8

Switching Linear Dynamical Systems with Count Observations

The past two chapters have explored different notions of latent state: a dynamic network in Chapter 6 and a discrete latent state in Chapter 7. These states are a powerful addition to the autoregressive models of the earlier chapters. In this chapter, we consider one final extension — a continuous latent state that evolves over time. These continuous latent state space models are one of the most common methods in computational neuroscience (Smith and Brown, 2003; Paninski et al., 2010; Macke et al., 2011; Buesing et al., 2012a; Petreska et al., 2011; Cunningham and Yu, 2014).

The simplest form of continuous state space model assumes that the latent state obeys linear dynamics. Here, however, we will consider a more general case in which the dynamics are only *conditionally* linear given a dynamic discrete latent state (Petreska et al., 2011). This is known as a *switching* linear dynamical system (Murphy, 2012; Fox, 2009). By switching between different linear dynamical regimes, we obtain highly nonlinear patterns of dynamics. Moreover, this switching linear dynamical system will recover a number of common models as special cases.

The challenge, as should be expected by now, is in performing efficient inference in the face of discrete observations. The aforementioned existing methods have relied upon a

Laplace approximation, which approximates the conditional distribution with a Gaussian. Given the tools developed in previous chapters, we can now develop asymptotically exact Gibbs sampling algorithms. In particular, the Pólya-gamma augmentations introduced in Chapter 5 will make it easy to develop efficient algorithms that leverage many of the standard tools that exist for Gaussian observation models. Once we have augmented our observations with Pólya-gamma auxiliary variables, the observations are conditionally Gaussian distributed. Thus, all of our tools for efficient Bayesian inference in linear Gaussian models are at our disposal.

Finally, we will consider a problem that we have given little consideration thus far, namely, the problem of model comparison. We have tacitly assumed that predictive likelihoods provide a sufficient means of comparing two models. In practice, this has led to some difficulty, as we encountered with the network model comparison in Chapters 3 and 5. The root of the problem is that predictive likelihood comparisons only implicitly depend on model complexity. More complex models are more prone to overfitting, which should manifest itself in decreased predictive performance. However, there are more direct means of assessing the balance between model complexity and predictive capability. In theory, the marginal likelihood — the denominator in Bayes' rule — should provide a better estimate of the trade-off between how well a model fits the data and the size of the hypothesis class (MacKay, 1992; Kass and Raftery, 1995).

We will show how the conditionally conjugate models derived via Pólya-gamma augmentation enable principled marginal likelihood estimation with annealed importance sampling (AIS) (Neal, 2001). In order to make this practically feasible, however, we must dive into the inner workings of the Pólya-gamma distribution and develop a novel sampling algorithm capable of efficiently generating random variates in the "small shape" regime required by AIS.

8.1 A Hierarchy of Latent State Space Models

Consider a general class of models with a continuous latent state, $\boldsymbol{x}_t \in \mathbb{R}^D$, that obeys affine, but potentially nonstationary, dynamics at discrete time t,

$$\boldsymbol{x}_t \sim \mathcal{N}(\boldsymbol{A}_t \boldsymbol{x}_{t-1} + \boldsymbol{b}_t,\ \boldsymbol{\Sigma}_t).$$

Let the initial state distribution have mean $\boldsymbol{\mu}_1$. Furthermore, assume a linear activation model $\boldsymbol{\psi}_t = \boldsymbol{C}\boldsymbol{x}_t$, where the mean spike count, $s_{t,n}$ is a nonlinear function of the activation, $\psi_{t,n}$, and neuron-specific parameters, ν_n. We refer to the collection of model parameters as,

$$\boldsymbol{\theta} = \left\{ \{\boldsymbol{A}_t, \boldsymbol{b}_t, \boldsymbol{\Sigma}_t\}_{t=1}^T, \boldsymbol{\mu}_1, \boldsymbol{C}, \{\nu_n\}_{n=1}^N \right\}$$

