Probabilistic sequential matrix factorization

Abstract

We introduce the probabilistic sequential matrix factorization (PSMF) method for factorizing time-varying and non-stationary datasets consisting of high-dimensional time-series. In particular, we consider nonlinear-Gaussian state-space models in which sequential approximate inference results in the factorization of a data matrix into a dictionary and time-varying coefficients with (possibly nonlinear) Markovian dependencies. The assumed Markovian structure on the coefficients enables us to encode temporal dependencies into a low-dimensional feature space. The proposed inference method is solely based on an approximate extended Kalman filtering scheme which makes the resulting method particularly efficient. The PSMF can account for temporal nonlinearities and, more importantly, can be used to calibrate and estimate generic differentiable nonlinear subspace models. We show that the PSMF can be used in multiple contexts: modelling time series with a periodic subspace, robustifying changepoint detection methods, and imputing missing-data in high-dimensional time-series of air pollutants measured across London.

1 Introduction

In the past decades, the problem of r-rank factorization of a data matrix \( Y \in \mathbb{R}^{d \times n} \) as

\[ Y \approx CX \]  

(1)

where \( C \in \mathbb{R}^{d \times r} \) is termed dictionary matrix and \( X \in \mathbb{R}^{r \times n} \) is termed coefficients, has received significant attention in multimedia signal processing and machine learning under the umbrella term of matrix factorizations (MFs). The classical method for solving problems of the form (1) is the nonnegative matrix factorization (NMF) (Lee and Seung, 1999), which is proposed for nonnegative data matrices and to obtain nonnegative factors. The interest was then extended to general MF problems for real-valued data and factors. Apart from optimization based formulations following the NMF, probabilistic approaches were introduced both for the nonnegative case based on variational inference (Cemgil, 2009) and the real-valued case based on Markov chain Monte Carlo (MCMC) (Mnih and Salakhutdinov, 2008; Salakhutdinov and Mnih, 2008).

Naturally, online and recursive implementations of these algorithms have received significant attention as they enable the practitioner to scale the algorithms up for big datasets. In this front, a number of algorithms have been proposed which are based either on stochastic optimization (Bucak and Günsel, 2009; Mairal et al., 2010; Gemulla et al., 2011) or within a probabilistic framework (Akyildiz and Míguez, 2019). However, these methods are for i.i.d data in general and cannot explicitly handle cases where the columns of \( Y \) possess a time-dependent structure. Extension of matrix factorization to the time-dependent case has been a subject of recent research. In particular, in one of the early works, Yildirim et al. (2012) propose a nonnegative matrix factorization model by introducing a state-space model with a Poisson likelihood where the inference is then carried out with sequential Monte Carlo. The estimation of the dictionary is posed as a static parameter estimation problem whereas the coefficients were inferred as latent variables. In a similar manner, Sun et al. (2012) propose a state-space based approach where the dictionary is estimated using an expectation-maximization (EM) algorithm. An extension of the nonnegative models to the dynamic settings was considered by Févotte et al. (2013) named as the nonnegative dynamical systems (NDS). Similar methods based on dynamic nonnegative models attracted significant attention which also use state-space formulations, see, e.g., Mohammadiha et al. (2013, 2014). We refer to Févotte et al. (2018) for a literature review of temporal NMF methods. An optimization based temporal matrix factorization was introduced by Yu et al. (2016) where the regularizers are used to induce structure on learned dictionary and coefficients.
The interesting application of the NMF for time series was considered in Weiderer et al. (2019) in which the authors demonstrated that structured subspaces can be very useful to model time-series.

**Contribution.** In this work, we formulate a nonlinear Gaussian state-space model (SSM) for sequential factorization of time-series. Our formulation is fully probabilistic in the sense that we place a Gaussian prior on the dictionary matrix and a general Markov model for the evolution of the coefficients. The inference procedure is based on an approximate extended Kalman filtering scheme which results in a sequential matrix factorization method. More precisely, our model assumes a time-dependent structure on the columns of the coefficient matrix. To this end, we formulate a matrix-variate general (Gaussian) graphical model for which tractable approximate inference based on extended Kalman filters (Kalman, 1960) is available in closed form. This analytical tractability is key to efficient implementation as we do not require any sampling procedure to approximate the posterior distributions. The inference method we provide is explicit and update rules are readily available to implement without further considerations on the practitioner’s side. Our method can be customized, i.e., the subspace model can be modified accordingly to the needs of the application at hand, yet, our method can be easily adapted provided that the needed derivatives can be computed (readily possible with the tools of automatic differentiation).

**Notation**

We denote the \(d \times d\) identity matrix with \(I_d\). The notation \(\mathcal{N}(x; \mu, \Sigma)\) denotes the Gaussian density over the variable \(x\) with mean \(\mu\) and covariance matrix \(\Sigma\). Similarly, \(\mathcal{MN}(X; M, U, V)\) denotes the matrix-variate Gaussian density with the mean-matrix \(M\), the row-covariance \(U\), and the column-covariance \(V\). We use the following notation to denote sequences: \(x_{1:n} = \{x_1, \ldots, x_n\}\). For a matrix \(Z\), \(z = \text{vec}(Z)\) denotes vectorisation of \(Z\). We note that if \(C \sim \mathcal{MN}(C; M, U, V)\), then \(c \sim \mathcal{N}(c; \text{vec}(M), V \otimes U)\) where \(c = \text{vec}(C)\).

2 The Probabilistic Model

Let \(Y \in \mathbb{R}^{d \times n}\) be the data matrix. The dictionary matrix \(C \in \mathbb{R}^{d \times r}\) is an \(d \times r\) matrix where \(r\) is the approximation rank. We denote the coefficient matrix with \(X \in \mathbb{R}^{r \times n}\) where \(n\) is the number of data samples. The notation \(y_k\) indicates the \(k\)th column of the data matrix \(Y\) and the corresponding coefficient vector is denoted \(x_k\) which is similarly the \(k\)th column of the coefficient matrix \(X\).

We first describe the state space model which consists of observations \((y_k)_{k \geq 1} \in \mathbb{R}^d\), latent coefficients \((x_k)_{k \geq 0} \in \mathbb{R}^r\) and latent dictionary matrix \(C \in \mathbb{R}^{d \times r}\) as follows

\[
\begin{align*}
p(C) &= \mathcal{MN}(C; C_0, I_d, V_0), \\
p(x_0) &= \mathcal{N}(x_0; \mu_0, F_0), \\
p(x_k | x_{k-1}) &= \mathcal{N}(x_k | f_\theta(x_{k-1}), Q_k), \\
p(y_k | x_k, C) &= \mathcal{N}(y_k | C x_k, R_k),
\end{align*}
\]

for \(k \geq 1\), where \(f_\theta: \mathbb{R}^r \times \Theta \rightarrow \mathbb{R}^r\) is a nonlinear mapping defining the dynamics of the coefficients where \(\Theta \subset \mathbb{R}^{d_0}\) is the parameter space, and the sequences \((Q_k, R_k)_{k \geq 0}\) are defining the noise covariances of the coefficient dynamics (4) and the observation model (5), respectively. The initial covariances of the state and the dictionary are denoted as \(P_0\) and \(V_0\), respectively.

