models via SEM; (b) this allows the simultaneous estimation of between-person and within-person structures; and (c) the approach offers great flexibility in terms of model specification, as illustrated by the inclusion of measurement error covariances across different measurement occasions.

Although the general idea to use SEM (i.e., factor analysis) to fit individual ( $N = 1$ ) time series dates back to the first half of the last century (Cattell et al., 1947), especially as compared to the use of SEM to fit between-person structures, there exists little research on this topic and no research on the simultaneous estimation of between- and within-person structures. In particular, it was Molenaar and Nesselroade (Molenaar, 1985; Nesselroade & Ford, 1985a; Nesselroade et al., 2002; Nesselroade & Molenaar, 2004) who advanced the person-centered approach in subsequent years. Typically, this was done by using time-delayed embedding to create block-Toeplitz covariance matrices that could be used as input for standard SEM programs. This approach works well for many practical situations, but the resulting parameter estimates are not ML estimates and their inferential properties are unknown (Hamaker, Dolan, & Molenaar, 2002; van Buuren, 1997; Zhang et al., 2008). A number of alternative approaches to fit individual time series that do not suffer from these problems exist (e.g., state-space models; cf. Chow et al., 2010; Durbin & Koopman, 2001). However, as previously discussed, we know of only two papers that investigate the use of ML estimation for single-subject models by means of SEM (Hamaker et al., 2003; Singer, 2010). The first Monte Carlo simulation reported here demonstrated that it is possible to use SEM to obtain ML estimates for dynamic factor models. When comparing the results to a recent simulation study by Zhang et al. (2008), we showed that the resulting parameter estimates are almost identical to those of existing procedures like the Kalman filter (see Table 1). Furthermore, given that the properties of the likelihood function are known, the usual fit indexes, including information-theoretical indexes, such as the Akaike's information criterion (AIC), can be computed. Their practical use in terms of assessing model fit, including possible cutoff criteria, however, remains to be investigated.

The biggest advantage of the ML-SEM approach to time series modeling is its enormous flexibility in model specification, which opens up a variety of new modeling options. For example, via multiple group analysis it becomes possible to simultaneously estimate (one or more) individual time series together with (one or more) cross-sectional models. This was demonstrated by our second Monte Carlo simulation. In this context we proposed a direct test of ergodicity; that is, an  $LR$  test of invariance between a within- and between-person model. We also showed how the *degree* of ergodicity for a given constellation of constructs and samples can be explored by rank-ordering individuals according to their likelihoods. In our view, examining the degree of ergodicity at the model level is a promising way for future research (for a different approach to identify homogeneous subgroups by comparing individual block-Toeplitz covariance matrices; see Nesselroade & Molenaar, 1999).

Without doubt, the best possible situation in applied research is a situation with information on many individuals observed at many time points. In such a situation, one might start by fitting an individual factor model and examining the degree to which the factor model is the same for all individuals. Unfortunately, however, researchers and practitioners find themselves often in a less luxurious position, by having to make claims about a within-person structure (e.g., for treatment purposes) without having many observation occasions. Given that the last 100 years of psychological research were almost exclusively restricted to the analysis of between-person variation (Molenaar, 2004) little knowledge exists on such within-person models and we can only echo the call for a “Kuhnian paradigm shift within the science of psychology” (Molenaar & Campbell, 2009, p. 112). Nevertheless, what is known from between-subject analyses could serve as a reference or starting point in this paradigm shift. The degree to which within-person structures deviate from between-person structures is an empirical question, and might differ across constellations of constructs and persons. We are currently investigating this topic in a different paper (Brose, Voelkle, Lövdén, Lindenberg, & Schmiedek, submitted) using data of the COGITO study (Schmiedek, Lövdén, & Lindenberg, 2010). The ML-SEM approach introduced here provides a statistical tool to address this question, and might foster efforts at developing a taxonomy of ergodicity for psychological constructs.<sup>4</sup>

The last part of the article discussed how to extend the ML-SEM approach to individual time series analysis to more complex models. This has been illustrated by the introduction of two measurement error covariances over time in the third Monte Carlo simulation. As expected, all parameter estimates converge on the population parameters (see Table 3). Note that due to its recursive nature, it is not possible to fit such a model with the Kalman filter.

We also noted that the advantage of increased flexibility comes at the expense of computation time. At present this limits the application of the ML-SEM approach to moderately complex models with a limited number of time points. Although the models employed in this article are not trivial, future research should focus on generalizing the approach to more complex models with more time points. For this purpose, it seems promising to modify prevalent optimization procedures to better account for the highly structured pattern of (sparse) matrices involved in the likelihood function. The challenge will be to find the right balance between assuming a predefined structure and retaining the flexibility of the approach.

This article can be viewed as a first step toward a more comprehensive approach to individual time series modeling within an SEM framework. It has shown how to use SEM to obtain direct (ML) estimates of dynamic factor models, and a number of new modeling options have been discussed, including an *LR* test of ergodicity, and the estimation of complex error structures.

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<sup>4</sup>Another potential advantage of the simultaneous estimation of between- and within-person models might be an improved initializing of the individual time series by borrowing information on the between-person model at the first time point. This remains to be explored in future research.

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