Given these parameters, we can summarize this probabilistic model. In keeping with standard texts (e.g. Murphy, 2012, Chapter 18), we use "Matlab" notation to refer to a sequence of spike count vectors, $\boldsymbol{s}_{1:T}$, and a sequence of latent state vectors, $\boldsymbol{x}_{1:T}$. We have,

$$p(\boldsymbol{s}_{1:T}, \boldsymbol{x}_{1:T} \mid \boldsymbol{\theta}) = p(\boldsymbol{\theta})\, p(\boldsymbol{x}_{1:T} \mid \boldsymbol{\theta})\, p(\boldsymbol{s}_{1:T} \mid \boldsymbol{x}_{1:T}, \boldsymbol{\theta})$$

where

$$\begin{aligned} p(\boldsymbol{x}_{1:T} \mid \boldsymbol{\theta}) &= \mathcal{N}(\boldsymbol{x}_1 \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \prod_{t=2}^{T} \mathcal{N}(\boldsymbol{x}_t \mid \boldsymbol{A}_t \boldsymbol{x}_{t-1} + \boldsymbol{b}_t, \boldsymbol{\Sigma}_t) \\ p(\boldsymbol{s}_{1:T} \mid \boldsymbol{x}_{1:T}, \boldsymbol{\theta}) &= \prod_{t=1}^{T} p(\boldsymbol{s}_t \mid \boldsymbol{C}\boldsymbol{x}_t, \{\nu_n\}) \\ &= \prod_{t=1}^{T} \prod_{n=1}^{N} p(s_{t,n} \mid \psi_{t,n}, \nu_n). \end{aligned} \tag{8.1}$$

Now consider the special case where there are only $K < T$ unique dynamics and covariance matrices, $\{\boldsymbol{A}_k, \boldsymbol{b}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$, and that at any instant in time, the chosen dynamics are specified by the discrete latent variable $z_t \in \{1, \ldots, K\}$. Moreover, suppose this discrete

latent variable follows a Markov model with initial state distribution $\boldsymbol{\pi}_0$ and transition probabilities $\{\boldsymbol{\pi}_k\}_{k=1}^K$, as in the last chapter. Then the dynamics for $\boldsymbol{z}_{1:T}$ and $\boldsymbol{x}_{1:T}$ are,

$$p(\boldsymbol{z}_{1:T} \mid \boldsymbol{\theta}) = \text{Discrete}(z_1 \mid \boldsymbol{\pi}_0) \prod_{t=2}^{T} \text{Discrete}(z_t \mid \boldsymbol{\pi}_{z_{t-1}}).$$

$$p(\boldsymbol{x}_{1:T} \mid \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{x}_1 \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{z_1}) \prod_{t=2}^{T} \mathcal{N}(\boldsymbol{x}_t \mid \boldsymbol{A}_{z_t}\boldsymbol{x}_{t-1} + \boldsymbol{b}_{z_t}, \boldsymbol{\Sigma}_{z_t}),$$

This is a *switching linear dynamical system* (SLDS) model (Murphy, 2012; Fox, 2009). At any point in time, the latent state obeys linear dynamics. The particular choice of dynamics switches between K discrete values according to a Markov model.

The SLDS contains a number of other models as special cases:

- When there is only one discrete latent state ($K = 1$), this reduces to a standard linear dynamical system (LDS).
- When there is one discrete latent state and no continuous dynamics ($\boldsymbol{A}_k \equiv 0$), this reduces to factor analysis (FA).
- When (i) the state dimensionality is equal to the number of neurons ($D = N$); (ii) there are no continuous dynamics ($\boldsymbol{A}_k \equiv 0$); and (iii) the emission matrix is the identity ($\boldsymbol{C} \equiv \boldsymbol{I}$), the SLDS reduces to a hidden Markov model. At each point in time, the firing rate is determined solely by $\boldsymbol{b}_{z_t}$.
- When the the conditions of the HMM are met *and* the discrete transition matrix, $\boldsymbol{P}$, has identical rows ($\boldsymbol{\pi}_k \equiv \boldsymbol{\pi}_0$), the SLDS further reduces to a simple mixture model. At each point in time, the discrete latent state is drawn from $z_t \sim \text{Discrete}(\boldsymbol{\pi}_0)$.

