Estimating Linear Mixed-effects State Space Model Based on Disturbance Smoothing

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Abstract

We extend the linear mixed-effects state space model to accommodate the correlated individuals and investigate its parameter and state estimation based on disturbance smoothing in this paper. For parameter estimation, EM and score based algorithms are considered. Intermediate quantity of EM algorithm is investigated firstly from which the explicit recursive formulas for the maximizer of the intermediate quantity are derived out for two given models. As for score based algorithms, explicit formulas for the score vector are achieved from which it is shown that the maximum likelihood estimation is equivalent to moment estimation. For state estimation we advocate it should be carried out without assuming the random effects being known in advance especially when the longitudinal observations are sparse. To this end an algorithm named kernel smoothing based mixture Kalman filter (MKF-KS) is proposed. Numerical studies are carried out to investigate the proposed algorithms which validate the efficacy of the proposed inference approaches.

Key words: State space model, Mixed-effects, Parameter estimation, State estimation, Disturbance smoothing

1. Introduction

State space models are widely used in various fields such as economics, engineering, biology et al. In particular structural time series models are just the special state space models. For linear state space model with Gaussian error, it is known that Kalman filter is optimal for state
estimation. For nonlinear state space model, there does not exist optimal algorithm and various suboptimal algorithms for state estimation have been proposed in literatures, see Harvey (1989), Durbin and Koopman (2012) for details about these algorithms. Traditionally the state space models are designed for the single processes.

In recent years in order to deal with the longitudinal data, the state space models for the multiple processes have been proposed and much attention has been attracted in this field. These models can be classified into two categories, i.e., the discrete and continuous models. For the single processes the discrete models are often referred as the hidden Markov models (HMMs). Historically the discrete models with random effects were introduced by Langeheine and van de Pol (1994) while Altman (2007) provided a general framework for implementing the random effects in the discrete models. For the parameter estimation, Altman (2007) evaluated the likelihood as a product of matrixes and performed numerical integration via Gaussian quadrature. A quasi-Newton method is used for maximum likelihood estimation. Maruotti (2011) discussed mixed hidden Markov models and their estimation using EM algorithm. Jackson et al (2014) extended the work of Altman (2007) by allowing the hidden state to jointly model longitudinal binary and count data. The likelihood was evaluated by forward-backward algorithm and adaptive Gaussian quadrature. For continuous state space models, Gamerman and Migon (1993) was the first to use the state space model to deal with multiple processes. They proposed dynamic hierarchical models for the longitudinal data. Unlike the usual hierarchical model where the parameters are modeled by hierarchical structure, the hierarchy in Gamerman and Migon (1993) is built for the state variables. Landim and Gamerman (2000) generalized such models to multiple processes. It should be noted that dynamic hierarchical models are still the linear state space models with Gaussian error and so the statistical inference for such model can be carried out using the traditional method. Lodewyckx et al (2011) proposed hierarchical linear state space model to model the emotion dynamics. Here the hierarchy is built for the parameters. Unlike the models in Gamerman and Migon (1993), these models are essentially the nonlinear state space model and Baysian approach was employed to estimate the unknown parameters. Liu et al (2011) proposed a similar model, which was called mixed-effects state space model (MESSM), to model the longitudinal observations of a group of HIV infected patients. As for the statistical inference of the model, both EM algorithm and Baysian approach were investigated. In order to justify their statistical inference, Liu et al (2011) assumed that the individuals in the group are
independent and the model should have a linear form of parameter. As for the state estimation, they took the predicted values of random effects as the true values and then estimate the state using Kalman filter.

In this paper we extend the models proposed in Liu et al (2011) and Lodewyckx et al (2011). The proposed models can accommodate the group with correlated individuals and do not require the models should possess the linear form of parameters. The model will still be named as MESSM just as in Liu et al (2011). For this generalized MESSM, both the parameter and state estimation are considered. As for parameter estimation, EM algorithm is firstly considered. Unlike Liu et al (2011) in which EM algorithm is based on state smoothing, we establish the EM algorithm based on the disturbance smoothing which greatly simplifies EM algorithm. Actually the proposed EM algorithm can be seen as the Rao-Blackwellized version of that proposed in Liu et al (2011). For two important special MESSM’s, we get the elegant recursive formula for the maximizer of intermediate quantity of EM algorithm. Since the convergence rate of EM algorithm is just linear, score based algorithms, e.g., quasi-Newton algorithm, are then investigated. Also based on the disturbance smoothing, an explicit and simple expression for the score vector is derived out for both the fixed effects and variance components involved in MESSM. Based on the score vector, it is shown that the maximum likelihood estimation of MESSM is in fact equivalent to a particular moment estimation.

As for state estimation, based on the predicted random effects Liu et al (2011) employed Kalman filter to estimate the state. Such prediction is based on the batch data and so it is not a recursive prediction. In many cases, e.g., clinical trial, the recursive prediction is more meaningful. Furthermore it is known that the predicting error of the random effects is rather large if longitudinal observations are sparse. Ignorance of the predicting error in this situation will result in a large bias and underestimate mean squared error of Kalman filter. In this paper we propose a algorithm adapted from the algorithm in Liu and West (2001) to estimate the state which is a recursive method and dose not require the random effects are known in advance. Thus the algorithm can apply whether the longitudinal observations are sparse or not.

In the last the models are further extended to accommodate several practical problems, including missing data, non-diagonal transition matrix and time-dependent effects et al. Simulation examples are carried out which validate the efficacy of the algorithms of parameter estimation. These approaches are applied to a real clinical trial data set and the results show that though the
state estimation is based on the data only up to the present time point, the resulted mean squared errors are comparable to the mean squared error that are resulted from Kalman filter proposed by Liu et al (2011).

This paper is organized as follows. In section 2 the data generating process for generalized MESSM is described; In section 3 the algorithms for both parameter and state estimation are detailed; Several further extensions of the MESSM are considered in section 4. In section 5 two numerical examples are investigated to illustrate the efficacy of proposed algorithms. Section 6 presents a brief discussion about the proposed algorithms.

2. Model Formulation

Consider a group of dynamic individuals. For \( i \)th individual \((i = 1, \cdots, m)\), the following linear state space model is assumed,

\[
\begin{align*}
x_{it} &= T(\theta_i)x_{i,t-1} + v_{it}, \quad v_{it} \sim N(0, Q), \\
y_{it} &= Z(\theta_i)x_{it} + w_{it}, \quad w_{it} \sim N(0, R),
\end{align*}
\]

(1)

(2)

where \( x_{it} \) and \( y_{it} \) are the \( p \times 1 \) state vector and \( q \times 1 \) observation vector for the \( i \)th individual at time \( t \); \( v_{it} \) is the \( p \times 1 \) state disturbance and \( w_{it} \) is the \( q \times 1 \) observational error, both of which are normally distributed with mean zero and variance matrix \( Q \) and \( R \) respectively. The \( p \times p \) state transition matrix \( T(\theta_i) \) and the \( q \times p \) observation matrix \( Z(\theta_i) \) are parameterized with the \( r \times 1 \) parameter vector \( \theta_i \).

For \( \{v_{it}, t = 1, 2, \cdots\} \), the following correlation structure are assumed

\[
Cov(v_{it}, v_{i't'}) = \begin{cases} Q(i,i')_{p\times p} & \text{if } t = t' \\ 0 & \text{else} \end{cases}
\]

i.e., at the same time point, the covariance between the different individuals \( i \) and \( i' \) is \( Q(i,i') \) and so the individuals in this group are correlated with each other. If \( i = i' \), then \( Q(i,i') = Q \). More complex relationship also can be possible, see section 4.2 for another modeling of the relationship among the individuals. For \( \{w_{it}, t = 1, 2, \cdots\} \), we assume

\[
Cov(w_{it}, w_{i't'}) = \begin{cases} R_{q\times q} & \text{if } i = i', t = t' \\ 0 & \text{else} \end{cases}
\]
There is another layer of complexity in model (1) ~ (2), i.e., we have to specify the correlation structure for \( \theta_i \), \( 1 \leq i \leq n \), for which we assume

\[
\theta_i = \psi_i a + b_i, \quad b_i \sim N(0, D),
\]

where \( \psi_i \) is the exogenous variable representing the characteristics of the \( i \)th individuals, \( a \) is the fixed effect and \( b_i \) the random effect. We assume \( b_i \)'s are independent with \( \text{Cov}(b_i, b_{i'}) = D \). Here an implicit assumption is that the individual parameter \( \theta_i \) is static. Time-dependent \( \theta_i \) may be more appropriate in some cases which will be considered in section 4.2. For the correlation structure among \( v_{it}, w_{it} \) and \( \theta_i \), we assume

\[
\text{Cov}(\theta_i, v_{it}) = \text{Cov}(\theta_i, w_{it}) = \text{Cov}(v_{it}, w_{it}) = 0
\]

for \( 1 \leq i \leq m, 1 \leq i' \leq m, t \geq 1, t' \geq 1 \).

