

SEPARABLE FACTOR ANALYSIS WITH APPLICATIONS TO MORTALITY DATA¹

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Human mortality data sets can be expressed as multiway data arrays, the dimensions of which correspond to categories by which mortality rates are reported, such as age, sex, country and year. Regression models for such data typically assume an independent error distribution or an error model that allows for dependence along at most one or two dimensions of the data array. However, failing to account for other dependencies can lead to inefficient estimates of regression parameters, inaccurate standard errors and poor predictions. An alternative to assuming independent errors is to allow for dependence along each dimension of the array using a separable covariance model. However, the number of parameters in this model increases rapidly with the dimensions of the array and, for many arrays, maximum likelihood estimates of the covariance parameters do not exist. In this paper, we propose a submodel of the separable covariance model that estimates the covariance matrix for each dimension as having factor analytic structure. This model can be viewed as an extension of factor analysis to array-valued data, as it uses a factor model to estimate the covariance along each dimension of the array. We discuss properties of this model as they relate to ordinary factor analysis, describe maximum likelihood and Bayesian estimation methods, and provide a likelihood ratio testing procedure for selecting the factor model ranks. We apply this methodology to the analysis of data from the Human Mortality Database, and show in a cross-validation experiment how it outperforms simpler methods. Additionally, we use this model to impute mortality rates for countries that have no mortality data for several years. Unlike other approaches, our methodology is able to estimate similarities between the mortality rates of countries, time periods and sexes, and use this information to assist with the imputations.

1. Introduction. Human mortality data are used extensively by researchers and policy makers to analyze historic and current population trends and assess long-term impacts of public policy initiatives. To enable such inference, numerous regression models have been proposed that estimate mortality rates as a function of age using a small number of parameters [Heligman and Pollard (1980), Mode and Busby (1982), Siler (1983)]. Practitioners using these methods typically model

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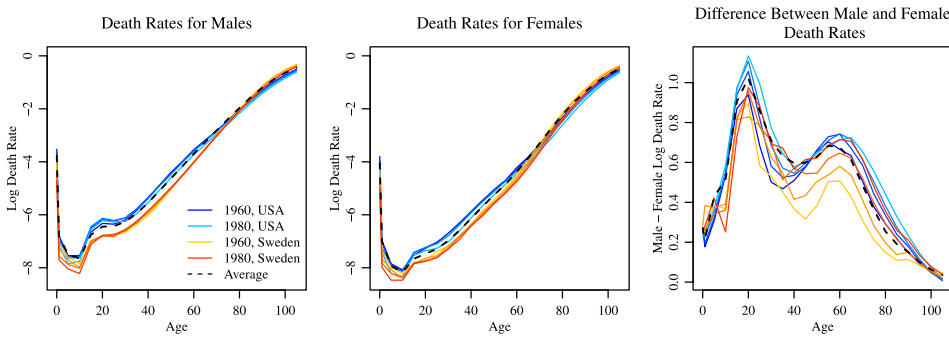


FIG. 1. *Mortality curves for the United States of America and Sweden. The gradient of colors for each country represents the log death rates in the four 5-year time periods from 1960 to 1980. The average sex-specific mortality curve over the four time periods and all countries is shown in black.*

the age-specific death rates for each country, year and sex combination separately and assume independent error distributions. Examples of death rates analyzed by such methods are shown in Figure 1 for the United States and Sweden. Each mortality curve is defined by 23 age-specific death rates and the average sex-specific mortality curve from 1960–1980 over thirty-eight countries is also displayed.

From the figure, it is clear that a country’s mortality rates in one time period are similar to its rates in adjacent time periods. Acknowledging this fact, several researchers have developed models for “dynamic life tables,” that is, matrices of mortality rates for combinations of ages and time periods, for single country–sex combinations. An example of such a life table is the male death rates in Sweden from 1960 to 1980 shown in Figure 1. Some of the models developed for these data specify ARIMA processes for the time-varying model parameters [McNown and Rogers (1989), Renshaw and Haberman (2003a)], while others smooth the death rates over age and time using a kernel smoother [Felipe, Guillen and Nielsen (2001)], p -splines [Currie, Durban and Eilers (2004)], nonseparable age–time period covariance functions [Martínez-Ruiz et al. (2010)] or multiplicative effects for age and time [Lee and Carter (1992), Renshaw, Haberman and Hatzopoulos (1996), Renshaw and Haberman (2003b, 2003c), Chiou and Müller (2009)].

Human mortality data sets typically provide mortality rates of populations corresponding to combinations of several factors. For example, the Human Mortality Database (HMD) [University of California, Berkeley and Max Planck Institute for Demographic Research (2011)] provides mortality rates of populations corresponding to combinations of 40 countries, 9 time periods, 23 age groups, and both male and female sexes. As is shown in Figure 1, mortality rates of men and women within a country will typically both be higher than or both lower than the sex-specific rates averaged across countries. Furthermore, differences between male and female mortality rates generally show trends that are consistent across countries and time periods. Such patterns suggest joint estimation of mortality rates

using a model that can share information across levels of two or more factors. Two models that consider death rates for more than one country or sex are that developed by [Li and Lee \(2005\)](#), which estimates common age and time period effects for a group of countries or both sexes, and [Carter and Lee \(1992\)](#), where male and female death rates within the same country share a time-varying mortality level. Although these methods consider either both sexes or multiple countries, the extreme similarity of the curves in [Figure 1](#) for males across countries and for a given country across sexes suggest that separately modeling death rates for different countries or sexes is inefficient, and inference may be improved by using a joint model that shares information across all factors.

With this in mind, we consider a regression model for the HMD data consisting of a mean model that is a piecewise-polynomial in age with additive effects for country, time period and sex (more details on this model, and its comparison to other models, are provided in [Section 4](#)). This mean model is extremely flexible: it contains over 370 parameters and an ordinary least squares (OLS) fit accounts for over 99% of the total variation in the data (coefficient of determination, $R^2 > 0.995$). Nonetheless, an analysis of the residuals from the OLS fit indicates that some clear patterns in the data are not captured by the regression model and, in particular, a model of independent errors is a poor representation of these data. To illustrate this, note that the residuals can be represented as a 4-way array, the dimensions of which are given by the number of levels of each of the four factors: country, time period, sex and age. To examine residual correlation across levels of a factor, the 4-way array of residuals can be converted into a matrix whose columns represent the levels of the factor, and a sample correlation matrix for the factor can be obtained. [Figure 2](#) summarizes the patterns in the residual correlations using the first two principal components of each sample correlation matrix. If a model of independent errors were to be adequate, we would expect the sample correlation values to be small and centered about zero, and no discernible patterns to exist in

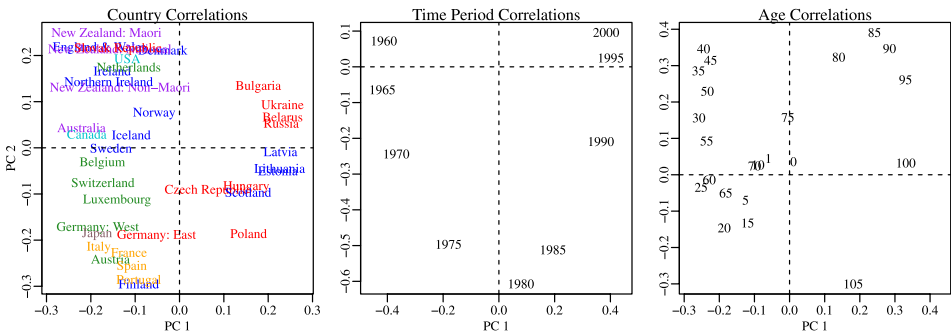


FIG. 2. The first two principal components of each sample correlation matrix are displayed, and countries in the same United Nations region are shown in the same color. Close proximity in the principal components space away from the origin is indicative of a positive correlation.

the principal components. However, the sample correlations are substantially more positive than would be expected under independence: 59% of the observed country correlations, 61% of time period correlations and 98% of age correlations are greater than the corresponding 95% theoretical percentiles under the independence assumption. Additionally, there are clear geographic, temporal and age trends in the principal components in Figure 2. For example, the residuals for the Ukrainian mortality rates are positively correlated to those for Russia, and the residuals for the year 2000 are positively correlated with those for 1995. This residual analysis suggests that an assumption of uncorrelated errors is inappropriate.

Failure to recognize correlated errors can lead to a variety of inferential problems, such as inefficient parameter estimates and inaccurate standard errors. For the analysis of the mortality data, an additional important consequence is that the accuracy of predictions of missing mortality rates may suffer. Predicting missing death rates is a primary application of modeling mortality data, as developing countries often lack reliable death registration data. It is possible that the residual dependence could be reduced by increasing the flexibility of the mean model, but since this is already fairly complex, we may instead prefer to represent residual dependence with a covariance model, leading to a general linear model for the data in which the mean function and residual covariance are estimated simultaneously.

The mortality data, like the residuals, can be represented as a 4-way array, each dimension of which corresponds to one of the factors of country, time period, sex and age. In the literature on multiway array data [see, e.g., [Kroonenberg \(2008\)](#)], each dimension is referred to as a mode of the array, so the 4-way array of mortality data consists of four modes. As described by [Hoff \(2011\)](#), a natural covariance model for a K -way data array is a separable covariance model, parameterized in terms of K covariance matrices, one for each mode of the array. If the array is also assumed to be normally distributed, the model is referred to as the array normal model and can be seen as an extension of the matrix normal model [[Dawid \(1981\)](#)].