Intuitively, the model (2)–(5) is a dimensionality reduction model where the dynamical structure of the learned subspace is explicitly modeled via the transition density (4). This means, inferring \(C\) and \((x_k)_{k \geq 0}\) will lead to a probabilistic dimensionality reduction scheme where the dynamical structure in the data will manifest itself in the dynamics of the coefficients \((x_k)_{k \geq 0}\). The model is a probabilistic state-space model for which standard inference tools may be helpful, however, one main difficulty in our case is that we assume \(C\) to be an unknown and random matrix, therefore, the (extended) Kalman filter cannot be applied directly for inference. To alleviate this problem, we formulate the prior in (2) with a Kronecker covariance structure which enables us to update (conditional on \(x_k\)) the posterior distribution of \(C\) analytically (Akyildiz and Míguez, 2019). Hence, this model can be seen as a temporal extension of the model proposed by Akyildiz and Míguez (2019) which is designed for the factorization of a data matrix consisting of (conditionally) independent data points.

3 Inference and Estimation

In this section, we describe the algorithm for performing sequential inference in the model (2)–(5). We first describe the optimal inference recursions to conduct inference in this model. Then, we describe our approximate inference scheme to approximate these optimal recursions.

3.1 Optimal sequential inference

In this section, we summarize the optimal inference recursions for our model when \(\theta\) is assumed to be fixed. For notational clarity, we drop the parameter \(\theta\) from the notation. In order to define one-step procedure of the method, we assume that we are given the filters \(p(x_{k-1} | y_{1:k-1})\) and \(p(c | y_{1:k-1})\) at time \(k - 1\).
Prediction. Considering the conditional independence relationships presented in the model (2)–(5), we first compute the predictive distribution via the Chapman-Kolmogorov equation

\[ p(x_k|y_{1:k-1}) = \int p(x_{k-1}|y_{1:k-1}) p(x_k|x_{k-1}) dx_{k-1}. \]  

(6)

We note that, given \( p(x_{k-1}|y_{1:k-1}) \), this step is independent of the dictionary and solely depends on the dynamical model at hand.

Update. Given this predictive distribution of \( x_k \), we can now define the update steps of the method. Differently than a regular Kalman filter, we have two main quantities to update: \( x_k \) and \( c \). We first define the incremental marginal likelihood:

\[ p(y_k|y_{1:k-1}) = \int \int p(y_k|c,x_k)p(x_k|y_{1:k-1}) p(c|y_{1:k-1}) dx_k dc. \]

Next, we define the optimal inference recursions for updating the dictionary \( C \) and coefficients \( (x_k)_{k\geq 1} \).

Dictionary Update: Given \( p(y_k|y_{1:k-1}) \), we can first update the dictionary as follows

\[ p(c|y_{1:k}) = \frac{p(c|y_{1:k-1}) p(y_k|c,y_{1:k-1})}{p(y_k|y_{1:k-1})}. \]  

(7)

where

\[ p(y_k|c,y_{1:k-1}) = \int p(y_k|c,x_k)p(x_k|y_{1:k-1}) dx_k. \]  

(8)

Coefficient Update: At the same time, we can also update the coefficients at time \( k \) (independent of the dictionary update):

\[ p(x_k|y_{1:k}) = \frac{p(x_k|y_{1:k-1}) p(y_k|x_k,y_{1:k-1})}{p(y_k|y_{1:k-1})}. \]  

(9)

where

\[ p(y_k|x_k,y_{1:k-1}) = \int p(y_k|x_k,c)p(c|y_{1:k-1}) dc. \]  

(10)

Perhaps not surprisingly, all these computations are rarely tractable. In the next section, we introduce successive approximations to make all these steps approximately tractable. Doing so leads to an efficient and explicit inference algorithm.

3.2 Approximate sequential inference

The recursions we presented in the last section are optimal. However, they involve intractable integrals, which are not possible to compute in closed form. In this section, we propose a sequence of approximations for intractable integrals. We note that the resulting method, an approximate extended Kalman filter, is sequential, i.e., uses a single observation at each iteration.

We start by assuming a special structure on the model to obtain a tractable structure. First, we note that a key assumption we make is on the prior: The matrix-Gaussian prior in (2) can be written as

\[ p(c) = \mathcal{N}(c; c_0, V_0 \otimes I_d). \]

The Kronecker structure in the covariance will be key to obtain an approximate and tractable posterior distribution with the same covariance structure. Now, in order to describe our inference scheme, assume that, we are given \( p(c|y_{1:k-1}) = \mathcal{N}(c; c_{k-1}, V_{k-1} \otimes I_d) \) and \( p(x_{k-1}|y_{1:k-1}) = \mathcal{N}(x_{k-1}; \mu_{k-1}, P_{k-1}) \). Departing from these two distributions, it is not possible to exactly update \( p(c|y_{1:k}) \) and \( p(x_k|y_{1:k}) \). Hence as we introduce some approximations, from now on, we denote approximate densities with the symbol \( \tilde{p}(\cdot) \) instead of \( p(\cdot) \) which indicates that the distribution under consideration is not exact. In what follows, starting from (exact) filters, we demonstrate the computations of a single time step of the method.

3.2.1 Prediction

In the prediction step, we need to compute (6). This is analytically tractable for \( f_0(x) = Ax \). More specifically, when \( f_0(x) = Ax \), given \( p(x_{k-1}|y_{1:k-1}) = \mathcal{N}(x_{k-1}; \mu_{k-1}, P_{k-1}) \), we obtain \( p(x_k|y_{1:k-1}) = \mathcal{N}(x_k; \tilde{\mu}_k, \tilde{P}_k) \) where \( \tilde{\mu}_k = A\mu_{k-1} \) and \( \tilde{P}_k = AP_{k-1}A^\top + Q_k \). However, if \( f_0(x) \) is a nonlinear function, no generic solution exists, and the integral in (6) becomes intractable. In this case, we can use an extended Kalman update. This update is based on the linearization of the transition model (Anderson and Moore, 1979). In this case, we obtain \( \tilde{p}(x_k|y_{1:k-1}) = \mathcal{N}(x_k; \tilde{\mu}_k, \tilde{P}_k) \)

\[ \tilde{\mu}_k = f_0(\mu_{k-1}) \quad \text{and} \quad \tilde{P}_k = F_k P_{k-1} F_k^\top + Q_k, \]

where \( F_k = \frac{\partial f_0(x)}{\partial x} |_{x=\tilde{\mu}_{k-1}} \) is a Jacobian matrix associated to \( f_0 \). We note that the unscented Kalman filter (UKF) can also be used in this step, if \( F_k \) is not available to compute.

3.2.2 Update

For the update step, we are interested in updating two main variables, namely, \( x_k \) and \( C \). Given the approximate predictive distribution \( \tilde{p}(x_k|y_{1:k-1}) \), we would like to obtain \( \tilde{p}(c|y_{1:k}) \) and \( \tilde{p}(x_k|y_{1:k}) \). We start by describing the update rule for the dictionary \( C \), then proceed to deriving the approximate posterior of \( x_k \). Given the prediction, update steps of \( C \) and \( x_k \) are independent of each other, to avoid the repeated
use of the data point $y_k$.