The graphical models corresponding to these special cases are shown in Figure 8.1, with the omission of some model parameters to conserve space. This figure is adapted from Figure 2.2. The only model that is not captured here is the autoregressive model since, here, all interaction between spike counts arises through the latent state. Next we show how a single, unified algorithm can support efficient inference in the SLDS and all its special cases.

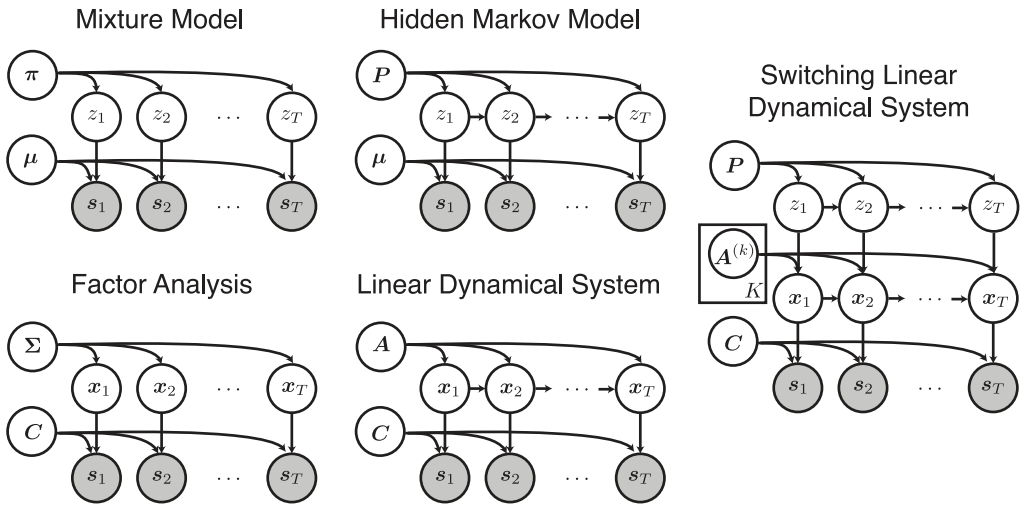

Figure 8.1: Special cases of the switching linear dynamical system. Adapted from Figure 2.2.

8.2 Markov chain Monte Carlo Inference

First we show how the continuous latent states, $\boldsymbol{x}_{1:T}$, can be updated with a block Gibbs sampler when the observations are conditionally Gaussian distributed. The key elements of the inference algorithm will be conserved when we move to discrete count observations. Given the Gaussian inference algorithm, we will show how the Pólya-gamma augmentation explored in Chapter 5 enables efficient Bayesian inference in discrete models as well.

8.2.1 Block Gibbs Sampling Latent States with Gaussian Observations

Suppose the spike counts, $\boldsymbol{s}_t$ are conditionally distributed according to a Gaussian distribution. Moreover, assume the distribution has nonstationary precision, $\boldsymbol{\Omega}_t$, such that

$$p(\boldsymbol{s}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{s}_t \mid \boldsymbol{C}\boldsymbol{x}_t, \boldsymbol{\Omega}_t^{-1}). \tag{8.2}$$

In this case, the conditional density over continuous latent states, $p(\boldsymbol{x}_{1:T} \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta})$, is jointly Gaussian as well. We perform a block Gibbs update for the entire latent state sequence, $\boldsymbol{x}_{1:T}$, using a forward filtering-backward sampling algorithm, just as we did for the HMM in Section 7.2.1.

