Expectation Correction for Smoothed Inference in Switching Linear Dynamical Systems

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Abstract

We introduce a method for approximate smoothed inference in a class of switching linear dynamical systems, based on a novel form of Gaussian Sum smoother. This class includes the switching Kalman 'Filter' and the more general case of switch transitions dependent on the continuous latent state. The method improves on the standard Kim smoothing approach by dispensing with one of the key approximations, thus making fuller use of the available future information. Whilst the central assumption required is projection to a mixture of Gaussians, we show that an additional conditional independence assumption results in a simpler but accurate alternative. Our method consists of a single Forward and Backward Pass and is reminiscent of the standard smoothing 'correction' recursions in the simpler linear dynamical system. The method is numerically stable and compares favourably against alternative approximations, both in cases where a single mixture component provides a good posterior approximation, and where a multimodal approximation is required.

Keywords: Gaussian sum smoother, switching Kalman filter, switching linear dynamical system, expectation propagation, expectation correction

1. Switching Linear Dynamical System

The Linear Dynamical System (LDS) (Bar-Shalom and Li, 1998; West and Harrison, 1999) is a key temporal model in which a latent linear process generates the observed time-series. For more complex time-series which are not well described globally by a single LDS, we may break the time-series into segments, each modeled by a potentially different LDS. This is the basis for the Switching LDS (SLDS) where, for each time-step t, a switch variable $s_t \in 1, ..., S$ describes which of the LDSs is to be used. The observation (or 'visible' variable) $v_t \in \mathcal{R}^V$ is linearly related to the hidden state $h_t \in \mathcal{R}^H$ by

$$v_t = B(s_t)h_t + \eta^{\nu}(s_t), \qquad \eta^{\nu}(s_t) \sim \mathcal{N}(\bar{v}(s_t), \Sigma^{\nu}(s_t))$$
(1)

where $\mathcal{N}(\mu, \Sigma)$ denotes a Gaussian distribution with mean μ and covariance Σ . The transition dynamics of the continuous hidden state h_t is linear

$$h_t = A(s_t)h_{t-1} + \eta^h(s_t), \qquad \quad \eta^h(s_t) \sim \mathcal{N}\left(\bar{h}(s_t), \Sigma^h(s_t)\right). \tag{2}$$

^{1.} These systems also go under the names Jump Markov model/process, switching Kalman Filter, Switching Linear Gaussian State-Space model, Conditional Linear Gaussian Model.

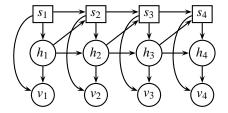


Figure 1: The independence structure of the aSLDS. Square nodes denote discrete variables, round nodes continuous variables. In the SLDS links from *h* to *s* are not normally considered.

The dynamics of the switch variables is Markovian, with transition $p(s_t|s_{t-1})$. The SLDS is used in many disciplines, from econometrics to machine learning (Bar-Shalom and Li, 1998; Ghahramani and Hinton, 1998; Lerner et al., 2000; Kitagawa, 1994; Kim and Nelson, 1999; Pavlovic et al., 2001). See Lerner (2002) and Zoeter (2005) for recent reviews of work.

AUGMENTED SWITCHING LINEAR DYNAMICAL SYSTEM

In this article, we will consider the more general model in which the switch s_t is dependent on both the previous s_{t-1} and h_{t-1} . We call this an *augmented Switching Linear Dynamical System*² (aSLDS), in keeping with the terminology in Lerner (2002). An equivalent probabilistic model is, as depicted in Figure (1),

$$p(v_{1:T}, h_{1:T}, s_{1:T}) = p(v_1|h_1, s_1)p(h_1|s_1)p(s_1)\prod_{t=2}^{T} p(v_t|h_t, s_t)p(h_t|h_{t-1}, s_t)p(s_t|h_{t-1}, s_{t-1}).$$

The notation $x_{1:T}$ is shorthand for x_1, \ldots, x_T . The distributions are parameterized as

$$p(v_t|h_t, s_t) = \mathcal{N}(\bar{v}(s_t) + B(s_t)h_t, \Sigma^{v}(s_t)), \quad p(h_t|h_{t-1}, s_t) = \mathcal{N}(\bar{h}(s_t) + A(s_t)h_{t-1}, \Sigma^{h}(s_t))$$

where $p(h_1|s_1) = \mathcal{N}(\mu(s_1), \Sigma(s_1))$. The aSLDS has been used, for example, in state-duration modeling in acoustics (Cemgil et al., 2006) and econometrics (Chib and Dueker, 2004).

Inference

The aim of this article is to address how to perform inference in both the SLDS and aSLDS. In particular we desire the so-called *filtered* estimate $p(h_t, s_t|v_{1:t})$ and the *smoothed* estimate $p(h_t, s_t|v_{1:T})$, for any t, $1 \le t \le T$. Both exact filtered and smoothed inference in the SLDS is intractable, scaling exponentially with time (Lerner, 2002). To see this informally, consider the filtered posterior, which may be recursively computed using

$$p(s_t, h_t|v_{1:t}) = \sum_{s_{t-1}} \int_{h_{t-1}} p(s_t, h_t|s_{t-1}, h_{t-1}, v_t) p(s_{t-1}, h_{t-1}|v_{1:t-1}).$$
(3)

At timestep 1, $p(s_1, h_1|v_1) = p(h_1|s_1, v_1)p(s_1|v_1)$ is an indexed set of Gaussians. At time-step 2, due to the summation over the states s_1 , $p(s_2, h_2|v_{1:2})$ will be an indexed set of S Gaussians; similarly at

^{2.} These models are closely related to *Threshold Regression Models* (Tong, 1990).

time-step 3, it will be S^2 and, in general, gives rise to S^{t-1} Gaussians. More formally, in Lauritzen and Jensen (2001), a general exact method is presented for performing stable inference in such hybrid discrete models with conditional Gaussian potentials. The method requires finding a strong junction tree which, in the SLDS case, means that the discrete variables are placed in a single cluster, resulting in exponential complexity.

The key issue in the (a)SLDS, therefore, is how to perform *approximate* inference in a numerically stable manner. Our own interest in the SLDS stems primarily from acoustic modeling, in which the time-series consists of many thousands of time-steps (Mesot and Barber, 2006; Cemgil et al., 2006). For this, we require a stable and computationally feasible approximate inference, which is also able to deal with state-spaces of high hidden dimension, *H*.

2. Expectation Correction

Our approach to approximate $p(h_t, s_t|v_{1:T}) \approx \tilde{p}(h_t, s_t|v_{1:T})$ mirrors the Rauch-Tung-Striebel (RTS) 'correction' smoother for the LDS (Rauch et al., 1965; Bar-Shalom and Li, 1998). Readers unfamiliar with this approach will find a short explanation in Appendix (A), which defines the important functions LDSFORWARD and LDSBACKWARD, which we shall make use of for inference in the aSLDS. Our correction approach consists of a single Forward Pass to recursively find the filtered posterior $\tilde{p}(h_t, s_t|v_{1:t})$, followed by a single Backward Pass to correct this into a smoothed posterior $\tilde{p}(h_t, s_t|v_{1:T})$. The Forward Pass we use is equivalent to Assumed Density Filtering (Alspach and Sorenson, 1972; Boyen and Koller, 1998; Minka, 2001). The main contribution of this paper is a novel form of Backward Pass, based on collapsing the smoothed posterior to a mixture of Gaussians.

Unless stated otherwise, all quantities should be considered as approximations to their exact counterparts, and we will therefore usually omit the tildes throughout the article.

2.1 Forward Pass (Filtering)

Readers familiar with Assumed Density Filtering (ADF) may wish to continue directly to Section (2.2). The basic idea is to represent the (intractable) posterior using a simpler distribution. This is then propagated forwards through time, conditioned on the new observation, and subsequently collapsed back to the tractable distribution representation—see Figure (2). Our aim is to form a recursion for $p(s_t, h_t|v_{1:t})$, based on a Gaussian mixture approximation of $p(h_t|s_t, v_{1:t})$. Without loss of generality, we may decompose the filtered posterior as

$$p(h_t, s_t|v_{1:t}) = p(h_t|s_t, v_{1:t})p(s_t|v_{1:t}).$$

We will first form a recursion for $p(h_t|s_t, v_{1:t})$, and discuss the switch recursion $p(s_t|v_{1:t})$ later. The full procedure for computing the filtered posterior is presented in Algorithm (1).

The exact representation of $p(h_t|s_t, v_{1:t})$ is a mixture with $O(S^t)$ components. We therefore approximate this with a smaller I_t -component mixture

$$p(h_t|s_t, v_{1:t}) \approx \tilde{p}(h_t|s_t, v_{1:t}) \equiv \sum_{i_t=1}^{I_t} \tilde{p}(h_t|i_t, s_t, v_{1:t}) \tilde{p}(i_t|s_t, v_{1:t})$$

where $\tilde{p}(h_t|i_t, s_t, v_{1:t})$ is a Gaussian parameterized with mean³ $f(i_t, s_t)$ and covariance $F(i_t, s_t)$. The Gaussian mixture weights are given by $\tilde{p}(i_t|s_t, v_{1:t})$. In the above, \tilde{p} represent approximations to the

^{3.} Strictly speaking, we should use the notation $f_t(i_t, s_t)$ since, for each time t, we have a set of means indexed by i_t, s_t . This mild abuse of notation is used elsewhere in the paper.

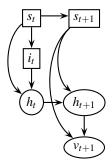


Figure 2: Structure of the mixture representation of the Forward Pass. Essentially, the Forward Pass defines a 'prior' distribution at time t which contains all the information from the variables $v_{1:t}$. This prior is propagated forwards through time using the exact dynamics, conditioned on the observation, and then collapsed back to form a new prior approximation at time t+1.

corresponding exact p distributions. To find a recursion for these parameters, consider

$$\tilde{p}(h_{t+1}|s_{t+1}, v_{1:t+1}) = \sum_{s_t, i_t} \tilde{p}(h_{t+1}, s_t, i_t|s_{t+1}, v_{1:t+1})
= \sum_{s_t, i_t} \tilde{p}(h_{t+1}|i_t, s_t, s_{t+1}, v_{1:t+1}) \tilde{p}(s_t, i_t|s_{t+1}, v_{1:t+1})$$
(4)

where each of the factors can be recursively computed on the basis of the previous filtered results (see below). However, this recursion suffers from an exponential increase in mixture components. To deal with this, we will later collapse $\tilde{p}(h_{t+1}|s_{t+1},v_{1:t+1})$ back to a smaller mixture. For the remainder, we drop the \tilde{p} notation, and concentrate on computing the r.h.s of Equation (4).