**Dictionary Update.** We start with the update of $\bar{p}(c|y_{1:k})$. First note that, the integral (8) has a closed form solution:

$$p(y_k|c, y_{1:k-1}) = \mathcal{N}(y_k; C\bar{\mu}_k, R_k + C\bar{P}_kC^T).$$  

(11)

This closed form is not helpful to us, however, because this distribution plays the role of the likelihood in update (7). Since both the mean and the covariance depend on $C$, the update (7) becomes intractable. To alleviate this problem, we first replace $C\bar{P}_kC^T \approx C_k^{-1}\bar{P}_kC_k^{-1}$ in (11). This enables us to obtain a tractable update where the likelihood is of the form $\mathcal{N}(y_k; C\mu_k, R_k + C_k^{-1}\bar{P}_kC_k^{-1})$. However, for an efficient update of $C$ in purely matrix-form, we need to obtain a likelihood with a diagonal covariance. Finally, if we choose the closest Gaussian with a constant diagonal covariance in the problem dimension $d$, we need to obtain a tractable update where the likelihood is of the form $\mathcal{N}(y_k; C\mu_k, \eta_k \otimes I_d)$. For this, we first construct the following approximation (see, e.g., Fernandez-Bes et al. (2015))

$$\bar{p}(y_k|c, y_{1:k-1}) = \mathcal{N}(y_k; C\mu_k, \eta_k \otimes I_d),$$  

(12)

where

$$\eta_k = \frac{\text{Tr}(R_k + C_k^{-1}\bar{P}_kC_k^{-1})}{d}.$$  

(13)

Now given the likelihood (12), we can obtain the approximate filter $\bar{p}(c|y_{1:k})$ as follows. We note that for the given previous posterior approximation and the likelihood, the update for the new posterior can be computed analytically, hence given formally in the following proposition based on Akylidiz and Miguez (2019).

**Proposition 1.** Given

$$\bar{p}(c|y_{1:k-1}) = \mathcal{N}(c; c_{k-1}, V_{k-1} \otimes I_d)$$

and the likelihood

$$\bar{p}(y_k|c, y_{1:k-1}) = \mathcal{N}(y_k; C\mu_k, \eta_k \otimes I_d)$$  

(14)

the approximate posterior distribution $\bar{p}(c|y_{1:k})$ is given by

$$\bar{p}(c|y_{1:k}) = \mathcal{N}(c; c_k, V_k \otimes I_d),$$

where $c_k = \text{vec}(C_k)$ and the posterior column-covariance matrix $V_k$ is given by

$$V_k = \left( V_{k-1} - \frac{V_{k-1}\bar{\mu}_k\bar{\mu}_k^T V_{k-1}}{\bar{\mu}_k^T V_{k-1}\bar{\mu}_k + \eta_k} \right), \text{ for } k \geq 1,$$  

(15)

where $V_0$ is given by the prior pdf in (2). Moreover, the posterior mean $c_k$ can be obtained in matrix-form and is given by

$$C_k = C_{k-1} + \frac{(y_k - C_{k-1}\bar{\mu}_k)\bar{\mu}_k^TV_{k-1}}{\bar{\mu}_k^TV_{k-1}\bar{\mu}_k + \eta_k}, \text{ for } k \geq 1,$$  

(16)

where $C_k$ is the posterior mean of the dictionary matrix $C$.

**Proof.** See Supplement B. \hfill \blacksquare

We note the main gain of this result is that we obtain matrix-variate update rules for the sufficient statistics of the posterior distribution. This is key to an efficient implementation of the method.

**Coefficient Update.** To update the posterior distribution of coefficients, we first derive the approximation of $p(y_k|y_{1:k-1}, x_k)$ by integrating out $c$, see Eq. (10). First, we have the following exact result.

**Proposition 2.** Given $p(y_k|c, x_k)$ as in (5) and

$$p(c|y_{1:k-1}) = \mathcal{N}(c; c_{k-1}, V_{k-1} \otimes I_d),$$

we obtain

$$p(y_k|y_{1:k-1}, x_k) = \mathcal{N}(y_k; C_{k-1}x_k, R_k + x_k^TV_{k-1}x_k \otimes I_d).$$  

(17)

**Proof.** See Supplement C. \hfill \blacksquare

We note that in practice this quantity will be approximate as, e.g., $\bar{p}(c|y_{1:k-1})$ (and other quantities) will be approximate. Moreover, even if they were exactly computable, the likelihood in (17) with its current form is not amenable for carrying out the exact inference step (9) as well, since it contains $x_k$ in both mean and covariance. Therefore, we first construct the following likelihood

$$\bar{p}(y_k|y_{1:k-1}, x_k) = \mathcal{N}(y_k; C_{k-1}x_k, \bar{R}_k),$$  

(18)

where $\bar{R}_k = R_k + \bar{\mu}_k^TV_{k-1}\bar{\mu}_k \otimes I_d$. With this form of the likelihood, we can now obtain the approximate posterior using (9), as an application of the standard Kalman update (Anderson and Moore, 1979), as

$$\bar{p}(x_k|y_{1:k}) = \mathcal{N}(x_k; \mu_k, P_k)$$

where

$$\mu_k = \bar{\mu}_k + \bar{P}_kC_{k-1}(C_{k-1}\bar{P}_kC_{k-1} + \bar{R}_k)^{-1}(y_k - C_{k-1}\bar{\mu}_k),$$

$$P_k = \bar{P}_k - \bar{P}_kC_{k-1}(C_{k-1}\bar{P}_kC_{k-1} + \bar{R}_k)^{-1}C_{k-1}\bar{P}_k.$$

Note that matrix inversions in these update rules are for $r \times r$ matrices where $r$ is the approximation rank which is typically small. Therefore, matrix inversions do not create a computational bottleneck with respect to the problem dimension $d$ and they stay easy to compute.
3.2.3 Parameter estimation

As we mentioned above, all prediction and update steps are conditional on $\theta$ which we dropped from the notation for clarity. Next, we describe the parameter estimation procedure explicitly. We would like to solve the maximum-likelihood estimation (MLE) problem

$$\theta^* \in \arg \max_{\theta \in \Theta} \log p_0(y_{1:n}),$$

(19)

in order to estimate the parameters of interest. However, this maximization is intractable for general models, therefore can only be attained through numerical optimization. In particular, we focus on gradient schemes for solving the problem (19), see, e.g., Kantas et al. (2015) for a review on parameter estimation methods for state-space models. We note that depending on the probabilistic model (particularly the choice of $f_\theta$), the problem (19) can be highly non-convex and difficult to solve numerically.

In this section, we first develop an offline and iterative gradient ascent scheme for the cases where the number of observations from the time-series is limited. In this case, the parameter can be updated after a single filtering pass conditional on the parameter and this procedure can be iterated. Then we introduce the recursive version which can be used for the online, streaming setting when the number of data points are large.