The marginal "filtered" distribution given observations up to time t is a Gaussian, which we will denote by,

$$p(\boldsymbol{x}_t \mid \boldsymbol{s}_{1:t}, \boldsymbol{z}_{1:t}, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{x}_t \mid \boldsymbol{m}_t, \boldsymbol{V}_t),$$

where $\boldsymbol{m}_t$ and $\boldsymbol{V}_t$ are the filtered mean and covariance, respectively. Kalman filtering is an iterative for computing the filtered means and variances of a Gaussian linear dynamical system, and it is analogous to the HMM filtering algorithms of the previous chapter. Here, we follow the presentation of Murphy (2012, Chapter 18). Kalman filtering consists of iterating forward in time from $t = 1$ to $t = T$. Assume that at iteration t we have already computed $\boldsymbol{m}_{t-1}$ and $\boldsymbol{V}_{t-1}$. As with the HMM, given the Markovian structure of the probabilistic model, the conditional distribution of $\boldsymbol{x}_t$ factors into,

$$p(\boldsymbol{x}_t \mid \boldsymbol{s}_{1:t}, \boldsymbol{z}_{1:t}, \boldsymbol{\theta}) \propto \underbrace{p(\boldsymbol{s}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta})}_{\text{condition}} \underbrace{p(\boldsymbol{x}_t \mid \boldsymbol{s}_{1:t-1}, \boldsymbol{z}_{1:t}, \boldsymbol{\theta})}_{\text{predict}}.$$

We will show that both of these factors are Gaussian distributions, and hence their product is as well.

The first step is to *predict* $\boldsymbol{x}_t$ given observations $\boldsymbol{s}_{1:t-1}$. To do so, we marginalize over the previous latent state, $\boldsymbol{x}_{t-1}$,

$$\begin{aligned} p(\boldsymbol{x}_t \mid \boldsymbol{s}_{1:t-1}, \boldsymbol{z}_{1:t}, \boldsymbol{\theta}) &\propto \int p(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, z_t, \boldsymbol{\theta})\, p(\boldsymbol{x}_{t-1} \mid \boldsymbol{s}_{1:t-1}, \boldsymbol{z}_{1:t-1}, \boldsymbol{\theta})\, \mathrm{d}\boldsymbol{x}_{t-1} \\ &= \mathcal{N}(\boldsymbol{x}_t \mid \boldsymbol{m}_{t|t-1}, \boldsymbol{V}_{t|t-1}), \end{aligned}$$

where

$$\begin{aligned} \boldsymbol{m}_{t|t-1} &\triangleq \boldsymbol{A}_t \boldsymbol{m}_{t-1} + \boldsymbol{b}_t \\ \boldsymbol{V}_{t|t-1} &\triangleq \boldsymbol{A}_t \boldsymbol{V}_{t-1} \boldsymbol{A}_t^\mathsf{T} + \boldsymbol{\Sigma}_t. \end{aligned}$$

Then, we *condition* on the current observations, $\boldsymbol{s}_t$, to get the parameters of the filtered

distribution,

$$\begin{aligned} \boldsymbol{m}_t &= \boldsymbol{m}_{t|t-1} + \boldsymbol{K}_t(\boldsymbol{s}_t - \boldsymbol{C}\boldsymbol{m}_{t|t-1}) \\ \boldsymbol{V}_t &= (\boldsymbol{I} - \boldsymbol{K}_t\boldsymbol{C})\boldsymbol{V}_{t|t-1}, \end{aligned} \tag{8.3}$$

where $\boldsymbol{K}_t$ is the "Kalman gain" matrix,

$$\boldsymbol{K}_t \triangleq \boldsymbol{V}_{t|t-1}\boldsymbol{C}^\mathsf{T}\left[\boldsymbol{C}\boldsymbol{V}_{t|t-1}\boldsymbol{C}^\mathsf{T} + \boldsymbol{\Omega}_t^{-1}\right]^{-1}.$$

Once we have computed the filtered means and covariances for all time bins, we can sample from the joint distribution over $\boldsymbol{x}_{1:T}$ by applying the chain rule,

$$\begin{aligned} p(\boldsymbol{x}_{1:T} \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) &= p(\boldsymbol{x}_T \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) \prod_t p(\boldsymbol{x}_t \mid \boldsymbol{x}_{t+1:T}, \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) \\ &\propto p(\boldsymbol{x}_T \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) \prod_t p(\boldsymbol{x}_t \mid \boldsymbol{s}_{1:t}, \boldsymbol{z}_{1:t}, \boldsymbol{\theta})\, p(\boldsymbol{x}_{t+1} \mid \boldsymbol{x}_t, z_{t+1}, \boldsymbol{\theta}). \end{aligned}$$