Even though the separable covariance model is not a full, unstructured covariance model, the array normal likelihood is unbounded for many array dimensions, prohibiting the use of maximum likelihood methods [[Manceur and Dutilleul \(2013\)](#)]. Estimates of the array normal covariance parameters can still be obtained by taking a Bayesian approach [[Hoff \(2011\)](#)] or by using a penalized likelihood [[Allen and Tibshirani \(2010\)](#)]. However, the lack of existence of the maximum likelihood estimates (MLEs) indicates that the data is unable to provide information about all of the parameters. In this article we propose an alternative modeling approach that parameterizes the covariance matrix of each mode by a reduced rank matrix plus a diagonal matrix, referred to here as factor analytic covariance structure. This new model, called Separable Factor Analysis (SFA), is an extension of factor analysis to array-valued data and provides a parsimonious representation of mode-specific covariance in an array-valued data set. The reduction in the number of parameters by using covariance matrices with factor analytic structure leads to

existence of MLEs for the SFA parameters in many cases when the MLEs of the array normal parameters do not exist.

This article is outlined as follows: in the next section we introduce and motivate SFA, as well as discuss its properties and similarities to ordinary factor analysis. We describe two estimation procedures in Section 3: an iterative maximum likelihood algorithm and a Metropolis–Hastings sampler for inference in a Bayesian framework. A likelihood ratio testing procedure for selecting the rank of the factor model for each mode is also presented. In Section 4 the SFA model is used to analyze the HMD mortality data and its performance is compared to simpler covariance models in a simulation study. We illustrate how SFA uses estimated similarities between country mortality rates to provide imputations for countries missing mortality data for several years. This prediction method extends the approach taken in [Coale and Demeny \(1966\)](#), [Brass \(1971\)](#), [United Nations \(1982\)](#) and [Murray et al. \(2003\)](#), where one country’s mortality curve is modeled a function of another’s. Our approach is novel in that it estimates the covariance between mortality rates across all countries, time periods and sexes, and uses these relationships to impute missing death rates. We conclude with a discussion in Section 5.

2. Extending factor analysis to arrays.

2.1. Motivating separable factor analysis. Suppose Y is a K -way array of dimension $m_1 \times m_2 \times \cdots \times m_K$. We are interested in relating the data Y to explanatory variables X through the model $Y = M(X, \beta) + E$, where β represents unknown regression coefficients and E represents the deviations from the mean. As was discussed in the preliminary analysis of the mortality data, it is often unreasonable to assume the elements of E are independent and identically distributed.

In cases where there is no independent replication, estimation of the $\text{Cov}[E]$ can be problematic, as it must be based on essentially a single sample. One solution is to approximate the covariance matrix with one with simplified structure. A frequently used model in spatio-temporal analysis is a separable covariance model [[Stein \(2005\)](#), [Genton \(2007\)](#)], which estimates a covariance matrix for each mode of the array. It is written $\text{Cov}[\text{vec}(E)] = \Sigma_K \otimes \Sigma_{K-1} \otimes \cdots \otimes \Sigma_1$, where “vec” and “ \otimes ” denote the vectorization and Kronecker operators, respectively. In the context of the mortality data, this model contains a covariance matrix for country (Σ_c), time period (Σ_t), age (Σ_a) and sex (Σ_s). A separable covariance model with the assumption that the deviations are normally distributed, $\text{vec}(E) \sim \text{normal}(0, \text{Cov}[\text{vec}(E)])$, is an array normal model and was developed by [Hoff \(2011\)](#) as an extension of the matrix normal [[Dawid \(1981\)](#), [Browne \(1984\)](#), [Oort \(1999\)](#)].

The mode covariance matrices in the array normal model are not estimable for certain array dimensions using standard techniques such as maximum likelihood estimation [[Manceur and Dutilleul \(2013\)](#)]. However, often the covariance matrices of large modes can be well approximated by matrices with simpler structure.

A common approach in the social sciences to modeling the covariance of a high-dimensional random vector $x \in \mathbb{R}^p$ is to use a k -factor model, which parameterizes the covariance matrix as $\text{Cov}[x] = \Lambda \Lambda^T + D^2$, where $\Lambda \in \mathbb{R}^{p \times k}$, $k < p$, and D is a diagonal matrix [Spearman (1904), Mardia, Kent and Bibby (1979)]. We will refer to this model as single mode factor analysis, as it models the covariance among one set of variables. When the number of independent observations n is less than p , the sample covariance matrix is not positive definite and hence cannot be used as an estimate of $\text{Cov}[x]$. Nevertheless, under the assumption that x follows a multivariate normal distribution with known mean, the maximum likelihood estimate of the factor analytic covariance matrix exists if $k < \min(p, n)$ [Robertson and Symons (2007)].

We propose a submodel of the array normal model where each mode covariance matrix potentially has factor analytic structure. We call this model *Separable Factor Analysis* (SFA) and it is written as follows:

$$\begin{aligned} \text{vec}(E) &\sim \text{normal}(0, \text{Cov}[\text{vec}(E)]), \\ (1) \quad \text{Cov}[\text{vec}(E)] &= \Sigma_K \otimes \Sigma_{K-1} \otimes \cdots \otimes \Sigma_1, \\ \text{where } \Sigma_i &= \Lambda_i \Lambda_i^T + D_i^2 \quad \text{for } 0 \leq k_i < m_i \end{aligned}$$

and Σ_i is unconstrained (i.e., equals any positive definite matrix) if $k_i = m_i$. SFA models are characterized by the covariance matrix structure chosen for each mode and can be represented by a K -vector of ranks (k_1, \dots, k_K) , where k_i equals the rank of Λ_i if mode i 's covariance matrix has factor analytic structure and equals m_i if the mode covariance matrix is unstructured. Note that we consider the $k_i = 0$ case where the covariance matrix is diagonal. A key advantage of the SFA model over the array normal model is that empirical evidence has shown that MLEs of the SFA covariance parameters exist for array dimensions where the MLEs of the array normal unstructured covariance matrices do not exist.

2.2. Properties of SFA. In this section we relate the SFA parameters to those in ordinary factor analysis, discuss indeterminacies in the model, and interpret the SFA parameters when the true covariance matrix in each mode is unstructured. This requires the concept of array matricization. Here we follow the convention set in Kolda and Bader (2009) where the matricization of an array in the i th mode is defined as the $(m_i \times \prod_{j \neq i} m_j)$ matrix $Y_{(i)}$, whose column indices vary faster for earlier mode indices than later mode indices [see Kiers (2000) and De Lathauwer, De Moor and Vandewalle (2000) for alternative definitions].

Latent variable representation. Although the primary motivation for the factor analytic structure of the mode covariance matrices in SFA is parameter reduction, the SFA has a convenient latent variable formulation similar to that in single mode factor analysis. A single mode k -factor model for a sample of n mean-zero p -variate random vectors is written $\{x_1, \dots, x_n\} \sim \text{i.i.d. normal}(0, \Lambda \Lambda^T + D^2)$,

where $\Lambda \in \mathbb{R}^{p \times k}$ and D is a diagonal matrix. Defining $X = [x_1, \dots, x_n]$ as the $p \times n$ matrix of observations, this model has an equivalent latent variable representation as a decomposition into common latent factors, $Z = [z_1, \dots, z_n]$, and variable specific latent factors, $E = [e_1, \dots, e_n]$, as follows:

$$\begin{aligned}
 X_{p \times n} &= \Lambda_{p \times k} Z_{k \times n} + D_{p \times p} E_{p \times n}, \\
 \{z_1, \dots, z_n\} &\sim \text{i.i.d. normal}(0, I_k), \quad \text{Cov}[z_i, e_j] = 0_{k \times p} \\
 \{e_1, \dots, e_n\} &\sim \text{i.i.d. normal}(0, I_p).
 \end{aligned}
 \tag{2}$$

for all i, j ,

This representation expresses the j th observation of the i th variable X_{ij} as a linear combination of common latent factors z_j with coefficients given by the i th row of Λ , plus a single variable specific factor E_{ij} , scaled by the i th diagonal element of D .

A similar representation exists for each mode with a factor analytic covariance structure in the SFA model. Consider a mean-zero array Y and an SFA model with a factor analytic covariance matrix in the i th mode. Define \tilde{Y}^i to be the array obtained by standardizing Y with all but the i th mode's covariance matrix:

$$(3) \quad \text{vec}(\tilde{Y}^i) := \text{vec}(Y)(\Sigma_K^{-1/2} \otimes \dots \otimes \Sigma_{i+1}^{-1/2} \otimes I_{m_i} \otimes \Sigma_{i-1}^{-1/2} \otimes \dots \otimes \Sigma_1^{-1/2}).$$

It follows that

$$\begin{aligned}
 \{y_1, \dots, y_{m_{-i}}\} &\sim \text{i.i.d. normal}(0, \Lambda_i \Lambda_i^T + D_i^2) \quad \text{and} \\
 \tilde{Y}_{(i)}^i &= [y_1, \dots, y_{m_{-i}}] \stackrel{d}{=} \Lambda_i Z^i + D_i E^i,
 \end{aligned}
 \tag{4}$$

where $m_{-i} = \prod_{j \neq i} m_j$, and Z^i and E^i are $k_i \times m_{-i}$ and $m_i \times m_{-i}$, respectively, with the same distributional properties as Z and E in (2). The superscript i on $\tilde{Y}_{(i)}^i$ indicates the i th mode has not been standardized and the subscript (i) indicates the array has been matricized along the i th mode. The representation in (4) suggests the parameters $\{\Lambda_i, D_i\}$ can be viewed as single mode factor analysis parameters for the i th mode of the array when the covariance in all other modes has been removed. This representation is used in the parameter estimation methods in Section 3.