Iterative estimation. When the number of data points is limited, it is possible to employ an iterative estimation procedure which results in multiple passes over the data. This can be done iteratively by implementing

$$\theta_i = \theta_{i-1} + \gamma \nabla \log \tilde{p}_0(y_{1:n})|_{\theta = \theta_{i-1}},$$

(20)

at the $i$’th iteration. We name this scheme as the iterative PSMF. We note that the exact computation of $\nabla \log \tilde{p}_0(y_{1:n})$ is not possible due to the aforementioned intractability. Instead, we propose an approximate gradient by observing that

$$\nabla \log \tilde{p}_0(y_{1:n}) = \sum_{k=1}^{n} \nabla \log \tilde{p}_0(y_k|y_{1:k-1}).$$

It is easy to see that this gradient can be computed while doing forward filtering without needing to store all gradients. We note that it is possible to obtain two different approximations of the incremental marginal likelihood $\tilde{p}_0(y_k|y_{1:k-1})$ depending on when it is computed. One can integrate out $c$ in (12) or one can integrate out $x_k$ in (18). However, the resulting quantities are closely related and we choose the former path for computational reasons. We refer to Sec. 3.2.4 for the derivation of the approximate log-marginal likelihood $\log \tilde{p}_0(y_k|y_{1:k-1})$.

Recursive estimation. For long sequences of data, it may not be necessary (and can be inefficient) to perform the iterative procedure (20). For this case, the parameter can be updated whenever a data point is received. In other words, one can perform the filtering steps by fixing $\theta = \theta_{k-1}$ and then update

$$\theta_k = \theta_{k-1} + \gamma \nabla \log \tilde{p}_0(y_k|y_{1:k-1})|_{\theta = \theta_{k-1}}.$$  

(21)

We name the resulting PSMF with this parameter update as the recursive PSMF. This is an adaptation of the online maximum-likelihood estimation procedure for state-space models (Kantas et al., 2015), also known as recursive maximum-likelihood\(^1\). This procedure has guarantees for finite-state space HMMs, but its convergence for general SSMs stays an open problem (Kantas et al., 2015).

The full procedure can be seen from Algorithm 1.

Remark 1. We note that the gradient descent schemes in (20) and (21) can be replaced by modern optimizers to improve the speed of convergence, such as Adam (Kingma and Ba, 2015). We take advantage of such optimizers in one of our numerical results.

3.2.4 Approximating the marginal likelihood

In this section, we provide the expression for the log marginal likelihood approximation. We consider the likelihood given in (12) which is of the form $\tilde{p}_0(y_k|y_{1:k-1}, c) = N((y_k; C f_\theta(\mu_{k-1}), y_k \otimes I_d)$. Given the prior $\tilde{p}(c|y_{1:k-1}) = N(c; c_{k-1}, V_{k-1} \otimes I_d)$, we obtain the marginal likelihood as

$$\tilde{p}_0(y_k|y_{1:k-1}) = \int \tilde{p}(y_k|y_{1:k-1}, c)\tilde{p}(c|y_{1:k-1})dc = N \left( y_k; C_{k-1} f_\theta(\mu_{k-1}), \left(\| f_\theta(\mu_{k-1})\|_2^2 V_{k-1} + \eta_k \right) \otimes I_d \right).$$

The negative log-likelihood is then given by

$$- \log \tilde{p}_0(y_k|y_{1:k-1}) = \frac{c}{2} d \log \left( \| f_\theta(\mu_{k-1})\|_2^2 V_{k-1} + \eta_k \right) + \frac{1}{2} \frac{\| y_k - C_{k-1} f_\theta(\mu_{k-1})\|^2}{\eta_k + \| f_\theta(\mu_{k-1})\|_2^2 V_{k-1}}$$

(22)

where $= c$ denotes this equality is up to some constants that are independent of $\theta$, hence irrelevant for the optimization. Eq. (22) can be seen as an optimization objective which arises from our model. We can compute the gradients of (22) using automatic differentiation for generic $f_\theta$.\(^1\)The main difference for our case, however, our gradients are not exact but approximate.
Algorithm 1 Iterative and recursive PSMF

1: Initialize $\theta_0$, $C_0$, $V_0$, $\mu_0$, $P_0$, $(Q)_{k \geq 0}$, $(R)_{k \geq 0}$.
2: for $i \geq 1$ do
3: $C_0 = C_T$, $\mu_0 = \mu_T$, $P_0 = P_T$, $V_0 = V_T$.
4: for $1 \leq k \leq T$ do
5: Predictive mean of $x_k$
   \[ \mu_k = f_{\theta_{i-1}}(\mu_{k-1}) \quad \text{or} \quad \mu_k = f_{\theta_{i-1}}(\mu_{k-1}) \]
6: Predictive covariance of $x_k$
   \[ \bar{P}_k = F_k P_{k-1} F_k^T + Q_k \]
   where $F_k = \frac{\partial f(x)}{\partial x}{|_{x = \bar{x}_{k-1}}}$.
7: Mean update of the dictionary
   \[ C_k = C_{k-1} + (y_k - C_{k-1} \mu_k) \bar{P}_k V_{k-1} \]
8: Covariance update of the dictionary
   \[ V_k = V_{k-1} - \frac{V_{k-1} \bar{P}_k \bar{P}_k V_{k-1}}{\mu_k \bar{P}_k V_{k-1} \mu_k + \eta_k} \]
9: Mean update of $x_k$
   \[ \mu_k = \bar{\mu}_k + \bar{P}_k C_{k-1} S_k^{-1} (y_k - C_{k-1} \bar{\mu}_k) \]
   where $S_k = C_{k-1} P_k C_{k-1}^T + \bar{R}_k$.
10: Covariance update of $x_k$
    \[ P_k = \bar{P}_k - \bar{P}_k C_{k-1} S_k^{-1} C_{k-1} \bar{P}_k + R_k \]
11: Parameter update \#recursive version
    \[ \theta_i = \theta_{i-1} + \gamma \nabla \log \bar{p}_{\theta}(y_k | y_{1:k-1}){|_{\theta = \theta_{i-1}}} \]
12: end for
13: Parameter update \#iterative version
    \[ \theta_i = \theta_{i-1} + \gamma \sum_{k=1}^T \nabla \log \bar{p}_{\theta}(y_k | y_{1:k-1}){|_{\theta = \theta_{i-1}}} \]
14: end for

3.3 Handling missing data

In order to obtain update rules which can explicitly handle missing data, we need to modify only the likelihood. When we receive an observation vector with missing entries, we model it as $z_k = m_k \otimes y_k$ where $m_k \in \{0, 1\}^d$ is a mask vector which contains zeros for missing entries and ones otherwise. We note that $z_k = M_k y_k$ where $M_k = \text{diag}(m_k)$. Therefore, we obtain the likelihood of $z_k$ as

\[ p(z_k | c, x_k) = \mathcal{N}(z_k; M_k C x_k, M_k R_k M_k^T) \]

The update rules of the method can be re-derived using this likelihood and essentially identical to the Algorithm 1 with masks. See Supplement D for details.

4 Experiments

4.1 A synthetic nonlinear periodic subspace

To simplify our setup and demonstrate the utility of the algorithm in order to learn a dictionary and a structured subspace jointly, we choose $x_0 = \mu_0$ and $P_0 = 0$ and

\[ x_t = f_\theta(x_{t-1}) = \cos(\theta t + x_{t-1}) \]

where $\theta \in \mathbb{R}_+^d$ and $Q_k = 0$ for all $k \geq 1$. This defines a deterministic subspace with highly periodic structure. We choose $d = 20$ and $r = 6$ and generate the data from the model (2)–(5) with

\[ \theta^* = [10^{-3}, 2 \times 10^{-3}, 3 \times 10^{-3}, 4 \times 10^{-3}, 5 \times 10^{-3}, 6 \times 10^{-3}]^T. \]

We initialize $C_0$ randomly and $\theta_0$ drawn from a uniform distribution on $[0, 0.1]^6$. We set $V_0 = v_0 \otimes I_r$ with

Figure 1: Orange: Noisy observed synthetic time series. Green: Unobserved future data. Red: Reconstruction & predictions. We show the method is able to learn the ground truth model when it is well-specified.