Thus, we can sample in reverse order, starting with $\boldsymbol{x}_T$ and ending with $\boldsymbol{x}_1$. The conditional distribution of $\boldsymbol{x}_t$

$$p(\boldsymbol{x}_t \mid \boldsymbol{x}_{t+1:T}, \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) \propto \mathcal{N}(\boldsymbol{x}_t \mid \boldsymbol{m}_t, \boldsymbol{V}_t)\, \mathcal{N}(\boldsymbol{x}_{t+1} \mid \boldsymbol{A}_{t+1}\boldsymbol{x}_t + \boldsymbol{b}_{t+1}, \boldsymbol{\Sigma}_{t+1}), \tag{8.4}$$

which is yet another Gaussian distribution. Now we can write the complete algorithm for block Gibbs sampling the continuous latent states, $\boldsymbol{x}_{1:T}$.

Require: $\boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}$
  for $t = 1, \ldots, T$ **do**
    Compute $\boldsymbol{m}_t$ and $\boldsymbol{V}_t$ ▷ Eq. 8.3
  end for
  for $t = T, \ldots, 1$ **do**
    Sample $\boldsymbol{x}_t \mid \boldsymbol{x}_{t+1}, \boldsymbol{m}_t, \boldsymbol{V}_t, \boldsymbol{\theta}$ ▷ Eq. 8.4
  end for

Algorithm 8.1: Forward filtering-backward sampling (FFBS) algorithm for the Gaussian linear dynamical system. Note the similarity to the FFBS algorithm for HMMs in Alg. 7.1.

8.2.2 Pólya-gamma Augmentation for Discrete Observations

The conditional distribution of the latent states is only Gaussian if the observations are as well. Fortunately, the observations become conditionally Gaussian after augmenting the data with Pólya-gamma auxiliary variables. Recall from Chapter 5 that the Pólya-gamma augmentation is an auxiliary variable scheme that applies to models with logistic link functions (Polson et al., 2013). Specifically, this augmentation can be used to develop Gibbs for models with likelihoods of the form,

$$\begin{aligned} p(s \mid \psi, \nu) &= c(s, \nu)\, \sigma(\psi)^{a(s,\nu)}\, (1 - \sigma(\psi))^{d(s,\nu)} \\ &= c(s, \nu) \frac{(e^{\psi})^{a(s,\nu)}}{(1 + e^{\psi})^{b(s,\nu)}}. \end{aligned}$$

These are called *logistic likelihoods* because the latent variables are transformed by a logistic function, $\sigma(\psi) = e^{\psi}/(1 + e^{\psi})$. Bernoulli, binomial, negative binomial, and multinomial likelihoods can all be put in this form. For example, in the Bernoulli case,

$$\mathrm{Bern}(s \mid \psi) = \sigma(\psi)^s (1 - \sigma(\psi))^{1-s} = \frac{(e^{\psi})^s}{(1 + e^{\psi})}.$$

Thus, $a(s, \nu) = s, b(s, \nu) \equiv 1$, and $c(s, \nu) \equiv 1$. We refer the reader back to Table 5.1 for the formulation of other count distributions.

The augmentation is based on an integral identity derived from the Laplace transform of the Pólya-gamma density. If $p_{\mathrm{PG}}(\omega \mid b, 0)$ is the density of the Pólya-gamma distribution, $\mathrm{PG}(b, 0)$, then,

$$\frac{(e^{\psi})^a}{(1 + e^{\psi})^b} = 2^{-b} e^{\kappa\psi} \int_0^{\infty} e^{-\omega\psi^2/2}\, p_{\mathrm{PG}}(\omega \mid b, 0)\, \mathrm{d}\omega, \tag{8.5}$$

where $\kappa = a - b/2$. The integral on the right-hand side is the Laplace transform of the Pólya-gamma density evaluated at $\psi^2/2$, and the left-hand side is the same form found in discrete distributions with logistic link functions. Importantly, viewed as a function of ψ for fixed ω, the right-hand side is an unnormalized Gaussian density. Thus, the identity in (8.5) transforms a logistic likelihood to a Gaussian likelihood conditioned on an auxiliary

variable, ω.