Model indeterminacies. SFA as parameterized in (1) has two indeterminacies, one of which is common to all factor models and one that is common to all array normal models. The first indeterminacy, which is also present in single mode factor analysis, is the orientation of the Λ matrices. The array covariance matrix in (1) is the same with mode i factor analytic parameters $\{\Lambda_i, D_i\}$ as it is with parameters $\{\Lambda_i G_i, D_i\}$, where G_i is any $k_i \times k_i$ orthogonal matrix. A common identifiable parameterization of Λ is that which restricts Λ to be lower-triangular with positive diagonal elements [Geweke and Zhou (1996), Carvalho et al. (2008); see Anderson

and Rubin (1956) for alternative identifiability conditions]. The formulation in (1) can be viewed as a model with parameter-expanded Λ_i matrices, similar to that in Bhattacharya and Dunson (2011), since it includes no identifiability constraints.

The second indeterminacy concerns the scales of the mode covariance matrices and stems from the model's separable covariance structure. For example, the transformation $\{\Sigma_i, \Sigma_j\} \mapsto \{c\Sigma_i, \Sigma_j/c\}$ does not affect the array covariance matrix in (1) for any $c > 0$. This scale nonidentifiability is eliminated if all mode covariance matrices are restricted to have trace equal to one and a scale parameter is included for the total variance of the array.

Pseudo-true parameters. In single mode factor analysis the goal is to represent the covariance among a large set of variables in terms of a small number of latent factors. However, often it is unlikely the true covariance matrix Σ has factor analytic structure. Therefore, there is interest in what k -factor analytic parameter values, Λ and D , best approximate the true covariance matrix Σ . These optimal parameter values, denoted $\bar{\Lambda}(\Sigma)$ and $\bar{D}(\Sigma)$, are those that minimize the Kullback–Leibler (KL) divergence between the k -factor model and the multivariate normal model. Minimizing the KL divergence is equivalent to maximizing the expected value of the k -factor analysis (FA) probability density with respect to the true multivariate normal (MN) distribution. Letting $X = [x_1, \dots, x_n]$ where $\{x_1, \dots, x_n\} \sim \text{i.i.d. normal}(0, \Sigma)$, $\bar{\Lambda}(\Sigma)$ and $\bar{D}(\Sigma)$ can be defined as

$$\begin{aligned} \{\bar{\Lambda}(\Sigma), \bar{D}(\Sigma)\} &:= \arg \max_{\Lambda, D} E_{MN}[p_{FA}(X|\Lambda, D)] \\ &= \arg \max_{\Lambda, D} c_{FA} - \frac{n}{2} \log(|\Lambda \Lambda^T + D^2|) - \frac{n}{2} \text{tr}[(\Lambda \Lambda^T + D^2)^{-1} \Sigma], \end{aligned}$$

where “tr” represents the trace operator and c_{FA} is a constant not depending on Λ or D . In the case of $k = 0$, the best approximating diagonal matrix \bar{D}^2 contains the diagonal elements of Σ .

Similarly, SFA is an approximation to a separable covariance structure where modes' true covariance matrices are unlikely to have factor analytic structure. Suppose the distribution of Y is array normal with mean zero and covariance matrices $\tilde{\Sigma} = \{\tilde{\Sigma}_i : 1 \leq i \leq K\}$. Consider a (k_1, \dots, k_K) SFA model for Y with parameters $\Lambda = \{\Lambda_i : 0 < k_i < m_i\}$, $D = \{D_i : 0 \leq k_i < m_i\}$ and $\Sigma = \{\Sigma_j : k_j = m_j\}$. The expected value of the SFA probability density with respect to the true array normal (AN) model is

$$(5) \quad E_{AN}[p_{SFA}(Y|\Sigma, D, \Lambda)] = c_{SFA} - \sum_{i=1}^K \frac{m}{2m_i} \log(|\Sigma_i|) - \frac{1}{2} \prod_{i=1}^K \text{tr}[\Sigma_i^{-1} \tilde{\Sigma}_i]$$

where $\Sigma_i = \Lambda_i \Lambda_i^T + D_i^2 \quad \text{for } 0 \leq k_i < m_i,$

c_{SFA} is a constant independent of the SFA parameters, and $m = \prod_{i=1}^K m_i$. Let $\bar{\Lambda}(\tilde{\Sigma})$, $\bar{D}(\tilde{\Sigma})$ and $\bar{\Sigma}(\tilde{\Sigma})$ denote the SFA parameters that maximize (5) and, hence,

provide the best approximation to the true separable covariance matrix based on $\tilde{\Sigma}$. It can be shown that for all appropriate i , j and k ,

$$(6) \quad \bar{\bar{\Lambda}}_i(\tilde{\Sigma}) = \bar{\Lambda}(\tilde{\Sigma}_i), \quad \bar{\bar{D}}_j(\tilde{\Sigma}) = \bar{D}(\tilde{\Sigma}_j) \quad \text{and} \quad \bar{\bar{\Sigma}}_k(\tilde{\Sigma}) = \tilde{\Sigma}_k.$$

This implies that the best factor analytic parameters, $\{\bar{\bar{\Lambda}}_i(\tilde{\Sigma}), \bar{\bar{D}}_j(\tilde{\Sigma})\}$, for a given mode in the SFA model are the closest fitting single mode factor analytic parameters to that mode's true covariance matrix, $\{\bar{\Lambda}_i(\tilde{\Sigma}_i), \bar{D}_j(\tilde{\Sigma}_i)\}$. As we might expect, the optimal values of the unstructured covariance matrices in the SFA model, $\bar{\bar{\Sigma}}_k(\tilde{\Sigma})$, are the modes' true covariance matrices $\tilde{\Sigma}_k$.

This implies that when the true model is array normal, the optimal SFA parameters for a given mode do not depend on the specified covariance structures in the other modes. Note that the scale indeterminacy of the covariance matrices is still present here, such that there is a set of optimal SFA parameter values that provide the same approximation. Asymptotically, as the number of replicates of the array increases, these optimal SFA parameter values are the limiting values of the SFA maximum likelihood estimates [White (1982)].

3. Estimation and testing. In this section we consider parameter estimation for the SFA model and propose a likelihood ratio testing procedure for selecting the ranks (k_1, \dots, k_K) . Two estimation methods are described here: an iterative algorithm for maximum likelihood estimation and a Metropolis–Hastings algorithm which approximates the posterior distribution of the parameters given the data. We present the case where the array has mean zero, however, both estimation methods and the testing procedure can be extended to allow for simultaneous estimation of a mean structure and the SFA covariance structure. Examples of such extensions are discussed in Section 4 for the mortality data.

3.1. Maximum likelihood estimation. While simultaneous maximization of the SFA log likelihood with respect to all parameters is difficult, maximizing the log likelihood with respect to a single mode's covariance parameters is feasible. Thus, we propose a block coordinate ascent algorithm that iteratively maximizes the SFA log likelihood over a single mode's covariance parameters using the latest values of all other modes' parameters and is guaranteed to increase the log likelihood at each step.

Let $\Lambda = \{\Lambda_i : 0 < k_i < m_i\}$, $\mathbf{D} = \{D_i : 0 \leq k_i < m_i\}$, and $\Sigma = \{\Sigma_j : k_j = m_j\}$ as in Section 2.2. Also, let $\Lambda_{-j} = \Lambda / \{\Lambda_j\}$ be the set Λ with Λ_j removed, and define \mathbf{D}_{-j} and Σ_{-i} analogously. The iterative maximum likelihood algorithm proceeds as follows:

0. Specify initial values for all covariance parameters $\{\Lambda, \mathbf{D}, \Sigma\}$.
1. For each mode $\{i : k_i = 0\}$, update the estimate of D_i .
2. For each mode $\{i : 0 < k_i < m_i\}$, update the estimates of Λ_i and D_i .

3. For each mode $\{i : k_i = m_i\}$, update the estimate of Σ_i .
4. Repeat steps 1–3 until a desired level of convergence is obtained.

The maximization of the SFA log likelihood for the updates in steps 1 and 3 are straightforward. Differentiating the log likelihood with respect to D_i or Σ_i , it can be shown the updates for steps 1 and 3, respectively, are

$$D_i^2 = \text{diag}\left(\frac{m_i}{m} \tilde{Y}_{(i)}^i (\tilde{Y}_{(i)}^i)^T\right) \quad \text{and} \quad \Sigma_i = \frac{m_i}{m} \tilde{Y}_{(i)}^i (\tilde{Y}_{(i)}^i)^T,$$

where the covariance matrices used to standardize Y in \tilde{Y}^i are the latest covariance matrix estimates and $m = \prod_i^K m_i$.