Figure 2: Left: Orange: True subspace functions where the data is generated from. Red: Estimated subspace functions (up to the label switching). Right: The reconstruction error $\|Y - CX\|_F^2$ over (outer) iterations of the iterative PSMF.
We generate 1000 such datasets to test the method. Furthermore, in addition to the standard Gaussian noise, the data is contaminated by heavy-tailed $t$-distributed noise with varying degrees of freedom from 1.5 to 1.9 (i.e., with infinite variance) in 5% of the entries on average, which makes the problem challenging. In order to learn the structural changes and be robust against the heavy-tailed noise, we design a smooth subspace model $(x_i(t))_{i \geq 0}$ for $i = 1, \ldots, r$ in continuous-time consisting of a Gaussian process (GP) prior, i.e., $x_i(t) \sim \mathcal{GP}(0, C(t-t'))$ with Matérn-$3/2$ kernel:

$$C(\tau) = \sigma^2 2^{1-\nu} \frac{\Gamma(\nu)}{\Gamma(\nu/2)} \frac{\nu}{\ell} K_{\nu} \left( \sqrt{\frac{2\nu}{\ell}} \frac{\tau}{\nu} \right),$$

where $\tau = |t-t'|$, $K_{\nu}$ is the modified Bessel function (Williams and Rasmussen, 2006) and $\nu = 3/2$. This particular GP admits a state-space representation which can then be used within a filtering framework (Hartikainen and Särkkä, 2010). In particular, Matérn-3/2 GP can be represented by the following stochastic differential equation (SDE) (Särkkä et al., 2013)

$$\frac{dx_i(t)}{dt} = \begin{bmatrix} 0 & 1 \\ -\kappa^2 & -2\kappa \end{bmatrix} x_i(t) + \begin{bmatrix} 0 \\ 1 \end{bmatrix} w_i(t)$$

(23)

where $x_i(t) = [x_i(t), dx_i(t)/dt]$ and $\kappa = \sqrt{2\nu/\ell}$. We choose $\sigma^2 = 0.1$ and $\ell = 0.1$ and discretize the equation (23) with the step-size $\gamma = 0.001$. We discretize the SDEs for $i = 1, \ldots, r$ and construct a joint state which leads to a linear dynamical system in $2r$ dimensions for which then we can run the PSMF. The details of the discretization and the corresponding PSMF model are given in Supplement E.2.

We run the PSMF with the discretized GP-subspace model with $r = 10$. We note that in this experiment our aim is not to reconstruct the data but to be able to obtain a representation which would be helpful in changepoint detection. We choose a standard off-the-shelf changepoint detection method which we abbreviate simply as CPD (Killick et al., 2012). We first run it on the generated time-series directly which we dub as CPD-Data. Then, we estimate a smooth GP-subspace via the PSMF and run the same standard CPD method on the columns of estimated $X$ matrix (learned GP features) instead of the data itself. The results can be seen from Table 1 which clearly shows the improved performance and robustness of the PSMF for changepoint applications.

### 4.3 Imputation of London Air Quality data

In this section, we test our method on a practical problem of imputation of time-series. The time-series under consideration is a dataset of pollutant measurements across London. To be precise, we consider three different datasets of pollutants. First, we consider the
We simply assume that the subspace model evolves according to a simple random walk model, i.e., $f_\theta(x) = x$. This formulation rids us from the parameter estimation problem. We use the filtered estimates for data imputation. Similarly, we use the same random walk model for the MLE-SMF. We formulate the TMF accordingly with the weight matrix set to identity to obtain a fair comparison. This particular form of the TMF is tractable. For both PSMF and MLE-SMF, we set $R_k := R = \lambda \otimes I$, with $\lambda = 10$. $P_0 = I$, $Q_k := Q = q \otimes I$, with $q = 0.1$. For the PSMF, we set $V_0 = v_0 \otimes I$, where $v_0 = 2$. We limit all methods to run only three iterations over data in order to limit run-times and create a challenging setting which can arise under time constraints. We run all methods 1000-times over different missing data patterns and average the results. From Table 2, it can be seen that the PSMF attains lower RMSE errors compared to the MLE-SMF and the TMF. Furthermore, Table 3 shows that the PSMF quantifies the uncertainty better than the MLE-based SMF which treats the dictionary $C$ as a static variable. In particular, Table 3 shows the added value of the prior we put on $C$.

### 5 Conclusion

We have recast the problem of probabilistic dimensionality reduction for time-series as a joint state filtering and parameter estimation problem in a probabilistic state-space model. Our model is fully probabilistic and we provide a tractable sequential inference algorithm to run the method with linear computational complexity with respect to the number of data points. Our algorithm is purely recursive and can be used in streaming settings as well. The state-space formulation of the problem opens many directions for future research such as (i) the use of general nonlinear models for $f_\theta$ or more general non-Gaussian likelihoods, (ii) the exploration of the use of switching state-space models, and (iii) the integration of more advanced inference techniques such as ensemble Kalman filters or Monte Carlo based methods for nonlinear and non-Gaussian generalizations of our model.

### Table 2: Average imputation performances on held-out data in terms of RMSEs on London air quality datasets with varying amount of missing data (over 1000 Monte Carlo runs). The standard deviations are indicated in parentheses.

|        | NO$_2$ | PM10 | PM25 | CPU times (secs) |
|--------|--------|------|------|------------------|
|        | 20%    | 30%  | 40%  |                  |
| PSMF   | 5.89   | 6.80 | 7.27 |                  |
|        | (0.02) | (0.07) | (0.14) |                  |
| MLE-SMF | 11.17 | 9.0 | 9.67 | 4.18 |
|        | (0.41) | (0.25) | (0.26) | 4.90 |
| TMF    | 7.53   | 7.54 | 8.22 | 3.70 |
|        | (0.13) | (0.09) | (0.15) | 4.76 |

### Table 3: Average coverage percentage of the missing data by the 2$\sigma$ uncertainty bars of the posterior predictive estimates. These ratios are only available for the probabilistic methods and not available for the TMF.

|        | NO$_2$ | PM10 | PM25 |
|--------|--------|------|------|
|        | 20%    | 30%  | 40%  |
| PSMF   | 0.81   | 0.82 | 0.80 | 0.94 |
|        | (0.49) | (0.65) | (0.62) | 0.93 |
| MLE-SMF| 0.49   | 0.63 | 0.62 | 0.87 |
|        | (0.48) | (0.63) | (0.62) | 0.84 |