Now, let us return to the likelihood of (8.1), where $\psi_{t,n} = [\boldsymbol{C}\boldsymbol{x}_t]_n = \boldsymbol{c}_n^\mathsf{T}\boldsymbol{x}_t$ is the activation of neuron n at time t. As a function of $\boldsymbol{x}_t$, the likelihood is proportional to,

$$\begin{aligned} p(\boldsymbol{s}_t \,|\, \boldsymbol{x}_t, \boldsymbol{\theta}) &\propto \prod_{n=1}^{N} \frac{(e^{\psi_{t,n}})^{a(s_{t,n},\nu_n)}}{(1+e^{\psi_{t,n}})^{b(s_{t,n},\nu_n)}} \\ &\propto \prod_{n=1}^{N} e^{\kappa(s_{t,n},\nu_n)\psi_{t,n}} \int_0^\infty e^{-\omega_{t,n}\psi_{t,n}^2/2}\, p_{\mathrm{PG}}(\omega_{t,n} \,|\, b(s_{t,n},\nu_n), 0)\, \mathrm{d}\omega_{t,n}. \end{aligned}$$

By introducing $\omega_{t,n}$ as auxiliary variables, the likelihood of $\boldsymbol{x}_t$ is proportional to a multivariate Gaussian distribution,

$$\begin{aligned} p(\boldsymbol{s}_t \,|\, \boldsymbol{x}_t, \boldsymbol{\omega}_t, \{\nu_n\}) &\propto \prod_{n=1}^{N} \mathcal{N}(\boldsymbol{c}_n^\mathsf{T}\boldsymbol{x}_t \,|\, \omega_{t,n}^{-1}\kappa(s_{t,n},\nu_n),\, \omega_{t,n}^{-1}) \\ &\propto \mathcal{N}(\widehat{\boldsymbol{s}}_t \,|\, \boldsymbol{C}\boldsymbol{x}_t,\, \boldsymbol{\Omega}_t^{-1}), \end{aligned} \tag{8.6}$$

where

$$\begin{aligned} \boldsymbol{\kappa}_t &= [\kappa(s_{t,1},\nu_1), \ldots, \kappa(s_{t,N},\nu_N)]^\mathsf{T} \\ \widehat{\boldsymbol{s}}_t &= \boldsymbol{\Omega}_t^{-1}\boldsymbol{\kappa}_t \\ \boldsymbol{\Omega}_t &= \mathrm{diag}\left([\omega_{t,1}, \ldots, \omega_{t,N}]\right). \end{aligned}$$

Note the similarity between the augmented likelihood of (8.6) and the Gaussian likelihood of (8.2). The only difference is that, here, the precision is given by the auxiliary variables, and the "effective" observations, $\widehat{s}_{t,n}$, are a function of $s_{t,n}$, $\omega_{t,n}$, and ν_n. Thus, given a set of Pólya-gamma auxiliary variables, the block Gibbs updates in Algorithm 8.1 will apply equally well to the setting with discrete count observations.

Moreover, by the exponential tilting property of the Pólya-gamma distribution, the

conditional distribution of $\omega_{t,n}$ is proportional to a Pólya-gamma distribution:

$$\begin{aligned} p(\omega_{t,n} \mid \psi_{t,n}, s_{t,n}, \nu_n) &\propto e^{-\omega_{t,n}\psi_{t,n}^2/2}\, p_{\mathrm{PG}}(\omega_{t,n} \mid b(s_{t,n}, \nu_n),\, 0) \\ &\propto p_{\mathrm{PG}}(\omega_{t,n} \mid b(s_{t,n}, \nu_n),\, \psi_{t,n}). \end{aligned} \tag{8.7}$$

These auxiliary variables are conditionally independent of each other, and hence amenable to block parallel Gibbs sampling. Efficient Pólya-gamma sampling algorithms have been developed for the regimes typically encountered in Bernoulli, binomial, and negative binomial models (Windle et al., 2014).