EVALUATING $p(h_{t+1}|s_t, i_t, s_{t+1}, v_{1:t+1})$

We find $p(h_{t+1}|s_t, i_t, s_{t+1}, v_{1:t+1})$ from the joint distribution $p(h_{t+1}, v_{t+1}|s_t, i_t, s_{t+1}, v_{1:t})$, which is a Gaussian with covariance and mean elements⁴

$$\Sigma_{hh} = A(s_{t+1})F(i_t, s_t)A^{\mathsf{T}}(s_{t+1}) + \Sigma^h(s_{t+1}), \quad \Sigma_{vv} = B(s_{t+1})\Sigma_{hh}B^{\mathsf{T}}(s_{t+1}) + \Sigma^v(s_{t+1})$$

$$\Sigma_{vh} = B(s_{t+1})F(i_t, s_t), \quad \mu_v = B(s_{t+1})A(s_{t+1})f(i_t, s_t), \quad \mu_h = A(s_{t+1})f(i_t, s_t).$$
 (5)

These results are obtained from integrating the forward dynamics, Equations (1,2) over h_t , using the results in Appendix (B). To find $p(h_{t+1}|s_t,i_t,s_{t+1},v_{1:t+1})$ we may then condition $p(h_{t+1},v_{t+1}|s_t,i_t,s_{t+1},v_{1:t+1})$ on v_{t+1} using the results in Appendix (C)—see also Algorithm (4).

EVALUATING $p(s_t, i_t | s_{t+1}, v_{1:t+1})$

Up to a trivial normalization constant the mixture weight in Equation (4) can be found from the decomposition

$$p(s_t, i_t | s_{t+1}, v_{1:t+1}) \propto p(v_{t+1} | i_t, s_t, s_{t+1}, v_{1:t}) p(s_{t+1} | i_t, s_t, v_{1:t}) p(i_t | s_t, v_{1:t}) p(s_t | v_{1:t}).$$

$$(6)$$

^{4.} We derive this for $\bar{h}_{t+1}, \bar{v}_{t+1} \equiv 0$, to ease notation.

Algorithm 1 aSLDS Forward Pass. Approximate the filtered posterior $p(s_t|v_{1:t}) \equiv \rho_t$, $p(h_t|s_t,v_{1:t}) \equiv \sum_{i_t} w_t(i_t,s_t) \mathcal{N}(f_t(i_t,s_t),F_t(i_t,s_t))$. Also we return the approximate log-likelihood log $p(v_{1:T})$. We require $I_1 = 1,I_2 \leq S,I_t \leq S \times I_{t-1}$. $\theta_t(s) = A(s),B(s),\Sigma^h(s),\Sigma^v(s),\bar{h}(s),\bar{v}(s)$ for t>1. $\theta_1(s) = A(s),B(s),\Sigma(s),\Sigma^v(s),\mu(s),\bar{v}(s)$

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for s_1 \leftarrow 1 to S do
     \{f_1(1,s_1), F_1(1,s_1), \hat{p}\} = LDSFORWARD(0,0,v_1;\theta(s_1))
     \rho_1 \leftarrow p(s_1)\hat{p}
end for
for t \leftarrow 2 to T do
     for s_t \leftarrow 1 to S do
           for i \leftarrow 1 to I_{t-1}, and s \leftarrow 1 to S do
                \{\mu_{x|y}(i,s), \Sigma_{x|y}(i,s), \hat{p}\} = \text{LDSFORWARD}(f_{t-1}(i,s), F_{t-1}(i,s), \nu_t; \theta_t(s_t))
                p^*(s_t|i,s) \equiv \langle p(s_t|h_{t-1},s_{t-1}=s) \rangle_{p(h_{t-1}|i_{t-1}=i,s_{t-1}=s,\nu_{1:t-1})}
                p'(s_t, i, s) \leftarrow w_{t-1}(i, s) p^*(s_t|i, s) \rho_{t-1}(s) \hat{p}
           Collapse the I_{t-1} \times S mixture of Gaussians defined by \mu_{x|y}, \Sigma_{x|y}, and weights
           p(i,s|s_t) \propto p'(s_t,i,s) to a Gaussian with I_t components, p(h_t|s_t,v_{1:t}) \approx
           \sum_{i_t=1}^{l_t} p(i_t|s_t,v_{1:t})p(h_t|s_t,i_t,v_{1:t}). This defines the new means f_t(i_t,s_t), covariances
           F_t(i_t, s_t) and mixture weights w_t(i_t, s_t) \equiv p(i_t | s_t, v_{1:t}).
           Compute \rho_t(s_t) \propto \sum_{i,s} p'(s_t, i, s)
     end for
     normalize \rho_t \equiv p(s_t|v_{1:t})
     L \leftarrow L + \log \sum_{s,i,s} p'(s_t,i,s)
end for
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The first factor in Equation (6), $p(v_{t+1}|i_t, s_t, s_{t+1}, v_{1:t})$, is a Gaussian with mean μ_v and covariance Σ_{vv} , as given in Equation (5). The last two factors $p(i_t|s_t, v_{1:t})$ and $p(s_t|v_{1:t})$ are given from the previous iteration. Finally, $p(s_{t+1}|i_t, s_t, v_{1:t})$ is found from

$$p(s_{t+1}|i_t, s_t, v_{1:t}) = \langle p(s_{t+1}|h_t, s_t) \rangle_{p(h_t|i_t, s_t, v_{1:t})}$$
(7)

where $\langle \cdot \rangle_p$ denotes expectation with respect to p. In the standard SLDS, Equation (7) is replaced by the Markov transition $p(s_{t+1}|s_t)$. In the aSLDS, however, Equation (7) will generally need to be computed numerically. A simple approximation is to evaluate Equation (7) at the mean value of the distribution $p(h_t|i_t,s_t,v_{1:t})$. To take covariance information into account an alternative would be to draw samples from the Gaussian $p(h_t|i_t,s_t,v_{1:t})$ and thus approximate the average of $p(s_{t+1}|h_t,s_t)$ by sampling.⁵

CLOSING THE RECURSION

We are now in a position to calculate Equation (4). For each setting of the variable s_{t+1} , we have a mixture of $I_t \times S$ Gaussians. In order to avoid an exponential explosion in the number of mixture

^{5.} Whilst we suggest sampling as part of the aSLDS update procedure, this does not render the Forward Pass as a form of sequential sampling procedure, such as Particle Filtering. The sampling here is a form of exact sampling, for which no convergence issues arise, being used only to numerically evaluate Equation (7).

components, we numerically collapse this back to I_{t+1} Gaussians to form

$$p(h_{t+1}|s_{t+1},v_{1:t+1}) \approx \sum_{i_{t+1}=1}^{I_{t+1}} p(h_{t+1}|i_{t+1},s_{t+1},v_{1:t+1}) p(i_{t+1}|s_{t+1},v_{1:t+1}).$$

Hence the Gaussian components and corresponding mixture weights $p(i_{t+1}|s_{t+1},v_{1:t+1})$ are defined implicitly through a numerical (Gaussian-Mixture to smaller Gaussian-Mixture) collapse procedure, for which any method of choice may be supplied. A straightforward approach that we use in our code is based on repeatedly merging low-weight components, as explained in Appendix (D).

A RECURSION FOR THE SWITCH VARIABLES

A recursion for the switch variables can be found by considering

$$p(s_{t+1}|v_{1:t+1}) \propto \sum_{i_t,s_t} p(i_t,s_t,s_{t+1},v_{t+1},v_{1:t}).$$

The r.h.s. of the above equation is proportional to

$$\sum_{s_t,i_t} p(v_{t+1}|i_t,s_t,s_{t+1},v_{1:t}) p(s_{t+1}|i_t,s_t,v_{1:t}) p(i_t|s_t,v_{1:t}) p(s_t|v_{1:t})$$

where all terms have been computed during the recursion for $p(h_{t+1}|s_{t+1},v_{1:t+1})$.

THE LIKELIHOOD $p(v_{1:T})$

The likelihood $p(v_{1:T})$ may be found by recursing $p(v_{1:t+1}) = p(v_{t+1}|v_{1:t})p(v_{1:t})$, where

$$p(v_{t+1}|v_{1:t}) = \sum_{i_t, s_t, s_{t+1}} p(v_{t+1}|i_t, s_t, s_{t+1}, v_{1:t}) p(s_{t+1}|i_t, s_t, v_{1:t}) p(i_t|s_t, v_{1:t}) p(s_t|v_{1:t}).$$

In the above expression, all terms have been computed in forming the recursion for the filtered posterior $p(h_{t+1}, s_{t+1}|v_{1:t+1})$.

2.2 Backward Pass (Smoothing)

The main contribution of this paper is to find a suitable way to 'correct' the filtered posterior $p(s_t, h_t|v_{1:t})$ obtained from the Forward Pass into a smoothed posterior $p(s_t, h_t|v_{1:T})$. We initially derive this for the case of a single Gaussian representation—the extension to the mixture case is straightforward and given in Section (2.3). Our derivation holds for both the SLDS and aSLDS. We approximate the smoothed posterior $p(h_t|s_t, v_{1:T})$ by a Gaussian with mean $g(s_t)$ and covariance $G(s_t)$, and our aim is to find a recursion for these parameters. A useful starting point is the exact relation:

$$p(h_t, s_t|v_{1:T}) = \sum_{s_{t+1}} p(s_{t+1}|v_{1:T}) p(h_t|s_t, s_{t+1}, v_{1:T}) p(s_t|s_{t+1}, v_{1:T}).$$

The term $p(h_t|s_t, s_{t+1}, v_{1:T})$ may be computed as

$$p(h_{t}|s_{t}, s_{t+1}, v_{1:T}) = \int_{h_{t+1}} p(h_{t}, h_{t+1}|s_{t}, s_{t+1}, v_{1:T})$$

$$= \int_{h_{t+1}} p(h_{t}|h_{t+1}, s_{t}, s_{t+1}, v_{1:T}) p(h_{t+1}|s_{t}, s_{t+1}, v_{1:T})$$

$$= \int_{h_{t+1}} p(h_{t}|h_{t+1}, s_{t}, s_{t+1}, v_{1:t}) p(h_{t+1}|s_{t}, s_{t+1}, v_{1:T})$$
(8)

which is in the form of a recursion. This recursion therefore requires $p(h_{t+1}|s_t, s_{t+1}, v_{1:T})$, which we can write as

$$p(h_{t+1}|s_t, s_{t+1}, v_{1:T}) \propto p(h_{t+1}|s_{t+1}, v_{1:T}) p(s_t|s_{t+1}, h_{t+1}, v_{1:t}). \tag{9}$$

