The Expectation-Maximization Algorithm for Continuous-time Hidden Markov Models

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Abstract

We propose a unified framework that extends the inference methods for classical hidden Markov models to continuous settings, where both the hidden states and observations occur in continuous time. Two different settings are analyzed: (1) hidden jump process with a finite state space; (2) hidden diffusion process with a continuous state space. For each setting, we first estimate the hidden state given the observations and model parameters, showing that the posterior distribution of the hidden states can be described by differential equations in continuous time. Then we consider the estimation of unknown model parameters, deriving the formulas for the expectation-maximization algorithm in the continuous-time setting. We also propose a Monte Carlo method for sampling the posterior distribution of the hidden states and estimating the unknown parameters.

1 Introduction

Hidden Markov models (HMM) are widely used for inferring the underlying dynamical process from observed data. The classical discrete-time hidden Markov model (DT-HMM) contains a pair of stochastic processes \( \{ (X_t, Y_t) : t = 0, \ldots, T \} \). The hidden process \( \{ X_t \} \) is a Markov chain with transition probability \( \Pr\{X_{t+1} | X_t; \theta \} \); the observations \( \{ Y_t \} \) are sampled independently at each time \( t \) based on the observation probability \( \Pr\{Y_t | X_t; \theta \} \). Here \( \theta \) denotes the model parameters. The following are two basic problems for HMM:

State estimation Given the observations \( \{ Y_t \} \) and the model parameters \( \theta \), calculate the posterior distribution of the hidden states \( \Pr\{X_t | Y_0, \ldots, Y_T; \theta \} \).

Parameter estimation Given the observations \( \{ Y_t \} \) with unknown model parameters \( \theta \), learn \( \theta \).

In the case of DT-HMM, there are already well-established theorems and algorithms to address both problems [38]. The Baum-Welch algorithm uses the forward-backward equations for state estimation, and the expectation-maximization (EM) algorithm for parameter estimation (see Section 2). Our goal is to extend the framework of the Baum-Welch algorithm to continuous-time hidden Markov models (CT-HMM), where both the hidden process \( \{ X_t \} \) and observations \( \{ Y_t \} \) occur in continuous time. We will apply this framework to two different settings: the hidden process \( \{ X_t \} \) can be either a jump process with finite state space, or a diffusion process with continuous state space.

Section 3 considers CT-HMM for hidden jump process, where both the hidden states and observations take a finite set of values. Consider a system where the underlying states can switch between several discrete values, and we have a sensor that monitors the system in continuous time, whose output also

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takes discrete values. It is reasonable to model the hidden states \( \{X_t\} \) as a jump process, and assume that the sensor output \( \{Y_t\} \) changes every time \( \{X_t\} \) jumps. Specifically, for each jumping time \( \tau \) of \( \{X_t\} \), resample \( Y_\tau \) from the observation probability condition on \( X_\tau \), and \( X_t, Y_t \) remain constant during the holding period \( [\tau, \tau') \), where \( \tau' \) is the next jumping time of \( \{X_t\} \). Here the holding time \( \tau' - \tau \) is an exponentially distributed random variable, therefore this can be regarded as an extension of DT-HMM whose holding time is always 1. Applying the Baum-Welch framework to this continuous setting, the state estimation, i.e., the posterior distribution \( \Pr \{X_t | Y_s, s \in [0, T]; \theta\} \) can be described by forward and backward piecewise ODEs. The parameter estimation can be obtained by the EM algorithm, and the parameter update formula consists of summation terms corresponding to each jumping time, and integral terms for the holding period.

Section 4 shows that the framework can also be applied to CT-HMM with hidden diffusion process, where the hidden states and observations take continuous values. Here we analyze the classical setting in the Stratonovitch-Kushner and Zakai equations. The Zakai equation solves the optimal nonlinear filtering problem, which is the forward part in our framework. We give the corresponding SPDE for the backward part. By combining those we can solve the smoothing problem for state estimation. Then we theoretically derive the continuous-time formula for the EM algorithm in parameter estimation. For linear Gaussian problem, we show that our results are consistent with the discrete-time Kalman filter and smoother as well as the EM algorithm under the limit \( \Delta t \to 0 \). For general nonlinear problems, we propose a Monte Carlo method based on particle filter and smoother to sample the posterior distribution of hidden states, and then update parameters from the samples in the EM algorithm.

While this work mainly focuses on the continuous-time states and observations, the Baum-Welch framework can also be applied to the setting where the observations occur at some discrete time points independently, and we show the results in Appendix A.

Our contributions

- We extend the classical DT-HMM to the CT-HMM with hidden jump process, and derive the forward-backward ODEs for state estimation and the EM algorithm for parameter estimation.
- We apply the same framework to the CT-HMM with hidden nonlinear diffusion process. Starting from the Zakai equation for the filtering problem, we solve the corresponding smoothing problem for state estimation, and propose the EM algorithm for parameter estimation.
- Based on the formulas for hidden diffusion process, we propose a Monte Carlo method to sample the posterior distribution of hidden states, and then estimate the parameters from the samples.

2 Preliminaries

2.1 Notations

In this paper, we use uppercase \( X_t, Y_i \) to denote random variables, lowercase \( x_t, y_t \) to denote the particular values of the random variables, and \( \{X_t\}, \{Y_i\} \) to denote the stochastic processes. Let \( \Pr \{\cdot\} \) be the probability distribution and \( p(\cdot) \) be the probability density. Let \( \Pr \{\cdot; \theta\} \) be the probability distribution corresponding to the parameters \( \theta \). Without ambiguity, we may simply denote the conditional probability \( \Pr \{X_t = x_t | Y_i = y_t\} \) as \( \Pr \{x_t | y_t\} \).

In continuous time, the subscript \( x_{0:t} \) denotes all the \( x_s \) for \( 0 \leq s \leq t \). In some parts of the paper we may need discretization of the time space with step \( \Delta t \). In this case we only consider \( x_t \) on the grid, i.e., \( t = k\Delta t \) for some integer \( k \), then \( x_{0:t} \) denotes all the \( x_{l\Delta t} \) for \( l = 0, 1, \ldots, k \), and \( \Delta x_t = x_{t+\Delta t} - x_t \). Let \( 1_{\{\cdot\}} \) be the indicator function. Let \( \text{diag}(a_1, \ldots, a_n) \) be the \( n \times n \) diagonal matrix with \( a_1, \ldots, a_n \) on the main diagonal.
2.2 Expectation-maximization algorithm

The expectation-maximization (EM) algorithm is an iterative method to estimate parameters in statistical models. Let $\theta$ be the unknown parameters, and the model generates a set of unobservable latent variables $X$ and a set of observed data $Y$. The goal is to calculate the maximum likelihood estimation of the parameters $\theta$ given the observations $Y = y$, i.e., $\theta^* = \text{argmax}_\theta L(\theta)$ where

$$ L(\theta) = \log p(Y = y; \theta) = \log \int p(X = x, Y = y; \theta)dx. \quad (2.1) $$

In the case where the integral cannot be calculated directly, the EM algorithm takes an iterative approach as following. Assume that we can find a function $Q(\theta, \theta')$ such that $L(\theta) \geq Q(\theta, \theta')$ and $L(\theta) = Q(\theta, \theta)$ for all $\theta$ and $\theta'$. For iterations $k = 0, 1, 2, \ldots$, let $\theta^{k+1} = \text{argmax}_\theta Q(\theta, \theta^k)$, then

$$ L(\theta^k) = L(\theta^k, \theta^k) \leq Q(\theta^{k+1}, \theta^k) \leq L(\theta^{k+1}), $$

i.e., $L(\theta^k)$ is nondecreasing during the iterations. If $L$ is upper bounded, the EM algorithm will converge to a local maximum.

Consider the following construction of $Q$:

$$ Q(\theta, \theta') = \int p(x|y; \theta') \log \frac{p(x, y; \theta)}{p(x|y; \theta')} dx. \quad (2.2) $$

Since

$$ L(\theta) = \log \int p(x, y; \theta)dx = \log \int p(x|y; \theta') \frac{p(x, y; \theta)}{p(x|y; \theta')} dx $$

and $\log(\cdot)$ is concave, we have $Q(\theta, \theta') \leq L(\theta)$. Meanwhile,

$$ Q(\theta, \theta) = \int p(x|y; \theta) \log \frac{p(x, y; \theta)}{p(x|y; \theta)} dx $$

$$ = \int p(x|y; \theta) \log p(y; \theta) dx $$

$$ = \log p(y; \theta) = L(\theta), $$

thus $Q$ is a qualified construction.

The EM algorithm repeats the following two steps until convergence. In the expectation step (E-step), calculate the conditional probability $p(X = x|Y = y; \theta^k)$; in the maximization step (M-step), update the parameter as $\theta^{k+1} = \text{argmax}_\theta Q(\theta, \theta^k)$. In practice we may use

$$ Q(\theta, \theta') = \int p(X = x|Y = y; \theta') \log p(X = x, Y = y; \theta) \quad (2.3) $$

instead of $(2.2)$, since they give the same result in the M-step.

2.3 Baum-Welch algorithm

The Baum-Welch algorithm solves both the state estimation and parameter estimation for the classical DT-HMM. In a DT-HMM $\{(X_t, Y_t): t = 0, \ldots, T\}$, the hidden states $X_t \in \{1, \ldots, n\}$ is a Markov chain with transition probability $P$, and the observations $Y_t \in \{1, \ldots, m\}$ are a set of independent and identically distributed (i.i.d.) observations according to the observation probability $r$, i.e.,

$$ P_{ij} = \Pr\{X_{t+1} = j|X_t = i\}, $$

$$ r_i(y) = \Pr\{Y_t = y|X_t = i\}, \quad (2.4) $$

for $i, j = 1, \ldots, n$ and $y = 1, \ldots, m$. 


**State estimation** Assume that the probabilities \(P\) and \(r\) and the initial distribution \(\pi_0(i) = \Pr\{X_0 = i\}\) are given, and we have observations \(Y_t = y_t, t = 0, \ldots, T\). The goal is to estimate the posterior distribution \(\Pr\{X_t|y_{0:T}\}\). The Baum-Welch algorithm introduces two sets of probabilities

\[
\alpha_t(i) = \Pr\{X_t = i, Y_{0:t}\}, \quad \beta_t(i) = \Pr\{y_{t+1:T}|X_t = i\},
\]

that can be solved by the forward and backward equations inductively:

\[
\alpha_0(i) = \pi_0(i)r_i(y_0), \quad \alpha_t(i) = \sum_{j=1}^{n}\alpha_{t-1}(j)P_{ij}r_j(y_t),
\]

\[
\beta_T(i) = 1, \quad \beta_t(i) = \sum_{j=1}^{n}P_{ij}\beta_{t+1}(j)r_j(y_{t+1}).
\]

Since

\[
\Pr\{X_t = i, y_{0:T}\} = \Pr\{y_{t+1:T}|X_t = i, y_{0:t}\} \Pr\{X_t = i, y_{0:t}\} = \alpha_t(i)\beta_t(i),
\]

the posterior distribution is given by

\[
\rho_t(i) = \Pr\{X_t = i|y_{0:T}\} = \frac{\alpha_t(i)\beta_t(i)}{\sum_{i'}^{n} \alpha_t(i')\beta_t(i')}.
\]

Here we also calculate

\[
\xi_t(i, j) = \Pr\{X_{t-1} = i, X_t = j|y_{0:T}\} = \frac{\alpha_{t-1}(i)P_{ij}\beta_t(j)r_j(y_t)}{\sum_{i'}^{n} \alpha_t(i')\beta_t(i')}.
\]