Estimation of a mode's factor analytic parameters in step 2 is more difficult, but can be accomplished using methods developed for single mode factor analysis. The SFA log likelihood as a function of the i th mode's factor analytic parameters is

$$(7) \quad \begin{aligned} \ell(\Lambda_i, D_i | \Sigma, \Lambda_{-i}, D_{-i}, Y) = & c_i - \frac{m}{2m_i} \log(|\Lambda_i \Lambda_i^T + D_i^2|) \\ & - \frac{1}{2} \text{tr}[(\Lambda_i \Lambda_i^T + D_i^2)^{-1} \tilde{Y}_{(i)}^i (\tilde{Y}_{(i)}^i)^T], \end{aligned}$$

where c_i is a constant not depending on Λ_i or D_i . The log likelihood for a single mode k_i -factor model for a $p \times n$ matrix X is written

$$(8) \quad \ell(\Lambda, D | X) = c - \frac{n}{2} \log(|\Lambda \Lambda^T + D^2|) - \frac{1}{2} \text{tr}[(\Lambda \Lambda^T + D^2)^{-1} X X^T].$$

Notice that the SFA log likelihood has the same form as that for single mode factor analysis where XX^T and n are replaced by $\tilde{Y}_{(i)}^i (\tilde{Y}_{(i)}^i)^T$ and m/m_i , respectively. Therefore, estimation methods for single mode factor analysis can be used to update Λ_i and D_i in step 2.

Numerous iterative algorithms have been developed to obtain the single mode factor model maximum likelihood estimates, however, many suffer from poor convergence behavior [Lawley (1940), Jöreskog (1967), Jennrich and Robinson (1969)]. An expectation–maximization (EM) algorithm was developed based on the model representation in (2) that treats Z as latent variables [Dempster, Laird and Rubin (1977), Rubin and Thayer (1982)]. The slow convergence of this algorithm led to expectation/conditional maximization either (ECME) algorithms, some of which rely on numerical optimization procedures [Liu and Rubin (1998), Zhao, Yu and Jiang (2008)]. Zhao, Yu and Jiang (2008) proposed an iterative algorithm that updates Λ , treating D as known, and then sequentially updates each diagonal element of D , treating Λ and all other elements of D as known. This algorithm has closed form expressions for all parameter updates and was shown to outperform the EM algorithm and its extensions in terms of convergence and computation time. For these reasons, we chose to use it for step 2 of the SFA estimation procedure.

Divergence of the SFA maximum likelihood algorithm, where the log likelihood continually grows at a nondecreasing rate, is evidence that the maximum likelihood estimates do not exist. While the update in step 1 for a mode with a diagonal covariance matrix is always well defined (i.e., the SFA log likelihood has a maximum in terms of D_i), step 2 of the algorithm for an unstructured covariance matrix is only well defined if $m_i < \prod_{j \neq i} m_j$. Similarly, step 3 is well defined for a mode i if $k_i < \text{rank}(\tilde{Y}_{(i)}^i (\tilde{Y}_{(i)}^i)^T)$. This latter requirement is effectively equivalent to $k_i < \min(m_i, \prod_{j \neq i} m_j)$ since $\tilde{Y}_{(i)}^i$ is unlikely to be rank deficient for a continuous array Y .

Since no identifiability constraints are placed on the mode covariance matrix scales or the factor analytic Λ_i parameters, the estimates that result from the above procedure correspond to a set of equivalent estimates obtained by reallocating the scale of the covariance matrices and rotating the Λ_i matrices. If interpretation of the Λ matrices is of interest, an identifiable parameterization can be obtained from the resulting estimate using the restrictions mentioned in Section 2.2. The iterative maximum likelihood estimation procedure can be extended to simultaneously estimate parameters β associated with an array mean model $M(X, \beta)$, if an additional step is added to the procedure that maximizes the normal log likelihood with respect to β and \tilde{Y} is redefined as the array that has been standardized by both the mean and covariance matrices.

3.2. Bayesian estimation. Maximum likelihood estimates of the SFA covariance parameters and any mean model parameters β can be obtained using the block coordinate ascent algorithm, however, obtaining standard errors of the estimates based on the Fisher information matrix requires complicated derivatives and large matrix inversion. While numerical estimation of the information matrix is possible [Spall (2005)], an alternative estimation procedure that readily provides parameter uncertainty estimates is that based on a Bayesian approach. In this framework inference for the parameters is based on the joint posterior distribution of the parameters given the data, $p(\Lambda, \mathbf{D}, \Sigma | Y) \propto p(Y | \Lambda, \mathbf{D}, \Sigma) p(\Lambda, \mathbf{D}, \Sigma)$, where $p(Y | \Lambda, \mathbf{D}, \Sigma)$ is the density of the (k_1, \dots, k_K) SFA model and $p(\Lambda, \mathbf{D}, \Sigma)$ is the joint prior distribution of the parameters. Again, we present this algorithm for the mean-zero array case, however, it can be trivially extended to include mean model parameters β .

Prior specification. In the absence of real prior information, we suggest a convenience prior composed of semiconjugate distributions for the parameters. For each mode i with an unstructured covariance matrix, the prior distribution for Σ_i^{-1} is Wishart($\kappa_i, \mathbf{I}_{m_i}$) with hyperparameter κ_i , where $\kappa_i \geq m_i$. For a mode i with a factor analytic covariance matrix, the joint prior distribution of $\{\Lambda_i, D_i\}$ is specified as follows:

$$(9) \quad \{\text{vec}(\Lambda_i) | D_i\} \sim \text{normal}(0, \mathbf{I}_{k_i} \otimes D_i^2),$$

$$(10) \quad \{D_i^{-2}[1, 1], \dots, D_i^{-2}[m_i, m_i]\} \sim \text{i.i.d. gamma}(v_0/2, \text{rate} = v_0 d_0^2/2),$$

where $v_0 > 0$ and $d_0^2 > 0$. A priori each mode's parameters are modeled as independent of all other modes' parameters given the hyperparameters v_0 , d_0^2 and $\{\kappa_i : k_i = m_i\}$.

The prior distribution of the factor analytic parameters given in (9)–(10) has nice properties related to the rotational indeterminacies in the $\mathbf{\Lambda}$ matrices. Recall that the SFA likelihood is invariant to rotation of Λ_i , meaning $L_{\text{SFA}}(\Lambda_i, D_i, \mathbf{\Sigma}, \mathbf{\Lambda}_{-i}, \mathbf{D}_{-i} | Y) = L_{\text{SFA}}(\Lambda_i G_i, D_i, \mathbf{\Sigma}, \mathbf{\Lambda}_{-i}, \mathbf{D}_{-i} | Y)$, where L_{SFA} is the SFA likelihood and G_i is any $k_i \times k_i$ orthogonal matrix. Integrating the joint prior distribution $p(\Lambda_i, D_i)$ over D_i , the marginal distribution of Λ_i is obtained and can be expressed as

$$p(\Lambda_i) \propto \prod_{j=1}^{m_i} [v_0 d_0^2 + \|\Lambda_i[j, :]\|^2]^{(k_i + v_0)/2},$$

where $\|\cdot\|^2$ denotes the Frobenius norm. Observe that $p(\Lambda_i) = p(\Lambda_i G_i)$, implying that the prior distribution is also invariant to rotations of Λ_i . This is a desirable property, as it indicates the prior does not favor one set of parameters over another if they are equivalent given the data (i.e., have the same SFA likelihood).

Metropolis–Hastings algorithm. The posterior distribution $p(\mathbf{\Lambda}, \mathbf{D}, \mathbf{\Sigma} | Y)$ is not a standard distribution and is difficult to sample from directly, so we propose approximating it using samples from a Metropolis–Hastings algorithm. This algorithm produces a Markov chain in $\{\mathbf{\Lambda}, \mathbf{D}, \mathbf{\Sigma}\}$, whose stationary distribution is equal to $p(\mathbf{\Lambda}, \mathbf{D}, \mathbf{\Sigma} | Y)$, and proceeds by iteratively proposing new values of each mode's parameters. Typically, in such an algorithm, proposals are accepted based on a probability that is a function of the data likelihood, prior and proposals, however, the parameter proposals in this algorithm all have acceptance probability equal to one. The algorithm can be described as follows:

0. Specify initial values for all covariance parameters $\{\mathbf{\Lambda}, \mathbf{D}, \mathbf{\Sigma}\}$.

1. For each mode $\{i : k_i = 0\}$, sample D_i from its full conditional distribution:

$$(11) \quad \begin{aligned} & \{D_i^{-2}[j, j] | \mathbf{D}_{-i}, \mathbf{\Lambda}, \mathbf{\Sigma}, Y\} \\ & \sim \text{gamma}((v_0 + m/m_i)/2, \text{rate} = (v_0 d_0^2 + S_i[j, j])/2) \end{aligned}$$

for $j \in \{1, \dots, m_i\}$ where $S_i = \tilde{Y}_{(i)}^i (\tilde{Y}_{(i)}^i)^T$.

2. For each mode $\{i : 0 < k_i < m_i\}$, sample new values of Λ_i and D_i using the following steps:

(a) Sample $\{\text{vec}(Z^i) | \Lambda_i, D_i, \tilde{Y}^i\} \sim \text{normal}(\text{vec}(\phi \Lambda_i^T D_i^{-2} \tilde{Y}_{(i)}^i), \mathbf{I}_{m/m_i} \otimes \phi)$ where $\phi = (\Lambda_i^T D_i^{-2} \Lambda_i + \mathbf{I})^{-1}$.