The above recursions represent the exact computation of the smoothed posterior. In our approximate treatment, we replace all quantities p with their corresponding approximations \tilde{p} . A difficulty is that the functional form of $\tilde{p}(s_t|s_{t+1},h_{t+1},v_{1:t})$ in the approximation of Equation (9) is not squared exponential in h_{t+1} , so that $\tilde{p}(h_{t+1}|s_t,s_{t+1},v_{1:T})$ will not be a mixture of Gaussians. One possibility would be to approximate the non-Gaussian $p(h_{t+1}|s_t,s_{t+1},v_{1:T})$ (dropping the \tilde{p} notation) by a Gaussian (mixture) by minimizing the Kullback-Leilbler divergence between the two, or performing moment matching in the case of a single Gaussian. A simpler alternative is to make the assumption $p(h_{t+1}|s_t,s_{t+1},v_{1:T}) \approx p(h_{t+1}|s_{t+1},v_{1:T})$, see Figure (3). This is a considerable simplification since $p(h_{t+1}|s_{t+1},v_{1:T})$ is already known from the previous backward recursion. Under this assumption, the recursion becomes

$$p(h_t, s_t|v_{1:T}) \approx \sum_{s_{t+1}} p(s_{t+1}|v_{1:T}) p(s_t|s_{t+1}, v_{1:T}) \left\langle p(h_t|h_{t+1}, s_t, s_{t+1}, v_{1:t}) \right\rangle_{p(h_{t+1}|s_{t+1}, v_{1:T})}. \tag{10}$$

We call the procedure based on Equation (10) Expectation Correction (EC) since it 'corrects' the filtered results which themselves are formed from propagating expectations. In Appendix (E) we show how EC is equivalent to a partial Discrete-Continuous factorized approximation.

Equation (10) forms the basis of the EC Backward Pass. However, similar to the ADF Forward Pass, the number of mixture components needed to represent the posterior in this recursion grows exponentially as we go backwards in time. The strategy we take to deal with this is a form of Assumed Density Smoothing, in which Equation (10) is interpreted as a propagated dynamics reversal, which will subsequently be collapsed back to an assumed family of distributions—see Figure (4). How we implement the recursion for the continuous and discrete factors is detailed below.⁷

^{6.} In the *exact* calculation, $p(h_{t+1}|s_t, s_{t+1}, v_{1:T})$ is a mixture of Gaussians since $p(s_t|s_{t+1}, h_{t+1}, v_{1:t}) = p(s_t, s_{t+1}, h_{t+1}, v_{1:T})/p(s_{t+1}, h_{t+1}, v_{1:T})$ so that the mixture of Gaussians denominator $p(s_{t+1}, h_{t+1}, v_{1:T})$ cancels with the first term in Equation (9), leaving a mixture of Gaussians. However, since in Equation (9) the two terms $p(h_{t+1}|s_{t+1}, v_{1:T})$ and $p(s_t|s_{t+1}, h_{t+1}, v_{1:t})$ are replaced by approximations, this cancellation is not guaranteed.

^{7.} Equation (10) has the pleasing form of an RTS Backward Pass for the continuous part (analogous to LDS case), and a discrete smoother (analogous to a smoother recursion for the HMM). In the Forward-Backward algorithm for the HMM (Rabiner, 1989), the posterior $\gamma_t \equiv p(s_t|v_{1:T})$ is formed from the product of $\alpha_t \equiv p(s_t|v_{1:t})$ and $\beta_t \equiv p(v_{t+1:T}|s_t)$. This approach is also analogous to EP (Heskes and Zoeter, 2002). In the correction approach, a direct recursion for γ_t in terms of γ_{t+1} and α_t is formed, without explicitly defining β_t . The two approaches to inference are known as $\alpha - \beta$ and $\alpha - \gamma$ recursions.

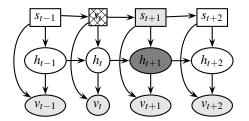


Figure 3: Our Backward Pass approximates $p(h_{t+1}|s_{t+1},s_t,v_{1:T})$ by $p(h_{t+1}|s_{t+1},v_{1:T})$. Motivation for this is that s_t only influences h_{t+1} through h_t . However, h_t will most likely be heavily influenced by $v_{1:t}$, so that not knowing the state of s_t is likely to be of secondary importance. The darker shaded node is the variable we wish to find the posterior state of. The lighter shaded nodes are variables in known states, and the hashed node a variable whose state is indeed known but assumed unknown for the approximation.

Evaluating $\langle p(h_t|h_{t+1}, s_t, s_{t+1}, v_{1:t}) \rangle_{p(h_{t+1}|s_{t+1}, v_{1:T})}$

 $\langle p(h_t|h_{t+1},s_t,s_{t+1},v_{1:t})\rangle_{p(h_{t+1}|s_{t+1},v_{1:T})}$ is a Gaussian in h_t , whose statistics we will now compute. First we find $p(h_t|h_{t+1},s_t,s_{t+1},v_{1:t})$ which may be obtained from the joint distribution

$$p(h_t, h_{t+1}|s_t, s_{t+1}, v_{1:t}) = p(h_{t+1}|h_t, s_{t+1})p(h_t|s_t, v_{1:t})$$
(11)

which itself can be found using the forward dynamics from the filtered estimate $p(h_t|s_t, v_{1:t})$. The statistics for the marginal $p(h_t|s_t, s_{t+1}, v_{1:t})$ are simply those of $p(h_t|s_t, v_{1:t})$, since s_{t+1} carries no extra information about h_t . The remaining statistics are the mean of h_{t+1} , the covariance of h_{t+1} and cross-variance between h_t and h_{t+1} ,

$$\langle h_{t+1} \rangle = A(s_{t+1}) f_t(s_t)$$

$$\Sigma_{t+1,t+1} = A(s_{t+1}) F_t(s_t) A^{\mathsf{T}}(s_{t+1}) + \Sigma^h(s_{t+1}), \qquad \Sigma_{t+1,t} = A(s_{t+1}) F_t(s_t).$$

Given the statistics of Equation (11), we may now condition on h_{t+1} to find $p(h_t|h_{t+1}, s_t, s_{t+1}, v_{1:t})$. Doing so effectively constitutes a reversal of the dynamics,

$$h_t = \overleftarrow{A}(s_t, s_{t+1})h_{t+1} + \overleftarrow{\eta}(s_t, s_{t+1})$$

where $\overleftarrow{A}(s_t, s_{t+1})$ and $\overleftarrow{\eta}(s_t, s_{t+1}) \sim \mathcal{N}(\overleftarrow{m}(s_t, s_{t+1}), \overleftarrow{\Sigma}(s_t, s_{t+1}))$ are easily found using the conditioned Gaussian results in Appendix (C)—see also Algorithm (5). Averaging the reversed dynamics we obtain a Gaussian in h_t for $\langle p(h_t|h_{t+1}, s_t, s_{t+1}, v_{1:t})\rangle_{p(h_{t+1}|s_{t+1}, v_{1:T})}$ with statistics

$$\mu_{t} = \overleftarrow{A}(s_{t}, s_{t+1})g(s_{t+1}) + \overleftarrow{m}(s_{t}, s_{t+1}), \quad \Sigma_{t,t} = \overleftarrow{A}(s_{t}, s_{t+1})G(s_{t+1})\overleftarrow{A}^{\mathsf{T}}(s_{t}, s_{t+1}) + \overleftarrow{\Sigma}(s_{t}, s_{t+1}).$$

These equations directly mirror the RTS Backward Pass, see Algorithm (5).

^{8.} Integrating over h_{t+1} means that the information from s_{t+1} passing through h_{t+1} via the term $p(h_{t+1}|s_{t+1},h_t)$ vanishes. Also, since s_t is known, no information from s_{t+1} passes through s_t to h_t .

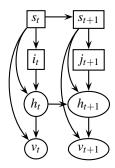


Figure 4: Structure of the Backward Pass for mixtures. Given the smoothed information at timestep t + 1, we need to work backwards to 'correct' the filtered estimate at time t.

EVALUATING $p(s_t|s_{t+1},v_{1:T})$

The main departure of EC from previous methods is in treating the term

$$p(s_t|s_{t+1},v_{1:T}) = \langle p(s_t|h_{t+1},s_{t+1},v_{1:t})\rangle_{p(h_{t+1}|s_{t+1},v_{1:T})}.$$
(12)

The term $p(s_t|h_{t+1}, s_{t+1}, v_{1:t})$ is given by

$$p(s_t|h_{t+1}, s_{t+1}, v_{1:t}) = \frac{p(h_{t+1}|s_t, s_{t+1}, v_{1:t})p(s_t, s_{t+1}|v_{1:t})}{\sum_{s_t'} p(h_{t+1}|s_t', s_{t+1}, v_{1:t})p(s_t', s_{t+1}|v_{1:t})}.$$
(13)

Here $p(s_t, s_{t+1}|v_{1:t}) = p(s_{t+1}|s_t, v_{1:t})p(s_t|v_{1:t})$, where $p(s_{t+1}|s_t, v_{1:t})$ occurs in the Forward Pass, Equation (7). In Equation (13), $p(h_{t+1}|s_{t+1}, s_t, v_{1:t})$ is found by marginalizing Equation (11).

Performing the average over $p(h_{t+1}|s_{t+1},v_{1:T})$ in Equation (12) may be achieved by any numerical integration method desired. Below we outline a crude approximation that is fast and often performs surprisingly well.

MEAN APPROXIMATION

A simple approximation of Equation (12) is to evaluate the integrand at the mean value of the averaging distribution. Replacing h_{t+1} in Equation (13) by its mean gives the simple approximation

$$\langle p(s_t|h_{t+1},s_{t+1},v_{1:t})\rangle_{p(h_{t+1}|s_{t+1},v_{1:T})} \approx \frac{1}{Z} \frac{e^{-\frac{1}{2}z_{t+1}^{\mathsf{T}}(s_t,s_{t+1})\Sigma^{-1}(s_t,s_{t+1}|v_{1:t})z_{t+1}(s_t,s_{t+1})}}{\sqrt{\det\Sigma(s_t,s_{t+1}|v_{1:t})}} p(s_t|s_{t+1},v_{1:t})$$

where $z_{t+1}(s_t, s_{t+1}) \equiv \langle h_{t+1} | s_{t+1}, v_{1:T} \rangle - \langle h_{t+1} | s_t, s_{t+1}, v_{1:t} \rangle$ and Z ensures normalization over s_t . This result comes simply from the fact that in Equation (12) we have a Gaussian with a mean $\langle h_{t+1} | s_t, s_{t+1}, v_{1:t} \rangle$ and covariance $\Sigma(s_t, s_{t+1} | v_{1:t})$, being the filtered covariance of h_{t+1} given s_t, s_{t+1} and the observations $v_{1:t}$, which may be taken from Σ_{hh} in Equation (5). Then evaluating this Gaussian at the specific point $\langle h_{t+1} | s_{t+1}, v_{1:T} \rangle$, we arrive at the above expression. An alternative to this simple mean approximation is to sample from the Gaussian $p(h_{t+1} | s_{t+1}, v_{1:T})$, which has the potential advantage that covariance information is used. Other methods such as variational

^{9.} This is a form of exact sampling since drawing samples from a Gaussian is easy. This should not be confused with meaning that this use of sampling renders EC a sequential Monte-Carlo sampling scheme.