The proposed algorithm for sampling the latent variables and parameters of an SLDS is summarized in Algorithm 8.2.

Require: $\boldsymbol{s}_{1:T}$ and $\boldsymbol{z}_{1:T}, \boldsymbol{x}_{1:T}$, and $\boldsymbol{\theta}$ from previous iteration
  Sample $\boldsymbol{\theta} \mid \boldsymbol{z}_{1:T}, \boldsymbol{x}_{1:T}, \boldsymbol{s}_{1:T}$
  Sample $\boldsymbol{z}_{1:T} \mid \boldsymbol{x}_{1:T}, \boldsymbol{\theta}$ ▷ Algorithm 7.1
  for $t = 1, \ldots, T$ **do** ▷ In parallel
    for $n = 1, \ldots, N$ **do** ▷ In parallel
      Sample $\omega_{t,n} \mid s_{t,n}, \boldsymbol{x}_t, \boldsymbol{\theta}$ ▷ Eq. 8.7
    end for
  end for
  Compute $\boldsymbol{\Omega}_{1:T}$ and $\widehat{\boldsymbol{s}}_{1:T}$ ▷ Eq. 8.6
  Sample $\boldsymbol{x}_{1:T} \mid \widehat{\boldsymbol{s}}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\Omega}_{1:T}, \boldsymbol{\theta}$ ▷ Algorithm 8.1

Algorithm 8.2: Single iteration of Gibbs sampler for an switching LDS with discrete count observations.

8.2.3 Missing Data

Sometimes we only have partial observations. For example, in some cases we have multiple recordings from the same circuit, but each recording only provides access to a subset of the population of neurons (Turaga et al., 2013). In other cases, we simply hold out some of the data for predictive likelihood comparisons. With Gaussian observations, we can implement this by replacing the missing data point, $s_{t,n}$, with a zero mean, zero precision observation. In the discrete count model, this can be implemented by setting the auxiliary variable, $\omega_{t,n}$, and the effective observation, $\widehat{s}_{t,n}$, to zero. Recall that the Pólya-gamma auxiliary variables

specify the precision of the effective observations. By setting this to zero, we effectively remove this data point.

8.3 Alternative Approaches

Most alternative approaches to performing Bayesian inference in latent state space models with discrete observations have relied on a Laplace approximation (Tierney and Kadane, 1986) to the conditional distribution, $p(\boldsymbol{x}_{1:T} \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta})$ (Smith and Brown, 2003; Paninski et al., 2010; Macke et al., 2011). * Given a Gaussian approximation, the model parameters, $\boldsymbol{\theta}$, can be optimized such that they maximize the *expected* joint log probability under the approximate Gaussian distribution on $\boldsymbol{x}_{1:T}$. This constitutes an approximate expectation-maximization (EM) algorithm (Dempster et al., 1977).

For completeness, we describe the fundamentals of this approach, largely following the presentation of Macke et al. (2011). Consider a generative model in which $s_{t,n} \sim \mathrm{Poisson}(\exp\{\boldsymbol{c}_n^\mathsf{T}\boldsymbol{x}_t\})$. The conditional log probability of $\boldsymbol{x}_{1:T}$ is given by,

$$\begin{aligned}\log p(\boldsymbol{x}_{1:T} \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) \simeq &\sum_{t=1}^{T}\sum_{n=1}^{N} s_{t,n}(\boldsymbol{c}_n^\mathsf{T}\boldsymbol{x}_t) - \exp\{\boldsymbol{c}_n^\mathsf{T}\boldsymbol{x}_t\} + \\ &- \frac{1}{2}(\boldsymbol{x}_1 - \boldsymbol{\mu}_1)^\mathsf{T}\boldsymbol{\Sigma}_{z_1}^{-1}(\boldsymbol{x}_1 - \boldsymbol{\mu}_1) + \\ &- \frac{1}{2}\sum_{t=2}^{T}(\boldsymbol{x}_t - \boldsymbol{A}_{z_t}\boldsymbol{x}_{t-1} - \boldsymbol{b}_{z_t})^\mathsf{T}\boldsymbol{\Sigma}_{z_t}^{-1}(\boldsymbol{x}_t - \boldsymbol{A}_{z_t}\boldsymbol{x}_{t-1} - \boldsymbol{b}_{z_t}),\end{aligned}$$

where $\simeq$ denotes equality up to an additive constant. This log probability is concave and can be efficiently maximized to obtain the mean of the Laplace approximation,

$$\boldsymbol{\mu}^* = \arg\max_{\boldsymbol{x}_{1:T}} \log p(\boldsymbol{x}_{1:T} \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}).$$