**Parameter estimation** Now assume that \(\theta = (P, r)\) are the unknown parameters to be estimated. Let \(\rho\) and \(\xi\) be the state estimation based on \(\theta = \theta^k\). From the EM algorithm \[^{[2.3]}\] the parameter update is given by \(\theta^{k+1} = \arg\max_\theta Q(\theta, \theta^k)\), and

\[
Q(\theta, \theta^k) = \sum_{x_{0:T}} \Pr\{x_{0:T}|y_{0:T}; \theta^k\} \log \Pr\{x_{0:T}, y_{0:T}; \theta\}
\]

\[
= \sum_{x_{0:T}} \Pr\{x_{0:T}|y_{0:T}; \theta^k\} \left[ \log \Pr\{x_0\} + \sum_{i=1}^{T} \log P_{x_{i-1}, x_i} + \sum_{t=0}^{T} \log r_{x_i}(y_t) \right]
\]

\[
= C + \sum_{x_{0:T}} \sum_{i=1}^{T} \Pr\{x_{i-1}, x_i|y_{0:T}; \theta^k\} \log P_{x_{i-1}, x_i} + \sum_{t=0}^{T} \Pr\{x_{i}|y_{0:T}; \theta^k\} \log r_{x_i}(y_t)
\]

\[
= C + \sum_{i,j} \sum_{t=1}^{T} \xi_{t}(i, j) \log P_{ij} + \sum_{i} \sum_{t=0}^{T} \rho_{t}(i) \log r_{i}(y_t),
\]

where \(C\) is a constant not depending on \((P, r)\). Solving the optimization problem, the transition probability is updated as

\[
P^{k+1}_{ij} = \frac{\sum_{t=1}^{T} \xi_t(i, j)}{\sum_{j'} \sum_{t=1}^{T} \xi_t(i, j')} = \frac{\sum_{t=1}^{T} \xi_t(i, j)}{\sum_{t=0}^{T-1} \rho_t(i)},
\]

and the observation probability is given by

\[
r^{k+1}_{i}(y) = \frac{\sum_{t=0}^{T} \rho_t(i)1_{y_t = y}}{\sum_{t=0}^{T} \rho_t(i)}.
\]
2.4 Filtering problem

The goal of the filtering problem is to estimate the state of a stochastic dynamical system given some noisy measurements of the system. The earliest results are the Stratonovich-Kushner and Zakai equations [45, 25, 26, 46] that solve the optimal nonlinear filtering problems, and this line of work focus more on the theoretical derivation (see Section 4.2). From the application prospective, most previous work considers the discrete-time dynamics

\[ X_{t+1} = f(X_t) + W_t, \]
\[ Y_t = h(X_t) + V_t. \]

(For real world problems in continuous time, one may discretize time first.) Two types of algorithms are widely used: Kalman filter and particle filter.

Kalman filter The Kalman filter [21] considers the linear case where the optimal filter has explicit solution. Assume that both \( f \) and \( h \) are linear and the initial distribution of \( X_0 \) is Gaussian, then the conditional distribution of the states is always Gaussian:

\[ X_t | Y_0:t \sim N(\mu_t, P_t). \]

The Kalman filter gives the update rule from \((\mu_t, P_t)\) to \((\mu_{t+1}, P_{t+1})\). [39] gives the formula of corresponding smoother (RTS). The extended Kalman filter (EKF) is a finite dimensional approximation of the nonlinear dynamics, which assumes that the conditional distribution of \( X_t \) is approximately Gaussian. [5] analyzes the EKF in continuous time.

Particle filter The particle filter [17] applies sequential Monte Carlo methods to generate a set of samples (particles) to represent the conditional distribution of the states. For instance, later in (4.19) we approximate \( \tilde{\pi}_t \) by \( \hat{\pi}_t(x) = \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi_i^t}(x) \) with samples \( \{\xi_i^t\} \). Here the dynamics \( f \) and \( h \) can be nonlinear and the noise \( \{W_t\} \) and \( \{V_t\} \) can be non-Gaussian. [10, 28, 27, 29] apply the particle filters to solve the Kushner equation. Extensions of particle filter include auxiliary particle filters [37], Gaussian sum particle filters [24], and Rao-Blackwellised particle filtering [8, 13]. The particle smoother is based on the samples in the filter with updated reweighting. The discrete-time particle smoother is proposed by [12], which is based on the update formula in [23].

3 CT-HMM with jump process

3.1 Problem settings

Definition. Denote a CT-HMM \( \{(X_t, Y_t) : t \in [0, T]\} \) as \( (Q, r, \pi_0) \) if the hidden states \( X_t \in \{1, \ldots, n\} \) and the observations \( Y_t \in \{1, \ldots, m\} \) are generated as following:

Hidden state \( \{X_t\} \) is a jump process given by the initial probability \( \pi_0(i) = \Pr\{X_0 = i\} \) and generator \( Q \in \mathbb{R}^{n \times n} \), i.e.

\[ Q_{ij} = \lim_{\Delta t \downarrow 0} \frac{\Pr\{X_{t+\Delta t} = j | X_t = i\}}{\Delta t}, \quad i, j \in \{1, \ldots, n\}, i \neq j, \]

(3.1)

and \( Q_{ii} = -\sum_{j \neq i} Q_{ij} \).

Observation Let \( 0 = \tilde{\tau}_0 < \tilde{\tau}_1 < \tilde{\tau}_2 < \cdots < \tilde{\tau}_S \leq T \) be the jumping time of \( \{X_t\} \). At each \( \tilde{\tau}_s \), the observation \( Y_{\tilde{\tau}_s} \) is generated from

\[ r_i(y) = \Pr\{Y_{\tilde{\tau}_s} = y | X_{\tilde{\tau}_s} = i\}, \]

(3.2)

where \( i = 1, \ldots, n, y = 1, \ldots, m \), and \( Y_t = Y_{\tilde{\tau}_s} \) for \( t \in [\tilde{\tau}_s, \tilde{\tau}_{s+1}) \).
According to the definition above, both $\{X_t\}$ and $\{Y_t\}$ are piecewise constant functions in $t$:

$$X_t = \sum_{s=0}^{S} X_{\bar{r}_s} 1_{[\bar{r}_s, \bar{r}_{s+1})}(t), \quad Y_t = \sum_{s=0}^{S} Y_{\bar{r}_s} 1_{[\bar{r}_s, \bar{r}_{s+1})}(t),$$

(3.3)

where $\{\bar{r}_s\}_{s=0}^{S}$ are the jumping time of $\{X_t\}$, and $\{\bar{r}_s\}_{s=0}^{S}$ are the discontinuities of $\{Y_t\}$. A key point is that $\{\bar{r}_s\}_{s=0}^{S} \subseteq \{\bar{r}_s\}_{s=0}^{S}$ since $\{X_t\}$ may jump at $\bar{r}_s$ but generate the same $Y_{\bar{r}_s} = Y_{\bar{r}_{s+1}}$. So the embedded Markov chain $\{(X_{\bar{r}_s}, Y_{\bar{r}_s})\}_{s=0}^{S}$ is a DT-HMM, but $\{(X_{\bar{r}_s}, Y_{\bar{r}_s})\}_{s=0}^{S}$ is not. Since we can only observe $\{Y_t\}$ and $\{\bar{r}_s\}_{s=0}^{S}$ instead of $\{\bar{r}_s\}_{s=0}^{S}$, we cannot apply the DT-HMM methods directly.

### 3.1.1 Comparison with related work

Before proceeding with the detailed calculation, we compare our setting with previous work where CT-HMM with hidden jump process are modeled under different assumptions.

The first line of previous work assumes that $\{Y_t\}$ can only be observed at some discrete time points $[6, 19, 30, 31]$. One of the applications is modeling disease progression, where the disease states can be described as a jump process, and the observations of patients are noisy and arrive irregularly in time. Under this setting, it is reasonable to assume that the observations are conditionally independent and may not be synchronized with the jumps. However, the discrete-observation setting cannot be extended to the continuous-observation setting by simply taking the continuous limit. Let $N$ be the number of observations. If we keep increasing $N$, the observations $\{Y_t\}$ cannot be continuous in $t$ if they are conditionally independent; meanwhile, the state estimation will be more and more accurate, and we will get perfect estimation $X_t = x_t$ almost surely as $N \to \infty$. Note that the discrete-observation setting can also be solved by the Baum-Welch framework, and we list the corresponding results in Appendix A.

The second line of work assumes continuous observations $\{Y_t\}$ that are not conditionally independent. Although here the number of observations $N = \infty$, the state estimation still has a proper posterior distribution. [41, 40] consider the Markov-modulated Poisson processes where $\{Y_t\}$ is a Poisson process whose rate is determined by $\{X_t\}$. [14] considers the Markov-modulated Markov processes where $\{Y_t\}$ is a non-homogeneous jump process whose generator is determined by $\{X_t\}$. [34] further considers the bivariate Markov chain where $\{(X_t, Y_t)\}$ together is a jump process. This can be regarded as a special case of our setting if we rewrite $\tilde{X}_t = (X_t, Y_t)$ together as the hidden state and $Y_t$ as the observation (now $Y_t$ is a partial observation of $\tilde{X}_t$). In our setting, $Y_t$ is not necessarily part of $X_t$, but contains partial information of $X_t$. It is also a natural extension of the classical case since the embedded chain $\{(X_{\bar{r}_s}, Y_{\bar{r}_s})\}_{s=0}^{S}$ is a DT-HMM. Note that [30] has similar settings except that they need to know the underlying jumping time $\{\bar{r}_s\}$, while we only require $\{\bar{r}_s\}$ from $\{Y_t\}$.

In addition, previous derivations usually follow standard approach of the parameter estimation for (non-hidden) jump process [35, 18], calculating the dwell time of each hidden state and the number of jumps between two states. Here we take a more straightforward approach by taking limit in the discrete-time Baum-Welch algorithm. Section 4 shows that it is an unified approach that can also be applied to hidden diffusion process.

### 3.2 State estimation

For state estimation, we assume that the model $(Q, r, \pi_0)$ are given, and we have continuous-time observations $Y_t = y_t$, $t \in [0,T]$. For parameter estimation, we assume that the generator $Q$ is unknown and needs to be calculated by the EM algorithm.

**Theorem 1.** For a CT-HMM $(Q, r, \pi_0)$ defined above, assume that the observations $Y_t = y_t$, $t \in [0,T]$. Let the row vector $\alpha_t = [\alpha_t(1) \cdots \alpha_t(n)] \in \mathbb{R}^{1 \times n}$ and the column vector $\beta_t = [\beta_t(1) \cdots \beta_t(n)]^\top \in \mathbb{R}^{n \times 1}$
be the solutions of the forward and backward piecewise ODEs respectively

\[
\begin{align*}
\alpha_0 &= \pi_0 R(y_0), \\
\alpha_t &= \alpha_t | D + (Q - D)R(y_{\tau_s})|, \quad t \in [\tau_s, \tau_{s+1}), \\
\alpha_{\tau_s} &= \alpha_{\tau_s} | Q - D)R(y_{\tau_s}), \\
\beta_T &= 1, \\
\beta_t &= -| D + (Q - D)R(y_{\tau_s})| \beta_t, \quad t \in [\tau_s, \tau_{s+1}), \\
\beta_{\tau_s} &= (Q - D)R(y_{\tau_s}) \beta_{\tau_s},
\end{align*}
\]

(3.4)

where \( D = \text{diag}(Q_{11}, \ldots, Q_{nn}) \), \( R(y) = \text{diag}(r_1(y), \ldots, r_n(y)) \) and the left limit \( \alpha_{\tau_s} = \lim_{t \uparrow \tau_s} \alpha_t \). Then the posterior distribution of the hidden states satisfies

\[
\rho_t(i) = \Pr[X_t = i | Y_s = y_s, s \in [0, T]] = \frac{\alpha_t(i) \beta_t(i)}{\alpha_0 \cdot \beta_0},
\]

(3.6)

where the inner product \( \alpha_0 \cdot \beta_0 = \sum_{i=1}^n \alpha_0(i) \beta_0(i) \).

To prove the theorem, we first discretize \([0, T]\) with time step \( \Delta t \) and then take limit \( \Delta t \to 0 \). During the proof we may omit some technical details, e.g., the convergence of the stochastic process under the limit.

An important property is that \( \{(X_t, Y_t)\} \) together is a Markov process with transition probability

\[
\Pr\{X_{t+\Delta t} = j, Y_{t+\Delta t} = y_t | X_t = i, y_t \} = \begin{cases} (1 + Q_{ii} \Delta t)1_{y_{t+\Delta t} = y_t}, & j = i, \\
Q_{ji} r_{j}(y_{t+\Delta t}) \Delta t, & j \neq i. \end{cases}
\]

(3.7)

Here we omit the \( o(\Delta t) \) terms on the right hand side. Then the Baum-Welch forward-backward algorithm for DT-HMM can be modified as follows.