Algorithm 2 aSLDS: EC Backward Pass (Single Gaussian case I = J = 1). Approximates $p(s_t|v_{1:T})$ and $p(h_t|s_t, v_{1:T}) \equiv \mathcal{N}(g_t(s_t), G_t(s_t))$. This routine needs the results from Algorithm (1) for I = 1.

```
G_T \leftarrow F_T, g_T \leftarrow f_T,
\mathbf{for} \ t \leftarrow T - 1 \ \mathbf{to} \ 1 \ \mathbf{do}
\mathbf{for} \ s \leftarrow 1 \ \mathbf{to} \ S, s' \leftarrow 1 \ \mathbf{to} \ S \ \mathbf{do},
(\mu, \Sigma)(s, s') = \mathsf{LDSBACKWARD}(g_{t+1}(s'), G_{t+1}(s'), f_t(s), F_t(s), \theta_{t+1}(s'))
p(s|s') = \langle p(s_t = s|h_{t+1}, s_{t+1} = s', v_{1:t}) \rangle_{p(h_{t+1}|s_{t+1} = s', v_{1:T})}
p(s, s'|v_{1:T}) \leftarrow p(s_{t+1} = s'|v_{1:T})p(s|s')
\mathbf{end} \ \mathbf{for}
\mathbf{for} \ s_t \leftarrow 1 \ \mathbf{to} \ S \ \mathbf{do}
\mathsf{Collapse} \ \mathsf{the} \ \mathsf{mixture} \ \mathsf{defined} \ \mathsf{by} \ \mathsf{weights} \ p(s_{t+1} = s'|s_t, v_{1:T}) \propto p(s_t, s'|v_{1:T}), \ \mathsf{means}
p(s_t, s') \ \mathsf{and} \ \mathsf{covariances} \ \Sigma(s_t, s') \ \mathsf{to} \ \mathsf{a} \ \mathsf{single} \ \mathsf{Gaussian}. \ \mathsf{This} \ \mathsf{defines} \ \mathsf{the} \ \mathsf{new} \ \mathsf{means}
g_t(s_t), \ \mathsf{covariances} \ G_t(s_t).
p(s_t|v_{1:T}) \leftarrow \Sigma_{s'} \ p(s_t, s'|v_{1:T})
\mathbf{end} \ \mathsf{for}
\mathbf{end} \ \mathsf{for}
```

approximations to this average (Jaakkola and Jordan, 1996) or the unscented transform (Julier and Uhlmann, 1997) may be employed if desired.

CLOSING THE RECURSION

We have now computed both the continuous and discrete factors in Equation (10), which we wish to use to write the smoothed estimate in the form $p(h_t, s_t|v_{1:T}) = p(s_t|v_{1:T})p(h_t|s_t, v_{1:T})$. The distribution $p(h_t|s_t, v_{1:T})$ is readily obtained from the joint Equation (10) by conditioning on s_t to form the mixture

$$p(h_t|s_t, v_{1:T}) = \sum_{s_{t+1}} p(s_{t+1}|s_t, v_{1:T}) p(h_t|s_t, s_{t+1}, v_{1:T})$$

which may be collapsed to a single Gaussian (or mixture if desired). As in the Forward Pass, this collapse implicitly defines the Gaussian mean $g(s_t)$ and covariance $G(s_t)$. The smoothed posterior $p(s_t|v_{1:T})$ is given by

$$p(s_{t}|v_{1:T}) = \sum_{s_{t+1}} p(s_{t+1}|v_{1:T}) p(s_{t}|s_{t+1}, v_{1:T})$$

$$= \sum_{s_{t+1}} p(s_{t+1}|v_{1:T}) \langle p(s_{t}|h_{t+1}, s_{t+1}, v_{1:t}) \rangle_{p(h_{t+1}|s_{t+1}, v_{1:T})}.$$
(14)

The algorithm for the single Gaussian case is presented in Algorithm (2).

NUMERICAL STABILITY

Numerical stability is a concern even in the LDS, and the same is to be expected for the aSLDS. Since the LDS recursions LDSFORWARD and LDSBACKWARD are embedded within the EC algorithm, we may immediately take advantage of the large body of work on stabilizing the LDS recursions, such as the Joseph form (Grewal and Andrews, 1993), or the square root forms (Park and Kailath, 1996; Verhaegen and Van Dooren, 1986).

RELAXING EC

The conditional independence assumption $p(h_{t+1}|s_t,s_{t+1},v_{1:T}) \approx p(h_{t+1}|s_{t+1},v_{1:T})$ is not strictly necessary in EC. We motivate it by computational simplicity, since finding an appropriate moment matching approximation of $p(h_{t+1}|s_t,s_{t+1},v_{1:T})$ in Equation (9) requires a relatively expensive non-Gaussian integration. If we therefore did treat $p(h_{t+1}|s_t,s_{t+1},v_{1:T})$ more correctly, the central assumption in this relaxed version of EC would be a collapse to a mixture of Gaussians (the additional computation of Equation (12) may usually be numerically evaluated to high precision). Whilst we did not do so, implementing this should not give rise to numerical instabilities since no potential divisions are required, merely the estimation of moments. In the experiments presented here, we did not pursue this option, since we believe that the effect of this conditional independence assumption is relatively weak.

INCONSISTENCIES IN THE APPROXIMATION

The recursion Equation (8), upon which EC depends, makes use of the Forward Pass results, and a subtle issue arises about possible inconsistencies in the Forward and Backward approximations. For example, under the conditional independence assumption in the Backward Pass, $p(h_T|s_{T-1},s_T,v_{1:T})\approx p(h_T|s_T,v_{1:T})$, which is in contradiction to Equation (5) which states that the approximation to $p(h_T|s_{T-1},s_T,v_{1:T})$ will depend on s_{T-1} . Similar contradictions occur also for the relaxed version of EC. Such potential inconsistencies arise because of the approximations made, and should not be considered as separate approximations in themselves. Furthermore, these inconsistencies will most likely be strongest at the end of the chain, $t \approx T$, since only then is Equation (8) in direct contradiction to Equation (5). Such potential inconsistencies arise since EC is not founded on a consistency criterion, unlike EP—see Section (3)—but rather an approximation of the exact recursions. Our experience is that compared to EP, which attempts to ensure consistency based on multiple sweeps through the graph, such inconsistencies are a small price to pay compared to the numerical stability advantages of EC.

2.3 Using Mixtures in the Backward Pass

The extension to the mixture case is straightforward, based on the representation

$$p(h_t|s_t, v_{1:T}) \approx \sum_{j_t=1}^{J_t} p(h_t|s_t, j_t, v_{1:T}) p(j_t|s_t, v_{1:T}).$$

Analogously to the case with a single component,

$$p(h_t, s_t|v_{1:T}) = \sum_{i_t, j_{t+1}, s_{t+1}} p(s_{t+1}|v_{1:T}) p(j_{t+1}|s_{t+1}, v_{1:T}) p(h_t|j_{t+1}, s_{t+1}, i_t, s_t, v_{1:T})$$

$$\cdot \langle p(i_t, s_t|h_{t+1}, j_{t+1}, s_{t+1}, v_{1:t}) \rangle_{p(h_{t+1}|j_{t+1}, s_{t+1}, v_{1:T})}.$$

The average in the last line of the above equation can be tackled using the same techniques as outlined in the single Gaussian case. To approximate $p(h_t|j_{t+1}, s_{t+1}, i_t, s_t, v_{1:T})$ we consider this as the marginal of the joint distribution

$$p(h_t, h_{t+1}|i_t, s_t, j_{t+1}, s_{t+1}, v_{1:T}) = p(h_t|h_{t+1}, i_t, s_t, j_{t+1}, s_{t+1}, v_{1:t})p(h_{t+1}|i_t, s_t, j_{t+1}, s_{t+1}, v_{1:T}).$$

Algorithm 3 aSLDS: EC Backward Pass. Approximates $p(s_t|v_{1:T})$ and $p(h_t|s_t,v_{1:T}) \equiv \sum_{j_t=1}^{J_t} u_t(j_t,s_t) \mathcal{N}(g_t(j_t,s_t),G_t(j_t,s_t))$ using a mixture of Gaussians. $J_T = I_T, J_t \leq S \times I_t \times J_{t+1}$. This routine needs the results from Algorithm (1).

```
 \begin{aligned} & \textbf{for } t \leftarrow F_T, g_T \leftarrow f_T, u_T \leftarrow w_T \; (*) \\ & \textbf{for } t \leftarrow T - 1 \; \textbf{to } 1 \; \textbf{do} \\ & \textbf{for } s \leftarrow 1 \; \textbf{to } S, s' \leftarrow 1 \; \textbf{to } S, i \leftarrow 1 \; \textbf{to } I_t, j' \leftarrow 1 \; \textbf{to } J_{t+1} \; \textbf{do} \\ & (\mu, \Sigma)(i, s, j', s') = \mathsf{LDSBACKWARD}(g_{t+1}(j', s'), G_{t+1}(j', s'), f_t(i, s), F_t(i, s), \theta_{t+1}(s')) \\ & p(i, s|j', s') = \langle p(s_t = s, i_t = i|h_{t+1}, s_{t+1} = s', j_{t+1} = j', v_{1:t}) \rangle_{p(h_{t+1}|s_{t+1} = s', j_{t+1} = j', v_{1:T})} \\ & p(i, s, j', s'|v_{1:T}) \leftarrow p(s_{t+1} = s'|v_{1:T})u_{t+1}(j', s')p(i, s|j', s') \\ & \textbf{end for} \\ & \textbf{for } s_t \leftarrow 1 \; \textbf{to } S \; \textbf{do} \\ & \text{Collapse the mixture defined by weights } p(i_t = i, s_{t+1} = s', j_{t+1} = j'|s_t, v_{1:T}) \propto \\ & p(i, s_t, j', s'|v_{1:T}), \; \text{means } \mu(i_t, s_t, j', s') \; \text{and covariances } \Sigma(i_t, s_t, j', s') \; \text{to a mixture with } \\ & J_t \; \text{components. This defines the new means } g_t(j_t, s_t), \; \text{covariances } G_t(j_t, s_t) \; \text{and mixture weights } u_t(j_t, s_t). \\ & p(s_t|v_{1:T}) \leftarrow \Sigma_{i_t,j',s'} p(i_t, s_t, j', s'|v_{1:T}) \; \\ & \textbf{end for} \\ & \textbf{end for} \end{aligned}
```

(*) If $J_T < I_T$ then the initialization is formed by collapsing the Forward Pass results at time T to J_T components.