The model given above is a generalized version of MESSM given in Liu et al (2011) and Lodewyckx et al (2011), in which they assume that the disturbance \( v_{it} \) is independent to \( v_{i't} \) for \( i \neq i' \). Here we assume there exists static correlation among the individuals. Another critical assumption in Liu et al (2011) is that both \( T(\theta_i) \) and \( Z(\theta_i) \) should be the linear functions of \( \theta_i \).

Here this restriction also is not required.

The following notations are adopted in this paper. \( \{ m \ a_{ij} \}_{i=1}^{p} \) denotes a \( p \times q \) matrix with elements \( a_{ij} \); \( \{ c \ w_{ij} \}_{i=1}^{n} \) denotes a \( n \) dimensional column vector; \( \{ r \ u_{ij} \}_{i=1}^{m} \) denotes a \( n \) dimensional row vector; diagonal matrix is denoted by \( \{ d \ a_{ii} \}_{i=1}^{n} \). All the elements can be replaced by matrices which will result in a block matrix. As for the model (1) ~ (2), define \( x_t = \{ c \ x_{it} \}_{i=1}^{m}, \ \theta = \{ d \ \theta_i \}_{i=1}^{m}, \ \bar{T}(\theta) = \{ d \ T(\theta_i) \}_{i=1}^{m}, \ \bar{Z}(\theta) = \{ d \ Z(\theta_i) \}_{i=1}^{m}, \ v_t = \{ c \ v_{it} \}_{i=1}^{m}, \ y_t = \{ c \ y_{it} \}_{i=1}^{m}, \ w_t = \{ c \ w_{it} \}_{i=1}^{m}, \) and then the model can be written in matrix form as

\[
x_t = \bar{T}(\theta)x_{t-1} + v_t, \quad (5)
\]
\[
y_t = \bar{Z}(\theta)x_t + w_t. \quad (6)
\]

Here \( \text{Var}(v(t)) \triangleq \bar{Q} = \{ d \ Q(i,i') \}_{i=1}^{m} \), \( \text{Var}(w(t)) \triangleq \bar{R} = \{ d \ R \}_{i=1}^{m} \), \( \text{Var}(\theta) = \{ d \ D \}_{i=1}^{m} \) and \( \text{Cov}(v_t, w_t) = \text{Cov}(\theta, v_t) = \text{Cov}(\theta, w_t) = 0 \). Equations (1) ~ (6) represent the data generating process. Given the observations up to time \( t, y_{1:t} = (y_{11}, \ldots, y_{m1}, \ldots, y_{1t}, \ldots, y_{mt}) \), we will study the following problems: (1) How to estimate the parameters involved in the model, including covariance matrix \( \bar{Q}, \bar{R}, D \) and fixed effects \( a \). (2) How to get the online estimate of the state \( x_{it} \).
for $1 \leq i \leq m$. Though these problems had been studied in literatures, we will adopt different ways to address these issues which turn out to be more efficient in most settings.

3. Model Estimation

The parameters involved in MESSM include the fixed effects $a$ and those involved in variance matrices $(Q, R, D)$ which is denoted by $\delta$. We write $(Q(\delta), R(\delta), D(\delta))$ to indicate explicitly such dependence of variance matrix on $\delta$. In this section we consider how to estimate parameter $\Delta^T \equiv (a^T, \delta^T)$ and the state $x_t$ based on the observations $y_{1:T}$. Lodewyckx et al (2011) and Liu et al (2011) had investigated these questions in details, including EM algorithm based maximum likelihood estimation and Baysian estimation. While these approaches are shown to be efficient for the given illustrations, they are cumbersome to be carried out. On the other hand it is also well known that the rate of convergence for EM algorithm is linear which is slower than quasi-Newton algorithm. In the following we will first consider a new version of EM algorithm which is simpler than the existed results. Then scores based algorithm is investigated. Explicit and simple expression for the score vector is derived out. State estimation also is investigated using an adapted filter algorithm proposed by Liu and West (2001).

3.1. Maximizing the likelihood via EM algorithm

For model (5)~(6), we take $(\theta^T, x_t^T, \cdots, x_t^T)^T$ as the missing data and $(\theta^T, x_t^T, \cdots, x_t^T, y_{1:T})^T$ the complete data. Note $f(\theta, x_{1:T}, y_{1:T}|\Delta) = f(\theta|\Delta)f(x_{1:T}|\theta, \Delta)f(y_{1:T}|\theta, x_{1:T}, \Delta)$ in which all the terms $f(\theta|\Delta)$, $f(x_{1:T}|\theta, \Delta)$ and $f(y_{1:T}|\theta, x_{1:T}, \Delta)$ are normal densities by assumption. For the sake of simplicity, we let $x_1 \sim N(a_1, P_1)$ with known $a_1$ and $P_1$. Then omitting constants, the log joint density can be written as

$$
\log f(\theta, x_{1:T}, y_{1:T}|\Delta) = -\frac{m}{2} \log |D(\delta)| - \frac{T}{2} \log |R(\delta)| - \frac{T}{2} \log |Q(\delta)|
$$

$$
- \frac{1}{2} \sum_{i=1}^m \text{tr} [D(\delta)^{-1}(\theta_i - \Psi_i a)(\theta_i - \Psi_i a)^T] - \frac{1}{2} \sum_{i=1}^T \text{tr} [R(\delta)^{-1}(y_i - \tilde{Z}(\theta)x_t)]
$$

$$
\leq \{y_i - \tilde{Z}(\theta)x_t\}^T - \frac{1}{2} \sum_{i=1}^T \text{tr} [Q(\delta)^{-1}\{x_t - \tilde{T}(\theta)x_{t-1}\}\{x_t - \tilde{T}(\theta)x_{t-1}\}^T]
$$

where for $t = 1$, $Q(\delta)^{-1}\{x_t - \tilde{T}(\theta)x_{t-1}\}\{x_t - \tilde{T}(\theta)x_{t-1}\}^T$ is explained as $P_1^{-1}(x_1 - a_1)(x_1 - a_1)^T$. Let $\Delta^* = (a^*, \delta^*)^T$ denote the value of $\Delta$ in the $j$th step of EM algorithm, then $Q(\Delta, \Delta^*)$, the intermediate quantity of EM algorithm, is defined as the expectation of $\log f(\theta, x_{1:T}, y_{1:T})$
conditional on $\Delta^*$ and the observations $y_{1:T}$. Let $E(\cdot)$ denote this conditional expectation and then with (7) and the normal assumption in hand, we have

$$Q(\Delta, \Delta^*) \triangleq E[\log f(\theta, y_{1:T}, y_{1:T} | \Delta)]$$

$$= \frac{m}{2} \log |D(\bar{\delta})| - \frac{T}{2} \log |\bar{\delta}| - \frac{T}{2} \log |Q(\bar{\delta})| - \frac{1}{2} \sum_{i=1}^{m} \text{tr}[D(\bar{\delta})^{-1} \{ (\Psi_i(a^* - a) + b_i|T) (\Psi_i(a^* - a) + b_i|T)^T \}]
+ \text{Var}(b_i|y_{1:T}, \Delta^*)] - \frac{1}{2} \sum_{i=1}^{T} \text{tr}[\bar{\delta}(\bar{\delta})^{-1} \{ w_{i|T} w_{i|T}^T + \text{Var}(w_i|y_{1:T}, \Delta^*) \}]
- \frac{1}{2} \sum_{i=1}^{T} \text{tr}[\bar{\delta}(\bar{\delta})^{-1} \{ v_{i|T} v_{i|T}^T + \text{Var}(v_i|y_{1:T}, \Delta^*) \}],$$

where $b_i|T = \bar{E}(b_i), w_{i|T} = \bar{E}(w_i), v_{i|T} = \bar{E}(v_i)$. In order to find the maximizer of $Q(\Delta, \Delta^*)$ with respect to $\Delta$, we have to compute these conditional expectations and variances firstly. Note that

$$b_{i|T} = \bar{E}(b_{i|T}(\theta)), \quad w_{i|T} = \bar{E}(w_{i|T}(\theta)), \quad v_{i|T} = \bar{E}(v_{i|T}(\theta)),$$

where

$$b_{i|T}(\theta) = E(b_i|y_{1:T}, \Delta^*, \theta), \quad w_{i|T}(\theta) = E(w_i|y_{1:T}, \Delta^*, \theta), \quad v_{i|T}(\theta) = E(v_i|y_{1:T}, \Delta^*, \theta)$$

and

$$\text{Var}(v_i|y_{1:T}, \Delta^*) = \bar{E}(\text{Var}(v_i|y_{1:T}, \Delta^*, \theta)) + \text{Var}(v_{i|T}(\theta)|y_{1:T}, \Delta^*),$$

$$\text{Var}(w_i|y_{1:T}, \Delta^*) = \bar{E}(\text{Var}(w_i|y_{1:T}, \Delta^*, \theta)) + \text{Var}(w_{i|T}(\theta)|y_{1:T}, \Delta^*).$$