In the forward equation, let

\[
\alpha_t(i) = \Pr\{X_t = i, y_{0:t} \} \Delta t^{-s}, \quad t \in [\tau_s, \tau_{s+1}),
\]

(Later we will show that the limit of the right hand side exists when taking \( \Delta t \to 0 \).) The initial probability \( \alpha_0(i) = \pi_0(i) r_i(y_0) \). Since

\[
\Pr\{X_{t+\Delta t} = i, y_{0:t+\Delta t} \} = \sum_{j=1}^n \Pr\{X_{t+\Delta t} = i, X_t = j, y_{0:t+\Delta t}\}
\]

\[
= \sum_{j=1}^n \Pr\{X_{t+\Delta t} = i, y_{t+\Delta t} | X_t = j, y_t \} \Pr\{X_t = j, y_{0:t}\}
\]

\[
= (1 + Q_{ii} \Delta t)1_{y_{t+\Delta t} = y_t} \Pr\{X_t = i, y_{0:t}\} + \sum_{j \neq i} Q_{ji} r_{j}(y_{t+\Delta t}) \Delta t \Pr\{X_t = j, y_{0:t}\},
\]

we have

\[
\alpha_{t+\Delta t}(i) = \frac{\alpha_t(i) + \left[ \alpha_t(i) Q_{ii} + \sum_{j \neq i} \alpha_t(j) Q_{ji} r_{j}(y_{t}) \right] \Delta t}{\sum_{j \neq i} \alpha_t(j) Q_{ji} r_{j}(y_{t+\Delta t})}, \quad y_{t+\Delta t} = y_t,
\]

(3.8)

\[
\alpha_{t+\Delta t}(i) = \frac{\alpha_t(i) + \left[ \alpha_t(i) Q_{ii} + \sum_{j \neq i} \alpha_t(j) Q_{ji} r_{j}(y_{t+\Delta t}) \right] \Delta t}{\sum_{j \neq i} \alpha_t(j) Q_{ji} r_{j}(y_{t+\Delta t})}, \quad y_{t+\Delta t} \neq y_t.
\]

Taking \( \Delta t \to 0 \), we get the forward piecewise ODE \( (3.4) \).

In the backward equation, let

\[
\beta_t(i) = \Pr\{y_{t+\Delta t:t} | X_t = i, y_t \} \Delta t^{-(S-s)}, \quad t \in [\tau_s, \tau_{s+1}).
\]
Then the boundary condition $\beta_T(i) = 1$. Since
\[
\Pr\{y_t|X_t = i, y_{t+1}\} = \sum_{j=1}^{n} \Pr\{X_t = j, y_{t+1}|X_t = i, y_{t+1}\}
\]
\[
= \sum_{j=1}^{n} \Pr\{y_{t+1}|X_t = j, y_t\} \Pr\{X_t = j, y_t|X_t = i, y_{t+1}\}
\]
\[
= \Pr\{y_{t+1}|X_t = i, y_t\}(1 + Q_{i} \Delta t)\mathbf{1}_{y_t = y_{t+1}}
\]
\[
+ \sum_{j \neq i} \Pr\{y_{t+1}|X_t = j, y_t\} Q_{ij} r_j(y_t) \Delta t,
\]
we have
\[
\beta_{t+1}(i) = \left\{ \begin{array}{l} \beta_t(i) + \left[ Q_{i} \beta_t(i) + \sum_{j \neq i} Q_{ij} r_j(y_t) \beta_t(j) \right] \Delta t, \quad y_{t+1} = y_t, \\
\sum_{j \neq i} Q_{ij} r_j(y_t) \beta_t(j), \quad y_{t+1} \neq y_t. \end{array} \right.
\]
Taking $\Delta t \to 0$, we get the backward piecewise ODE (3.5).
Now calculate $\rho_t = \Pr\{X_t = i|y_0:T\}$ in (3.6) from $\alpha_t$ and $\beta_t$. Since
\[
\Pr\{X_t = i, y_0:T\} = \Pr\{y_{t+1}|X_t = i, y_t\} \Pr\{X_t = i, y_{0:t}\} = \alpha_t(i) \beta_t(i) \Delta t^S,
\]
and
\[
\Pr\{y_{0:T}\} = \sum_{i} \Pr\{X_t = i, y_{0:T}\} = \sum_{i} \alpha_t(i) \beta_t(i) \Delta t^S = \alpha_t \cdot \beta_t \Delta t^S,
\]
the inner product $\alpha_t \cdot \beta_t$ is constant for all $t$. Therefore,
\[
\rho_t(i) = \frac{\Pr\{X_t = i, y_{0:T}\}}{\Pr\{y_{0:T}\}} = \frac{\alpha_t(i) \beta_t(i)}{\alpha_0 \cdot \beta_0}.
\]

### 3.3 Parameter estimation

In case when the generator $Q$ is an unknown parameter in the model, it can be estimated by the following EM algorithm.

**Algorithm 2.** For a CT-HMM $(Q, r, \pi_0)$ defined above, assume that the observations $Y_t = y_t, t \in [0, T]$, and $Q$ is the unknown parameter. Let $Q^0$ be the initialization of the generator, then repeat the following E-step and M-step to update $Q^k, k = 0, 1, \ldots$ until convergence.

**E-step** Under the current estimate $Q = Q^k$, solve the forward and backward piecewise ODEs (3.4) and (3.5) for $\alpha_t$ and $\beta_t$, and calculate the posterior distribution $\rho_t$ from (3.6).

**M-step** Update the generator from $Q^k$ to $Q^{k+1}$ using
\[
Q^{k+1}_{ij} = \frac{1}{(\alpha_0 \cdot \beta_0) T} \int_0^T \rho_t(i) dt \left[ \sum_{s=0}^{S} \int_{\tau_s}^{\tau_{s+1}} \alpha_t(i) Q^k_{ij} r_j(y_{\tau_s}) \beta_t(j) dt + \sum_{s=1}^{S} \alpha_{t-1} Q^k_{ij} r_j(y_{\tau_s}) \beta_{t-1}(j) \right]
\]
for $j \neq i$, and $Q^{k+1}_{ii} = -\sum_{j \neq i} Q^{k+1}_{ij}$.

The goal of the E-step is to calculate the posterior distribution $\Pr\{X_t|y_0:T; Q^k\}$ under the current generator $Q^k$. This is equivalent to the previous state estimation problem if we replace the true generator $Q$ by $Q^k$. Besides $\alpha_t, \beta_t$ and $\rho_t$, here we also need to calculate
\[
\xi_t(i, j) = \Pr\{X_t = i, X_{t+1} = j|y_0:T\}.
\]
under the time discretization. Since
\[
Pr\{X_{t-\Delta t} = i, X_t = j, y_{0:T}\} = Pr\{y_{t+\Delta t:T}|X_t = j, y_t\} \cdot Pr\{X_t = j, y_t|X_{t-\Delta t} = i, y_{-\Delta t}\} \cdot Pr\{X_{t-\Delta t} = i, y_{0:T-\Delta t}\},
\]
we can show that
\[
(\alpha_0 \cdot \beta_0)\xi_t(i, j) = \begin{cases} 
\alpha_{t-\Delta t}(i)(1 + Q_{ij}\Delta t)\beta_t(i), & y_{-\Delta t} = y_t, j = i, \\
\alpha_{t-\Delta t}(i)Q_{ij}r_j(y_t)\beta_t(j)\Delta t, & y_{-\Delta t} = y_t, j \neq i, \\
0, & y_{-\Delta t} \neq y_t, j = i, \\
\alpha_{t-\Delta t}(i)Q_{ij}r_j(y_t)\beta_t(j), & y_{-\Delta t} \neq y_t, j \neq i.
\end{cases}
\]

The goal of the M-step is to calculate the maximum-likelihood estimation of the parameter $Q$ given the current estimation of $\{(X_t, Y_t)\}$. Under the time discretization, the update formula of the EM algorithm \[2,3\] gives $Q^{k+1} = \operatorname{argmax}_Q Q(Q, Q^k)$, where
\[
Q(Q, Q^k) = \sum_{x_{0:T}} Pr\{x_{0:T}|y_{0:T}; Q^k\} \log Pr\{x_{0:T}, y_{0:T}; Q\}.
\]

Let $\alpha_t$, $\beta_t$, $\rho_t$ and $\xi_t$ are calculated in the E-step with respect to $Q^k$. Since $\{(X_t, Y_t)\}$ together is a Markov process with transition probabilities \[3,7\],
\[
Pr\{x_{0:T}, y_{0:T}; Q\} = Pr\{x_{0}, y_{0}\} \prod_{t=\Delta t}^T Pr\{x_t, y_t|x_{t-\Delta t}, y_{t-\Delta t}; Q\},
\]
then
\[
Q(Q, Q^k) = \sum_{x_{0:T}} Pr\{x_{0:T}|y_{0:T}; Q^k\} \left[ \log Pr\{x_{0}, y_{0}\} + \sum_{t=\Delta t}^T \log Pr\{x_t, y_t|x_{t-\Delta t}, y_{t-\Delta t}; Q\} \right]
\]
\[
= \sum_{x_{0:T}} Pr\{x_{0}|y_{0}; Q^k\} \log Pr\{x_{0}, y_{0}\}
+ \sum_{t} \sum_{x_{t-\Delta t}, x_t} Pr\{x_{t-\Delta t}, x_t|y_{0:T}; Q^k\} \log Pr\{x_t, y_t|x_{t-\Delta t}, y_{t-\Delta t}; Q\}.
\]

Since $Pr\{x_{0}, y_{0}\}$ in the first term does not depend on $Q$, we only need to maximize the second term
\[
\sum_{t} \sum_{x_{t-\Delta t}, x_t} Pr\{x_{t-\Delta t}, x_t|y_{0:T}; Q^k\} \log Pr\{x_t, y_t|x_{t-\Delta t}, y_{t-\Delta t}; Q\}
\]
\[
= \sum_{i,j} \sum_{t} \xi_t(i, j) \log Pr\{X_t = j, y_t|X_{t-\Delta t} = i, y_{t-\Delta t}; Q\}
\]
\[
= \sum_{i} \sum_{t} \xi_t(i, i) \log(1 + Q_{ii}\Delta t) + \sum_{j \neq i} \sum_{t} \xi_t(i, j) \log(Q_{ij}\Delta t + \log r_j(y_t)).
\]

Notice that $(1 + Q_{ii}\Delta t) + \sum_{j \neq i} Q_{ij}\Delta t = 1$ and $\sum_{j=1}^n \xi_t(i, j) = \rho_{t-\Delta t}(i)$, then
\[
Q^{k+1}_{ij} = \frac{\sum_{t} \xi_t(i, j)}{\sum_{j'=1}^n \sum_{t} \xi_t(i, j')\Delta t} = \frac{1}{(\alpha_0 \cdot \beta_0) \sum_{t} \rho_{t-\Delta t}(i)\Delta t}
\cdot \left[ \sum_{y_{t-\Delta t} = y_t} \alpha_{t-\Delta t}(i)Q^k_{ij}r_j(y_t)\beta_t(j)\Delta t + \sum_{y_{t-\Delta t} \neq y_t} \alpha_{t-\Delta t}(i)Q^k_{ij}r_j(y_t)\beta_t(j) \right]
\]
for $j \neq i$. Taking $\Delta t \to 0$, we will have the update \[3,8\] in Algorithm \[2\]
4 CT-HMM with diffusion process

4.1 Problem settings

In this section, we analyze another type of CT-HMM where the hidden process is a diffusion process, and the hidden states and observations take continuous values. We consider the same setting as the Stratonovich-Kushner and Zakai equations. Assume that the hidden process $X_t \in \mathbb{R}^n$ and the observations $Y_t \in \mathbb{R}^m$ are given by SDEs

$$
dX_t = f(X_t)dt + \sigma dW_t, \\
dY_t = h(X_t)dt + \eta dB_t,
$$

(4.1)

where the drift terms $f: \mathbb{R}^n \to \mathbb{R}^n$, $h: \mathbb{R}^n \to \mathbb{R}^m$; the noise terms $\{W_t\}$ and $\{B_t\}$ are independent $n$-dimensional and $m$-dimensional Brownian motions respectively. Here we assume that $\sigma$ and $\eta$ are scalars for brevity, and all the results can be easily extended to the case when they are matrices. Let the initial distribution of $X_0$ be $\pi_0(x) = p(X_0 = x)$, and the time period $t \in [0,T]$.