As in the case of a single mixture, the problematic term is $p(h_{t+1}|i_t, s_t, j_{t+1}, s_{t+1}, v_{1:T})$. Analogously to before, we may make the assumption

$$p(h_{t+1}|i_t, s_t, j_{t+1}, s_{t+1}, v_{1:T}) \approx p(h_{t+1}|j_{t+1}, s_{t+1}, v_{1:T})$$

meaning that information about the current switch state s_t, i_t is ignored. We can then form

$$p(h_t|s_t, v_{1:T}) = \sum_{i_t, j_{t+1}, s_{t+1}} p(i_t, j_{t+1}, s_{t+1}|s_t, v_{1:T}) p(h_t|i_t, s_t, j_{t+1}, s_{t+1}, v_{1:T}).$$

This mixture can then be collapsed to smaller mixture using any method of choice, to give

$$p(h_t|s_t, v_{1:T}) \approx \sum_{j_t=1}^{J_t} p(h_t|j_t, s_t, v_{1:T}) p(j_t|s_t, v_{1:T})$$

The collapse procedure implicitly defines the means $g(j_t, s_t)$ and covariances $G(j_t, s_t)$ of the smoothed approximation. A recursion for the switches follows analogously to the single component Backward Pass. The resulting algorithm is presented in Algorithm (3), which includes using mixtures in both Forward and Backward Passes. Note that if $J_T < I_T$, an extra initial collapse is required of the I_T component Forward Pass Gaussian mixture at time T to J_T components.

EC has time complexity $O(S^2IJK)$ where S are the number of switch states, I and J are the number of Gaussians used in the Forward and Backward passes, and K is the time to compute the exact Kalman smoother for the system with a single switch state.

^{10.} As in the single component case, in principle, this assumption may be relaxed and a moment matching approximation be performed instead.

3. Relation to Other Methods

Approximate inference in the SLDS is a long-standing research topic, generating an extensive literature. See Lerner (2002) and Zoeter (2005) for reviews of previous work. A brief summary of some of the major existing approaches follows.

Assumed Density Filtering Since the exact filtered estimate $p(h_t|s_t,v_{1:t})$ is an (exponentially large) mixture of Gaussians, a useful remedy is to project at each stage of the recursion Equation (3) back to a limited set of K Gaussians. This is a Gaussian Sum Approximation (Alspach and Sorenson, 1972), and is a form of Assumed Density Filtering (ADF) (Minka, 2001). Similarly, Generalized Pseudo Bayes2 (GPB2) (Bar-Shalom and Li, 1998) also performs filtering by collapsing to a mixture of Gaussians. This approach to filtering is also taken in Lerner et al. (2000) which performs the collapse by removing spatially similar Gaussians, thereby retaining diversity.

Several smoothing approaches directly use the results from ADF. The most popular is Kim's method, which updates the filtered posterior weights to form the smoother (Kim, 1994; Kim and Nelson, 1999). In both EC and Kim's method, the approximation

 $p(h_{t+1}|s_t, s_{t+1}, v_{1:T}) \approx p(h_{t+1}|s_{t+1}, v_{1:T})$, is used to form a numerically simple Backward Pass. The other approximation in EC is to numerically compute the average in Equation (14). In Kim's method, however, an update for the discrete variables is formed by replacing the required term in Equation (14) by

$$\langle p(s_t|h_{t+1},s_{t+1},v_{1:t})\rangle_{p(h_{t+1}|s_{t+1},v_{1:T})} \approx p(s_t|s_{t+1},v_{1:t}).$$
 (15)

This approximation¹¹ decouples the discrete Backward Pass in Kim's method from the continuous dynamics, since $p(s_t|s_{t+1},v_{1:t}) \propto p(s_{t+1}|s_t)p(s_t|v_{1:t})/p(s_{t+1}|v_{1:t})$ can be computed simply from the filtered results alone (the continuous Backward Pass in Kim's method, however, does depend on the discrete Backward Pass). The fundamental difference between EC and Kim's method is that the approximation (15) is not required by EC. The EC Backward Pass therefore makes fuller use of the future information, resulting in a recursion which intimately couples the continuous and discrete variables. The resulting effect on the quality of the approximation can be profound, as we will see in the experiments.

Kim's smoother corresponds to a potentially severe loss of future information and, in general, cannot be expected to improve much on the filtered results from ADF. The more recent work of Lerner et al. (2000) is similar in spirit to Kim's method, whereby the contribution from the continuous variables is ignored in forming an approximate recursion for the smoothed $p(s_t|v_{1:T})$. The main difference is that for the discrete variables, Kim's method is based on a correction smoother (Rauch et al., 1965), whereas Lerner's method uses a Belief Propagation style Backward Pass (Jordan, 1998). Neither method correctly integrates information from the continuous variables. How to form a recursion for a mixture approximation which does not ignore information coming through the continuous hidden variables is a central contribution of our work.

Kitagawa (1994) used a two-filter method in which the dynamics of the chain are reversed. Essentially, this corresponds to a Belief Propagation method which defines a Gaussian sum

^{11.} In the HMM this is exact, but in the SLDS the future observations carry information about s_t .

	EC	Relaxed EC	EP	Kim
Mixture Collapsing to Single			X	
Mixture Collapsing to Mixture	X	X		X
Cond. Indep. $p(h_{t+1} s_t, s_{t+1}, v_{1:T}) \approx p(h_{t+1} s_{t+1}, v_{1:T})$	X			х
Approx. of $p(s_t s_{t+1},v_{1:T})$, average Equation (12)	X	X		
Kim's Backward Pass				X
Mixture approx. of $p(h_{t+1} s_t, s_{t+1}, v_{1:T})$, Equation (9)		X		

Table 1: Relation between methods. In the EC methods, the mean approximation may be replaced by an essentially exact Monte Carlo approximation to Equation (12). EP refers to the Single Gaussian approximation in Heskes and Zoeter (2002). In the case of using Relaxed EC with collapse to a single Gaussian, EC and EP are not equivalent, since the underlying recursions on which the two methods are based are fundamentally different.

approximation for $p(v_{t+1:T}|h_t, s_t)$. However, since this is not a density in h_t, s_t , but rather a conditional likelihood, formally one cannot treat this using density propagation methods. In Kitagawa (1994), the singularities resulting from incorrectly treating $p(v_{t+1:T}|h_t, s_t)$ as a density are heuristically finessed.

Expectation Propagation EP (Minka, 2001), as applied to the SLDS, corresponds to an approximate implementation of Belief Propagation¹² (Jordan, 1998; Heskes and Zoeter, 2002). EP is the most sophisticated rival to Kim's method and EC, since it makes the least assumptions. For this reason, we'll explain briefly how EP works. Unlike EC, which is based on an approximation of the exact filtering and smoothing recursions, EP is based on a consistency criterion.

First, let's simplify the notation, and write the distribution as $p = \prod_t \phi(x_{t-1}, v_{t-1}, x_t, v_t)$, where $x_t \equiv h_t \otimes s_t$, and $\phi(x_{t-1}, v_{t-1}, x_t, v_t) \equiv p(x_t | x_{t-1}) p(v_t | x_t)$. EP defines 'messages' ρ , λ^{13} which contain information from past and future observations respectively. Explicitly, we define $\rho_t(x_t) \propto p(x_t | v_{1:t})$ to represent knowledge about x_t given all information from time 1 to t. Similarly, $\lambda_t(x_t)$ represents knowledge about state x_t given all observations from time t to time t+1. In the sequel, we drop the time suffix for notational clarity. We define $\lambda(x_t)$ implicitly through the requirement that the marginal smoothed inference is given by

$$p(x_t|v_{1:T}) \propto \rho(x_t)\lambda(x_t). \tag{16}$$

Hence $\lambda(x_t) \propto p(v_{t+1:T}|x_t, v_{1:t}) = p(v_{t+1:T}|x_t)$ and represents all future knowledge about $p(x_t|v_{1:T})$. From this

$$p(x_{t-1}, x_t | v_{1:T}) \propto \rho(x_{t-1}) \phi(x_{t-1}, v_{t-1}, x_t, v_t) \lambda(x_t). \tag{17}$$

^{12.} Non-parametric belief propagation (Sudderth et al., 2003), which performs approximate inference in general continuous distributions, is also related to EP applied to the aSLDS, in the sense that the messages cannot be represented easily, and are approximated by mixtures of Gaussians.

^{13.} These correspond to the α and β messages in the Hidden Markov Model framework (Rabiner, 1989).

^{14.} In this Belief Propagation/EP viewpoint, the backward messages, traditionally labeled as β , correspond to conditional likelihoods, and not distributions. In contrast, in the EC approach, which is effectively a so-called $\alpha - \gamma$ recursion, the backward γ messages correspond to posterior distributions.