For the smoothed disturbances $w_{i|T}(\theta), v_{i|T}(\theta)$ and the relevant variances we have,

$$w_{i|T}(\theta) = \bar{R}(\delta^*) e_i(\theta), \quad \text{Var}(w_i|y_{1:T}, \Delta^*, \theta) = \bar{R}(\delta^*) - \bar{R}(\delta^*) D_i(\theta) \bar{R}(\delta^*),$$

$$v_{i|T}(\theta) = \bar{Q}(\delta^*) r_{i-1}(\theta), \quad \text{Var}(v_i|y_{1:T}, \Delta^*, \theta) = \bar{Q}(\delta^*) - \bar{Q}(\delta^*) N_{i-1}(\theta) \bar{Q}(\delta^*),$$

where the backward recursions for $e_i(\theta), r_{i-1}(\theta), D_i(\theta)$ and $N_{i-1}(\theta)$ are given by

$$e_i(\theta) = F_i(\theta)^{-1} v_i - K_i(\theta)^T r_i(\theta),$$

$$r_{i-1}(\theta) = Z(\theta)^T F_{i-1}(\theta)^{-1} v_i + L_i(\theta)^T r_i(\theta),$$

$$D_i(\theta) = F_i(\theta)^{-1} + K_i(\theta)^T N_i(\theta) K_i(\theta),$$

$$N_{i-1}(\theta) = Z(\theta)^T F_i(\theta)^{-1} Z(\theta) + L_i(\theta)^T N_i(\theta) L_i(\theta).$$
for $t = T, \cdots, 1$. These terms are calculated backwardly with $r_T = 0$ and $N_T = 0$. Here $F_i(\theta), K_i(\theta)$ are respectively the variance matrix of innovation and gain matrix involved in Kalman filter. The recursions for these matrix can be stated as follows,

$$P_{t+1|T}(\theta) = T(\theta)P_{t-1|T}(\theta) + \tilde{Q}(\delta^*), \quad F_t(\theta) = Z(\theta)P_{t-1|T}(\theta)Z(\theta)^T + \tilde{R}(\delta^*), \quad (18)$$

$$K_t(\theta) = T(\theta)P_{t-1|T}(\theta)Z(\theta)^T F_t(\theta)^{-1}, \quad L_t(\theta) = T(\theta) - K_t(\theta)Z(\theta). \quad (19)$$

The recursions (12)~(19) can be found in Durbin and Koopman (2012). Combining these recursive formulas with (9)~(11) yields

$$w_{t|T}w_{t|T}^T = \tilde{R}(\delta^*)E(e_i(\theta))^T(\delta^*),$$

$$v_{t|T}v_{t|T} = \tilde{Q}(\delta^*)E(r_{t-1}(\theta))^T(\delta^*),$$

$$\text{Var}(w_i|y_{1:T}, \Delta^*) = \tilde{R}(\delta^*) - \tilde{R}(\delta^*)E(D_i(\theta))\tilde{R}(\delta^*) + \tilde{R}(\delta^*)\text{Var}(e_i(\theta)|y_{1:T}, \Delta^*)\tilde{R}(\delta^*),$$

$$\text{Var}(v_i|y_{1:T}, \Delta^*) = \tilde{Q}(\delta^*) - \tilde{Q}(\delta^*)E(N_{t-1}(\theta))\tilde{Q}(\delta^*) + \tilde{Q}(\delta^*)\text{Var}(r_{t-1}(\theta)|y_{1:T}, \Delta^*)\tilde{Q}(\delta^*).$$

Substituting these expression into (5) we have

$$Q(\Delta, \Delta^*) = -\frac{m}{2}\log|D(\delta)| - T\frac{1}{2}\log|\tilde{R}(\delta)| - \frac{T}{2}\log|\tilde{Q}(\delta)|$$

$$-\frac{1}{2}\sum_{i=1}^m \text{tr} \left[ D(\delta)^{-1} \{ (\Psi_i(a^* - a) + b_i)^T(\Psi_i(a^* - a) + b_i) \} \right]$$

$$-\frac{1}{2}\sum_{i=1}^m \text{tr} \left[ \tilde{R}(\delta)^{-1} \{ \tilde{R}(\delta^*) + \tilde{R}(\delta^*)E(e_i^2(\theta) - D_i(\theta))\tilde{R}(\delta^*) \} \right]$$

$$-\frac{1}{2}\sum_{i=1}^m \text{tr} \left[ \tilde{Q}(\delta)^{-1} \{ \tilde{Q}(\delta^*) + \tilde{Q}(\delta^*)E(r_{t-1}(\theta) - N_{t-1}(\theta))\tilde{Q}(\delta^*) \} \right].$$

Now we have obtained the expression for the intermediate quantity of EM algorithm. Except conditional expectations and variances, all the quantities involved can be easily computed by Kalman filter. These conditional expectations and variances include $h_{i|T}$, $ED_i(\theta)$, $EN_i(\theta)$, $E\{e_i(\theta)e_i(\theta)^T\}$, $E\{r_{t-1}(\theta)r_{t-1}(\theta)^T\}$ and $\text{Var}(b_i|y_{1:T}, \Delta^*)$. Here we adopt the Monte Carlo method to approximate the expectations and variances. Specifically given the random samples $\{\theta_j^{(j)}, j = 1, \cdots, M\}$ from the posterior $f(\theta|y_{1:T}, \Delta^*)$, all the population expectation is approximated by the sample expectation. For example we approximate $b_{i|T}$ by $\frac{1}{M}\sum_{j=1}^M \theta_j^{(j)} - \Psi_i a^*$. The same approximation applies to other expectations and variances. As for the sampling from the posterior $f(\theta|y_{1:T}, \Delta^*)$, the random-walk Metropolis algorithm is employed in this paper to
generate the samples. Certainly it is also possible to use other sampling scheme such as importance sampling to generate the random samples from \( f(\theta | y_{1:T}, \Delta^*) \). In our finite experiences MCMC algorithm is superior to the importance sampling in present situations. It is meaningful to compare the proposed EM algorithm with that in Liu et al (2011). Recall the EM algorithm in Liu et al (2011) have to sample both \( x_t \) and \( \theta \) from their joint distribution \( f(\theta, x_t | y_{1:T}, \Delta^*) \) where Gibbs sampler was proposed to implement the sampling in their study. Here only the random samples of \( \theta \) from \( f(\theta | y_{1:T}, \Delta^*) \) are needed for running the EM algorithm and thus the proposed EM algorithm can be seen as a Rao-Blackwellized version of that in Liu et al (2011). Note the dimension of \( x_t \) increases as the number of the individuals increases and consequently a faster and more stable convergence rate of the proposed algorithm can be expected especially when the number of the correlated individuals is large.

For the purpose of illustration consider the following autoregressive plus noise model,

\[
y_t = x_t + w_t, w_t \sim \text{i.i.d.} \ N(0, \delta_1), x_t = \theta x_{t-1} + v_t, v_t \sim \text{i.i.d.} \ N(0, \delta_2)
\]  

(21)

where

\[
\theta_i = \mu_0 + b_i, b_i \sim \text{i.i.d.} \ N(0, \delta_3), i = 1, \cdots, m.
\]  

(22)

Here we assume all the individuals in this group are independent with each other. This model can be rewritten in the matrix form as

\[
y_t = \tilde{Z}(\theta)x_t + w_t, w_t \sim \text{i.i.d.} \ N_m(0, \delta I_m), \quad x_t = \tilde{T}(\theta)x_{t-1} + v_t, v_t \sim \text{i.i.d.} \ N_m(0, \delta I_m)
\]

with \( y_t = (y_{1t}, \cdots, y_{mt})^T, x_t = (x_{1t}, \cdots, x_{mt})^T, w_t = (w_{1t}, \cdots, w_{mt})^T, v_t = (v_{1t}, \cdots, v_{mt})^T, \theta = (\theta_1, \cdots, \theta_m)^T, \delta = (\delta_1, \delta_2, \delta_3)^T, \tilde{Z}(\theta) = I_m, \tilde{T}(\theta) = \text{diag}(\theta_1, \cdots, \theta_m), \tilde{R}(\delta) = \delta I_m, \tilde{Q} = \delta_2 I_m, \Psi_I = 1, D(\delta) = \delta_3 \).