4.2 State estimation

State estimation is closely related to the filtering and smoothing problem (see Section 2.4). The optimal nonlinear filtering of the diffusion model (4.1) is solved by the Stratonovich-Kushner equation [15, 25, 26] that describes the dynamics of the density of the states condition on the previous observations $\tilde{\pi}_t(x) = p(X_t = x|Y_{0:t})$.

$$
d\tilde{\pi}_t(x) = \mathcal{L}^* \tilde{\pi}_t(x) + \frac{1}{\eta^2} \tilde{\pi}_t(x) [h(x) - \mathbb{E}_{X \sim \tilde{\pi}_t} h(X)]^T [dY_t - \mathbb{E}_{X \sim \tilde{\pi}_t} h(X) dt].
$$

(4.2)

(See Theorem 3 for the definition of the operators $\mathcal{L}$ and $\mathcal{L}^*$.) The Zakai equation [46] introduces a simplified dynamics for the unnormalized conditional distribution $\pi_t(x) = \tilde{\pi}_t(x) Z_t$ with some constant $Z_t$, and we take it as the forward part [4, 4]. The corresponding smoothing problem considers the density of the states condition on the whole observation process $\rho_t(x) = p(X_t = x|Y_{0:T})$. [2] derives the differential equation

$$
\frac{d\rho_t(x)}{dt} = \frac{\rho_t(x)}{\tilde{\pi}_t(x)} \mathcal{L}^* \tilde{\pi}_t(x) - \tilde{\pi}_t(x) \mathcal{L} \left[ \frac{\rho_t(x)}{\tilde{\pi}_t(x)} \right].
$$

(4.3)

Unlike [4, 4] where the equation of the smoother $\rho_t$ contains the filtered $\tilde{\pi}_t$, here we follow the Baum-Welch framework, writing the smoother as the product of two terms that are the solutions of the forward and backward SPDEs respectively.

**Theorem 3.** For a CT-HMM with hidden diffusion process defined above, let $\pi_t$ and $\beta_t$ be the solutions of the forward and backward SPDEs respectively

$$
\pi_0(x) = p(X_0 = x), \quad d\pi_t(x) = \mathcal{L}^* \pi_t(x) dt + \eta^{-2} \pi_t(x) h^T(x) dY_t, \\
\beta_T(x) = 1, \quad d\beta_t(x) = -\mathcal{L} \beta_t(x) dt - \eta^{-2} \beta_t(x) h^T(x) [dY_t - h(x) dt],
$$

(4.4)

(4.5)

where

$$
\mathcal{L}^* \pi_t(x) = - \nabla \cdot [f(x) \pi_t(x)] + \frac{\sigma^2}{2} \nabla^2 \pi_t(x),
$$

$$
\mathcal{L} \beta_t(x) = f(x) \cdot \nabla \beta_t(x) + \frac{\sigma^2}{2} \nabla^2 \beta_t(x);
$$
the gradient operator $\nabla = \left[ \frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n} \right]$, and the Laplace operator $\nabla^2 = \nabla \cdot \nabla = \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2}$. Then the posterior distribution of the hidden states is given by

$$\rho_t(x) = p(X_t = x|Y_s = y_s, s \in [0,T]) = \frac{1}{Z_T} \pi_t(x) \beta_t(x)$$

(4.6)

for some normalization factor $Z_T$.

The proof is based on the derivation of the Zakai equation and we give the sketch here. (See [36] for more details.)

Since $dY_t = h(X_t)dt + \eta dB_t$, from Girsanov theorem, define an equivalent measure $Q$ by

$$dQ = M_T^{-1}dP, \quad M_t = \exp \left[ -\frac{1}{2\eta^2} \int_0^t h^\top(X_s)h(X_s)ds + \frac{1}{\eta^2} \int_0^t h^\top(X_s)dY_s \right].$$

Then under measure $Q$, $\{Y_t/\eta\}$ is a Brownian motion and $\{M_t\}$ is a martingale, while $\{X_t\}$ and $\{Y_t\}$ are independent. For any function $g$, let

$$\psi_t[g] = \mathbb{E}_P[g(X_t)|Y_{0:t}], \quad \phi_t[g] = \mathbb{E}_Q[g(X_t)M_t|Y_{0:t}], \quad Z_t = \phi_t[1] = \mathbb{E}_Q[M_t|Y_{0:t}],$$

one can show that

$$\psi_t[g] = \phi_t[g]/Z_t.$$

Since $\{X_t\}$ and $\{Y_t\}$ are independent under $Q$, we can derive the dynamics of $\phi_t[g]$ as

$$d\phi_t[g] = \phi_t[\mathcal{L}g]dt + \phi_t \left[ \frac{h^\top}{\eta^2} \right] dY_t.$$  

(4.7)

Assume that we can write $\phi_t[g] = \int_{\mathbb{R}^n} g(x)\pi_t(x)dx$, then $\pi_t(x) = p(X_t = x|Y_{0:t})Z_t$, and satisfies the adjoint of (4.7), i.e., the Zakai equation (4.4).

Furthermore, let the smoothing component be

$$\beta_t(x) = \mathbb{E}_Q[M_T/M_t|X_t = x, Y_{0:T}],$$

then one can show that $\rho_t(x) = \pi_t(x)\beta_t(x)/Z_T$, and $\beta_t$ satisfies the backward SPDE (4.5). We can also calculate that

$$\frac{d\rho_t(x)}{dt} = \frac{1}{Z_T} [\beta_t(x)\mathcal{L}^\top\pi_t(x) - \pi_t(x)\mathcal{L}\beta_t(x)],$$

(4.8)

which is equivalent to (4.3).

### 4.3 Parameter estimation

For simplicity, we assume that only $f$ contains unknown parameter $f = f(x; \theta)$. The following is the EM algorithm.

**Algorithm 4.** For a CT-HMM with hidden diffusion process defined above, assume that the observations $Y_t = y_t$, $t \in [0,T]$, and $f = f(x; \theta)$ where $\theta$ is the unknown parameter. Let $\theta^0$ be the initialization of $\theta$, then repeat the following E-step and M-step to update $\theta^k$, $k = 0, 1, \ldots$ until convergence.

**E-step** Using the current value of the estimated $\theta = \theta^k$, solve the forward and backward SPDEs (4.4) and (4.5) for $\pi_t$ and $\beta_t$ respectively, and calculate the posterior distribution $\rho_t$ from (4.3).

**M-step** Update the parameter by $\theta^{k+1} = \arg\min_{\theta} \hat{Q}(\theta, \theta^k)$ where

$$\hat{Q}(\theta, \theta^k) = \int_0^T \int_{\mathbb{R}^n} \rho_t(x) \left[ \|f(x; \theta^k)\|^2_2 - 2f(x; \theta^k)^T f(x; \theta) + \frac{\sigma^2 \nabla \beta_t(x)}{\beta_t(x)} \right] dx dt.$$  

(4.9)
The E-step is equivalent to the state estimation discussed above. So we will focus on the M-step. We still discretize $[0, T]$ with time step $\Delta t$ and then take limit $\Delta t \to 0$. The parameter update formula (2.3) gives $\theta^{k+1} = \arg\max_{\theta} Q(\theta, \theta^k)$ where

$$Q(\theta, \theta^k) = \int p(x_{0:T}|y_{0:T}; \theta^k) \log p(x_{0:T}, y_{0:T}; \theta) dx_{0:T}$$

(4.10)

(thе integral takes over $dx_{0:T} = dx_0 dx_{\Delta t} dx_{2\Delta t} \cdots dx_T$). Notice that

$$p(x_{0:T}, y_{0:T}; \theta) = p(x_0) \prod_{t=0}^{T-\Delta t} p(\Delta x_t | x_t; \theta) \prod_{t=0}^T p(\Delta y_t | x_t),$$

where

$$p(\Delta x_t | x_t; \theta) = \frac{1}{Z_f} \exp \left[ -\frac{\|\Delta x_t - f(x_t; \theta)\Delta t\|^2}{2\sigma^2 \Delta t} \right]$$

for $Z_f = (2\pi \sigma^2)^{n/2}$, and $p(x_0), p(\Delta y_t | x_t)$ do not depend on $\theta$. So we have

$$Q(\theta, \theta^k) = \int p(x_{0:T}|y_{0:T}; \theta^k) \left[ \log p(x_0) + \sum_{t=0}^{T-\Delta t} \log p(\Delta x_t | x_t; \theta) + \sum_{t=0}^T \log p(\Delta y_t | x_t) \right] dx_{0:T}$$

$$= \int p(x_0|y_{0:T}; \theta^k) \log p(x_0) dx_0 + \sum_{t=0}^{T-\Delta t} \int p(x_t, \Delta x_t|y_{0:T}; \theta^k) \log p(\Delta x_t|x_t; \theta) dx_t dx_{t+\Delta t}$$

$$+ \sum_{t=0}^T \int p(x_t|y_{0:T}; \theta^k) \log p(\Delta y_t|x_t) dx_t.$$ 

Only the second summation term depends on $\theta$, whose integral becomes

$$\int p(x_t, \Delta x_t|y_{0:T}; \theta^k) \log p(\Delta x_t|x_t; \theta) dx_t dx_{t+\Delta t}$$

$$= -\log Z_f - \int \rho_t(x_t)p(\Delta x_t|x_t, y_{0:T}; \theta^k) \frac{\|\Delta x_t - f(x_t; \theta)\Delta t\|^2}{2\sigma^2 \Delta t} dx_t dx_{t+\Delta t}$$

$$= C - \frac{1}{2\sigma^2} \int \rho_t(x_t) [\|f(x_t; \theta)\|^2 \Delta t - 2f^T(x_t; \theta)E[\Delta x_t|x_t, y_{0:T}; \theta^k]] dx_t$$

$$= C - \frac{1}{2\sigma^2} \int \rho_t(x) [\|f(x; \theta)\|^2 \Delta t - 2f^T(x; \theta)E[\Delta x|x_{t} = x, y_{0:T}; \theta^k]] dx,$$

where $C$ is a constant and not depending on $\theta$. Therefore, $\theta^{k+1} = \arg\min_{\theta} \tilde{Q}(\theta, \theta^k)$ where

$$\tilde{Q}(\theta, \theta^k) = \int_{\mathbb{R}^n} \sum_{t=0}^{T-\Delta t} \rho_t(x) [\|f(x; \theta)\|^2 \Delta t - 2f^T(x; \theta)E[\Delta x|x_{t} = x, y_{0:T}; \theta^k]] dx.$$ 

Now take $\Delta t \to 0$, we have

$$\tilde{Q}(\theta, \theta^k) = \int_0^T \int_{\mathbb{R}^n} \rho_t(x) \left[ \|f(x; \theta)\|^2 - 2f^T(x; \theta) \frac{d}{dt} \right]_{t=0} E[X_{t+\tau}|X_t = x, y_{0:T}; \theta^k] dx dt,$$

and from (4.6) we can calculate that

$$\frac{d}{dt} \bigg|_{t=0} E[X_{t+\tau}|X_t = x, y_{0:T}] = f(x) + \frac{\sigma^2 \nabla \beta_t(x)}{\beta_t(x)}.$$ 

Therefore, (4.9) holds in Algorithm 3.
### 4.4 Linear Gaussian dynamics

In this section, we apply our algorithm to the linear Gaussian dynamics. Here both \( f \) and \( h \) are linear and the initial distribution \( \pi_0 \) is Gaussian, thus the posterior distribution of the hidden state is always Gaussian. We will see that the SPDEs in state estimation and the optimization in parameter estimation have explicit solutions, and are consistent with the discrete-time Kalman filter and smoother as well as the EM algorithm under the limit \( \Delta t \to 0 \).

Let \( f(x) = Fx \) and \( h(x) = Hx \) where the matrices \( F \in \mathbb{R}^{n \times n} \) and \( H \in \mathbb{R}^{m \times n} \). We also consider \( \sigma \in \mathbb{R}^{n \times n} \) and \( \eta \in \mathbb{R}^{m \times n} \) to be matrices. The dynamics of the hidden process \( \{X_t\} \) and the observation \( \{Y_t\} \) becomes

\[
\begin{align*}
\text{d}X_t &= FX_t \text{d}t + \sigma \text{d}W_t, \\
\text{d}Y_t &= HX_t \text{d}t + \eta \text{d}B_t.
\end{align*}
\] (4.11)

Assume that the initial distribution is Gaussian \( X_0 \sim \mathcal{N}(\mu_0, P_0) \). So the posterior distribution of \( X_t \) is always Gaussian.