Taking the above equation as a starting point, we have

$$p(x_t|v_{1:T}) \propto \int_{x_{t-1}} \rho(x_{t-1}) \phi(x_{t-1}, v_{t-1}, x_t, v_t) \lambda(x_t).$$

Consistency with Equation (16) requires (neglecting irrelevant scalings)

$$\rho(x_t)\lambda(x_t) \propto \int_{x_{t-1}} \rho(x_{t-1}) \phi(x_{t-1}, v_{t-1}, x_t, v_t) \lambda(x_t).$$

Similarly, we can integrate Equation (17) over x_t to get the marginal at time x_{t-1} which, by consistency, should be proportional to $\rho(x_{t-1})\lambda(x_{t-1})$. Hence

$$\rho(x_t) \propto \frac{\int_{x_{t-1}} \rho(x_{t-1}) \phi(x_{t-1}, x_t) \lambda(x_t)}{\lambda(x_t)}, \lambda(x_{t-1}) \propto \frac{\int_{x_t} \rho(x_{t-1}) \phi(x_{t-1}, x_t) \lambda(x_t)}{\rho(x_{t-1})}$$
(18)

where the divisions can be interpreted as preventing over-counting of messages. In an exact implementation, the common factors in the numerator and denominator cancel. EP addresses the fact that $\lambda(x_t)$ is not a distribution by using Equation (18) to form the projection (or 'collapse'). In the numerator, $\int_{x_{t-1}} \rho(x_{t-1}) \phi(x_{t-1}, x_t) \lambda(x_t)$ and $\int_{x_t} \rho(x_{t-1}) \phi(x_{t-1}, x_t) \lambda(x_t)$ represent $p(x_t|v_{1:T})$ and $p(x_{t-1}|v_{1:T})$. Since these *are* distributions (an indexed mixture of Gaussians in the SLDS), they may be projected/collapsed to a single indexed Gaussian. The update for the ρ message is then found from division by the λ potential, and vice versa. In EP the explicit division of potentials only makes sense for members of the exponential family. More complex methods could be envisaged in which, rather than an explicit division, the new messages are defined by minimizing some measure of divergence between $\rho(x_t)\lambda(x_t)$ and $\int_{x_{t-1}} \rho(x_{t-1}) \phi(x_{t-1}, x_t) \lambda(x_t)$, such as the Kullback-Leibler divergence. In this way, non-exponential family approximations (such as mixtures of Gaussians) may be considered. Whilst this is certainly feasible, it is somewhat unattractive computationally since this would require for each time-step an expensive minimization.

For the single Gaussian case, in order to perform the division, the potentials in the numerator and denominator are converted to their canonical representations. To form the ρ update, the result of the division is then reconverted back to a moment representation. The resulting recursions, due to the approximation, are no longer independent and Heskes and Zoeter (2002) show that using more than a single Forward and Backward sweep often improves on the quality of the approximation. This coupling is a departure from the exact recursions, which should remain independent.

Applied to the SLDS, EP suffers from severe numerical instabilities (Heskes and Zoeter, 2002) and finding a way to minimize the corresponding EP free energy in an efficient, robust and guaranteed way remains an open problem. Our experience is that current implementations of EP are unsuitable for large scale time-series applications. Damping the parameter updates is one suggested approach to heuristically improve convergence. The source of these numerical instabilities is not well understood since, even in cases when the posterior appears uni-modal, the method is problematic. The frequent conversions between moment and canonical parameterizations of Gaussians are most likely at the root of the difficulties. An interesting comparison here is between Lauritzen's original method for exact computation on conditional Gaussian distributions (for which the SLDS is a special case) Lauritzen (1992),

which is numerically unstable due to conversion between moment and canonical representations, and Lauritzen and Jensen (2001), which improves stability by avoiding using canonical parameterizations.

Variational Methods Ghahramani and Hinton (1998) used a variational method which approximates the joint distribution $p(h_{1:T}, s_{1:T}|v_{1:T})$ rather than the marginal $p(h_t, s_t|v_{1:T})$ —related work is presented in Lee et al. (2004). This is a disadvantage when compared to other methods that directly approximate the marginal. The variational methods are nevertheless potentially attractive since they are able to exploit structural properties of the distribution, such as a factored discrete state-transition. In this article, we concentrate on the case of a small number of states S and hence will not consider variational methods further here. ¹⁵

Sequential Monte Carlo (Particle Filtering) These methods form an approximate implementation of Equation (3), using a sum of delta functions to represent the posterior—see, for example, Doucet et al. (2001). Whilst potentially powerful, these non-analytic methods typically suffer in high-dimensional hidden spaces since they are often based on naive importance sampling, which restricts their practical use. ADF is generally preferential to Particle Filtering, since in ADF the approximation is a mixture of non-trivial distributions, which is better at capturing the variability of the posterior. Rao-Blackwellized Particle Filters (Doucet et al., 2000) are an attempt to alleviate the difficulty of sampling in high-dimensional state spaces by explicitly integrating over the continuous state.

Non-Sequential Monte Carlo

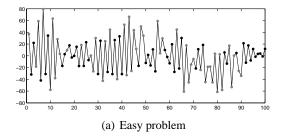
For fixed switches $s_{1:T}$, $p(v_{1:T}|s_{1:T})$ is easily computable since this is just the likelihood of an LDS. This observation raises the possibility of sampling from the posterior $p(s_{1:T}|v_{1:T}) \propto p(v_{1:T}|s_{1:T})p(s_{1:T})$ directly. Many possible sampling methods could be applied in this case, and the most immediate is Gibbs sampling, in which a sample for each t is drawn from $p(s_t|s_{\setminus t},v_{1:T})$ —see Neal (1993) for a general reference and Carter and Kohn (1996) for an application to the SLDS. This procedure may work well in practice provided that the initial setting of $s_{1:T}$ is in a region of high probability mass—otherwise, sampling by such individual coordinate updates may be extremely inefficient.

4. Experiments

Our experiments examine the stability and accuracy of EC against several other methods on long time-series. In addition, we will compare the absolute accuracy of EC as a function of the number of mixture components on a short time-series, where exact inference may be explicitly evaluated.

Testing EC in a problem with a reasonably long temporal sequence, T, is important since numerical stabilities may not be apparent in time-series of just a few time-steps. To do this, we sequentially generate hidden states h_t , s_t and observations v_t from a given model. Then, given only the parameters of the model and the observations (but not any of the hidden states), the task is to infer $p(h_t|s_t, v_{1:T})$ and $p(s_t|v_{1:T})$. Since the exact computation is exponential in T, a formally exact evaluation of the method is infeasible. A simple alternative is to assume that the original sample states $s_{1:T}$ are the 'correct' inferred states, and compare our most probable posterior smoothed

^{15.} Lerner (2002) discusses an approach in the case of a large structured discrete state transition. Related ideas could also be used in EC.



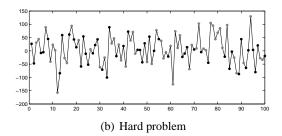


Figure 5: SLDS: Throughout, S=2, V=1 (scalar observations), T=100, with zero output bias. A(s)=0.9999* orth(randn(H,H)), B(s)= randn(V,H), $\bar{v}_t\equiv 0$, $\bar{h}_1=10*$ randn(H,1), $\bar{h}_{t>1}=0$, $\Sigma_1^h=I_H$, $p_1=$ uniform. The figures show typical examples for each of the two problems: (a) Easy problem. H=3, $\Sigma^h(s)=I_H$, $\Sigma^v(s)=0.1I_V$, $p(s_{t+1}|s_t) \propto 1_{S\times S}+I_S$. (b) Hard problem. H=30, $\Sigma^v(s)=30I_V$, $\Sigma^h(s)=0.01I_H$

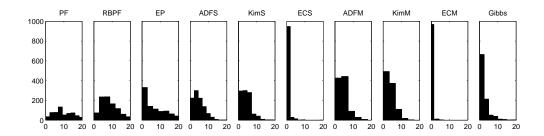


Figure 6: SLDS 'Easy' problem: The number of errors in estimating a binary switch $p(s_t|v_{1:T})$ over a time series of length T=100. Hence 50 errors corresponds to random guessing. Plotted are histograms of the errors over 1000 experiments. The histograms have been cutoff at 20 errors in order to improve visualization. (PF) Particle Filter. (RBPF) Rao-Blackwellized PF. (EP) Expectation Propagation. (ADFS) Assumed Density Filtering using a Single Gaussian. (KimS) Kim's smoother using the results from ADFS. (ECS) Expectation Correction using a Single Gaussian (I=J=1). (ADFM) ADF using a multiple of I=4 Gaussians. (KimM) Kim's smoother using the results from ADFM. (ECM) Expectation Correction using a mixture with I=J=4 components. In Gibbs sampling, we use the initialization from ADFM.

estimates $\arg\max_{s_t} p(s_t|v_{1:T})$ with the assumed correct sample s_t .¹⁶ We look at two sets of experiments, one for the SLDS and one for the aSLDS. In both cases, scalar observations are used so that the complexity of the inference problem can be visually assessed.

^{16.} We could also consider performance measures on the accuracy of $p(h_t|s_t, v_{1:T})$. However, we prefer to look at approximating $\arg\max_{s_t} p(s_t|v_{1:T})$ since the sampled discrete states are likely to correspond to the exact $\arg\max_{s_t} p(s_t|v_{1:T})$. In addition, if the posterior switch distribution is dominated by a single state $s_{1:T}^*$, then provided they are correctly estimated, the model reduces to an LDS, for which inference of the continuous hidden state is trivial.

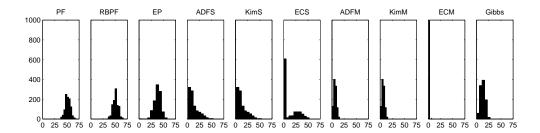


Figure 7: SLDS 'Hard' problem: The number of errors in estimating a binary switch $p(s_t|v_{1:T})$ over a time series of length T = 100. Hence 50 errors corresponds to random guessing. Plotted are histograms of the errors over 1000 experiments.

SLDS EXPERIMENTS

We chose experimental conditions that, from the viewpoint of classical signal processing, are difficult, with changes in the switches occurring at a much higher rate than the typical frequencies in the signal. We consider two different toy SLDS experiments: The 'easy' problem corresponds to a low hidden dimension, H=3, with low observation noise; The 'hard' problem corresponds to a high hidden dimension, H=30, and high observation noise. See Figure (5) for details of the experimental setup.

We compared methods using a single Gaussian, and methods using multiple Gaussians, see Figure (6) and Figure (7). For EC we use the mean approximation for the numerical integration of Equation (12). For the Particle Filter 1000 particles were used, with Kitagawa re-sampling (Kitagawa, 1996). For the Rao-Blackwellized Particle Filter (Doucet et al., 2000), 500 particles were used, with Kitagawa re-sampling. We included the Particle Filter merely for a point of comparison with ADF, since they are not designed to approximate the smoothed estimate.