NO$_2$ dataset which is collected from 83 different sites between 01/06/2018 – 01/12/2018. This dataset therefore is $83 \times 4393$ dimensional time-series. The second dataset consists of measurements of PM10 from 74 sites between 01/06/2018 – 01/12/2018 resulting in $74 \times 4393$ dimensional time-series. Finally, we consider a PM25 dataset which is collected from 26 sites between the same dates, resulting in $26 \times 4393$ dimensional time-series. All datasets contain a high number of missing points due to sensor failures and maintenance operations. In order to test the accuracy of imputations, we further remove blocks of data consisting of segments of length 20 and construct datasets with 20%, 30%, and 40% missing data. We then run our algorithm and compare it to two different baselines. The first baseline we consider is a standard MLE approach to probabilistic matrix factorization which is in similar spirit to Yildirim et al. (2012); Sun et al. (2012). In other words, we construct an SSM where $C$ is regarded as a static parameter and estimated using an online MLE procedure, named as MLE-SMF. The resulting method is a probabilistic and sequential matrix factorization method which gives us a good baseline to compare our uncertainty quantification performance. The second method is the temporal matrix factorization (TMF) which is an adaptation of the optimisation-based method proposed in Yu et al. (2016).
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References

Ömer Deniz Akyildiz and Joaquín Míguez. Dictionary filtering: a probabilistic approach to online matrix factorisation. *Signal, Image and Video Processing*, 13(4):737–744, June 2019.

Brian D.O. Anderson and John B. Moore. *Optimal filtering*. Englewood Cliffs, N.J. Prentice Hall, 1979.

Christopher M. Bishop. *Pattern Recognition and Machine Learning*. Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2006. ISBN 0387310738.

Serhat Selcuk BucaK and Bilge GünSel. Incremental subspace learning via non-negative matrix factorization. *Pattern Recognition*, 42(5):788–797, 2009.

Ali Taylan Cemgil. Bayesian inference for nonnegative matrix factorisation models. *Computational Intelligence and Neuroscience*, pages 4:1–4:17, January 2009. ISSN 1687-5265.

Jesus Fernandez-Bes, Víctor Elvira, and Steven Van Vaerenbergh. A probabilistic least-mean-squares filter. In *IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 2199–2203. IEEE, 2015.

Cédric Févotte, Jonathan Le Roux, and John R Hershey. Non-negative dynamical system with application to speech and audio. In *2013 IEEE International Conference on Acoustics, Speech and Signal Processing*, pages 3158–3162. IEEE, 2013.

Cédric Févotte, Paris Smaragdis, Nasser Mohammadiha, and Gautham J Mysore. Temporal extensions of nonnegative matrix factorization. *Audio Source Separation and Speech Enhancement*, pages 161–187, 2018.

Rainer Gemulla, Erik Nijkamp, Peter J Haas, and Yannis Sismanis. Large-scale matrix factorization with distributed stochastic gradient descent. In *Proceedings of the 17th ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 69–77. ACM, 2011.

Jouni Hartikainen and Simo Särkkä. Kalman filtering and smoothing solutions to temporal gaussian process regression models. In *2010 IEEE International Workshop on Machine Learning for Signal Processing*, pages 379–384. IEEE, 2010.

David A Harville. *Matrix algebra from a statistician’s perspective*, volume 1. Springer, 1997.

Rudolph Emil Kalman. A new approach to linear filtering and prediction problems. *Journal of Fluids Engineering*, 82(1):35–45, 1960.

Nikolas Kantas, Arnaud Doucet, Sumetpal S Singh, Jan Maciejowski, and Nicolas Chopin. On particle methods for parameter estimation in state-space models. *Statistical Science*, 30(3):328–351, 2015.

Rebecca Killick, Paul Fearnhead, and Idris A Eckley. Optimal detection of changepoints with a linear computational cost. *Journal of the American Statistical Association*, 107(500):1590–1598, 2012.

Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *International Conference on Learning Representations (ICLR)*, 2015.

Daniel D. Lee and H. Sebastian Seung. Learning the parts of objects by non-negative matrix factorization. *Nature*, 401(6755):788–791, October 1999.

Julien Mairal, Francis Bach, Jean Ponce, and Guillermo Sapiro. Online learning for matrix factorization and sparse coding. *The Journal of Machine Learning Research*, 11:19–60, 2010.

Andriy Mnih and Ruslan R Salakhutdinov. Probabilistic matrix factorization. In *Advances in neural information processing systems*, pages 1257–1264, 2008.

Nasser Mohammadiha, Paris Smaragdis, and Arne Lejon. Prediction based filtering and smoothing to exploit temporal dependencies in nmf. In *2013 IEEE International Conference on Acoustics, Speech and Signal Processing*, pages 873–877. IEEE, 2013.

Nasser Mohammadiha, Paris Smaragdis, Ghazaleh Panahandeh, and Simon Doclo. A state-space approach to dynamic nonnegative matrix factorization. *IEEE Transactions on Signal Processing*, 63(4):949–959, 2014.

Ruslan Salakhutdinov and Andriy Mnih. Bayesian probabilistic matrix factorization using markov chain monte carlo. In *Proceedings of the 25th international conference on Machine learning*, pages 880–887. ACM, 2008.

Simo Särkkä, Arno Solin, and Jouni Hartikainen. Spatiotemporal learning via infinite-dimensional bayesian filtering and smoothing: A look at gaussian process regression through kalman filtering. *IEEE Signal Processing Magazine*, 30(4):51–61, 2013.

John Z Sun, Kush R Varshney, and Karthik Subbian. Dynamic matrix factorization: A state space approach. In *Acoustics, Speech and Signal Processing (ICASSP)*, 2012 IEEE International Conference on, pages 1897–1900. IEEE, 2012.
Peter Weiderer, Ana Maria Tomê, and Elmar Wolfgang Lang. Decomposing temperature time series with non-negative matrix factorization. *arXiv preprint arXiv:1904.02217*, 2019.

Christopher KI Williams and Carl Edward Rasmussen. *Gaussian processes for machine learning*, volume 2. MIT press Cambridge, MA, 2006.

Sinan Yildirim, A Taylan Cemgil, and Sumeetpal S Singh. An online expectation-maximisation algorithm for nonnegative matrix factorisation models. *IFAC Proceedings Volumes*, 45(16):494–499, 2012.

Hsiang-Fu Yu, Nikhil Rao, and Inderjit S Dhillon. Temporal regularized matrix factorization for high-dimensional time series prediction. In *Advances in Neural Information Processing Systems*, pages 847–855, 2016.
**Supplementary Material**

**A Preliminaries**

In this section, we list some linear algebra properties related to Kronecker products, which will be used in proofs. We denote the Kronecker product $\otimes$. Let $A$ be of dimension $m \times r$ and $B$ be of dimension $r \times n$; then (Harville, 1997),

$$A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1r}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mr}B \end{bmatrix}.$$

For matrices $A, B$ and $X$, it holds that

$$\text{vec}(AXB) = (B^\top \otimes A)\text{vec}(X). \quad (A.1)$$

We can particularize this formula for an $r \times 1$ vector $x$ as

$$Ax = \text{vec}(Ax) = (x^\top \otimes I_d)\text{vec}(A). \quad (A.2)$$

Kronecker product has the following mixed product property (Harville, 1997)

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD), \quad (A.3)$$

and the inversion property (Harville, 1997)