#### 4.4.1 Continuous-time Kalman filter and smoother

Given the Gaussian property in the linear case, to describe the posterior distribution of \( X_t \), we only need to find the mean and variance from the SDEs (4.4) and (4.5). Here the SPDEs become

\[
\begin{align*}
\frac{\text{d}}{\text{d}t} \mu_t &= FX_t \mu_t + HP_t \eta \eta^\top, \\
\frac{\text{d}}{\text{d}t} P_t &= P_t h h^\top + \sigma \sigma^\top.
\end{align*}
\] (4.12)

Solving the SPDEs, we have

\[
\begin{align*}
\frac{\text{d}}{\text{d}t} \mu_t &= FX_t \mu_t + HP_t \eta \eta^\top, \\
\frac{\text{d}}{\text{d}t} P_t &= P_t h h^\top + \sigma \sigma^\top.
\end{align*}
\] (4.13)

and

\[
\begin{align*}
\mu_t &= (P_t^\sigma)^{-1} \left[ (P_t^\eta)^{-1} \mu_t + (P_t^\beta)^{-1} \mu_t^\beta \right], \\
P_t^\sigma &= \left[ (P_t^\eta)^{-1} + (P_t^\beta)^{-1} \right]^{-1}.
\end{align*}
\] (4.14)

For the initial conditions, \( X_0 \sim \mathcal{N}(\mu_0, P_0) \) gives \( \mu_0^\sigma = \mu_0 \) and \( P_0^\sigma = P_0 \). However, since \( \beta_T(x) = 1 \), we have \( P_T^\beta = +\infty \) and \( \mu_T^\beta \) is undefined. We can instead use \( (P_T^\beta)^{-1} \mu_T^\beta = 0 \), \( (P_T^\beta)^{-1} = 0 \) and

\[
\begin{align*}
\frac{\text{d}}{\text{d}t} \left[ (P_t^\beta)^{-1} \mu_t^\beta \right] &= -F (P_t^\beta)^{-1} \mu_t^\beta \text{d}t + (P_t^\beta)^{-1} \sigma \sigma^\top (P_t^\beta)^{-1} \mu_t^\beta \text{d}t - H^\top \eta \eta^\top \text{d}Y_t, \\
\frac{\text{d}}{\text{d}t} (P_t^\beta)^{-1} &= -F (P_t^\beta)^{-1} - (P_t^\beta)^{-1} F^\top (P_t^\beta)^{-1} \sigma \sigma^\top (P_t^\beta)^{-1} - H^\top \eta \eta^\top H.
\end{align*}
\]
As a comparison, in the following we consider Kalman filter and smoother under the limit $\Delta t \to 0$. We will see that the result is consistent with the differential equations above.

The discretization of the model gives
\[
X_{t+\Delta t} = (I + F\Delta t)X_t + \sigma\Delta W_t, \\
\Delta Y_t = HX_t\Delta t + \eta\Delta B_t,
\]
where we omit the $o(\Delta t)$ term. Here we use the notations in Kalman filter: for $t \leq s$, let
\[
X_t|Y_{0:s} \sim \mathcal{N}\left(\mu_{t|s}, P_{t|s}\right)
\]
be the distribution of $X_t$ condition on $\Delta Y_0, \Delta Y_1, \ldots, \Delta Y_{s-\Delta t}$ without $\Delta Y_s$. We will prove that $\mu_{t|t} = \mu^T_t$, $P_{t|t} = P^T_t$ and $\mu_{t|T} = \mu^T_0$, $P_{t|T} = P^T_0$.

For the filtering problem, we calculate $\mu_{t|t}$ and $P_{t|t}$. The discrete-time Kalman filter gives
\[
K_t = P_{t|t}H^T\Delta t \left(HP_{t|t}H^T\Delta t^2 + \eta\eta^T\Delta t\right)^{-1}, \\
\mu_{t+\Delta t} = \mu_{t|t} + K_t \left(\Delta Y_t - H\mu_{t|t}\Delta t\right), \\
P_{t+\Delta t} = (I - K_tH\Delta t)P_{t|t},
\]
and
\[
\mu_{t+\Delta t|t+\Delta t} = (I + F\Delta t)\mu_{t|t+\Delta t}, \\
P_{t+\Delta t|t+\Delta t} = (I + F\Delta t)P_{t|t+\Delta t}(I + F\Delta t)^T + \sigma\sigma^T\Delta t.
\]
We also have
\[
K_t = P_{t|t}H^T\eta^{-T}\eta^{-1} + O(\Delta t), \\
\mu_{t+\Delta t|t+\Delta t} - \mu_{t|t} = F\mu_{t|t}\Delta t + K_t \left(\Delta Y_t - H\mu_{t|t}\Delta t\right) + o(\Delta t), \\
P_{t+\Delta t|t+\Delta t} - P_{t|t} = [FP_{t|t} + P_{t|t}F^T - K_tHP_{t|t} + \sigma\sigma^T]\Delta t + o(\Delta t).
\]
We get the continuous-time Kalman filter by taking $\Delta t \to 0$, where $\mu_{t|t}$ and $P_{t|t}$ satisfy the same differential equations as $\mu^T_t$ and $P^T_t$ (4.13) respectively.

For the smoothing problem, we need to calculate $\mu_{t|T}$ and $P_{t|T}$. According to the Rauch-Tung-Striebel smoother [39],
\[
C_t = P_{t-\Delta t|t}(I + F\Delta t)^TP_{t|t}^{-1}, \\
\mu_{t-\Delta t|T} = \mu_{t-\Delta t|t} + C_t \left(\mu_{t|T} - \mu_{t|t}\right), \\
P_{t-\Delta t|T} = P_{t-\Delta t|t} + C_t \left(P_{t|T} - P_{t|t}\right) C^T_t.
\]
Then
\[
C_t = I - \left(F + \sigma\sigma^TP_{t|t}^{-1}\right)\Delta t + o(\Delta t), \\
\mu_{t-\Delta t|T} - \mu_{t|T} = -\left[\left(F + \sigma\sigma^TP_{t|t}^{-1}\right)\mu_{t|T} - \sigma\sigma^TP_{t|t}^{-1}\mu_{t|t}\right]\Delta t + o(\Delta t), \\
P_{t-\Delta t|T} - P_{t|T} = -\left[\left(F + \sigma\sigma^TP_{t|t}^{-1}\right)P_{t|T} + P_{t|T} \left(F + \sigma\sigma^TP_{t|t}^{-1}\right)^T - \sigma\sigma^T\right]\Delta t + o(\Delta t).
\]
Taking $\Delta t \to 0$, we get the backward ODEs
\[
\frac{d\mu_{t|T}}{dt} = \left(F + \sigma\sigma^TP_{t|t}^{-1}\right)\mu_{t|T} - \sigma\sigma^TP_{t|t}^{-1}\mu_{t|t}, \\
\frac{dP_{t|T}}{dt} = \left(F + \sigma\sigma^TP_{t|t}^{-1}\right)P_{t|T} + P_{t|T} \left(F + \sigma\sigma^TP_{t|t}^{-1}\right)^T - \sigma\sigma^T, \quad (4.16)
\]
where the initial conditions $\mu_{T|T}$ and $P_{T|T}$ are given by the previous filter.

Compare with our previous results, by plugging (4.13) in (4.14) we see that the ODEs for $\mu_t^\rho$ and $P_t^\rho$ are exactly the same as (4.16). Notice that for Kalman smoother (4.16), the ODEs for $\mu_{t|T}$ and $P_{t|T}$ depend on the filter $\mu_{t|t}$ and $P_{t|t}$, while in our solution (4.13) and (4.14), the smoother $\rho_t \propto \pi_t \beta_t$, where the differential equations for $\pi_t$ and $\beta_t$ are independent. Later we will see that $\beta_t$ plays an important role in the EM algorithm.

4.4.2 The EM algorithm for Kalman filter

In the linear dynamics (4.11), we assume that $H$, $\sigma$ and $\eta$ are given and $F$ is the unknown parameter to be estimated. We further assume that $\sigma$ and $\eta$ are scalars instead of matrices for simplicity. With the current estimation $F = F^k$, let the solution of the E-step be $\mu_t^\pi$, $P_t^\pi$, $\mu_t^\beta$, $P_t^\beta$ and $\mu_t^\rho$, $P_t^\rho$. In the M-step, the parameter update (4.9) becomes $F^{k+1} = \arg\min_F \tilde{Q}(F, F^k)$ where

$$
\tilde{Q}(F, F^k) = \int_0^T \int_{\mathbb{R}^n} \rho_t(x) \left[ x^T F^k F x - 2x^T F^T \left( F^k x + \sigma^2 \nabla \beta_t(x) \right) \right] dx dt.
$$

Since $\beta_t(x)$ is unnormalized Gaussian, i.e., $\beta_t(x)Z_t^\beta \sim \mathcal{N}(\mu_t^\beta, P_t^\beta)$, we have

$$
\nabla \beta_t(x) = -(P_t^\beta)^{-1} (x - \mu_t^\beta).
$$

Furthermore,

$$
\int_{\mathbb{R}^n} x \rho_t(x) dx = \mu_t^\pi, \quad \int_{\mathbb{R}^n} xx^T \rho_t(x) dx = \mu_t^\rho \mu_t^\rho^T + P_t^\rho,
$$

the objective function

$$
\tilde{Q}(F, F^k) = \int_0^T \int_{\mathbb{R}^n} \rho_t(x) \left[ x^T F^k F x - 2x^T F^T \left( F^k x - \sigma^2 (P_t^\beta)^{-1} (x - \mu_t^\beta) \right) \right] dx dt
$$

$$
= \int_0^T \int_{\mathbb{R}^n} \rho_t(x) \left[ x^T \left( F^T F - 2F^T F^k + 2\sigma^2 F^T (P_t^\beta)^{-1} \right) x - 2\sigma^2 x^T F^T (P_t^\beta)^{-1} \right] dx dt
$$

$$
= \int_0^T \left[ (\mu_t^\rho \mu_t^\rho^T + P_t^\rho) : \left( F^T F - 2F^T F^k + 2\sigma^2 F^T (P_t^\beta)^{-1} \right) - 2\sigma^2 \mu_t^\rho F^T (P_t^\beta)^{-1} \mu_t^\rho \right] dt
$$

$$
= (F^T F) : \int_0^T (\mu_t^\rho \mu_t^\rho^T + P_t^\rho) dt
$$

$$
- 2F : \left[ F^k \int_0^T (\mu_t^\rho \mu_t^\rho^T + P_t^\rho) dt - \sigma^2 \int_0^T (P_t^\beta)^{-1} \left( (\mu_t^\rho - \mu_t^\beta) \mu_t^\rho^T + P_t^\rho \right) dt \right].
$$

Therefore,

$$
F^{k+1} = \arg\min_F \tilde{Q}(F, F^k)
$$

$$
= F^k - \sigma^2 \left[ \int_0^T (P_t^\beta)^{-1} \left( (\mu_t^\rho - \mu_t^\beta) \mu_t^\rho^T + P_t^\rho \right) dt \right]^{-1} \left[ \int_0^T (\mu_t^\rho \mu_t^\rho^T + P_t^\rho) dt \right]^{-1}.
$$

(4.17)

In the following, we will show that our result is consistent with the discrete-time EM algorithm for linear dynamics.