An alternative MCMC procedure is to perform Gibbs sampling of $p(s_{1:T}|v_{1:T})$ using $p(s_t|s_{\setminus t},v_{1:T}) \propto p(v_{1:T}|s_{1:T})p(s_{1:T})$, where $p(v_{1:T}|s_{1:T})$ is simply the likelihood of an LDS—see for example Carter and Kohn (1996). We initialize the state $s_{1:T}$ by using the most likely states s_t from the filtered results using a Gaussian mixture (ADFM), and then swept forwards in time, sampling from the state $p(s_t|s_{\setminus t},v_{1:T})$ until the end of the chain. We then reversed direction, sampling from time T back to time 1, and continued repeating this procedure 100 times, with the mean over the last 80 sweeps used as the posterior mean approximation. This procedure is expensive since each sample requires computing the likelihood of an LDS defined on the whole time-series. The procedure therefore scales with GT^2 where G is the number of sweeps over the time series. Despite using a reasonable initialization, Gibbs sampling struggles to improve on the filtered results.

We found that EP was numerically unstable and often struggled to converge. To encourage convergence, we used the damping method in Heskes and Zoeter (2002), performing 20 iterations with a damping factor of 0.5. The disappointing performance of EP is most likely due to conflicts

^{17.} Carter and Kohn (1996) proposed an overly complex procedure for computing the likelihood $p(v_{1:T}|s_{1:T})$. This is simply the likelihood of an LDS (since $s_{1:T}$ are assumed known), and is readily computable using any of the standard procedures in the literature.

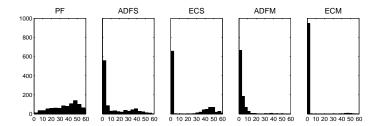


Figure 8: aSLDS: Histogram of the number of errors in estimating a binary switch $p(s_t|v_{1:T})$ over a time series of length T=100. Hence 50 errors corresponds to random guessing. Plotted are histograms of the errors over 1000 experiments. Augmented SLDS results. ADFM used I=4 Gaussians, and ECM used I=J=4 Gaussians. We used 1000 samples to approximate Equation (12).

I	1	4	4	16	16	64	64	256	256
J	1	1	4	1	16	1	64	1	256
error	0.0989	0.0624	0.0365	0.0440	0.0130	0.0440	4.75e-4	0.0440	3.40e-8

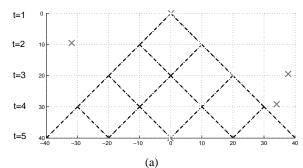
Table 2: Errors in approximating the states for the multi-path problem, see Figure (9). The mean absolute deviation $|p^{ec}(s_t|v_{1:T}) - p^{exact}(s_t|v_{1:T})|$ averaged over the S=4 states of s_t and over the times $t=1,\ldots,5$, computed for different numbers of mixture components in EC. The mean approximation of Equation (12) is used. The exact computation uses $S^{T-1}=256$ mixtures.

resulting from numerical instabilities introduced by the frequent conversions between moment and canonical representations.

The various algorithms differ widely in performance, see Figures (6,7). Not surprisingly, the best filtered results are given using ADF, since this is better able to represent the variance in the filtered posterior than the sampling methods. Unlike Kim's method, EC makes good use of the future information to clean up the filtered results considerably. One should bear in mind that both EC, Kim's method and the Gibbs initialization use the same ADF results. These results show that EC may dramatically improve on Kim's method, so that the small amount of extra work in making a numerical approximation of $p(s_t|s_{t+1}, v_{1:T})$, Equation (12), may bring significant benefits.

AUGMENTED SLDS EXPERIMENTS

In Figure (8), we chose a simple two state S = 2 transition distribution $p(s_{t+1} = 1 | s_t, h_t) = \sigma(h_t^\mathsf{T} w(s_t))$, where $\sigma(x) \equiv 1/(1 + e^{-x})$. Some care needs to be taken to make a model so for which even exact inference would produce posterior switches close to the sampled switches. If the switch variables s_{t+1} changes wildly (which is possible given the above formula since the hidden state h may have a large projected change if the hidden state changes) essentially no information is left in the signal for any inference method to produce reasonable results. We therefore set $w(s_t)$ to a zero vector except for the first two components, which are independently sampled from a zero mean Gaussian with standard deviation 5. For each of the two switch states, s, we have a transition matrix A(s), which



	t=1	t=2	t=3	t=4	t=5
s=1	0.495	0.000	0.000	0.000	0.269
s=2	0.495	0.000	0.000	0.000	0.682
s=3	0.005	0.507	0.713	0.509	0.022
s=4	0.005	0.493	0.287	0.491	0.027

Figure 9: (a) The multi-path problem. The particle starts from (0,0) at time t=1. Subsequently, at each time-point, either the vector (10,10) (corresponding to states s=1 and s=3) or (-10,10) (corresponding to states s=2 and s=4), is added to the hidden dynamics, perturbed by a small amount of noise, $\Sigma^h=0.1$. The observations are $\nu=h+\eta^\nu(s)$. For states s=1,2 the observation noise is small, $\Sigma^\nu=0.1I$, but for s=3,4 the noise in the horizontal direction has variance 1000. The visible observations are given by the x'. The true hidden states are given by '+'. (b) The exact smoothed state posteriors $p^{exact}(s_t|\nu_{1:T})$ computed by enumerating all paths (given by the dashed lines).

we set to be block diagonal. The first 2×2 block is set to $0.9999R_{\theta}$, where R_{θ} is a 2×2 rotation matrix with angle θ chosen uniformly from 0 to 1 radians. This means that s_{t+1} is dependent on the first two components of h_t which are rotating at a restricted rate. The remaining $H - 2 \times H - 2$ block of A(s) is chosen as (using MATLAB notation) $0.9999 * \operatorname{orth}(\operatorname{rand}(H - 2))$, which means a scaled randomly chosen orthogonal matrix. Throughout, S = 2, V = 1, H = 30, T = 100, with zero output bias. Using partly MATLAB notation, $B(s) = \operatorname{randn}(V, H)$, $\bar{v}_t \equiv 0$, $\bar{h}_1 = 10 * \operatorname{randn}(H, 1)$, $\bar{h}_{t>1} = 0$, $\Sigma_1^h = I_H$, $p_1 = \operatorname{uniform}$. $\Sigma^v = 30I_V$, $\Sigma^h = 0.1I_H$.

We compare EC only against Particle Filters using 1000 particles, since other methods would require specialized and novel implementations. In ADFM, I = 4 Gaussians were used, and for ECM, I = J = 4 Gaussians were used. Looking at the results in Figure (8), we see that EC performs well, with some improvement in using the mixture representation I, J = 4 over a single Gaussian I = J = 1. The Particle Filter most likely failed since the hidden dimension is too high to be explored well with only 1000 particles.

EFFECT OF USING MIXTURES

Our claim is that EC should cope in situations where the smoothed posterior $p(h_t|s_t, v_{1:T})$ is multimodal and, consequently, cannot be well represented by a single Gaussian. We therefore constructed an SLDS which exhibits multi-modality to see the effect of using EC with both I and J greater than 1. The 'multi-path' scenario is described in Figure (9), where a particle traces a path through a two dimensional space. A small number of time-steps was chosen so that the exact $p(s_t|v_{1:T})$ can be computed by direct enumeration. The observation of the particle is at times extremely noisy in the horizontal direction. This induces multi-modality of $p(h_t|s_t, v_{1:T})$ since there

^{18.} This should not be confused with the multi-modality of $p(h_t|v_{1:T}) = \sum_{s_t} p(h_t|s_t, v_{1:T}) p(s_t|v_{1:T})$.

are several paths that might plausibly have been taken to give rise to the observations. The accuracy with which EC predicts the exact smoothed posterior is given in Table (2). For this problem we see that both the number of Forward (I) and Backward components (J) affects the accuracy of the approximation, generally with improved accuracy as the number of mixture components increases. For a 'perfect' approximation method, one would expect that when $I = J = S^{T-1} = 256$, then the approximation should become exact. The small error for this case in Table (2) may arise for several reasons: the extra independence assumption used in EC, or the simple mean approximation used to compute Equation (12), or numerical roundoff. However, at least in this case, the effect of these assumptions on the performance is very small.

5. Discussion

Expectation Correction is a novel form of Backward Pass which makes less approximations than the widely used approach from Kim (1994). In Kim's method, potentially important future information channeled through the continuous hidden variables is lost. EC, along with Kim's method, makes the additional assumption $p(h_{t+1}|s_t,s_{t+1},v_{1:T}) \approx p(h_{t+1}|s_{t+1},v_{1:T})$. However, our experience is that this assumption is rather mild, since the state of h_{t+1} will be most heavily influenced by its immediate parent s_{t+1} .

Our approximation is based on the idea that, although exact inference will consist of an exponentially large number of mixture components, due to the forgetting which commonly occurs in Markovian models, a finite number of mixture components may provide a reasonable approximation. In tracking situations where the visible information is (temporarily) not enough to specify accurately the hidden state, then representing the posterior $p(h_t|s_t, v_{1:T})$ using a mixture of Gaussians may improve results significantly. Clearly, in systems with very long correlation times our method may require too many mixture components to produce a satisfactory result, although we are unaware of other techniques that would be able to cope well in that case.

We hope that the straightforward ideas presented here may help facilitate the practical application of dynamic hybrid networks to machine learning and related areas. Whilst models with Gaussian emission distributions such as the SLDS are widespread, the extension of this method to non-Gaussian emissions $p(v_t|h_t,s_t)$ would clearly be of considerable interest.

Software for Expectation Correction for this augmented class of Switching Linear Gaussian models is available from www.idiap.ch/~barber.

Acknowledgments

I would like to thank Onno Zoeter and Tom Heskes for kindly providing their Expectation Propagation code, Silvia Chiappa for helpful discussions, and Bertrand Mesot for many discussions, help with the simulations and for suggesting the relationship between the partial factorization and independence viewpoints of EC. I would also like to thank the reviewers for their many helpful comments and suggestions.