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}. \quad (A.4)$$

**B Proof of Proposition 1**

We adapt the proof in Akyildiz and Míguez (2019). We first note that for a Gaussian prior $p(c|y_{1:k-1}) = \mathcal{N}(c; c_{k-1}, P_{k-1})$ and likelihood of the form $p(y_k|y_{1:k-1}, c) = \mathcal{N}(y_k; H_k c, R_k)$, we can write the posterior analytically $p(c|y_{1:k}) = \mathcal{N}(c; c_k, P_k)$ where (see, e.g., Bishop (2006))

$$c_k = c_{k-1} + P_{k-1} H_k^\top (H_k P_{k-1} H_k^\top + R_k)^{-1}(y_k - H_k c_{k-1}), \quad (B.1)$$

$$P_k = P_{k-1} - P_{k-1} H_k^\top (H_k P_{k-1} H_k^\top + R_k)^{-1} H_k P_{k-1}. \quad (B.2)$$

In order to obtain an efficient matrix-variate update rule using this vector-form update, we first rewrite the likelihood (14) as

$$p(y_k|y_{1:k-1}, c) = \mathcal{N}(y_k; H_k c, R_k) \quad (B.3)$$

where $H_k = \bar{\mu}_k^\top \otimes I_d$ and $R_k = \eta_k \otimes I_d$. We note that, we have $P_0 = V_0 \otimes I_d$ and we assume as an induction hypothesis that $P_{k-1} = V_{k-1} \otimes I_d$. We start by showing that the update (B.2) can be greatly simplified using the special structure we impose. First, substituting $H_k = \bar{\mu}_k^\top \otimes I_d$, we get

$$P_k = (V_{k-1} \otimes I_d) - (V_{k-1} \otimes I_d)(\bar{\mu}_k \otimes I_d) \times ((\bar{\mu}_k \otimes I_d)(V_{k-1} \otimes I_d)(\bar{\mu}_k \otimes I_d) + \lambda \otimes I_d)^{-1} \times (\bar{\mu}_k \otimes I_d)(V_{k-1} \otimes I_d).$$

Using mixed product property (A.3) and the property (A.4), we obtain

$$P_k = (V_{k-1} \otimes I_d) - (V_{k-1} \bar{\mu}_k \otimes I_d) \times ((\bar{\mu}_k V_{k-1} \bar{\mu}_k + \lambda)^{-1} \otimes I_d)(\bar{\mu}_k V_{k-1} \otimes I_d).$$

One more use of the mixed product property (A.3) yields

$$P_k = \left(V_{k-1} - \frac{V_{k-1} \bar{\mu}_k \bar{\mu}_k V_{k-1}}{\bar{\mu}_k V_{k-1} \bar{\mu}_k + \lambda}\right) \otimes I_d. \quad (B.4)$$

Thus, we have $P_k = V_k \otimes I_d$ where,

$$V_k = V_{k-1} - \frac{V_{k-1} \bar{\mu}_k \bar{\mu}_k V_{k-1}}{\bar{\mu}_k V_{k-1} \bar{\mu}_k + \lambda}. \quad (B.5)$$
We have shown that the sequence \((P_k)_{k \geq 1}\) preserves the Kronecker structure. Next, we substitute \(P_{k-1} = V_{k-1} \otimes I_d\), \(H_k = \bar{\mu_k} \otimes I_d\) and \(R_k = \lambda \otimes I_d\) into (B.1) and we obtain

\[
c_k = c_{k-1} + (V_{k-1} \otimes I_d)(\bar{\mu_k} \otimes I_d) \times \left( (\bar{\mu_k}^\top \otimes I_d)(V_{k-1} \otimes I_d)(\bar{\mu_k} \otimes I_d) + \lambda \otimes I_d \right)^{-1} \times (y_k - (\bar{\mu_k}^\top \otimes I_d)c_{k-1}).
\]

The use of the mixed product property (A.3) multiple times leaves us with

\[
c_k = c_{k-1} + (V_{k-1} \bar{\mu_k} \otimes I_d) \left( (\bar{\mu_k} V_{k-1} \bar{\mu_k} + \lambda) \otimes I_d \right)^{-1} \times (y_k - (\bar{\mu_k}^\top \otimes I_d)c_{k-1}).
\]

Using (A.4) and again (A.3) yields

\[
c_k = c_{k-1} + \left[ \frac{V_{k-1} \mu_k}{\bar{\mu_k} V_{k-1} \bar{\mu_k} + \lambda} \otimes I_d \right] \times (y_k - (\bar{\mu_k}^\top \otimes I_d)c_{k-1}). \tag{B.6}
\]

Using (A.2), we get

\[
c_k = c_{k-1} + \left[ \frac{V_{k-1} \mu_k}{\bar{\mu_k} V_{k-1} \bar{\mu_k} + \lambda} \otimes I_d \right] (y_k - C_{k-1} \bar{\mu_k}).
\]

We now note that \((y_k - C_{k-1} \bar{\mu_k})\) and \(\frac{V_{k-1} \mu_k}{\bar{\mu_k} V_{k-1} \bar{\mu_k} + \lambda}\) are vectors. Hence, rewriting the above expression as

\[
c_k = c_{k-1} + \left[ \text{vec} \left( \frac{V_{k-1} \mu_k}{\bar{\mu_k} V_{k-1} \bar{\mu_k} + \lambda} \otimes I_d \right) \right] \times \text{vec}(y_k - C_{k-1} \bar{\mu_k}),
\]

we can apply (A.2) and obtain

\[
c_k = c_{k-1} + \text{vec} \left( \frac{(y_k - C_{k-1} \bar{\mu_k}) \bar{\mu_k} V_{k-1}^\top}{\bar{\mu_k} V_{k-1} \bar{\mu_k} + \lambda} \right). \tag{B.7}
\]

Hence up to a reshaping operation, we have the update rule (16) and conclude the proof.

\[\blacksquare\]

\[\textbf{C} \quad \textbf{Proof of Proposition 2}\]

Recall that we have a posterior of the form at time \(k-1\)

\[
p(c|y_{1:k-1}) = \mathcal{N}(c; c_{k-1}, V_{k-1} \otimes I_d),
\]

and we are given the likelihood

\[
p(y_k|c, x_k) = \mathcal{N}(y_k; (x_k \otimes I_d)c, \eta_k \otimes I_d).
\]

We are interested in computing

\[
p(y_k|y_{1:k-1}, x_k) = \int p(c|y_{1:k-1})p(y_k|c, x_k)dc.
\]

This integral is analytically tractable since both distributions are Gaussian and it is given by (Bishop, 2006)

\[
p(y_k|y_{1:k-1}, x_k) = \mathcal{N}(y_k; (x_k^\top \otimes I_d)c_k, (\lambda \otimes I_d) + (x_k^\top \otimes I_d)(V_{k-1} \otimes I_d)(x_k \otimes I_d)).
\]

Using the mixed product property (A.3), one obtains

\[
p(y_k|y_{1:k-1}, x_k) = \mathcal{N}(y_k; C_{k-1} x_k, (\lambda + x_k^\top V_{k-1} x_k) \otimes I_d).
\]

\[\textbf{D} \quad \textbf{The probabilistic model to handle missing data}\]

We define the probabilistic model with missing data

\[
p(C) = \mathcal{M}\mathcal{N}(C; C_0, I_d, V_0), \tag{D.1}
p(x_0) = \mathcal{N}(x_0; \mu_0, P_0), \tag{D.2}
p(y_k|x_{k-1}) = \mathcal{N}(y_k; f_0(x_{k-1}), Q_k), \tag{D.3}
p(z_k|x_k, C) = \mathcal{N}(z_k; M_k C x_k, M_k R_k M_k^\top). \tag{D.4}
\]
This model can explicitly handle the missing data when \((M_k)_{k \geq 1}\) (the missing data patterns) are given. The update rules for this model are defined using masks and are similar to the full data case. In what follows, we derive the update rules for this model by explicitly handling the masks and placing them into our updates formally. For the missing-data case, however, we need a minor approximation in the covariance update rule in order to keep the method efficient.