First, we calculate the joint distribution of $(X_t, X_{t+\Delta t})$ condition on the whole observation $Y_{0:T}$. We know that

$$
\pi_t(x) \propto p(X_t = x, Y_{0:t}), \quad \beta_t(x) \propto p(Y_{t:T} | X_t = x),
$$
thus
\[
p(X_t = x, X_{t+\Delta t} = x' | Y_{0:T}) \propto \pi_t(x)p(X_{t+\Delta t} = x', \Delta Y_t | X_t = x)\beta_{t+\Delta t}(x)
\]
\[
\propto \exp \left[ -\frac{1}{2} (x - \mu_t^\circ)^\top (P_t^\beta)^{-1} (x - \mu_t^\circ) - \frac{1}{2\eta^2\Delta t} \| \Delta Y_t - Hx\Delta t \|^2 \right] \\
- \frac{1}{2\sigma^2\Delta t} \| x' - (I + F\Delta t)x \|^2 - \frac{1}{2} (x' - \mu_{t+\Delta t}^\circ)^\top (P_{t+\Delta t}^\beta)^{-1} (x' - \mu_{t+\Delta t}^\circ) \right].
\]
So \((X_t, X_{t+\Delta t})\) are joint Gaussian. We can see that
\[
E[X_{t+\Delta t} | X_t = x, Y_{0:T}] = \left[ \frac{1}{\sigma^2\Delta t} + (P_t^\beta)^{-1} \right]^{-1} \left[ \frac{1}{\sigma^2\Delta t} (I + F\Delta t)x + (P_t^\beta)^{-1}\mu_t^\circ \right]
\]
\[
= x + F x\Delta t - \sigma^2(P_t^\beta)^{-1}(x - \mu_t^\circ)\Delta t + o(\Delta t)
\]
which is consistent with our result. On the other hand, consider the covariance between \(X_{t+\Delta t}\) and \(X_t\), i.e.,
\[
P_{t+\Delta t,t} = E \left[ (X_{t+\Delta t} - \mu_{t+\Delta t}^\circ)(X_t - \mu_t^\circ)^\top | Y_{0:T} \right],
\]
then
\[
E[X_{t+\Delta t} | X_t = x, Y_{0:T}] = \mu_{t+\Delta t}^\circ - P_{t+\Delta t,t}(P_t^\beta)^{-1}(x - \mu_t^\circ).
\]
Denote
\[
\mu_t^\circ = \left. \frac{d\mu_t^\circ}{dt} \right|_{\tau = 0}, \quad S_t = \left. \frac{dP_{t+\tau,t}}{dt} \right|_{\tau = 0}.
\]
One can calculate that \(S_t = (F - \sigma^2(P_t^\beta)^{-1})P_t^\circ\). Now the objective function
\[
\hat{Q}(F, F^k) = \int_0^T \int_{\mathbb{R}^n} \rho_t(x) \left[ x^\top F_t^\top F_t x - 2x^\top F_t \frac{d}{dt} \left. E[X_{t+\tau} | X_t = x, Y_{0:T}; F^k] \right|_{\tau = 0} \right] \, dx \, dt 
\]
\[
= \int_0^T \int_{\mathbb{R}^n} \rho_t(x) \left[ x^\top F_t^\top F_t x - 2x^\top F_t \left[ \mu_t^\circ - S_t(P_t^\circ)^{-1}(x - \mu_t^\circ) \right] \right] \, dx \, dt 
\]
\[
= \int_0^T \int_{\mathbb{R}^n} \rho_t(x) \left[ x^\top (F_t^\top F_t + 2F_t S_t(P_t^\circ)^{-1}) x - 2x^\top F_t \left[ \mu_t^\circ - S_t(P_t^\circ)^{-1}\mu_t^\circ \right] \right] \, dx \, dt 
\]
\[
= \int_0^T \left[ (\mu_t^\circ \mu_t^\circ^\top + P_t^\circ) : (F_t^\top F_t + 2F_t S_t(P_t^\circ)^{-1}) - 2\mu_t^\circ F_t^\top \left[ \mu_t^\circ - S_t(P_t^\circ)^{-1}\mu_t^\circ \right] \right] \, dt 
\]
\[
= (F^\top F) : \int_0^T (\mu_t^\circ \mu_t^\circ^\top + P_t^\circ) \, dt - 2F : \int_0^T (\mu_t^\circ \mu_t^\circ^\top + S_t) \, dt.
\]
Therefore,
\[
F^{k+1} = \arg\min_F \hat{Q}(F, F^k) = \left[ \int_0^T (\mu_t^\circ \mu_t^\circ^\top + S_t) \, dt \right]^{-1} \left[ \int_0^T (\mu_t^\circ \mu_t^\circ^\top + P_t^\circ) \, dt \right]^{-1} 
\]
\[
= \left[ \int_0^T \left( \frac{d\mu_t^\circ}{dt} \mu_t^\circ^\top + \frac{dP_{t+\tau,t}}{dt} \right|_{\tau = 0} \right) \, dt \right]^{-1} \left[ \int_0^T (\mu_t^\circ \mu_t^\circ^\top + P_t^\circ) \, dt \right]^{-1}. \quad (4.18)
\]
Comparing with the EM algorithm for discrete-time linear dynamics \[43\], the parameter update

\[
I + F^{k+1} \Delta t = \left[ \sum_{t=0}^{T} (\mu_t^\rho_{t+\Delta t} \mu_t^\rho_T + P_{t+\Delta t,t}) \right]^{-1} \left[ \sum_{t=0}^{T} (\mu_t^\rho \mu_t^\rho_T + P_t) \right].
\]

We can see that the formula (4.18) is the limit of the discrete case.

### 4.5 Monte Carlo method

For some simple cases like the linear Gaussian dynamics, we may have explicit solutions of the SPDEs (4.4) and (4.5). In general cases, however, we have to resort to numerical solutions of the Stratonovich-Kushner and Zakai equations. A direct approach is the finite-difference splitting. One can take a fixed non-random grid \( \{x_1, \ldots, x_N\} \) in the state space, and calculate \( \pi_t(x_i) \) to approximate the evolving measure. See the line of work [3, 4, 16, 20] for the theoretical proof of the convergence of this kind of numerical schemes. The finite difference approach suffers from the curse of dimensionality, thus is not suitable for high dimensional state space.

In the following we propose a Monte Carlo sampling method. For state estimation, notice that \( \pi_t(x_t) \propto p(X_t = x_t | y_{0:t}) \) and \( \rho_t(x_t) = p(X_t = x_t | y_{0:T}) \), we can modify the particle filter and smoother to generate samples to describe those posterior distributions. Then for the objective (4.9) in the parameter estimation, the integral over \( x \) can be calculated by the summation over the samples.

First, we solve the filtering problem \( \tilde{\pi}_t(x) = p(X_t = x | y_{0:t}) \). Discretize \([0, T]\) with time step \( \Delta t \). For each \( t = 0, \Delta t, 2\Delta t, \ldots, T \), we will have \( N \) samples \( \xi^i_t, i = 1, \ldots, N \), such that the filtered \( \tilde{\pi}_t(x) \) can be approximated by

\[
\hat{\pi}_t(x) = \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi^i_t}(x).
\]

(4.19)

Let \( \xi^0_i \sim \pi_0 \) be i.i.d. samples of the initial distribution. Assume that we already have \( \xi^i_t \). Resample

\[
\tilde{\xi}_i^i \sim \sum_{i=1}^{N} \frac{p(\Delta y_t | X_t = \xi^i_t)}{\sum_{i'=1}^{N} p(\Delta y_t | X_t = \xi^{i'}_t)} \delta_{\xi_t}(x)
\]

independently, then the distribution of \( \tilde{\xi}_i^i \) satisfies \( p(X_t | y_{0:t+\Delta t}) \). Thus we can sample

\[
\xi^i_{t+\Delta t} = \tilde{\xi}_i^i + f(\tilde{\xi}_i^i) \Delta t + \sigma \Delta W_i^t, \quad \Delta W_i^t \sim \mathcal{N}(0, \Delta t) \text{ i.i.d.,}
\]

and \( \xi^i_{t+\Delta t} \) is a set of samples for \( t + \Delta t \).

Next, we solve the smoothing problem \( \rho(x) = p(X_t = x | y_{0:T}) \), approximating it by weighting the samples

\[
\hat{\rho}(x) = \sum_{i=1}^{N} w^i_t \delta_{\xi^i_t}(x).
\]

(4.20)

We calculate the weight \( w^i_t \) backwards for \( t = T, T - \Delta t, T - 2\Delta t, \ldots, 0 \). Since \( \tilde{\pi}_T = \rho_T \), we have \( w^i_T = 1/N \).
Notice that

\[
\rho_t(x_t) = p(X_t = x_t|y_{0:T}) = \int p(x_t|x_{t+\Delta t}, y_{0:T})p(x_{t+\Delta t} = x_{t+\Delta t}|y_{0:T})dx_{t+\Delta t}
\]

\[
= \int p(x_{t+\Delta t}, y_{0:T}|x_t)p(x_t|y_{0:T})dx_t
\]

\[
= \int \frac{p(x_{t+\Delta t}, \Delta y_t|x_t)p(x_t|y_{0:T})}{\pi_t(x_t)}dx_t
\]

\[
= \hat{\pi}_t(x_t) \int \frac{p(x_{t+\Delta t}|x_t)p(\Delta y_t|x_t)}{\pi_t(x_t)}dx_t \rho_{t+\Delta t}(x_{t+\Delta t})dx_{t+\Delta t}.
\]

Replace \(\hat{\pi}_t\) and \(\rho_{t+\Delta t}\) by \(\tilde{\pi}_t\) and \(\tilde{\rho}_{t+\Delta t}\) respectively, we have

\[
\hat{\rho}_t(x_t)\tilde{\rho}_t(x_t) = \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi^i}(x_t) \sum_{j=1}^{N} \frac{p(\xi^j_{t+\Delta t}|x_t)p(\Delta y_t|x_t)w_{t+\Delta t}^j}{\frac{1}{N} \sum_{i'=1}^{N} p(\xi^j_{t+\Delta t}|\xi^{i'}_t)p(\Delta y_t|\xi^{i'}_t)}
\]

\[
= \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{p(\xi^j_{t+\Delta t}|\xi^i_t)p(\Delta y_t|\xi^i_t)w_{t+\Delta t}^j}{\sum_{i'=1}^{N} p(\xi^j_{t+\Delta t}|\xi^{i'}_t)p(\Delta y_t|\xi^{i'}_t)} \delta_{\xi^i}(x_t)
\]

Therefore, the weights are calculated as

\[
w_t^i = \sum_{j=1}^{N} \frac{p(\xi^j_{t+\Delta t}|\xi^i_t)p(\Delta y_t|\xi^i_t)w_{t+\Delta t}^j}{\sum_{i'=1}^{N} p(\xi^j_{t+\Delta t}|\xi^{i'}_t)p(\Delta y_t|\xi^{i'}_t)}.
\]

(4.21)

In addition, since

\[
\beta_t(x_t) \propto \frac{\rho_t(x_t)}{\tilde{\pi}_t(x_t)} = \int \frac{p(x_{t+\Delta t}|x_t)p(\Delta y_t|x_t)}{p(x_{t+\Delta t}|x_t)\tilde{\pi}_t(x_t)\rho_{t+\Delta t}(x_{t+\Delta t})dx_{t+\Delta t}}
\]

let

\[
\tilde{\beta}_t(x_t) = \sum_{j=1}^{N} \frac{p(\xi^j_{t+\Delta t}|x_t)p(\Delta y_t|x_t)w_{t+\Delta t}^j}{\sum_{i'=1}^{N} p(\xi^j_{t+\Delta t}|\xi^{i'}_t)p(\Delta y_t|\xi^{i'}_t)}
\]

(4.22)

then \(\beta_t\) can be approximated by \(\tilde{\beta}_t\) (times a constant factor, which will be eliminated in the \(\nabla \beta_t/\beta_t\) term in (4.9)). Since both \(p(\xi^j_{t+\Delta t}|x_t)\) and \(p(\Delta y_t|x_t)\) are Gaussian, the gradient \(\nabla \tilde{\beta}_t(x_t)\) can be calculated analytically. Notice that \(w_t^i = \tilde{\beta}_t(\xi^i_t)\).