From (20), we get the following recursive formulas,

\[
\hat{\mu}_\theta = \frac{1}{m} \sum_{i=1}^m \tilde{E}(\theta_i), \quad \hat{\delta}_1 = \frac{1}{m} \sum_{i=1}^m [\hat{\mu}_\theta - \tilde{E}(\theta_i)]^2,
\]

\[
\hat{\delta}_2 = \frac{1}{m} \sum_{i=1}^m \sum_{t=1}^T [\hat{\delta}_1^2 + \hat{\delta}_2^2 \tilde{E} \{ x_{it}^2(\theta) - D_{it}(\theta) \}]
\]

\[
\hat{\delta}_3 = \frac{1}{m} \sum_{i=1}^m \sum_{t=1}^T [\hat{\delta}_1^2 + \hat{\delta}_2^2 \tilde{E} \{ x_{it}^2(\theta) - N_{\Delta - 1}(\theta) \}]
\]

(23)

After getting \( (\hat{\mu}_\theta, \hat{\delta}_1, \hat{\delta}_2, \hat{\delta}_3)^T \) from (23), we take it as the new \( \Delta^* \) and use it to compute the next maximizer of \( Q(\Delta, \Delta^*) \) until the convergence is achieved. The convergent point is defined as the estimator of \( \Delta \).
The second illustration we consider is the damped local linear model which can be expressed as

\[ y_{it} = z_{it} + \varepsilon_{it}, \quad z_{it} = z_{i(t-1)} + u_{it} + \eta_{it}, \quad u_{it} = \theta_i t u_{i(t-1)} + \tau_{it}, \quad (24) \]

with \( \theta_i = \mu + b_i \) and

\[ \varepsilon_{it} \sim \text{i.i.d.} N(0, \delta_1), \quad \eta_{it} \sim \text{i.i.d.} N(0, \delta_2), \quad \tau_{it} \sim \text{i.i.d.} N(0, \delta_3), \quad b_i \sim \text{i.i.d.} N(0, \delta_4). \quad (25) \]

We also assume that the individuals in the group are independent with each other. Defining the state variable as \( x_{it} = (z_{it}, u_{it})^T \), then the damped local linear model can be rewritten as the state space model \( (11) \sim (13) \) with

\[ T = (1, 0), \quad Z = \begin{pmatrix} 1 & 1 \\ 0 & \theta_i \end{pmatrix}, \quad Q = \begin{pmatrix} \delta_2 & 0 \\ 0 & \delta_3 \end{pmatrix}, \quad R = \delta_1. \]

Here the unknown parameters include \( \Delta \hat{=} (\mu, \delta_1, \delta_2, \delta_3, \delta_4)^T \). Let

\[ r_{it} \hat{=} \begin{pmatrix} r_{it}^{(z)} \\ r_{it}^{(u)} \end{pmatrix}, \quad N_{it} \hat{=} \begin{pmatrix} N_{it}^{(zz)} & N_{it}^{(zu)} \\ N_{it}^{(zu)} & N_{it}^{(uu)} \end{pmatrix}, \]

then from \( (26) \), the recursive formula of EM algorithm turns out to be

\[ \hat{\mu}_\theta = \frac{1}{m} \sum_{t=1}^{m} \hat{E}(\theta_i), \quad \hat{\delta}_t = \frac{1}{m} \sum_{t=1}^{m} [\hat{\mu}_\theta - \hat{E}(\theta_i)]^2, \]

\[ \hat{\delta}_1 = \frac{1}{Tm} \sum_{t=1}^{m} \sum_{t=1}^{T} [\delta_{i}^t + \delta_{i}^{z^2} \hat{E}(c_{i}^2(\theta) - D_{it}(\theta))] , \]

\[ \hat{\delta}_2 = \frac{1}{Tm} \sum_{t=1}^{m} \sum_{t=1}^{T} [\delta_{i}^t + \delta_{i}^{z^2} \hat{E}((r_{it}^{(z)})^2(\theta) - N_{it}^{(zz)}(\theta))] , \]

\[ \hat{\delta}_3 = \frac{1}{Tm} \sum_{t=1}^{m} \sum_{t=1}^{T} [\delta_{i}^t + \delta_{i}^{z^2} \hat{E}((r_{it}^{(u)})^2(\theta) - N_{it}^{(uu)}(\theta))] . \]

3.2. Maximizing the likelihood via score based algorithms

In this section we consider the score-based algorithms which include quasi-Newton algorithm, steepest ascent algorithm et al. The core of such algorithms is how to compute the score vector. Here the likelihood \( L(\Delta|y_{1:T}) \) is a complex function of \( \Delta \) and the direct computation of score is difficult both analytically and numerically. We consider the following transformation of \( L(\Delta|y_{1:T}) \),

\[ \log L(\Delta|y_{1:T}) = \log f(\theta, x_{1:T}, y_{1:T}|\Delta) - \log f(\theta, x_{1:T}|y_{1:T}, \Delta) \quad (26) \]
Recall in section [3] $f(\theta, x_{1:T}, y_{1:T}\mid \Delta)$ denotes the joint distribution of $(\theta, x_{1:T}, y_{1:T})$ conditional on $\Delta$ and $E(\cdot)$ the conditional expectation $E(\cdot \mid y_{1:T}, \Delta^*)$. In present situation we let $\Delta^*$ denote the present value of $\Delta$ in quasi-Newton algorithm. Then taking $E$ of both sides of (26) yields

$$\log L(\Delta \mid y_{1:T}) = E[\log f(\theta, x_{1:T}, y_{1:T} \mid \Delta)] - E[\log f(\theta, x_{1:T} \mid y_{1:T}, \Delta)].$$  

Under the assumption that the exchange of integration and differentiation is legitimate it can be shown that

$$E\left[\frac{\partial \log f(\theta, x_{1:T} \mid y_{1:T}, \Delta)}{\partial \Delta}\bigg|_{\Delta=\Delta^*}\right] = 0,$$  

Consequently we have

$$\frac{\partial \log L(\Delta \mid y_{1:T})}{\partial \Delta}\bigg|_{\Delta=\Delta^*} = \frac{\partial}{\partial \Delta} E[\log f(\theta, x_{1:T}, y_{1:T} \mid \Delta)]\bigg|_{\Delta=\Delta^*}.$$  

Note the expectation in the right-hand side has the same form as the intermediate quantity of EM algorithm in the previous section. And so substituting (20) into (29) we get

$$\frac{\partial \log L(\Delta \mid y_{1:T})}{\partial \Delta}\bigg|_{\Delta=\Delta^*} = \sum_{i=1}^{m} \psi_i^T D(\delta^*)^{-1} b_{i\mid T},$$  

$$\frac{\partial \log L(\Delta \mid y_{1:T})}{\partial \delta_j}\bigg|_{\Delta=\Delta^*} = -\frac{1}{2} \sum_{i=1}^{m} \text{tr}\left[D(\delta^*)^{-1} \frac{\partial D(\delta^*)}{\partial \delta_j} \right]$$  

$$- D(\delta^*)^{-1} \left\{b_{i\mid T} b_{i\mid T}^T + \text{Var}(b_{i\mid y_{1:T}, \Delta^*}) \right\} D(\delta^*)^{-1} \frac{\partial D(\delta^*)}{\partial \delta_j} \right\}$$  

$$+ \frac{1}{2} \sum_{i=1}^{T} \text{tr}\left[E\left\{e_i(\theta)e_i(\theta)^T - D(\delta^*) \right\} \frac{\partial \hat{R}(\delta^*)}{\partial \delta_j}\right]\right]$$  

$$+ \frac{1}{2} \sum_{i=1}^{T} \text{tr}\left[E\left\{r_{i-1}(\theta)r_{i-1}(\theta)^T - N_{i-1}(\theta) \right\} \frac{\partial \hat{Q}(\delta^*)}{\partial \delta_j}\right]\right].$$  

Inspection of the score vector $\frac{\partial \log L(\Delta \mid y_{1:T})}{\partial \Delta}$ shows that in order to evaluate the score vector in present value $\Delta^*$, we need (1) a single pass of Kalman filter and smoother, (2) to run a MCMC algorithm to get the random samples $\theta_j^{(j)} (j = 1, \ldots, M)$ from $f(\theta \mid y_{1:T}, \Delta^*)$. These calculation can be carried out readily. It is interesting to compare this result with the existed results for the fixed-effects state space models. Engle and Watson (1981) had constructed a set of filter for computing the score vector analytically. However, as pointed out by Koopman and Shephard (1992), this approach is cumbersome, difficult to program and typically much more expensive to use than numerically differentiating the likelihood. Koopman and Shephard (1992) and Koopman (1993) also obtained an analytical expression for the score vector. But those expressions are only
feasible for the variance components and the scores for the parameters in observational matrix and state transition matrix should be computed by numerically differentiating. On the contrary the exact expressions of score vectors given in (30)−(31) not only can be used to compute the scores for variance components but also can be used to compute the scores for fixed effects straightforwardly.