(b) Sample

$$\begin{aligned} & \{\text{vec}(\Lambda_i) | Z^i, Y, \mathbf{D}, \mathbf{\Lambda}_{-i}, \mathbf{\Sigma}\} \\ & \sim \text{normal}(\gamma(Z_{(i)}^i \otimes D_i^{-2}) \text{vec}(\tilde{Y}_{(i)}^i), \gamma = [(Z_{(i)}^i (Z_{(i)}^i)^T + \mathbf{I}_{m_i}) \otimes D_i^{-2}]^{-1}). \end{aligned}$$

- (c) Sample $\{\text{vec}(Z^i) | \Lambda_i, D_i, \tilde{Y}^i\}$ as in 2(a).
- (d) Sample the elements of D_i^2 independently from

$$\{D_i^{-2}[j, j] | Z^i, Y, \mathbf{D}_{-i}, \Lambda, \Sigma\}$$

$$\sim \text{gamma}((v_0 + m/m_i + k_i)/2, \text{rate} = (v_0 d_0^2 + J[j, j] + \|\Lambda_i[j, \cdot]\|^2)/2),$$

where $J = (\tilde{Y}_{(i)}^i - \Lambda_i Z^i)(\tilde{Y}_{(i)}^i - \Lambda_i Z^i)^T$ and $\|\cdot\|^2$ denotes the Frobenius norm.

- 3. For each mode $\{i : k_i = m_i\}$, sample Σ_i from its full conditional distribution:

$$(12) \quad \{\Sigma_i^{-1} | \mathbf{D}, \Lambda, \Sigma_{-i}, Y\} \sim \text{Wishart}(\kappa_i + m/m_i, (\mathbf{I}_{m_i} + \tilde{Y}_{(i)}^i (\tilde{Y}_{(i)}^i)^T)^{-1}).$$

- 4. Repeat steps 1–3 until a sufficiently accurate approximation of the posterior distribution is obtained.

The covariance matrices used to standardize Y in \tilde{Y}^i in each of the updates above are the most current parameter updates. The updates of the factor analytic parameters $\{\Lambda_i, D_i\}$ in step 2 are based on the latent variable representation of SFA introduced in (4), which expresses Y as $\tilde{Y}_{(i)}^i \stackrel{d}{=} \Lambda_i Z^i + D_i E^i$, where the elements of Z^i and E^i are independent standard normal random variables. Proof that the acceptance probabilities are equal to one for the proposals of Λ_i and D_i is provided in [Appendix](#). Note that the Z^i variables involved in step 2 are not included as parameters, as is done in a parameter-augmented sampler, but instead are simply used to propose new factor analytic parameters.

Since no identifiability restrictions are placed on the scales of the mode covariance matrices or on the orientation of the Λ matrices, the model can be viewed as a parameter-expanded model, similar to the single-mode factor model in [Bhattacharya and Dunson \(2011\)](#). Working with this parameterization greatly simplifies the estimation procedure and avoids the index order dependence issues that arise from performing estimation with an identifiable parameterization where choice of the index order within a mode becomes an important modeling decision [see [Carvalho et al. \(2008\)](#) and [Bhattacharya and Dunson \(2011\)](#) for further discussion]. Note that identifiability of the Λ matrices is irrelevant when the goal in the analysis is covariance matrix estimation, mean model inference or prediction of missing values. However, if interpretation of the factor analytic parameters is of interest, the samples from the Markov chain can be transformed to identifiable parameters using the restrictions mentioned in [Section 2.2](#). Similarly, posterior inference on the total variance of the array can be based on the combined scales of each sample of covariance matrices, obtained by scaling all mode covariance matrices to have trace one.

Unlike in the frequentist setting where divergence of the maximum likelihood estimation procedure indicates a lack of information in the data about the parameters, the posterior distribution of the parameters given the data will always exist.

Although Bayesian parameter estimates are available, we should be aware of what information the estimates reflect. Extreme similarity between the prior distribution and the posterior distribution suggests that little information is gained from the data and inference based on the posterior distribution is primarily a reflection of the information in the prior.

Hyperparameters. When there is little prior information about the parameters, it is common to choose hyperparameter values that result in diffuse prior distributions. We propose $v_0 = 3$ and $\kappa_i = m_i + 2$ for $\{i : k_i = m_i\}$ as default values, as they correspond to prior distributions whose first moments are finite and represent some of the most diffuse distributions in the Wishart and gamma families, respectively. They also have the following properties:

$$(13) \quad E[\Sigma_i] = I_{m_i}, \quad E[D_i^2[j, j]] = 3d_0^2, \quad E[\text{tr}(\Lambda_i \Lambda_i^T)] = 3k_i m_i d_0^2.$$

Prior information about specific mode covariance matrices may be limited, however, an estimate $\hat{\psi}$ of the total variance of the array, $\psi = \text{tr}(\text{Cov}[\text{vec}(Y)]) = \prod_{i=1}^K \text{tr}(\Sigma_i)$, may be available. This information can improve parameter estimation by centering the prior distribution of the total variance of the array around a reasonable value. Based on the expectations in (13) and the independence of the mode covariance matrices in the prior, the prior expected value of the total variance of the array will equal the estimate, $E[\text{tr}(\text{Cov}[\text{vec}(Y)])] = \hat{\psi}$, if

$$(14) \quad d_0^2 = \hat{\psi}^{1/R} \left[\left(\prod_{j: 0 < k_j < m_j} [k_j + 1] \right) \left(\prod_{i=1}^K m_i \right) 3^R \right]^{-1/R},$$

where $R = \sum_{i=1}^K \mathbb{1}\{0 \leq k_i < m_i\}$ is the number of modes with factor analytic covariance structure. In the event there is no prior knowledge about ψ and it is not of interest in the analysis, we propose taking an empirical Bayes approach and obtaining an estimate of it based on the data. Possible estimates include $\hat{\psi} = \|Y\|^2$ or $\hat{\psi} = \|Y - \widehat{M}(X, \beta)\|^2$ if the model has a nonzero mean. In the latter case, $\widehat{M}(X, \beta)$ represents an initial estimate of the mean, such as the ordinary least squares estimate. A similar approach was suggested in Hoff (2011) for the array normal model.

3.3. Accommodating missing data. Mortality information is limited for many undeveloped countries that do not have reliable death registration data. Thus, it is not uncommon to be missing a country's death rates for specific ages or at all ages in a given year. Both the maximum likelihood and Bayesian estimation procedures can be modified to accommodate missing data, however, such modifications are often computationally expensive.

In the maximum likelihood estimation, expectation–maximization algorithms are often employed to obtain parameter estimates in the presence of missing data. The proposed coordinate ascent algorithm with an additional step that computes the expectation of the log probability of the data under the SFA model given the

current values of the parameters and observed data would correspond to an expectation/conditional maximization (ECM) algorithm [Meng and Rubin (1993)]. Allen and Tibshirani (2010) discuss such an algorithm in detail for the matrix normal ($K = 2$), when additional penalties are placed on the covariance matrices, and find that such an algorithm is not computationally feasible for high-dimensional data due to the complicated expectations required. An analogous algorithm for array data and the SFA model would likely suffer from the same burdens. Allen and Tibshirani (2010) further propose an approximation of the ECM procedure to obtain estimates of the missing values that involves the following three steps: initialize the missing values, compute maximum likelihood estimates of the parameters, and use an iterative procedure to compute the expectation of the missing values conditional on the observed data and parameters. While an analogous approximation could be developed for the SFA model, the procedure for the matrix case lacks theoretical guarantees and was also shown to require complete iteration of all three steps to obtain estimates that sufficiently match those from the ECM.

Accommodating missing data in a Bayesian framework is straightforward and provides predictive distributions for the missing values. The proposed Metropolis–Hastings algorithm can easily be adapted by including additional steps that sample portions of the missing data from their full conditional distributions. Although the full conditional distribution of all missing data elements conditional on the parameters and observed data can be expressed as a multivariate normal, calculating the parameters for this distribution is often computationally expensive due to the large matrices involved in computing the distribution’s covariance matrix. However, using results from Hoff (2011), the conditional distribution of a slice of an array (where one mode index is fixed) can be written as an array normal distribution. The missing data within the slice conditional on the observed data in the slice follows a multivariate normal distribution, which can be sampled from to update the missing values. Calculating the conditional distribution of the missing elements in a slice of the array via this two-step conditioning procedure (once for the slice and once for the missing data within the slice) circumvents computation with unnecessarily large matrices. Allen and Tibshirani (2010) used a similar procedure to obtain expected values of missing elements in a matrix normal model in their ECM approximation. Section 4 illustrates the use of a Metropolis–Hastings algorithm that has been modified to accommodate and provide predictions for missing mortality data.