Now we can apply the Monte Carlo approach to the Algorithm 4 for parameter estimation. In the E-step, the posterior distributions can be sampled as above. Then in the M-step, the parameter update (4.9) can be modified as \(\theta^{k+1} = \arg\min_{\theta} \hat{Q}(\theta, \theta^k)\) where

\[
\hat{Q}(\theta, \theta^k) = \sum_{t=0}^{T} \sum_{i=1}^{N} w_t^i \left[ \|f(\xi^i_t; \theta)\|_2^2 - 2 f^T(\xi^i_t; \theta) \left[ f(\xi^i_t; \theta^k) + \frac{\sigma^2}{w_t^i} \nabla \tilde{\beta}_t(\xi^i_t) \right] \right].
\]

(4.23)

If \(f(x; \theta)\) is linear in \(\theta\) (may be nonlinear in \(x\)): \(f(x; \theta) = A(x)\theta + b(x)\), then

\[
\hat{Q}(\theta, \theta^k) = \sum_{t=0}^{T} \sum_{i=1}^{N} w_t^i \left[ \theta^T A^T(\xi^i_t) A(\xi^i_t) \theta - 2 A(\xi^i_t) \theta + b(\xi^i_t) \right]^T \left[ A(\xi^i_t) \theta^k + \frac{\sigma^2}{w_t^i} \nabla \tilde{\beta}_t(\xi^i_t) \right] - \|b(\xi^i_t)\|_2^2,
\]

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and we have explicit solution

\[
\theta^{k+1} = \arg\min_\theta \hat{Q}(\theta, \theta^k)
\]

\[
= \theta^k + \sigma^2 \left[ \sum_{t=0}^T \sum_{i=1}^N w_i^t A^T (\xi^t_i) A (\xi^t_i) \right]^{-1} \left[ \sum_{t=0}^T \sum_{i=1}^N A^T (\xi^t_i) \nabla \beta_t (\xi^t_i) \right].
\] (4.24)

In general cases when (4.23) has no explicit solution, we may solve \(\theta^{k+1}\) using gradient methods.

### 4.6 Related work in parameter estimation

In general, parameter estimation is a more challenging problem than state estimation since it always relies on the latter. The first line of work \cite{9, 7} regards the parameter \(\theta\) as part of the hidden state. These papers consider \(\tilde{X}_t = (X_t, \theta)\) with dynamics

\[
\begin{bmatrix}
X_{t+1} \\
\theta_{t+1}
\end{bmatrix} = \begin{bmatrix}
f(X_t) \\
\theta_t
\end{bmatrix} + \begin{bmatrix}
W_t \\
0
\end{bmatrix},
\]

and apply state estimation methods for \(\{\tilde{X}_t\}\). The second line of work uses the EM algorithm that takes state estimation and parameter update alternately. \cite{43} proposes the EM algorithm for discrete-time Kalman filter. \cite{11} considers continuous diffusion process, and gives explicit formula for linear dynamics. For nonlinear dynamics, previous work only considers discrete-time settings. \cite{42, 47, 15, 33} all take the following approach. Recall the parameter update \(\theta^{k+1} = \arg\max_\theta Q(\theta, \theta^k)\) for \(Q\) defined in (4.10). The E-step uses the particle filter and smoother to sample from \(p(X_0:T | y_0:T; \theta^k)\). Instead of simplify the objective, they calculate \(Q(\theta, \theta^k)\) directly as a sum over the discrete time grid and samples. Then the M-step maximizes over \(\theta\) using the gradient \(\nabla \theta Q(\theta, \theta^k)\). As a comparison, we rewrite \(Q(\theta, \theta^k)\) in the continuous form, then it implies the explicit solution of the linear case as a straightforward result. In the nonlinear case, here we use the standard particle filter and smoother, and the continuous formulation may have more freedom to adaptively choose proper discretization and sampling scheme (like the extensions of particle filter) for better performance.

### 5 Simulation results

#### 5.1 Generator of hidden jump process

We first implement our algorithm for the CT-HMM with hidden jump process in Section 3. Notice that the piecewise ODEs (3.4) and (3.5) for state estimation, if solved directly, may lead to overflow or underflow of \(\alpha_t\) and \(\beta_t\) for large \(T\), and we modify the implementation as follows: at each \(\tau_s\), adaptively choose \(\kappa_s \in \mathbb{R}_+\), then update

\[
\alpha_{\tau_s} = \kappa_s \alpha_{\tau_{s-}} (Q - D) R(y_{\tau_s}), \quad \beta_{\tau_{s-}} = (Q - D) R(y_{\tau_s}) \beta_{\tau_s} / \kappa_s.
\]

The dynamics between \((\tau_s, \tau_{s+1})\) remains the same.

Here we test two simulation models:

1. A complete graph with \(n = 5\) states as \cite{31}. The generator \(Q\) is randomly drawn as \(-Q_{ii} \sim \mathcal{U}[1, 5], Q'_{ij} \sim \mathcal{U}[0, 1]\) and \(Q_{ij} = \frac{Q'_{ij}}{\sum_{j' \neq i} Q'_{ij'}} (-Q_{ii})\) for \(i, j \in \{1, \ldots, 5\}, i \neq j\), where \(\mathcal{U}\) is the uniform distribution. We initialize \(Q^0_{ii} = -3\) and \(Q^0_{ij} = 3/4\) for the EM algorithm.
Complete graph with $n = 5$ states

Sparse graph with $n = 20$ states

Figure 1: The simulation results for the CT-HMM with hidden jump process. Top: the distance $\|Q^k - Q\|_F$ under the Frobenius norm during the EM iterations for different noise levels $\sigma$ and total time $T$. Complex models may require larger $T$ to avoid overfitting, and the convergence is faster for smaller noise level $\sigma$. Bottom: the posteriors distribution $\rho_t(i)$ for each $i$ based on the true generator $Q$ and estimated $\hat{Q}$. The EM algorithm indeed converges. $\rho_t$ jumps at each $\tau_s$, but may still have significant changes between $(\tau_s, \tau_{s+1})$. Here $n = 5$, $\sigma = 0.2$, $T = 1000$ and we only show the results for $t \in [0, 20]$. 
Figure 2: The simulation results for bearings-only tracking [5.1]. Top: the estimated acceleration during the EM iterations. Here we repeat the simulations 5 times, and plot the mean and standard deviation. Bottom: the true trajectories and the estimation based on estimated \((a^k_x, a^k_y)\). The 3 figures show 3 of the 5 simulations. The light green lines are the trajectories for \(k = 175, 180, 185, \ldots, 200\), and the dark green line is their average. We also mark the positions at time points \(t = 0, 0.5, 1, \ldots, 3\) to compare the bearings.

2. A sparse graph with \(n = 20\) states. For each state \(i = 1, \ldots, 20\), randomly choose another 5 states \(V_i \subset \{1, \ldots, 20\} \setminus \{i\}\), \(|V_i| = 5\), and let \(Q_{ij} \sim \mathcal{U}(0, 1)\) for \(j \in V_i\), \(Q_{ii} = -\sum_{j \in V_i} Q_{ij}\) and \(Q_{ij} = 0\) for \(j \notin V_i \cup \{i\}\). The initialization \(Q^0_{ii} = -19/8\) and \(Q^0_{ij} = 1/8\).

For both of the models, the observations \(Y_t \in \{1, \ldots, n\}\) are given by \(r_i(i) = 1 - 2\sigma\) and \(r_i(i - 1) = r_i(i + 1) = \sigma\) (let \(r_1(0) = r_1(n)\) and \(r_n(n + 1) = r_n(1)\)). Assume that the state starts from \(X_0 = 1\), i.e., \(\pi_0 = [1, 0, \ldots, 0]\). We test different noise level \(\sigma\) and total time \(T\).

Figure 1 shows the simulation results. The top two figures show the convergence of \(Q^k\) for both models. Complex models may require larger \(T\) to avoid overfitting, and the convergence is faster for smaller noise level \(\sigma\). The bottom two figures compare the state estimation \(\rho_t(i)\) for each \(i\) based on the true generator \(Q\) and estimated \(\hat{Q}\). We can see that the EM algorithm indeed converges. In addition, \(\rho_t\) jumps at each \(\tau_s\), but may still have significant changes between \((\tau_s, \tau_{s+1})\).

5.2 Bearings-only tracking

The bearings-only tracking is a widely used simulation problem for filtering methods. The goal is to track an object moving in the \(x-y\) plane, and a fixed observer at the origin takes noisy measurements of the target bearings. The problem can be tracked back to [1]. [17, 37] analyze its linear discrete-time dynamics,
and [28, 27] consider the continuous-time hidden process with discrete-time observation. Here we assume that both the hidden states and observation occur in continuous-time as
\[
\begin{bmatrix}
x \\
\dot{x} \\
y \\
\dot{y}
\end{bmatrix}_t = \begin{bmatrix} a_x \\ \dot{a}_x \\ a_y \\ \dot{a}_y \end{bmatrix}_t \, dt + \sigma dW_t,
\]
\[
d\varphi_t = \arctan(y_t/x_t)dt + \eta dB_t. \tag{5.1}
\]
Here the position and volatility \((x, \dot{x}, y, \dot{y})\), is the hidden state, the acceleration \((a_x, a_y)\) is the unknown parameter, and the angle \(\varphi_t\) is the observation. (Unlike our general notations, in this problem we sometimes use lower case letters as random variables).

Assume that the initial position \((x_0, y_0) = (0, 1)\), the initial volatility \((\dot{x}_0, \dot{y}_0) = (1, 0)\), the noise \(\sigma = 0.1\), \(\eta = 0.02\), and the total time \(T = 3\). The true value of the acceleration is \((a_x, a_y) = (-0.5, -1)\), and we initialize \(a_0^x = a_0^y = 0\). The time discretization \(\Delta t = 0.01\) and the number of samples \(N = 128\). We simulate the true trajectory and observations 5 times, and run the EM algorithm for each of them. Figure 2 (top) shows the mean and standard deviation of estimated \((a^k_x, a^k_y)\) during the 5 runs. The estimations converge to near the true values, and we can expect that more repeated simulations and longer \(T\) may improve the accuracy.

We are also interested in recovering the true trajectory. Let \((\hat{a}_x, \hat{a}_y)\) be the estimation from the EM algorithm. Taking the Monte Carlo state estimation under \((a_x, a_y) = (\hat{a}_x, \hat{a}_y)\), we have samples \(\{\xi^i_t\}\) for the filter and weights \(\{w^i_t\}\) for the smoother. Then the true states \(x_t\) can be estimated by the simple or weighted average as
\[
\hat{x}^\text{filter}_t = \frac{1}{N} \sum_{i=1}^N \xi^i_t, \quad \hat{x}^\text{smooth}_t = \sum_{i=1}^N w^i_t \xi^i_t, \quad t = 0, \Delta t, \ldots, T. \tag{5.2}
\]
For the bearings-only tracking problem, since we only observe the angle but not the radius, a single estimation path may not exactly coincide with the true trajectory. Here we take the last few iterations \(k = 175, 180, 185, \ldots, 200\). For each \(k\), repeat the Monte Carlo smoother estimation (5.2) 5 times, and calculate the average of the 5 estimated trajectories. In Figure 2 (bottom), the light green lines are the average trajectories for each \(k\), and the dark green line is the average of the light green lines. We also mark the positions for time points \(t = 0, 0.5, 1, \ldots, 3\) to compare the bearings. We can see that after the averaging, the dark green line is close to the true trajectory (blue), and shares similar bearing at the same time points.

### 5.3 Cubic sensor problems for matrix estimation

In the cubic sensor problems [41, 22], the observation has the same dimension as the hidden state, and is given by \(h([x_1, \ldots, x_d]) = [x_1^3, \ldots, x_d^3]\). Here we assume that \(f\) is linear, then the dynamics is given by
\[
\begin{align*}
\text{d}X_t &= FX_t \, dt + \sigma dW_t, \\
\text{d}Y_t &= X_t^3 \, dt + \eta dB_t. \tag{5.3}
\end{align*}
\]

First consider the case that the whole matrix \(F\) is the unknown parameter to be estimated, i.e., \(\theta = F\). Then the parameter update (4.23) in our Monte Carlo method becomes
\[
F^{k+1} = \arg\min_F \hat{Q}(F, F^k) = F^k + \sigma^2 \left[ \sum_{t,i} \nabla \hat{\beta}(\xi^i_t) \xi^i_t \right] \left[ \sum_{t,i} w^i_t \xi^i_t \xi^i_t^\top \right]^{-1}. \tag{5.4}
\]
Figure 3: The cubic sensor problem for the matrix parameter estimation \(5.3\). The upper left figure shows the distance \(\|F^k - F\|_F\) under the Frobenius norm during the iterations. The EM algorithm converges fast for all the noise levels, while the larger noise level has faster convergence rate but lower accuracy. Then we calculate the solutions of the filter and smoother based on \(\hat{F}\). The other three figures compare the solutions and the true trajectories under different noise levels. The solution of the smoothing is indeed smoother and closer to the true trajectory.
Now let the dimension \( d = 2 \), the true matrix \( F = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \), the initial condition \( X_0 = [1, 0] \) at \( t = 0 \), and \( T = 10 \). We test different noise levels \( \sigma = \eta = 0.2, 0.5, 1.0 \). For each level, take the discretization \( \Delta t = 0.02 \), the number of samples \( N = 128 \), and the initialization \( F^0 = 0 \). Figure 3 shows that of \( F^k \) converges fast for all the noise levels, while larger noise level has faster convergence rate but lower accuracy.