As an illustration consider the autoregressive plus noise model given by (21)−(22). The scores defined in (30)−(31) can be shown to be

$$\frac{\partial \log L(\Delta | y_{1:T})}{\partial \mu_\theta} = \sum_{i=1}^{m} E(\theta_i | y_{1:T}, \Delta^*) - \mu_\theta^*, \quad (32)$$

$$\frac{\partial \log L(\Delta^* | y_{1:T})}{\partial \delta_1} = \frac{1}{2} \sum_{i=1}^{T} \sum_{j=1}^{m} [\bar{E} \{ e^2_i(\theta_i) - D_\theta(\theta_i) \}], \quad (33)$$

$$\frac{\partial \log L(\Delta^* | y_{1:T})}{\partial \delta_2} = \frac{1}{2} \sum_{i=1}^{T} \sum_{j=1}^{m} [\bar{E} \{ \hat{r}_{i-1}(\theta_i) - N_{\theta_i}(\theta_i) \}], \quad (34)$$

$$\frac{\partial \log L(\Delta^* | y_{1:T})}{\partial \delta_3} = \frac{1}{2} \sum_{i=1}^{T} \sum_{j=1}^{m} \frac{\delta_i^2 - b^2_{i,T} - \text{Var}(b_i | y_{1:T}, \Delta^*)}{\delta_3^2}. \quad (35)$$

Here $e_i(\theta_i), r_{\theta_i}(\theta_i), D_\theta(\theta_i)$ and $N_{\theta}(\theta_i)$ have been defined in (14)−(17) which correspond to the $i$th individual. If we denote the MLE of $\Delta$ by $\hat{\Delta} = (\hat{\mu}_\theta, \hat{\delta}_1, \hat{\delta}_2, \hat{\delta}_3)^T$, then by equating these scores at $\hat{\Delta}$ to zero we have

$$\bar{\mu}_\theta = \frac{1}{m} \sum_{i=1}^{m} E(\theta_i | y_{1:T}, \bar{\Delta}), \quad \hat{\delta}_1 = \frac{1}{m} \sum_{i=1}^{m} \left( b^2_{i,T} + \text{Var}(b_i | y_{1:T}, \bar{\Delta}) \right), \quad (36)$$

$$\sum_{i=1}^{m} \sum_{j=1}^{T} \sum_{i=1}^{T} [\bar{E} \{ e^2_i(\theta_i) \}] = \sum_{i=1}^{m} \sum_{j=1}^{T} [\bar{E}D_\theta(\theta_i)], \quad (37)$$

$$\sum_{i=1}^{m} \sum_{j=1}^{T} \sum_{i=1}^{T} [\bar{E} \{ \hat{r}_{i-1}(\theta_i) \}] = \sum_{i=1}^{m} \sum_{j=1}^{T} [\bar{E}N_{\theta_i}(\theta_i)]. \quad (38)$$

Equations (36) says that $\bar{\mu}_\theta$ is the sample mean of posterior mean $\bar{E}(\theta_i)$ at $\Delta = \bar{\Delta}$; As for the second term in (36), note at the true parameter $\Delta_0$,

$$E \{ b^2_{i,T} + \text{Var}(b_i | y_{1:T}, \Delta_0) \} = \text{Var}(E(b_i | y_{1:T}, \Delta_0)) + E\text{Var}(b_i | y_{1:T}, \Delta_0),$$

where the right hand side is just equal to $\delta_1$ and so $\hat{\delta}_1$ can also be seen as a moment estimator.

As for equation (37) and (38), it can be easily checked that for given $\theta \in \Theta$

$$E \{ e^2_i(\theta) | \bar{\Delta}, \theta \} = D_\theta(\theta), \quad E \{ \hat{r}_{i}^2(\theta) | \bar{\Delta}, \theta \} = N_{\theta}(\theta), \quad (39)$$
i.e., (37) and (38) are the moment equation for estimating $\delta_1$ and $\delta_2$. Consequently $\hat{\Delta}$ can be regarded as a moment estimator.

As another illustration consider the damped local linear model defined by (24) $\sim$ (25). The score vectors can also be obtained by formulas (30) $\sim$ (31). In fact it turns out the scores with respect to $\mu$, $\delta_1$ and $\delta_4$ have the same form as the scores given in (32), (33) and (35) respectively. As for $\delta_2$ and $\delta_3$ we have

$$
\frac{\partial \log L(\Delta^*|y_{1:T})}{\partial \delta_2} = \frac{1}{2} \sum_{t=1}^{T} \sum_{i=1}^{m} \left[ \tilde{E} \left\{ (r^{(z)}_{it-1})^2 (\theta_i) - N_{zz}(\theta_i) \right\} \right],
$$

(40)

$$
\frac{\partial \log L(\Delta^*|y_{1:T})}{\partial \delta_3} = \frac{1}{2} \sum_{t=1}^{T} \sum_{i=1}^{m} \left[ \tilde{E} \left\{ (r^{(u)}_{it-1})^2 (\theta_i) - N_{zu}(\theta_i) \right\} \right],
$$

(41)

Here $r^{(z)}_{it}$, $r^{(u)}_{it}$, $N^{(zz)}_{it}$ and $N^{(zu)}_{it}$ have been defined in section 3.1.

From these two illustrations it can be seen that for i.i.d. individuals, the maximum likelihood estimation of MESSM is equivalent to the moment estimation. For the general cases where the individuals may be correlated, this conclusion also holds but more complex moment equations are needed in those situations.

### 3.3. State estimation

In this section we discuss the algorithms for state estimation of MESSM under the assumption that the true parameter $\Delta_0$ is known. If the random effects $b_i$’s are also assumed to be known, then Kalman filter can yields the optimal state estimator. Just as mentioned in section 1, it is inappropriate to assume $b_i$’s being known in the setting of sparse longitudinal data and consequently Kalman filter should not be applied directly.

One way out is to define the random effects as the new state variables, then MESSM turns out to be a nonlinear state space model. Consequently for the state filter, we can employ the usual nonlinear filter or Monte Carlo filter to estimate the state. Though being straightforward, this approach is thought to be suboptimal because it does not utilize the structure information contained in MESSM (1) $\sim$ (2) in an efficient way.

Note that given the random effects, MESSM is a conditional linear state space model and so the mixture Kalman filter proposed in Chen and Liu (2001) seems to be a good candidate for state estimation. However because the parameter $\theta$ is static in present settings, the re-sampling step in mixture Kalman filter will make the sample $\{\theta_i^{(1)}, \cdots, \theta_i^{(M)}\}$ at time $t$ being a sub-sample of the sample $\{\theta_{i-1}^{(1)}, \cdots, \theta_{i-1}^{(M)}\}$ at time $t-1$. This will make $\{\theta_i^{(1)}, \cdots, \theta_i^{(M)}\}$ a poor representative of
the posterior $f(\theta|y_{1:t})$ as time $t$ passes. In order to get an improved representative of $f(\theta|y_{1:t})$, in the following we will present another algorithm which can overcome the problem of particle degeneracy and usually has a better performance in the aspect of representation of $f(\theta|y_{1:t})$ than usual mixture Kalman filter. This filter algorithm is adapted from the work in Liu and West (2001). The idea is to approximate the posterior distribution $f(\theta|y_{1:t})$ sequentially by a proper mixture of normal distribution. Then the problem of sampling from the complex posterior $f(\theta|y_{1:t})$ becomes a problem of sampling from a mixture distribution, which can be carried out straightforwardly. Specifically at time $t$ we assume the following approximation is appropriate

$$f(\theta|y_{1:t}) \approx \sum_{j=1}^{M} w_t^{(j)} N(m_t^{(j)}, h^2 V_t)$$

(42)

for some proper $w_t^{(j)}$, $m_t^{(j)}$ and $V_t$. The choices of $w_t^{(j)}$, $m_t^{(j)}$ and $V_t$ depend on the last particles $\{\theta_{t-1}^{(1)}, \ldots, \theta_{t-1}^{(M)}\}$ and the present observation $y_t$. The smoothing parameter $h$ controls the overall scale. We denote the Kalman filter at time $t \geq 1$ corresponding to $\theta_t^{(j)}$ by $KF_t^{(j)} = (x_{t|t}^{(j)}, p_{t|t}^{(j)}, x_{t+1|t}^{(j)}, p_{t+1|t}^{(j)})$ where $x_{t|t}^{(j)}$ denotes the filter estimator of $x_t$ with variance $p_{t|t}^{(j)}$; $x_{t+1|t}^{(j)}$ denotes the one-step-ahead predictor of $x_{t+1}$ with variance $p_{t+1|t}^{(j)}$. The filter algorithm can then be stated as follows.