3.4. Testing for the mode ranks. It is often difficult to choose the number of factors for a single mode factor model. This problem is only more pronounced in the array case where the rank k_i must be specified for each mode. As in single mode factor analysis [Mardia, Kent and Bibby (1979)], a likelihood ratio test can be constructed to test between nested SFA models with ranks (k_1, \dots, k_K) and (k_1^*, \dots, k_K^*) , where $k_i \leq k_i^*$ for all i . However, due to the large number of possible combinations of ranks, choosing the ranks using these likelihood ratio

tests is challenging. In the Bayesian framework, alternative approaches to specifying the factor rank in single mode factor analysis are to estimate it along with the model parameters using MCMC estimation methods such as reversible jump [Lopes and West (2004)] and path sampling [Lee and Song (2002)], or specify an infinite number of factors [Bhattacharya and Dunson (2011)]. While it is possible to extend these methods to the array case and SFA model, they would greatly increase the computational complexity of estimation. Maximum likelihood parameter estimates via the coordinate ascent algorithm can be obtained in minutes even for a large array such as the mortality data, while the MCMC Bayesian estimation procedure can take hours to run depending on the size of the array and complexity of the mean model. Therefore, here we propose an alternative mode-by-mode rank selection procedure based on the maximum likelihood parameter estimates that suggests when the rank specified for a given mode is sufficient for capturing the dependence within that mode.

As in Section 2.2, let \tilde{Y} denote a K -way array that has been standardized by all mode covariance matrices. To determine whether the dependence in mode i is captured by a proposed (k_1, \dots, k_K) SFA model, we can compute \tilde{Y} using the SFA mode covariance matrix estimates as in (1) and test whether the covariance matrix of the rows of $\tilde{Y}_{(i)}$ equals the identity. The likelihood ratio test statistic for this test is

$$(15) \quad t = \frac{m}{m_i} [\text{tr}(\hat{V}) - \log |\hat{V}| - m_i],$$

where $\hat{V} = \frac{m_i}{m} \tilde{Y}_{(i)} \tilde{Y}_{(i)}^T$, and has an asymptotic $\chi^2_{m_i(m_i+1)/2}$ distribution under the null hypothesis of an identity row covariance matrix. Note that rejecting this test suggests that a more complex covariance structure is needed for the i th mode. This motivates the following rank selection procedure for the entire array:

0. Consider an SFA model with all $k_i = 0$. Obtain estimates of the covariance parameters D_i using the maximum likelihood procedure in Section 3.1 and compute \tilde{Y} using the estimates.

1. For each mode i , define $R_i = \text{Cov}[\text{vec}(\tilde{Y}_{(i)})]$ and test $H_0: R_i = \mathbf{I}_{m/m_i} \otimes \mathbf{I}_{m_i}$ vs $H_1: R_i = \mathbf{I}_{m/m_i} \otimes V$, where V is an unstructured $m_i \times m_i$ covariance matrix, using a likelihood ratio test with test statistic given by (15).

2. If the test for mode i rejects and

$$\begin{cases} \delta(m_i, k_i + 1) > 0, & \text{increase the rank } k_i \text{ by one,} \\ \delta(m_i, k_i + 1) \leq 0, & \text{set the rank equal to } m_i. \end{cases}$$

If the test for mode i does not reject, fix k_i at its current value and perform no further tests on the mode. Obtain maximum likelihood estimates $\{\hat{\Sigma}, \hat{\mathbf{A}}, \hat{\mathbf{D}}\}$ for an SFA model with the new ranks (k_1, \dots, k_K) and compute \tilde{Y} using these new estimates.

3. Repeat steps 1–2 until each mode has failed to reject a test.

The suggested ranks (k_1, \dots, k_K) are those that result at the end of this procedure. In step 2 $\delta(m, k) = [(m - k)^2 - (m + k)]/2$ represents the reduction in the number of parameters when using a k -factor analytic covariance matrix instead of an $m \times m$ unstructured covariance matrix. When $\delta(m, k) \leq 0$, a factor analytic covariance structure no longer provides a reduction in the number of covariance parameters and an unstructured covariance matrix should be specified. Note that if a nonzero mean model was specified, its parameters β would be simultaneously estimated with the covariance matrices at each iteration of the procedure.

The maximum number of SFA models that could be considered using this procedure is bounded by the largest value of k_l such that $\delta(m_l, k_l) > 0$, where l denotes the array mode with the largest dimension m_l . To control the type I error rate of all mode tests to be α for an iteration of steps 1 and 2, the level of each mode test can be set to α^r , where r is the number of modes being tested (i.e., the number that have rejected every test thus far). An example of this procedure is described in Section 4.2 for the mortality data.

4. Application to Human Mortality Database death rates. In this section we analyze death rates from the Human Mortality Database (HMD) using an SFA model, compare our model to other covariance models, and obtain predictions for over four hundred missing death rates. We focus on death rates for 5-year time periods for populations corresponding to combinations of sex, age and country of residence. Specifically, we consider death rates from 1960 to 2005 for 40 countries, both sexes and twenty-three age groups, $\{0, 1-4, 5-9, 10-14, \dots, 105+\}$. These data are represented in a 4-way array $Y = \{y_{ctsa}\}$ of dimension $(40 \times 9 \times 2 \times 23)$, where y_{ctsa} is the log death rate for country c , time period t , sex s and age group a . We will refer to a set of age-specific death rates for a combination of country, time period and sex as a mortality curve.

We begin this section by introducing a flexible piecewise polynomial mean model and show the residuals from this mean model exhibit dependence within each mode: age, time period, country, and sex. Using the likelihood ratio testing procedure presented in Section 3.4, we select ranks for an SFA model. The resulting SFA model is compared to models with simpler covariance structures using out-of-sample cross-validation and is used to impute multiple years of missing death rates for Chile and Taiwan.

4.1. Mean model selection. As discussed in the [Introduction](#), existing methods for analyzing mortality data model the death rates for different countries, sexes and/or time periods separately. Such an approach can be inefficient due to the strong similarities between mortality rates within the same country, time period and sex. For this reason, we propose a new joint mean model for the HMD data that exploits these relationships between mortality rates that share levels of one or more of these factors.

Figure 1 shows mortality curves defined by the twenty-three age-specific death rates for the United States and Sweden in four time periods. The large spikes at age zero represent infant mortality, and the humps around age twenty, which are especially evident in males, are attributed to teenage and young adult accident mortality. The overall shapes of the mortality curves for each sex are similar across countries and time periods, however, Sweden has considerably lower mortality levels during childhood and young adulthood compared to the United States. This suggests that a mean model for the data should allow for different curves across countries and time periods, yet still take advantage of the similarity between death rates within the same country, age group or sex.

Drawing from the mortality literature and viewing mortality rates as function of age, we propose the following piecewise polynomial (PP) mean model:

$$(16) \quad E[y_{ctsa}] = \begin{cases} \phi^0, & a = 0, \\ \phi^1 + a\phi^{11} + a^2\phi^{12}, & 1 \leq a < 20, \\ \phi^2 + a\phi^{21} + a^2\phi^{22} + a^3\phi^{23}, & 20 \leq a, \end{cases}$$

$$\phi^i = \alpha_c^i + \beta_t^i + \gamma_s^i.$$

This model distinguishes between the infant, childhood and adult stages of mortality by fitting each with a separate polynomial, whose coefficients are composed of additive effects for country, time period and sex. The constant term at age zero is necessary to model the steep decline from infant mortality to child mortality that is not well represented by a low degree polynomial.

One of the most commonly used models in demography for age-specific mortality measures is the Heligman–Pollard (HP) model [Heligman and Pollard (1980)]. This model also uses eight parameters to parameterize a mortality curve, however, it is typically used to model each mortality curve individually and is nonlinear and nonconvex in the parameters, making estimation extremely difficult [Hartmann (1987), Congdon (1993)]. When the HP model is fit separately to the 684 HMD mortality curves for the 38 countries missing no death rates using OLS, it requires over 5400 parameters and under the assumption of independent, homoscedastic errors has a Bayesian Information Criterion (BIC) value of $-17,288$. However, when the PP model is fit jointly to the same data using OLS, it contains 376 parameters and has a BIC of $-52,436$. Due to the relative parsimony of the PP model, its superior fit in terms of BIC, and its straightforward estimation as a linear model, it was selected as the mean model.

4.2. Excess dependence and SFA rank selection. The piecewise polynomial model in (16) is extremely flexible. To investigate its fit to the HMD mortality rates, we focused on a subset of the original data that contains no missing observations, specifically the $(38 \times 9 \times 2 \times 23)$ array that does not contain death rates for Chile or Taiwan. The OLS fit explains 99.5% of the variation in the mortality rates (coefficient of determination, $R^2 = 0.995$). However, there is interest in

whether excess correlation exists in the residuals since modeling it can improve both predictions of missing values and the efficiency of parameter estimates. OLS estimates of the parameters in (16) are equivalent to maximum likelihood estimates assuming independent normal errors. To evaluate this latter assumption, we computed the empirical correlation matrix for each mode based on the mean model residuals.

As mentioned in the [Introduction](#), the distributions of these correlations have substantially more large positive values than would be expected under the assumption of independent errors. For example, speaking specifically to the temporal dependence, the average correlation between adjacent time periods, those one time period apart and those two periods apart is 0.79, 0.54 and 0.26, respectively. The first two principal components of each correlation matrix are shown in Figure 2. The horseshoe pattern in the time period principal components and the clustering of countries within the same region suggest temporal and geographic trends in the data are not captured by the mean [[Diaconis, Goel and Holmes \(2008\)](#)]. This indicates that even though the mean model contains several country-specific and time period-specific parameters, similarities between the mortality curves of certain countries and time periods is not being accounted for. The mean model already contains over 370 parameters and it would likely be nontrivial to modify it to capture all of the dependence seen in the residuals. For this reason, we consider incorporating a covariance structure to model this excess dependence. An array normal separable covariance structure could be specified, however, it would add over one thousand parameters to the model. Therefore, we instead consider an SFA model for the data with the PP mean with the belief that the residual dependence within some modes may be well approximated by a low rank factor analytic structured covariance matrix.