Assume that we are given

\[
\tilde{p}(c|z_{1:k-1}) = \mathcal{N}(c; c_{k-1}, V_{k-1} \otimes I_d)
\]

and the likelihood

\[
\tilde{p}(z_k|c, z_{1:k-1}) = \mathcal{N}(z_k; M_k \tilde{\mu}_k, \eta_k \otimes I_d)
\]

where

\[
\eta_k = \frac{\text{Tr}(M_k R_k M_k^\top + M_k C_{k-1} \tilde{P}_k C_{k-1}^\top M_k^\top)}{m}.
\]

In the sequel, we derive the update rules corresponding to the our method with missing data. The derivation relies on the proof of Prop. 1. We note that, using (A.1), we can obtain the likelihood

\[
\tilde{p}(z_k|c, z_{1:k-1}) = \mathcal{N}(z_k; H_k c, \eta_k \otimes I_d)
\]

where \(c = \text{vec}(C)\) and \(H_k = \tilde{\mu}_k^\top \otimes M_k\). Deriving the posterior in the same way as in the proof of Prop. 1 leaves us with the covariance update in the form

\[
P_k = V_{k-1} \otimes I_d - \frac{V_{k-1} \tilde{\mu}_k \tilde{\mu}_k^\top V_{k-1}}{\tilde{\mu}_k^\top V_{k-1} \tilde{\mu}_k + \lambda} \otimes M_k.
\]

Unlike the previous case, this covariance does not simplify to a form \(P_k = V_k \otimes I_d\) easily. For this reason, we approximate it as

\[
P_k \approx V_k \otimes I_d,
\]

where \(V_k\) is in the same form of missing-data free updates. To update the mean, we proceed in a similar way as in the proof of Prop. 1 as well. Straightforward calculations lead to the update

\[
C_k = C_{k-1} + \frac{(z_k - M_k C_{k-1} \tilde{\mu}_k) \tilde{\mu}_k^\top V_{k-1}}{\tilde{\mu}_k^\top V_{k-1} \tilde{\mu}_k + \eta_k}, \quad \text{for } k \geq 1.
\]

To update \(x_k\), once we fix \(C_{k-1}\), everything straightforwardly follows by replacing \(C_{k-1}\) by \(M_k C_{k-1}\) in the update rules for \((x_k)_{k \geq 1}\).

### E Additional details for the experiments

#### E.1 Experiment 1

In this experiment, we have used the Adam optimizer for optimization (Kingma and Ba, 2015). In particular, instead of implementing the gradient step (20), we replace it with the Adam optimizer. In order to do so, we define the gradient

\[
g_i = \nabla \log \tilde{p}_\theta(y_{1:n}) |_{\theta=\theta_{i-1}}.
\]

Upon computing the gradient \(g_i\), we first compute the running averages

\[
m_i = \beta_1 m_{i-1} + (1 - \beta_1) g_i,
\]

\[
v_i = \beta_2 v_{i-1} + (1 - \beta_2) (g_i \otimes g_i),
\]

which is then corrected as

\[
\hat{m}_i = \frac{m_i}{1 - \beta_1},
\]

\[
\hat{v}_i = \frac{v_i}{1 - \beta_2}.
\]

Finally the parameter update is computed as

\[
\theta_i = \text{Proj}_{\Theta} \left( \theta_{i-1} + \gamma \frac{\hat{m}_i}{\sqrt{\hat{v}_i + \epsilon}} \right),
\]

where \(\text{Proj}\) denotes the projection operator which constrains the parameter to stay positive in each dimension where \(\Theta = \mathbb{R}_+ \times \cdots \times \mathbb{R}_+ \subset \mathbb{R}^d\) which is implemented by simple max operators.

We choose the standard parameterization with \(\gamma = 10^{-3}, \beta_1 = 0.9, \beta_2 = 0.999\) and \(\epsilon = 10^{-8}\).
E.2 Experiment 2

E.2.1 Data generation and the experimental setup

We generate periodic time series using pendulum differential equations as the true subspace. For this experiment, we generate $d = 20$ dimensional data where $d_2 = 3$ of them undergo a structural change. In order to test the method, we generate 1000 synthetic datasets. One such dataset is given in Fig. 1. We generate data with $n = 1200$ and use the data after the data point $n_0 = 400$ to estimate changepoints, as the PSMF has to converge to a stable regime before it can be used to detect changepoints. The true changepoint is at $n_c = 601$.

E.2.2 The GP subspace model

In this subsection, we provide the details of the discretization of the Matérn-3/2 SDE. Particularly, we consider the SDE (Särkkä et al., 2013)

$$\frac{dx_i(t)}{dt} = Fx_i(t) + \begin{bmatrix} 0 \\ 1 \end{bmatrix} w_i(t)$$

(E.1)

where $x_i(t) = [x_i(t), dx_i(t)/dt]$ and $\kappa = \sqrt{2}\nu/\ell$ and

$$F = \begin{bmatrix} 0 & 1 \\ -\kappa^2 & -2\kappa \end{bmatrix}.$$ 

Given a step-size $\gamma$, the SDE (E.1) can be written as a linear dynamical system

$$x_{i,k} = A_i x_{i,k-1} + Q_i^{1/2} u_{i,k}$$
where \( A_i = \expm(\gamma F) \) where \( \expm \) denotes the matrix exponential and \( Q_i = P_\infty - A_i P_\infty A_i^\top \) and
\[
P_\infty = \begin{bmatrix}
\sigma^2 & 0 \\
0 & 3\sigma^2/\ell^2
\end{bmatrix}.
\]

Finally, we construct our dynamical system as
\[
x_k = Ax_{k-1} + Q^{1/2}u_k
\]
where \( x_k = [x_{1,k}, \ldots, x_{r,k}]^\top \in \mathbb{R}^{2r} \) and
\[
A = I_r \otimes A_i \quad \text{and} \quad Q = I_r \otimes Q_i.
\]

Using these system matrices, we define \( H_i = [1, 0] \) and \( H = I_r \otimes H_i \) and finally define the probabilistic model
\[
\begin{align*}
p(C) &= \mathcal{MN}(C; C_0, I_d, V_0), \\
p(x_0) &= \mathcal{N}(x_0; \mu_0, P_0), \\
p(x_k|x_{k-1}) &= \mathcal{N}(x_k; Ax_{k-1}, Q), \\
p(y_k|x_k, C) &= \mathcal{N}(y_k; CHx_k, R).
\end{align*}
\]

Inference in this model can be done via a simple modification of the Algorithm 1 where \( H \) matrix is involved in the computations.