Suppose the Monte Carlo sample $\theta_{t-1}^{(j)}$ and weights $w_{t-1}^{(j)}$ ($j=1, \ldots, M$), representing the posterior $f(\theta|y_{1:t-1})$, are available. Also the Kalman filter $KF_{t-1}^{(j)}$ has been derived out. $\bar{\theta}_{t-1}$ and $V_{t-1}$ denote the weighted sample mean and variance of the particles $\{\theta_{t-1}^{(1)}, \ldots, \theta_{t-1}^{(M)}\}$ respectively. Then at time $t$ when the observation $y_t$ is brought in,

- For each $j=1, \ldots, M$, compute $m_{t-1}^{(j)} = a \theta_{t-1}^{(j)} + (1-a) \bar{\theta}_{t-1}$ where $a = \sqrt{1-h^2}$.
- Sample an auxiliary integer variable from set $\{1, \ldots, M\}$ with probabilities proportional to $w_{t-1}^{(j)} f(y_t|x_{t|t-1}^{(j)}, \theta_{t|t-1}^{(j)})$, which is referred as $k$.
- Sample a new parameter vector $\theta_{t}^{(k)}$ from the $k$th normal component of the kernel density, i.e., $\theta_{t}^{(k)} \sim N(m_{t-1}^{(k)}, h^2 V_{t-1})$.
- For $\theta_{t}^{(k)}$, compute $KF_t^{(k)}$ and evaluate the corresponding weight
  $$w_t^{(k)} = \frac{f(y_t|x_{t|t}^{(k)}, \theta_{t}^{(k)})}{f(y_t|x_{t|t-1}^{(k)}, m_{t-1}^{(k)})}.$$
- Repeat step (2)-(4) a large number of times to produce a final posterior approximation $\theta_{t|t}^{(k)}$ and Kalman filter $KF_{t}^{(k)}$, both of which are associated with weights $w_{t}^{(k)}$. 

14
We call the algorithm above mixture Kalman filter with kernel smoothing (MKF-KS). Historically using kernel smoothing of density to approximate the posterior distribution of dynamic system originated from West (1993a, 1993b). MKF-KS assumes that the posterior can be well approximated by a mixture of normal distribution which in many cases is a reasonable assumption. More important is that MKF-KS can solve the problem of particle degeneration satisfyingly in most settings. From the Example 2 in section it can be seen MKF-KS does have a good performance. Therefore we recommend to use MKF-KS to estimate state for MESSM when the observations are sparse.

In additional to state estimation, MKF-KS can also be used as a basis to estimate the observed information matrix whose inverse usually is taken as the estimate of the variance matrix of the maximum likelihood estimator in literatures. Poyiadjis et al (2011) is the first to use the particle filter to approximate the observed information matrix. Nemeth et al (2013) improved the efficiency of such algorithms by using the idea of kernel smoothing of Liu and West (2001). The details of this algorithm will be omitted for brevity, for further details see Nemeth et al (2013). In the section we will combine MKF-KS with the algorithms 3 in Nemeth et al (2013) to estimate the observed information matrix.

4. Extensions

4.1. Incomplete observations

In previous sections, we have assumed all the individuals can be observed at all the time points. For longitudinal data however such assumption does not hold in many settings and the observations for some or even all of individuals may be missing at given time point. In this section we show that the mixed-effects state space model can be easily adapted to accommodate such situations.

Assume first the observations for all of the individuals are missing at time \( t \) for \( \tau \leq t \leq \tau^* - 1 \). As for the EM algorithm in section the intermediate quantity now is given by minus the following terms,

\[
-\frac{\tau^* - \tau}{2} \log |\tilde{R}(\delta)| - \frac{\tau^* - \tau}{2} \log |\tilde{Q}(\delta)| - \frac{1}{2} \sum_{i=1}^{\tau^* - 1} \text{tr} \left[ \tilde{R}(\delta) \left\{ \tilde{R}(\delta^*) + \tilde{R}(\delta^*) \tilde{E}(e_i^2(\theta) - D_i(\theta)\tilde{R}(\delta^*)) \right\} \right]
\] (43)
\[ -\frac{1}{2} \sum_{t=1}^{\tau_s-1} \text{tr} \left[ \tilde{Q}(\delta)^{-1} \left\{ \tilde{Q}(\delta^*) + \tilde{Q}(\delta^*)\tilde{E}(\theta_{t-1}(\theta) - N_{t-1}(\theta))\tilde{Q}(\delta^*) \right\} \right]. \]

Note here \( \tilde{E}(\cdot) \) is interpreted as \( \tilde{E}(\cdot) = E(\cdot|y_1, \tau_{s-1}, \tau, \Delta^*) \). As for the quasi-Newton algorithm in section 3, the equation (29) still holds in the present situation with the new interpretation of \( \text{covariance matrix} \), the correlation within the group can also be modeled by adopting a different \( E \text{MKF-KS from w} \).

While for weights involved in MKF-KS, we only need to modify the weight in the second step in (44) to \( w_{t-1}f(y_t|x_{t-1}, \theta^{(j)}_{t-1}) \) to \( w_{t-1} \). The weight in the fourth step will be unchanged.

Another type of the missing data is that only some of the individuals are not observed at given time point. In order to accommodate such case, we only need to allow the observation matrix \( \tilde{Z}(\theta) \) being time-dependent. Now model (31) becomes

\[ x_t = \tilde{T}(\theta)x_{t-1} + v_t, \quad (44) \]

\[ y_t = \tilde{Z}(\theta)x_t + w_t. \quad (45) \]

(44)–(45) allow \( \tilde{Z}(\theta) \) can possess different dimension at different time point and thus can accommodate this type of missing data. The algorithms for parameter and state estimation given in section 3 can be extended straightforwardly to accommodate this more general model. Example 2 in the next section involves a real data set which contains both types of missing data.

4.2. General transition matrix

In section 2, we have assumed the individuals in the group can be correlated, i.e., the covariance matrix \( Q(i,j^*) \) may be a non-diagonal matrix. In addition to allowing the non-diagonal covariance matrix, the correlation within the group can also be modeled by adopting a different
form of $F(\theta)$, the state transition matrix. In section [2] we have assumed $F(\theta)$ is a diagonal matrix, i.e., $F(\theta) = \{d(\theta_i)\}_{i=1}^m$. It can be seen that the algorithms of the parameter and state estimation in the previous sections can apply regardless of $F(\theta)$ being a diagonal matrix or not. Non-diagonal transition matrix can occur in many different situations. Consider the following target tracking model,

$$
\begin{align*}
    dS_a &= \{ -\alpha[S_a - h(S_t)] - \gamma S_a - \beta[S_a - g(S_t)] \} dt + dW_a + dB_t,
\end{align*}
$$

(46)

where $S_a = (S_{a1}^{(x)}, S_{a1}^{(y)})^T$ denotes the position of target $i$ at time $t$; $S_a = (S_{a1}^{(x)}, S_{a1}^{(y)})^T$ denotes the velocity of target $i$ at time $t$; $h(S_t) = \frac{1}{m} \sum_{i=1}^{m} S_a$ and $g(S_t) = \frac{1}{m} \sum_{i=1}^{m} S_a$ denotes the average position and velocity at time $t$. $B_t$ is a 2-dimensional Brownian motion common to all targets; $W_{it}$ is another 2-dimensional Brownian motion assumed to be independently generated for each target $i$ in the group; $\alpha$ denotes the rate at which $\dot{S}_a$ restores to the average position $h(S_t)$; $\beta$ denotes the rate at which $\dot{S}_a$ restores to the average velocity $g(S_t)$; $\gamma$ denotes the rate at which $\dot{S}_a$ restores to zero. Model (46) is the fundamental model for the group tracking problem. In present literatures, e.g., Khan et al (2005), Pang et al (2008, 2011), three restoring parameters $\alpha_i, \beta_i, \gamma_i$ are assumed to be identical across different individuals, i.e., $\alpha_1 = \cdots = \alpha_m$, $\beta_1 = \cdots = \beta_m$, $\gamma_1 = \cdots = \gamma_m$. Here with MESSM in hand we can relax this restriction and allow different restoring parameters for different individuals which is more reasonable in most situations. Let $\theta_i = (\alpha_i, \beta_i, \gamma_i)$ and $\theta^T = (\theta_1^T, \cdots, \theta_m^T)$. For $i = 1, \cdots, m$, let

$$
A_{i2} = \begin{pmatrix}
0 & 1 \\
-\alpha_i + \frac{\alpha}{m} & -\beta_i - \frac{\beta}{m}
\end{pmatrix},
A_{i4} = \begin{pmatrix}
0 & 0 \\
\frac{\alpha}{m} & \frac{\beta}{m}
\end{pmatrix},
$$

and $A_{i1} = \{d_{A_{i2}, A_{i2}}\}, A_{i3} = \{d_{A_{i4}, A_{i4}}\}$,

$$
A(\theta) = \begin{pmatrix}
A_{11} & A_{13} & \cdots & A_{13} \\
A_{23} & A_{21} & \cdots & A_{23} \\
\vdots & \vdots & \ddots & \vdots \\
A_{m3} & A_{m3} & \cdots & A_{m1}
\end{pmatrix}_{4m \times 4m}.
$$