Algorithm 4 LDS Forward Pass. Compute the filtered posteriors $p(h_t|v_{1:t}) \equiv \mathcal{N}(f_t, F_t)$ for a LDS with parameters $\theta_t = A, B, \Sigma^h, \Sigma^v, \bar{h}, \bar{v}$, for t > 1. At time t = 1, we use parameters $\theta_1 = A, B, \Sigma, \Sigma^v, \mu, \bar{v}$, where Σ and μ are the prior covariance and mean of h. The log-likelihood $L = \log p(v_{1:T})$ is also returned.

```
\begin{aligned} &\textbf{for}\ t \leftarrow 0, f_0 \leftarrow 0, L \leftarrow 0 \\ &\textbf{for}\ t \leftarrow 1, T\ \textbf{do} \\ & \{f_t, F_t, p_t\} = \texttt{LDSFORWARD}(f_{t-1}, F_{t-1}, \nu_t; \theta_t) \\ & L \leftarrow L + \log p_t \\ &\textbf{end for} \\ &\textbf{function}\ \texttt{LDSFORWARD}(f, F, \nu; \theta) \\ & \text{Compute joint } p(h_t, \nu_t | \nu_{1:t-1}) \text{:} \\ & \mu_h \leftarrow Af + \bar{h}, \qquad \mu_\nu \leftarrow B\mu_h + \bar{\nu} \\ & \Sigma_{hh} \leftarrow AFA^\mathsf{T} + \Sigma^h, \qquad \Sigma_{\nu\nu} \leftarrow B\Sigma_{hh}B^\mathsf{T} + \Sigma^\nu, \qquad \Sigma_{\nu h} \leftarrow B\Sigma_{hh} \\ & \text{Find } p(h_t | \nu_{1:t}) \text{ by conditioning:} \\ & f' \leftarrow \mu_h + \Sigma^\mathsf{T}_{\nu h} \Sigma^\mathsf{T}_{\nu \nu} (\nu - \mu_\nu), \qquad F' \leftarrow \Sigma_{hh} - \Sigma^\mathsf{T}_{\nu h} \Sigma^\mathsf{T}_{\nu \nu} \Sigma_{\nu h} \\ & \text{Compute } p(\nu_t | \nu_{1:t-1}) \text{:} \\ & p' \leftarrow \exp\left(-\frac{1}{2}\left(\nu - \mu_\nu\right)^\mathsf{T} \Sigma^\mathsf{-1}_{\nu \nu}\left(\nu - \mu_\nu\right)\right) / \sqrt{\det 2\pi \Sigma_{\nu \nu}} \\ & \textbf{return } f', F', p' \\ & \textbf{end function} \end{aligned}
```

Appendix A. Inference in the LDS

The LDS is defined by Equations (1,2) in the case of a single switch S=1. The LDS Forward and Backward passes define the important functions LDSFORWARD and LDSBACKWARD, which we shall make use of for inference in the aSLDS.

FORWARD PASS (FILTERING)

The filtered posterior $p(h_t|v_{1:t})$ is a Gaussian which we parameterize with mean f_t and covariance F_t . These parameters can be updated recursively using $p(h_t|v_{1:t}) \propto p(h_t,v_t|v_{1:t-1})$, where the joint distribution $p(h_t,v_t|v_{1:t-1})$ has statistics (see Appendix (B))

$$\mu_h = A f_{t-1} + \bar{h}, \quad \mu_v = B \mu_h + \bar{v}$$

$$\Sigma_{hh} = A F_{t-1} A^\mathsf{T} + \Sigma^h, \quad \Sigma_{vv} = B \Sigma_{hh} B^\mathsf{T} + \Sigma^v, \quad \Sigma_{vh} = B \Sigma_{hh}.$$

We may then find $p(h_t|v_{1:t})$ by conditioning $p(h_t, v_t|v_{1:t-1})$ on v_t , see Appendix (C). This gives rise to Algorithm (4).

BACKWARD PASS

The smoothed posterior $p(h_t|v_{1:T}) \equiv \mathcal{N}(g_t, G_t)$ can be computed recursively using:

$$p(h_t|v_{1:T}) = \int_{h_{t+1}} p(h_t|h_{t+1}, v_{1:T}) p(h_{t+1}|v_{1:T}) = \int_{h_{t+1}} p(h_t|h_{t+1}, v_{1:t}) p(h_{t+1}|v_{1:T})$$

where $p(h_t|h_{t+1},v_{1:t})$ may be obtained from the joint distribution

$$p(h_t, h_{t+1}|v_{1:t}) = p(h_{t+1}|h_t)p(h_t|v_{1:t})$$
(19)

Algorithm 5 LDS Backward Pass. Compute the smoothed posteriors $p(h_t|v_{1:T})$. This requires the filtered results from Algorithm (4).

```
G_{T} \leftarrow F_{T}, g_{T} \leftarrow f_{T}
\mathbf{for} \ t \leftarrow T - 1, 1 \ \mathbf{do}
\{g_{t}, G_{t}\} = \mathsf{LDSBACKWARD}(g_{t+1}, G_{t+1}, f_{t}, F_{t}; \theta_{t+1})
\mathbf{end} \ \mathbf{for}
\mathbf{function} \ \mathsf{LDSBACKWARD}(g, G, f, F; \theta)
\mu_{h} \leftarrow Af + \bar{h}, \qquad \Sigma_{h'h'} \leftarrow AFA^{\mathsf{T}} + \Sigma^{h}, \qquad \Sigma_{h'h} \leftarrow AF
\Sigma \leftarrow F_{t} - \Sigma^{\mathsf{T}}_{h'h} \Sigma^{-1}_{h'h'} \Sigma_{h'h}, \qquad \overline{A} \leftarrow \Sigma^{\mathsf{T}}_{h'h} \Sigma^{-1}_{h'h'}, \qquad \overline{m} \leftarrow f - \overline{A} \mu_{h}
g' \leftarrow \overline{A} \ g + \overline{m}, \qquad G' \leftarrow \overline{A} \ \overline{G} \ \overline{A}^{\mathsf{T}} + \overline{\Sigma}
\mathbf{return} \ g', G'
\mathbf{end} \ \mathbf{function}
```

which itself can be obtained by forward propagation from $p(h_t|v_{1:t})$. Conditioning Equation (19) to find $p(h_t|h_{t+1},v_{1:t})$ effectively reverses the dynamics,

$$h_t = \overleftarrow{A_t} h_{t+1} + \overleftarrow{\eta_t}$$

where $\overleftarrow{A_t}$ and $\overleftarrow{\eta}_t \sim \mathcal{N}(\overleftarrow{m_t}, \overleftarrow{\Sigma_t})$ are found using the conditioned Gaussian results in Appendix (C)—these are explicitly given in Algorithm (5). Then averaging the reversed dynamics over $p(h_{t+1}|v_{1:T})$ we find that $p(h_t|v_{1:T})$ is a Gaussian with statistics

$$g_t = \overleftarrow{A_t} g_{t+1} + \overleftarrow{m_t}, \quad G_t = \overleftarrow{A_t} G_{t+1} \overleftarrow{A_t}^\mathsf{T} + \overleftarrow{\Sigma_t}.$$

This Backward Pass is given in Algorithm (5). For parameter learning of the A matrix, the smoothed statistic $\langle h_t h_{t+1}^\mathsf{T} \rangle$ is required. Using the above formulation, this is given by $\overleftarrow{A_t} G_{t+1} + \langle h_t \rangle \langle h_{t+1}^\mathsf{T} \rangle$. This is much simpler than the standard expressions cited in Shumway and Stoffer (2000) and Roweis and Ghahramani (1999).

Appendix B. Gaussian Propagation

Let y be linearly related to x through $y = Mx + \eta$, where $\eta \sim \mathcal{N}(\mu, \Sigma)$, and $x \sim \mathcal{N}(\mu_x, \Sigma_x)$. Then $p(y) = \int_x p(y|x)p(x)$ is a Gaussian with mean $M\mu_x + \mu$ and covariance $M\Sigma_x M^T + \Sigma$.

Appendix C. Gaussian Conditioning

For a joint Gaussian distribution over the vectors x and y with means μ_x , μ_y and covariance elements Σ_{xx} , Σ_{xy} , Σ_{yy} , the conditional p(x|y) is a Gaussian with mean $\mu_x + \Sigma_{xy} \Sigma_{yy}^{-1} (y - \mu_y)$ and covariance $\Sigma_{xx} - \Sigma_{xy} \Sigma_{yy}^{-1} \Sigma_{yx}$.

Appendix D. Collapsing Gaussians

The user may provide any algorithm of their choice for collapsing a set of Gaussians to a smaller set of Gaussians (Titterington et al., 1985). Here, to be explicit, we present a simple one which is fast, but has the disadvantage that no spatial information about the mixture is used.

First, we describe how to collapse a mixture to a *single* Gaussian: We may collapse a mixture of Gaussians $p(x) = \sum_i p_i \mathcal{N}(x|\mu_i, \Sigma_i)$ to a single Gaussian with mean $\sum_i p_i \mu_i$ and covariance $\sum_i p_i \left(\sum_i + \mu_i \mu_i^\mathsf{T} \right) - \mu \mu^\mathsf{T}$.

To collapse a mixture to a K-component mixture we retain the K-1 Gaussians with the largest mixture weights—the remaining N-K Gaussians are simply merged to a single Gaussian using the above method. The alternative of recursively merging the two Gaussians with the lowest mixture weights gave similar experimental performance.

More sophisticated methods which retain some spatial information would clearly be potentially useful. The method presented in Lerner et al. (2000) is a suitable approach which considers removing Gaussians which are spatially similar (and not just low-weight components), thereby retaining diversity over the possible solutions.

Appendix E. The Discrete-Continuous Factorization Viewpoint

An alternative viewpoint is to proceed analogously to the Rauch-Tung-Striebel correction method for the LDS (Grewal and Andrews, 1993):

$$p(h_{t}, s_{t}|v_{1:T}) = \sum_{s_{t+1}} \int_{h_{t+1}} p(s_{t}, h_{t}, h_{t+1}, s_{t+1}|v_{1:T})$$

$$= \sum_{s_{t+1}} p(s_{t+1}|v_{1:T}) \int_{h_{t+1}} p(h_{t}, s_{t}|h_{t+1}, s_{t+1}, v_{1:t}) p(h_{t+1}|s_{t+1}, v_{1:T})$$

$$= \sum_{s_{t+1}} p(s_{t+1}|v_{1:T}) \left\langle p(h_{t}|h_{t+1}, s_{t+1}, s_{t}, v_{1:t}) p(s_{t}|h_{t+1}, s_{t+1}, v_{1:t}) \right\rangle$$

$$\approx \sum_{s_{t+1}} p(s_{t+1}|v_{1:T}) \left\langle p(h_{t}|h_{t+1}, s_{t+1}, s_{t}, v_{1:t}) \right\rangle \underbrace{\left\langle p(s_{t}|s_{t+1}, v_{1:T}) \right\rangle}_{p(s_{t}|s_{t+1}, v_{1:T})}$$
(20)

where angled brackets $\langle \cdot \rangle$ denote averages with respect to $p(h_{t+1}|s_{t+1},v_{1:T})$. Whilst the factorized approximation in Equation (20) may seem severe, by comparing Equations (20) and (10) we see that it is equivalent to the apparently milder assumption $p(h_{t+1}|s_t,s_{t+1},v_{1:T}) \approx p(h_{t+1}|s_{t+1},v_{1:T})$. Hence this factorized approximation is equivalent to the 'standard' EC approach in which the dependency on s_t is dropped.

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