In the end we get estimation

\[
\hat{F} = \begin{bmatrix} 0.00 & 0.88 \\ -0.98 & -0.01 \end{bmatrix}, \quad \sigma = \eta = 0.2, \\
\hat{F} = \begin{bmatrix} -0.10 & 0.83 \\ 1.02 & -0.01 \end{bmatrix}, \quad \sigma = \eta = 0.5, \\
\hat{F} = \begin{bmatrix} -0.19 & 0.87 \\ -1.12 & 0.10 \end{bmatrix}, \quad \sigma = \eta = 1.
\]

We further calculate the solutions of the filter and smoother (5.2) based on \( \hat{F} \). Instead of taking average of trajectories as the previous problem, here we only generate a single estimated trajectory for each noise level. Comparing with the true trajectory of \( X_t \). We can see that the solution of the smoothing is indeed smoother and closer to the true trajectory.

### 5.4 High dimensional linear dynamics

Here we apply our Monte Carlo method to a problem with high dimensional state space. In the cubic sensor dynamics (5.3), let \( F \in \mathbb{R}^{d \times d} \) be the tridiagonal matrix

\[
F = \lambda \begin{bmatrix} -1 & 1 \\ 1 & -2 & 1 \\ & \ddots & \ddots & \ddots \\ & & 1 & -2 & 1 \\ & & & 1 & -1 \end{bmatrix}, \quad (5.5)
\]

where the scalar \( \lambda \) is the unknown parameter to be estimated. We consider different dimensions \( d = 5, 15, 25 \), and take \( \lambda = 5, 25, 50 \) respectively. For each dimension, consider different noise levels \( \sigma = 0.2, 0.5, 1.0 \) and fix \( \eta = 0.01 \). Let the initial condition

\[
X_0 = \begin{bmatrix} -1, -1 + \frac{2}{d - 1}, -1 + \frac{4}{d - 1}, \ldots, 1 - \frac{2}{d - 1}, 1 \end{bmatrix},
\]

and \( T = 1 \). In Figure 4 we generate hidden processes \( \{X_t\} \) for different \( d, \lambda \) and \( \sigma \).

For each experiment, take \( \Delta t = 0.005 \), the number of samples \( N = 128 \), and the initialization \( \lambda^0 = 0 \). Figure 4 shows the simulation results. The EM algorithm with Monte Carlo method is efficient even for high dimensional problem. The higher the dimension, the more iterations are required. We also see that at larger noise level the convergence is faster at the beginning but is more volatile afterwards. The solutions of the filter and smoother (5.2) based on the estimated \( \hat{\lambda} \) are also close to the true path of \( \{X_t\} \).

### 5.5 Lorenz 96 model

The Lorenz 96 model is a dynamical system proposed by Edward Lorenz in 1996 [32], and is commonly used in data assimilation. Denote the components of the hidden state as \( X_t = [X_{1,t}, X_{2,t}, \ldots, X_{d,t}] \). Consider the following dynamics

\[
\frac{dX_{i,t}}{dt} = (X_{i+1,t} - X_{i-1,t})X_{i-1,t} - X_{i,t} + F + \sigma W_t, \quad i = 1, 2, \ldots, d, \quad (5.6)
\]
Figure 4: The hidden process \( \{X_t\} \) for the scalar parameter estimation problem (5.5). Each line shows the dynamics of one component of \( X_t \). Here we take different dimension \( d \), parameter \( \lambda \) and noise \( \sigma \).
Figure 5: The cubic sensor problem (5.3) for the scalar parameter estimation (5.5). Top: $d = 5$, $\lambda = 5$; middle: $d = 15$, $\lambda = 25$; bottom: $d = 25$, $\lambda = 50$. The first row shows the update of $\lambda_k$ during the iterations. The solutions of the filter and smoother calculated using $\hat{\lambda}$, and the relative error $\|\hat{x}_t - x_t\|_2 / \|x_t\|_2$ is shown in the second column.
Figure 6: The Lorenz 96 model \((5.6)\) with cubic sensor observations \((5.3)\). The upper left figure is the dynamics of the components of \(X_t\) under the force \(F = 8\) and initialization \(X_{i,0} = F\), which shows the chaotic behavior after starting from the equilibrium. The upper right figure shows that the distance \(|F^k - F|\) converges fast during the iterations. Then we calculate the solutions of the filter and smoother based on \(\hat{F}\). The bottom left figure shows that the smoother solution is close to the true trajectory, and indeed captures the chaotic behavior. The bottom right figure gives the relative error \(\|\hat{x}_t - x_t\|_2/\|x_t\|_2\).
where $X_{-1,t} = X_{d-1,t}$, $X_{0,t} = X_{d,t}$ and $X_{d+1,t} = X_{1,t}$. The scalar $F$ is a forcing constant. The observations still follow the cubic sensor (5.3).

Assume that the force $F$ is the unknown parameter to be estimated. Following [33], set the true value $F = 8$ that is commonly known to cause chaotic behavior. Let the dimension $d = 10$ and initialize the state from the equilibrium $X_{i,0} = F$, $i = 1, \ldots, d$. Let the noise $\sigma = 1$, $\eta = 5$ and the total time $T = 1$. Take the discretization $\Delta t = 0.05$ and the number of samples $N = 128$.

Figure [3] shows the simulation results. We can see that the hidden states show chaotic behavior after starting from the equilibrium. The parameter estimation $\hat{F}$ nevertheless converges fast to the true value. We also calculated the solution of the filter and smoother (5.2) based on the estimated $\hat{F}$. The relative error is small, and the state estimation indeed captures the chaotic behavior.

6 Conclusion

In this paper, we extend the classical Baum-Welch framework in HMM to continuous-time settings. For CT-HMM with hidden jump process or hidden diffusion process, we solve both the state estimation and parameter estimation problem. We also propose a Monte Carlo approach based on the standard particle filter and smoother, which may be further improved by using more advanced filtering methods. Instead of discretizing the time from the beginning, now one can first derive the continuous equations following our framework, then choose the proper discretization and sampling scheme for better performance. Our numerical results demonstrate that the proposed algorithms are quite effective.

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A CT-HMM with discrete-time observations

While this paper mainly focuses on the continuous-time states and observations, in some applications like disease progression, we may only have observations at some discrete time points and they are assumed to be independent (see Section 3.1.1). The Baum-Welch framework can also be applied to this setting as we now show.

A.1 Hidden jump process

Here we modify the CT-HMM \((Q, r, \pi_0)\) with hidden jump process in Section 3. The hidden states \(\{X_t\}\) remains to be a jump process with generator \(Q\) and initial probability \(\pi_0\). Instead of continuous-time observations, here we assume that we only can observe at discrete time points \(0 \leq \tau_1 < \cdots < \tau_S \leq T\), and \(Y_{\tau_s} \in \{1, \ldots, m\}\) are independently generated from \(r_i(y) = \Pr\{Y_{\tau_s} = y | X_{\tau_s} = i\}\). (A.1)

The following are the results for state estimation and parameter estimation given observations \(Y_{\tau_s} = y_{\tau_s}, s = 1, \ldots, S\).

**State estimation** Let \(\alpha_t = [\alpha_t(1) \cdots \alpha_t(n)] \in \mathbb{R}^{1 \times n}\) and \(\beta_t = [\beta_t(1) \cdots \beta_t(n)]^T \in \mathbb{R}^{n \times 1}\) be the solutions of the forward and backward piecewise ODEs respectively

\[
\begin{align*}
\alpha_0 &= \pi_0, \\
\dot{\alpha}_t &= \alpha_t Q, \quad t \in [\tau_s, \tau_{s+1}), \\
\alpha_{\tau_s} &= \alpha_{\tau_s-} R(y_{\tau_s}), \\
\beta_T &= 1, \\
\dot{\beta}_t &= -Q \beta_t, \quad t \in [\tau_s, \tau_{s+1}), \\
\beta_{\tau_s} &= R(y_{\tau_s}) \beta_{\tau_s},
\end{align*}
\]

(A.2)

where the left limit \(\alpha_{\tau_s-} = \lim_{t \uparrow \tau_s} \alpha_t\), and \(R(y) = \text{diag}(r_1(y), \ldots, r_n(y))\). Then the posterior distribution of the hidden states satisfies

\[
\rho_t(i) = \Pr\{X_t = i | Y_{\tau_s} = y_{\tau_s}, s = 1, \ldots, S\} = \frac{\alpha_t(i) \beta_t(i)}{\alpha_0 \cdot \beta_0},
\]

(A.4)

**Parameter estimation** Assume that the generator \(Q\) is the unknown parameter to be estimated. The EM algorithm can be applied: in the E-step, using the current estimate \(Q = Q^k\), we solve the state estimation for \(\alpha_t, \beta_t\) and \(\rho_t\); in the M-step, update the generator using

\[
Q_{ij}^{k+1} = \frac{\int_0^T \alpha_t(i) Q_t^k \beta_t(j) dt}{(\alpha_0 \cdot \beta_0) \int_0^T \rho_t(i) dt},
\]

for \(j \neq i\), and \(Q_{ii}^{k+1} = -\sum_{j \neq i} Q_{ij}^{k+1}\).
A.2 Hidden diffusion process

For the CT-HMM with hidden diffusion process in Section 3, take the same hidden process
\[ dX_t = f(X_t)dt + \sigma dW_t, \]
with initial distribution \( \pi_0 \), and assume discrete-time observations \( Y_{\tau_s}, s = 1, \ldots, S \) from
\[ r(y|x) = p(Y_{\tau_s} = y|X_{\tau_s} = x). \] (A.6)

State estimation

For the filtering problem, the unnormalized distribution
\[ \pi_t(x) = p(X_t = x|Y_{\tau_s} = y_{\tau_s}, \tau_s < t)Z_t \] (for some constant \( Z_t \)) satisfies the forward piecewise PDE
\[
\begin{aligned}
\pi_0(x) &= p(X_0 = x), \\
d\pi_t(x) &= \mathcal{L}^* \pi_t(x) dt, \quad t \in [\tau_s, \tau_{s+1}), \\
\pi_{\tau_s}(x) &= \lim_{t \uparrow \tau_s} \pi_t(x),
\end{aligned}
\]
(A.7)

where \( \pi_{\tau_s}(x) = \lim_{t \uparrow \tau_s} \pi_t(x) \). For the smoothing problem, let \( \beta_t(x) \) be the solution of the backward piecewise PDE
\[
\begin{aligned}
\beta_T(x) &= 1, \\
d\beta_t(x) &= -\mathcal{L} \pi_t(x) dt, \quad t \in [\tau_s, \tau_{s+1}), \\
\beta_{\tau_s}(x) &= \beta_{\tau_s}(x) r(y_{\tau_s}|x),
\end{aligned}
\]
(A.8)

then the posterior distribution of the hidden states is given by
\[ \rho_t(x) = p(X_t = x|Y_{\tau_s} = y_{\tau_s}, s = 1, \ldots, S) = \frac{1}{Z_T} \pi_t(x) \beta_t(x). \] (A.9)

Parameter estimation

Assume \( f(x) = f(x; \theta) \) where \( \theta \) is the unknown parameter to be estimated. The EM algorithm is similar to the continuous-time observations. In the E-step, using the current estimate \( \theta = \theta^k \), we solve the state estimation for \( \pi_t, \beta_t \) and \( \rho_t \); in the M-step, update the parameter using \( \theta^{k+1} = \arg\min_{\theta} \tilde{Q}(\theta, \theta^k) \) where
\[
\tilde{Q}(\theta, \theta^k) = \int_0^T \int_{\mathbb{R}^d} \rho_t(x) \left[ \|f(x; \theta)\|^2_2 - 2 f^T(x; \theta) \left[ f(x; \theta^k) + \frac{\sigma^2 \nabla \beta_t(x)}{\beta_t(x)} \right] \right] dxdt.
\]
(A.10)