Defining the non-diagonal matrix $T(\theta) = \exp(A(\theta)\tau)$ where $\tau$ is the time between successive observations, then we have the following discretized version of model (46) for $m$ targets,

$$
x_t = T(\theta)x_{t-1} + \nu_t,
$$

(47)
where \( x_t = (S_{1t}^{(1)}, S_{1t}^{(2)}, S_{1t}^{(3)}, \ldots, S_{mt}^{(1)}, S_{mt}^{(2)}, S_{mt}^{(3)})^T \), \( v(t) = (v_{1t}^T, \ldots, v_{mt}^T)^T \) and \( v_i \) denotes the state disturbance for the \( i \)th target with \( v_i \sim \mathcal{N}(0, Q) \) and \( \text{Cov}(v_i, v_j) = \Sigma_{i \neq j} \). Consequently \( \text{Var}(v(i)) = (1_m \otimes 1_m)\Sigma + \{d \ Q - \Sigma\}_{i=1}^m \) where \( 1_m \) denotes the \( m \)-dimensional vector with entry one. Furthermore for \( \theta_i \ (i = 1, \ldots, m) \), we assume

\[
\theta_i = \mu_\theta + b_i \sim \text{i.i.d.} \mathcal{N}(\mu_\theta, D),
\]

where \( \mu_\theta^T = (\alpha, \beta, \gamma) \) represents the fixed effects and \( b_i \sim \mathcal{N}(0, D) \) the random effects. In matrix form we have \( \theta = 1_m \otimes \mu_\theta + b \) where \( b^T = (b_{11}, \ldots, b_{1m}) \sim \mathcal{N}(0, \{d \ D\}_{i=1}^m) \). Model (47)~(48) constitute the state equations for MESSM. The measurement model is more complex and we refer to Khan et al (2005), Pang et al (2008, 2011) for more details in this respect. These state equations are meaningful generalization of the present group target tracking models.

### 4.3. Time-dependent effects

In the previous sections both the fixed effects \( a \) and random effects \( b \) are assumed to be static, i.e., constant across the time range. In some situations, as can be seen in Example 2 in the next section, \( a \) and \( b \) can be time-dependent. It turns out that the results given in previous sections can be easily adapted to accommodate the time-dependent effects. For the illustrative purpose, consider the case in which there exists a time point \( 1 < T' < T \) that for \( 1 \leq t \leq T' \) we have \( \theta_i = \Psi_i^{(1)}a_1 + b_{i1} \sim \mathcal{N}(0, D_1) \); while for \( T' < t \leq T \) we have \( \theta_i = \Psi_i^{(2)}a_2 + b_{i2} \sim \mathcal{N}(0, D_2) \). For ease of exposition, we assume the individuals are independent with each other. The unknown parameters include \( \Delta = (a_1, a_2, \delta^T)^T \) where \( \delta \) denotes the unknown parameter contained in \( D_1, D_2, Q \) and \( R \). In this situation, the intermediate quantity of EM algorithm can be shown to be

\[
Q(\Delta, \Delta^*) = -\frac{m}{2} \log |D_1(\delta)| - \frac{m}{2} \log |D_2(\delta)| - \frac{Tm}{2} \log |R(\delta)| - \frac{Tm}{2} \log |Q(\delta)|
\]

\[
- \frac{1}{2} \sum_{i=1}^m \text{tr} \left[ D_1(\delta)^{-1} \left\{ (\Psi_i^{(1)}(a_1 - a_i) + b_{i1}^T) \right. \right.
\]

\[
\left. \times (\Psi_i^{(1)}(a_1 - a_i) + b_{i1}^T)^T + \text{Var}(b_{i1}[y_{i1:T}, \Delta^*]) \left\} \right. \right]
\]

\[
- \frac{1}{2} \sum_{i=1}^m \text{tr} \left[ D_2(\delta)^{-1} \left\{ (\Psi_i^{(2)}(a_2 - a_i) + b_{i2}^T) \right. \right.
\]

\[
\left. \times (\Psi_i^{(2)}(a_2 - a_i) + b_{i2}^T)^T + \text{Var}(b_{i2}[y_{i1:T}, \Delta^*]) \left\} \right. \right]
\]
\[-\frac{1}{2} \sum_{i=1}^{m} \sum_{t=1}^{T} \text{tr} \left[ R(\delta)^{-1} \left\{ w_{i,T} w_{i,T}^T + \text{Var}(w_u | y_{1:T}, \Delta^*) \right\} \right] \]

\[-\frac{1}{2} \sum_{i=1}^{m} \sum_{t=1}^{T} \text{tr} \left[ Q(\delta)^{-1} \left\{ v_{i,T} v_{i,T}^T + \text{Var}(v_u | y_{1:T}, \Delta^*) \right\} \right], \]

where \(b_{i1|T}, b_{i2|T}, w_{i|T}, v_{i|T}\) have the same expression as \(b_{i|T}, w_{i|T}, v_{i|T}\) in section \[3\]. As for quasi-Newton algorithm, the score vector now can be shown to be

\[
\frac{\partial \log L(\Delta | y_{1:T})}{\partial \alpha_1} \bigg|_{\Delta = \Delta^*} = \sum_{i=1}^{m} w_i^T D_1(\delta^*)^{-1} b_{i1|T},
\]

\[
\frac{\partial \log L(\Delta | y_{1:T})}{\partial \alpha_2} \bigg|_{\Delta = \Delta^*} = \sum_{i=1}^{m} w_i^T D_2(\delta^*)^{-1} b_{i2|T},
\]

\[
\frac{\partial \log L(\Delta | y_{1:T})}{\partial \delta_j} \bigg|_{\Delta = \Delta^*} = -\frac{1}{2} \sum_{i=1}^{m} \text{tr} \left[ D_1(\delta^*)^{-1} \frac{\partial D_1(\delta^*)}{\partial \delta_j} ight] \\
-D_1(\delta^*)^{-1} \left\{ b_{i1|T} b_{i1|T}^T + \text{Var}(b_{i1|T}, \Delta^*) \right\} D_1(\delta^*)^{-1} \frac{\partial D_1(\delta^*)}{\partial \delta_j} \\
-\frac{1}{2} \sum_{i=1}^{m} \sum_{t=1}^{T} \text{tr} \left[ D_2(\delta^*)^{-1} \frac{\partial D_2(\delta^*)}{\partial \delta_j} \right] \\
-D_2(\delta^*)^{-1} \left\{ b_{i2|T} b_{i2|T}^T + \text{Var}(b_{i2|T}, \Delta^*) \right\} D_2(\delta^*)^{-1} \frac{\partial D_2(\delta^*)}{\partial \delta_j} \\
+ \frac{1}{2} \sum_{i=1}^{m} \sum_{t=1}^{T} \text{tr} \left[ \hat{E} \left\{ e_i(\theta) e_i(\theta)^T - D_i(\theta) \right\} \frac{\partial R(\delta^*)}{\partial \delta_j} \right] \\
+ \frac{1}{2} \sum_{i=1}^{m} \sum_{t=1}^{T} \text{tr} \left[ \hat{E} \left\{ r_{t-1}(\theta) r_{t-1}(\theta)^T - N_{t-1}(\theta) \right\} \frac{\partial Q(\delta^*)}{\partial \delta_j} \right].
\]

Liu et al (2011) used time-dependent effects to model the dynamics of load of HIV in vivo. Their model can be formulated as that defined in (21)–(23) with the modification that for \(1 \leq t \leq T', \ \theta_t = \mu_{\theta_1} + b_{\theta_1} \sim N(0, \delta_1)\); while for \(T' < t \leq T, \ \theta_t = \mu_{\theta_2} + b_{\theta_2} \sim N(0, \delta_2)\). For this model, recursive formulas for EM and quasi-Newton algorithm can be derived straightforwardly from those expressions given above. It turns out these formulas are similar to those given in section \[3\] and so the details are omitted.

5. Numerical Studies

In this section we investigate the performance of the proposed algorithms by two numerical examples. The first example uses the simulated data which is generated from the autoregressive
with noise model; The second example involves a clinical trial data set which had been investigated by several other authors. For parameter estimation both the EM and BFGS algorithms will be carried out while only the results of BFGS will be reported because of the similarity of the results. The variances are calculated from the observed information matrix based on MKF-KS and the algorithm 3 in Nemeth et al (2013).