As outlined in Section 3.4, suggestions for the SFA ranks can be obtained from a repeated likelihood ratio testing procedure. For the mortality data, we consider (k_c, k_t, k_s, k_a) SFA models where the ranks correspond to the country, time period, sex and age covariance matrices, respectively. The standardized residual array \tilde{Y} for a (k_c, k_t, k_s, k_a) SFA model is defined as $\text{vec}(\tilde{Y}) = (\text{vec}(Y) - \text{vec}(\widehat{M}))(\widehat{\Sigma}_a^{-1/2} \otimes \widehat{\Sigma}_s^{-1/2} \otimes \widehat{\Sigma}_t^{-1/2} \otimes \widehat{\Sigma}_c^{-1/2})$, where \widehat{M} represents the PP mean model estimate and $\widehat{\Sigma}_i$ is the SFA mode i covariance matrix estimate from the maximum likelihood estimation procedure (modified to estimate the mean model and covariance parameters simultaneously). The results from the iterative testing procedure are shown in Table 1. The first step in this process is to consider a $(0, 0, 0, 0)$ SFA model where all covariance matrices are diagonal. The likelihood ratio test statistics for this model are shown in the first row of Table 1 and the corresponding 0.05 level critical values are shown in the last row. Since the test for each mode rejects the null hypothesis of independent, variance one errors, the rank of each mode is increased by one in the subsequent model, except for that for the sex mode. A rank one factor analytic structure for a (2×2) covariance matrix has more

TABLE 1

Iterative testing procedure for the SFA ranks. Each row represents an SFA model and each entry is the likelihood ratio test statistic based on (15). The 0.05 level critical value for each test is given in the last row. A box around a statistic indicates that the mode does not reject the test for the first time and the rank is fixed in subsequent models

SFA ranks (k_c, k_t, k_s, k_a)	Likelihood ratio test statistic			
	Country	Time period	Sex	Age
(0, 0, 0, 0)	21,852	14,482	702	27,883
(1, 1, 2, 1)	9526	5853	0	14,451
(2, 2, 2, 2)	4425	1722	0	6374
(3, 3, 2, 3)	2776	716	0	3762
(4, 4, 2, 4)	1946	17	0	2422
(5, 4, 2, 5)	1556	14	0	1833
(6, 4, 2, 6)	1287	10	0	1340
(7, 4, 2, 7)	1040	8	0	967
(8, 4, 2, 8)	892	5	0	540
(9, 4, 2, 9)	762	8	0	363
(9, 4, 2, 10)	737	8	0	257
$\chi^2_{0.95}$ critical value	805	62	8	316

parameters than an unstructured covariance matrix, so the sex covariance matrix is unstructured in the next model. A box around a test statistic in the table indicates the mode failed to reject the test for the first time. Recall that when a mode's test does not reject, the rank for that mode is fixed and not increased in later models. The table shows where the sex, time period, country and age ranks become fixed at two, four, nine and ten, respectively. Observe that after a mode's rank is fixed, the test statistic for that mode stays below the critical value in all subsequent models. Although the mode tests are not independent of the covariance structures fit in the other modes, this consistency supports the suggested ranks.

4.3. Out-of-sample cross-validation. We evaluate the SFA model by comparing its out-of-sample predictive performance with two simpler covariance models that share the same PP mean model. The three covariance models considered are the following:

M1: Independent and identically distributed (i.i.d.) model.

M2: Time covariance model.

M3: SFA model (9, 4, 2, 10).

M1 corresponds to the conventional ordinary least squares (OLS) approach where all errors are assumed independent and identically distributed with a common variance. In general, country mortality rates are relatively stable over time, so if the

observed mortality for a given country, year and age deviates from the mean model in one year, it is likely the observations deviate in the same direction in neighboring years. Thus, a natural first step to incorporating a covariance model is to consider an unstructured covariance matrix for time as in M2.

Fifty cross-validations were performed by removing a random 25% of the array, estimating each of the three covariance models with the PP mean model on the remaining data, and computing the mean squared error (MSE) between the observed values and the predicted values for the withheld entries. The predicted values for M1 are those from the OLS PP mean estimate. For M2 and M3, the predictions are the posterior mean estimates of the missing values from the Bayesian estimation procedure described in Section 3.2, modified to accommodate missing data.

A prior distribution for the parameters in the PP model is needed to perform simultaneous Bayesian estimation for the mean and covariance parameters. The prior on the vector of PP coefficients is a mean-zero normal distribution with covariance matrix $m(X^T X)^{-1}$, where X is the design matrix for the PP model for $\text{vec}(Y)$ and $m = \prod_{i=1}^K m_i$. This is a relatively uninformative prior, as it is over 30 times more diffuse than the corresponding unit-information prior [Kass and Wasserman (1995)]. The hyperparameters were specified as described in Section 3.2 where the mean estimate \hat{M} used in $\hat{\psi}$ is the OLS estimate of the PP model. Since M2 has no modes with factor analytic structure, the prior on the time covariance matrix is

$$\Sigma_t^{-1} \sim \text{Wishart}\left(n_t = m_t + 2, \frac{m\hat{\psi}}{m_t} I_{m_t}\right).$$

This specification is necessary to preserve the property that $E[\text{tr}(\text{Cov}[\text{vec}(Y)])] = \hat{\psi}$ under the prior.

The results from the 50 cross-validations are shown in Table 2. The MSE for the SFA model was less than that of the time covariance model for each of the 50 cross-validations, and the MSE for the time covariance model was always less than that of the i.i.d. model. In terms of average MSE, both the time covariance model and the SFA model significantly improve upon the i.i.d. model, and the SFA model outperforms the time covariance model by nearly a factor of two. This is evidence that even with the extremely flexible PP mean model, the SFA covariance structure still improves model fit, as it is able to estimate the similarity between mortality

TABLE 2
Average and standard deviation of the mean squared errors from 50 out-of-sample cross-validation experiments

	M1 (i.i.d.)	M2 (time covariance)	M3 (SFA)
Average MSE	0.02996	0.00729	0.00385
Standard deviation of MSEs	0.00084	0.00049	0.00034

rates across countries, time periods, age groups and sexes, and use this information in its predictions.

4.4. Prediction of missing data. The imputation of missing death rates is an important application of modeling mortality data, as information is often incomplete for countries lacking accurate death registration data. We now consider the original $(40 \times 9 \times 2 \times 23)$ array of mortality rates with observations for Chile and Taiwan. Seven time periods of mortality information are missing for Chile (1960–1995) and two time periods for Taiwan (1960–1970), combining for a total of 414 missing entries in the array. This larger data array contains only two additional countries, so the SFA ranks (9, 4, 2, 10) selected for the reduced data are used again here. Predictions for the missing death rates were based on samples from the Metropolis–Hastings procedure, for which the effective sample sizes for the Monte Carlo estimates of all missing values were greater than 500.

In the left column of Figure 3, posterior mean predicted death rates and 95% prediction intervals are shown for Chile in 1990 and Taiwan in 1965. To visualize the impact of the SFA covariance model on the predicted death rates, we

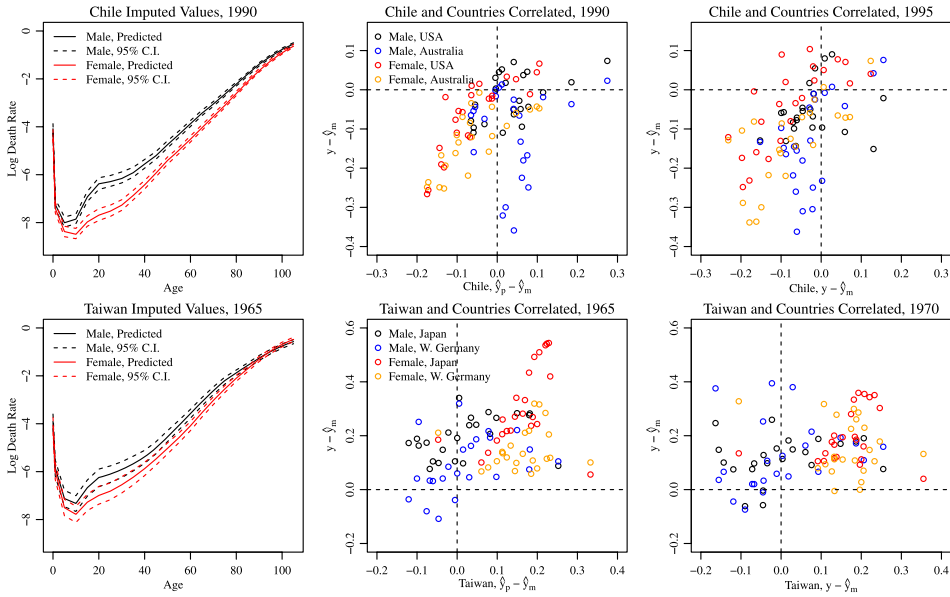


FIG. 3. The first column of plots shows the predicted values and corresponding 95% prediction intervals for the missing death rates for Chile and Taiwan. The middle column shows the difference between the posterior mean predicted value and the piecewise polynomial mean function fitted value, $\hat{y}_p - \hat{y}_m$, for Chile and Taiwan, along with empirical mean model residuals, $y - \hat{y}_m$, for countries that are highly correlated with them in the posterior mean country covariance matrix. The last column contains empirical residuals for the following time period when Chile and Taiwan mortality is observed.

investigate the difference between the SFA predicted values and the fitted values based on the PP mean model. The SFA predictions, \hat{y}_p , are conditional on the observed mortality rates for all other countries and time periods, while the mean model fitted values, \hat{y}_m , are based only on the estimate of the PP mean model. These differences, $\hat{y}_p - \hat{y}_m$, are called “predictive residuals” since they are based on predicted values instead of observed values and illustrate the changes in the predicted values by using the SFA covariance model compared to only using the mean model. The empirical residuals based on the PP mean model, $y - \hat{y}_m$, were computed for the United States and Australia, the two countries most highly correlated with Chile (estimated correlations around 0.40). These residuals were also computed for Japan and West Germany, the two countries most highly correlated with Taiwan (estimated correlations of around 0.13). The middle column of Figure 3 shows the predictive residuals for Chile and Taiwan and the empirical residuals for these select countries. The last column contains the empirical residuals in 1995 and 1970 when mortality information is available for all countries. Observe that the plots in the middle column and last column are similar, demonstrating an overall positive association for both sexes and all country pairs. This demonstrates how the model uses the relationship between the empirical residuals of Chile and other countries to predict Chile’s deviations from the mean model in years when Chile data is missing. The ability to draw information across multiple country, year and sex residuals to impute missing values is a critical strength of the SFA model that is not shared by other mortality models or simpler covariance structures.

The empirical residuals for Chile shown in the last column may not show as strong of an association with the United States and Australia as one would expect from a posterior mean correlation estimate of 0.4. However, recall that the estimate of the country correlations is based on all time periods, sexes and ages. Although we show adjacent time periods in this plot, the correlation between the country residuals in the period adjacent to the missing time period and the correlations in time periods furthest away are weighted equally in the estimate of the country correlation, and hence weighted equally in the imputation of the missing data. This property is a consequence of the separability of the SFA covariance matrix. A more complicated nonseparable covariance model would be required for the correlations between countries, ages and sexes to be differentially weighted in the imputation based on the proximity of the observed data to the missing data.

5. Discussion. In this article we introduced the separable factor analysis model for array-valued data. Unlike the array normal model where all mode covariance matrices are unstructured, SFA parameterizes mode covariance matrices by those with factor analytic structure. Using covariance matrices with reduced structure decreases the number of parameters in the model considerably and allows mode covariance matrices to be estimated using maximum likelihood methods for any array dimension. Including a covariance structure in a model for multiway data

can drastically improve mean model parameter estimation and missing data predictions in situations where dependence exists within modes that is not captured by the mean model. In an out-of-sample cross-validation study with a large set of mortality data, the SFA model was shown to have superior fit compared to models with simpler covariance structures, even in the presence of an extremely flexible mean model. The SFA model was also shown to estimate which countries have similar deviations from the mean model and was able to use this information in its predictions of multiple years of missing death rates.

We propose reducing the number of covariance parameters in the array normal model by modeling mode covariance matrices with factor analytic structure, however, other simplified covariance structures are possible. For example, the Bayesian graphical lasso [Wang (2012)] and covariance matrices derived from Gaussian graphical models [Wang and West (2009), Dobra, Lenkoski and Rodriguez (2011)] estimate or assume conditional independencies between pairs of indices (reflected by zeros in the precision matrix) and are commonly used to represent covariance among index sets which have a natural spatial structure. Similarly, for temporal data, a covariance matrix derived from an autoregressive model is commonly used. Nevertheless, in many cases there may not be a clear choice of a reduced structured covariance matrix, and in these cases specifically we propose the factor analytic structure as an agnostic approach to covariance matrix parameter reduction. It was suggested that an autoregressive covariance structure may be appropriate for the time and/or age mode covariance matrices in the mortality data application in Section 4. Figure 4 shows boxplots of the residual correlations discussed in the Introduction, grouped by time period lag and age group lag. If an autoregressive model of order-1 were appropriate for either of these modes, we would expect the correlations to monotonically decrease toward zero with lag. However, the negative correlations exhibited by the time periods and asymptoting behavior of the age correlations cannot be captured by such structure. This illustrates that even in instances when traditional covariance structures may seem appropriate, they may

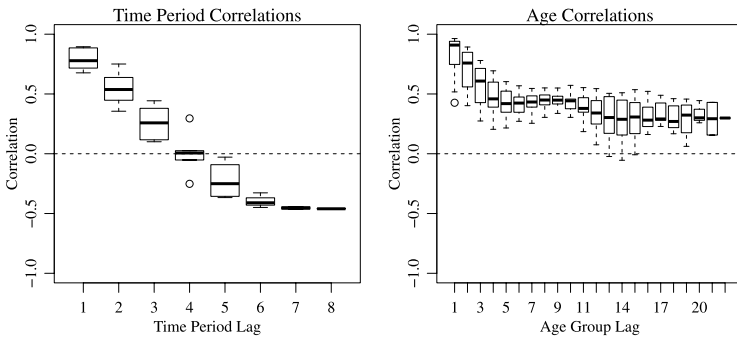


FIG. 4. Sample residual correlations between time periods and age groups from the OLS fit of the model in (16) grouped by lag.

not be given the mean model, and it may be preferable to take a more agnostic approach to modeling and assume a factor analytic structure.

A trivial extension of the SFA model would be to relax the separability assumption for groups of modes of the array. For example, in the mortality data, if we believed the residual correlation between sexes and across time periods was not separable, the four-way array could be unfolded into a three-way array whose dimensions are age, country and time period/sex. An SFA model could then be specified for the resulting three-way array. Relaxing the separability assumption between some modes is likely to improve model fit for specific data sets when the assumption of separability is not appropriate, however, this also increases the potential number of covariance parameters in the corresponding array normal model. Therefore, in order to gain a sufficient reduction in the number of covariance parameters, a small factor model rank is likely to be necessary for combined modes. Investigation of the empirical residual correlations may help suggest when relaxing the separable assumption is warranted.

APPENDIX: SAMPLING Λ AND D

Let Λ_i^* be the proposed value of Λ that results from 2(a–b). The acceptance probability for this proposal is

$$\begin{aligned}\alpha(\Lambda_i^*, \Lambda_i) &= \frac{p(\Lambda_i^*|Y, \Lambda_{-i}, D, \Sigma)p(\Lambda_i|\Lambda_i^*, D, \Sigma, \Lambda_{-i}, Y)}{p(\Lambda_i|Y, \Lambda_{-i}, D, \Sigma)p(\Lambda_i^*|\Lambda_i, D, \Sigma, \Lambda_{-i}, Y)} \\ &= \frac{p(Y|\Lambda_i^*, \Lambda_{-i}, D, \Sigma)p(\Lambda_i^*|D_i)p(\Lambda_i|\Lambda_i^*, D, \Sigma, \Lambda_{-i}, Y)}{p(Y|\Lambda_i, \Lambda_{-i}, D, \Sigma)p(\Lambda_i|D_i)p(\Lambda_i^*|\Lambda_i, D, \Sigma, \Lambda_{-i}, Y)}.\end{aligned}$$

The proposal probability can be written

$$\begin{aligned}&p(\Lambda_i^*|\Lambda_i, D, \Sigma, \Lambda_{-i}, Y) \\ &= \int p(\Lambda_i^*, Z^i|\Lambda_i, D, \Sigma, \Lambda_{-i}, Y) dZ^i \\ &= \int p(\Lambda_i^*|Z^i, D, \Sigma, \Lambda_{-i}, Y)p(Z^i|\Lambda_i, D, \Sigma, \Lambda_{-i}, Y) dZ^i \\ &= p(\Lambda_i^*|D, \Sigma, \Lambda_{-i}, Y) \\ &\quad \times \int \frac{p(Z^i|\Lambda_i^*, D, \Sigma, \Lambda_{-i}, Y)}{p(Z^i|D, \Sigma, \Lambda_{-i}, Y)} p(Z^i|\Lambda_i, D, \Sigma, \Lambda_{-i}, Y) dZ^i \\ &= \frac{p(Y|\Lambda_i^*, D, \Sigma, \Lambda_{-i})p(\Lambda_i^*, D, \Sigma, \Lambda_{-i})}{p(D, \Sigma, \Lambda_{-i}, Y)} \cdot c(\Lambda_i, \Lambda_i^*|D, \Sigma, \Lambda_{-i}, Y) \\ &= \frac{p(Y|\Lambda_i^*, D, \Sigma, \Lambda_{-i})p(\Lambda_i^*|D_i)p(D)p(\Sigma)p(\Lambda_{-i}|D_{-i})}{p(D, \Sigma, \Lambda_{-i}, Y)} \\ &\quad \times c(\Lambda_i, \Lambda_i^*|D, \Sigma, \Lambda_{-i}, Y),\end{aligned}$$

where $c(\Lambda_i, \Lambda_i^* | D, \Sigma, \Lambda_{-i}, Y)$ represents the integral, which is symmetric in Λ_i and Λ_i^* . Plugging the last expression into the acceptance probability, we obtain $\alpha(\Lambda_i^*, \Lambda_i) = 1$. Analogous logic can be used to show the acceptance probability for a proposed D_i from $2(c - d)$ is also one.

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