Example 1. Consider the model given by (21)\sim (22). The unknown parameters include $\Delta = (\mu_0, \delta_1, \delta_2, \delta_3)$. To generate the simulated data, the true parameters are set to be $\Delta_0 = (0.3, 0.3, 3, 0.1)$; initial state satisfies $x_0 \sim N(0, 3.2)$. We only consider the problem of parameter estimation in this example and three sample sizes, $m = 15, 30, 50$ will be investigated. In each case, three kinds of time series, $T = 10, 20, 30$, are considered. The repetition for each combination is set to be 500. The number of the random samples generated from the posterior distribution of random effects is set to be $M = 200$. The results are reported in Table 1 which include the parameter estimates and the corresponding standard errors. From Table 1 it can be seen that the proposed inference approaches can provide the reasonable estimates for the unknown parameters.

Example 2. A data set from the clinical trial of AIDS had been investigated in Liu et al (2011), Wu and Ding (1999) and Lederman et al (1998). This data set contains the records of 48 HIV infected patients who are treated with potent antiviral drugs. Dynamic models with mixed effects for this data set had been constructed in literatures, see Wu and Ding (1999), Liu et al (2011). In particular the model proposed in Liu et al (2011) is just the model given in the last paragraph in section 4.3. For parameter estimation, they investigated the EM algorithm and Baysian method. For state estimation, they took the estimates as the true values of the parameters and then employed the Kalman filter to estimate the state. Here the same model will be investigated and the focus is put on the statistical inference of such model. The observations $y_{it}$’s are the base 10 logarithm of the viral load for patient $i$ at week $t$. Unknown parameters include $\Delta = (\mu_0, \mu_2, \delta_1, \delta_2, \delta_3, \delta_4)^T$. Note for each patient, there exist some time points that the corresponding records $y_{it}$’s are missing. Thus the models in section 4.1 and 4.3 need to be combined together to analyze this data set.

For parameter estimation the results are reported in Table 2 which include the parameter estimates and the corresponding standard errors. Table 3 presents the estimated individual parameters using the particles $\{(\theta_{ij}^{(j)}, w_{ij}^{(j)}), j = 1, \cdots, M\}$ generated by MKF-KS algorithm at the last
time point. These estimates are just the weighted means of $\theta_t^{(j)}$ with weights $w_t^{(j)}$. With the estimated population parameters in hand, the state estimation is carried out using the MKF-KS algorithm. The resulted filter estimate and the one-step ahead prediction are plotted in Figure 1 for four patients who have the most observations among these 48 patients. For the purpose of comparison we also run Kalman filter with the individual parameters replaced by their estimates. Figure 2 presents the box plots of mean squared errors of MKF-KS and Kalman filter for 48 patients. It seems that these two MSE’s are similar in magnitude. This can be explained as follows. On the one hand, Kalman filter uses all the observations and should outperform MKF-KS algorithm which only uses the observations up to the present time point. On the other hand the predicted random effects are taken as the true random effects in Kalman filter which will results in bias in state estimation. While for MKF-KS the random effects are integrated out when the states are estimated and so less affected by estimating errors. Both factors affect the magnitude of the MSE’s. Recall contrary to Kalman filter the main advantages of MKF-KS is that without the known random effects it also can provide the recursive state estimation. This point is more important in the setting of sparse data in which the random effects can not be estimated accurately.

6. Conclusion

We consider both the parameter and state estimation for the linear mixed-effects state space model which can accommodate the correlated individuals. For parameter estimation EM and score based algorithms are investigated based on disturbance smoothing. The implementation of EM and score based algorithms only require the random samples of random effects from the posterior distribution. Particularly the proposed EM algorithm can be regarded as a Rao-Blackwellized version of that proposed in Liu et al (2011). For state estimation, because longitudinal data set usually involves sparse data with which random effects can not be estimated accurately, we advocate state estimation should be carried out without assuming the random effects being known. To this end a kernel smoothing based mixture Kalman filter is proposed to estimate the state. Numerical studies show the proposed inferences perform well in the setting of finite samples. The proposed models and statistical inferences can be extended by different ways. For example nonlinear mixed-effects state space model with additive Gaussian error can be handled by the similar ideas in this paper without much difficulty. But for the general
nonlinear/non-Gaussian state space model with mixed-effects, the proposed algorithms can not apply and new inference techniques need to be developed. Another interesting problem is how to carry out the parameter estimation in a recursive manner. For the ordinary fixed-effect state space models, there have existed some studies in this respect. Extending such inferences to state space model with mixed effects also is meaningful.

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Table 1: Parameter estimates and standard errors with true parameter $\mu = 0.3, \delta_1 = 0.3, \delta_2 = 3, \delta_3 = 0.1$.

| Cases | $\mu_\theta$ | SE | $\delta_1$ | SE | $\delta_2$ | SE | $\delta_3$ | SE |
|-------|-------------|----|-----------|----|------------|----|------------|----|
| $m=15$ | $T=10$ | 0.27 | 0.05 | 0.40 | 0.1 | 4.70 | 0.52 | 0.14 | 0.007 |
| | $T=20$ | 0.26 | 0.04 | 0.38 | 0.08 | 3.21 | 0.47 | 0.07 | 0.006 |
| | $T=30$ | 0.28 | 0.04 | 0.34 | 0.03 | 3.17 | 0.27 | 0.07 | 0.006 |
| $m=30$ | $T=10$ | 0.27 | 0.02 | 0.37 | 0.07 | 3.82 | 0.29 | 0.13 | 0.005 |
| | $T=20$ | 0.28 | 0.02 | 0.34 | 0.03 | 2.43 | 0.17 | 0.12 | 0.006 |
| | $T=30$ | 0.31 | 0.01 | 0.24 | 0.02 | 2.71 | 0.20 | 0.08 | 0.005 |
| $m=50$ | $T=10$ | 0.30 | 0.01 | 0.34 | 0.06 | 3.51 | 0.27 | 0.12 | 0.004 |
| | $T=20$ | 0.31 | 0.01 | 0.32 | 0.04 | 3.22 | 0.21 | 0.11 | 0.005 |
| | $T=30$ | 0.31 | 0.01 | 0.32 | 0.04 | 2.87 | 0.20 | 0.11 | 0.001 |

Table 2: Population parameter estimates and standard errors

| Estimates | $\mu_\theta_1$ | $\mu_\theta_2$ | $\delta_1$ | $\delta_2$ | $\delta_3$ | $\delta_4$ |
|-----------|---------------|----------------|-----------|-----------|-----------|-----------|
| SE’s      | 0.06 | 0.04 | 0.08 | 0.23 | 0.002 | 0.01 |
Table 3: Estimation of the individual parameters for 48 patients

| $\theta_i^{(1)}$ |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |
|-----------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 0.868915        | 0.849607 | 0.868957 | 0.827189 | 0.851339 | 0.847058 | 0.848824 | 0.851733 |
| 0.849319        | 0.868136 | 0.838490 | 0.835906 | 0.859012 | 0.825839 | 0.846816 | 0.859276 |
| 0.867417        | 0.857401 | 0.843068 | 0.835888 | 0.837270 | 0.852747 | 0.832048 | 0.842219 |
| 0.850987        | 0.852832 | 0.835151 | 0.856031 | 0.872748 | 0.873013 | 0.840243 | 0.851437 |
| 0.893272        | 0.865324 | 0.853658 | 0.858038 | 0.863467 | 0.836726 | 0.837801 | 0.846284 |
| 0.809998        | 0.844643 | 0.846764 | 0.848282 | 0.846723 | 0.833354 | 0.837123 | 0.828165 |

| $\theta_i^{(2)}$ |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |
|-----------------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| 0.852200        | 0.841703 | 0.947872 | 0.894520 | 0.848136 | 0.975277 | 0.862129 | 0.925632 |
| 0.859690        | 0.865170 | 0.762160 | 0.921414 | 0.932375 | 0.892159 | 0.858365 | 0.776656 |
| 0.938613        | 0.870105 | 0.900053 | 0.844046 | 0.962848 | 0.872085 | 0.826155 | 0.900559 |
| 0.843995        | 0.712202 | 0.901383 | 0.924811 | 0.910035 | 0.957107 | 0.920373 | 0.878261 |
| 0.868421        | 0.928374 | 0.867860 | 0.915143 | 0.849401 | 0.908050 | 0.944003 | 0.925122 |
| 0.936315        | 0.905399 | 0.872215 | 0.858642 | 0.821628 | 0.875818 | 0.753861 | 0.948502 |
Figure 1: Estimation of viral load for four patients in the HIV dynamic study. The circles represent base 10 logarithm of the viral loads. The green solid lines represent the one-step ahead prediction; The dotted lines represent the filtering estimates; The dashed lines represent the 95% confidence interval of the filtering estimates; The pink solid lines represent the 95% confidence interval of the one-step ahead prediction.
Figure 2: Mean square errors of the one-step ahead prediction for 48 patients. The left panel corresponds to the MKF-KS algorithm. The right panel corresponds to the Kalman filter with the estimated individual parameters.