Once the mean has been found, the optimal covariance is given by the inverse Hessian of

* While the Laplace approximation is most common, see Buesing et al. (2012b) and Pfau et al. (2013) for some interesting new directions.

the log posterior evaluated at $\boldsymbol{\mu}^*$,

$$\boldsymbol{\Sigma}^* = -\left[\nabla^2_{\boldsymbol{x}_{1:T}} \log p(\boldsymbol{x}_{1:T} \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) \Big|_{\boldsymbol{x}_{1:T}=\boldsymbol{\mu}^*}\right]^{-1}.$$

By exploiting the chain structure of the graphical model, this inverse Hessian can be computed in time linear in T using essentially the same forward-backward approaches used during sampling.

The mean and covariance parameterize a Gaussian approximation,

$$p(\boldsymbol{x}_{1:T} \mid \boldsymbol{s}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta}) \approx q(\boldsymbol{x}_{1:T}) = \mathcal{N}(\boldsymbol{x}_{1:T} \mid \boldsymbol{\mu}^*, \boldsymbol{\Sigma}^*).$$

Given this approximation, the parameters are updated by maximizing the expected log probability,

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathbb{E}_q \left[\log p(\boldsymbol{s}_{1:T}, \boldsymbol{x}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta})\right].$$

For example, consider this expectation as a function of the emission matrix, $\boldsymbol{C}$,

$$\begin{aligned}
\mathbb{E}_q \left[\log p(\boldsymbol{s}_{1:T}, \boldsymbol{x}_{1:T}, \boldsymbol{z}_{1:T}, \boldsymbol{\theta})\right] &\simeq \sum_{t=1}^{T} \sum_{n=1}^{N} s_{t,n} (\boldsymbol{c}_n^\mathsf{T} \mathbb{E}_q[\boldsymbol{x}_t]) - \mathbb{E}_q \left[\exp\{\boldsymbol{c}_n^\mathsf{T} \boldsymbol{x}_t\}\right], \\
&= \sum_{t=1}^{T} \sum_{n=1}^{N} s_{t,n} (\boldsymbol{c}_n^\mathsf{T} \boldsymbol{\mu}_t^*) - \exp\left\{\boldsymbol{c}_n^\mathsf{T} \boldsymbol{\mu}_t^* + \frac{1}{2} \boldsymbol{c}_n^\mathsf{T} \boldsymbol{\Sigma}_{tt}^* \boldsymbol{c}_n\right\}.
\end{aligned}$$

The last line follows from the moment generating function of the multivariate Gaussian distribution. This objective function is concave in $\boldsymbol{c}_n$. Note that closed form, concave expectations arise from the particular choice of exponential link function. Other models may require Monte Carlo estimates of the expectation inside the optimization. As more and more approximation is required, the performance of these methods tends to suffer.

Finally, we must handle the discrete latent states, $\boldsymbol{z}_{1:T}$. The simplest approach would be to alternate between updating the discrete and continuous latent states, as in the MCMC algorithm presented above. Alternatively, Petreska et al. (2011) have suggested a joint update

for both $\boldsymbol{x}_{1:T}$ and $\boldsymbol{z}_{1:T}$ based on an approximate filtering technique.

From our perspective, the principal advantages of the Pólya-gamma augmentation are: (i) it allows for simple block Gibbs updates that leverage off-the-shelf code for Gaussian models; (ii) it provides an asymptotically unbiased MCMC algorithm; (iii) the stochasticity of the MCMC transitions allows the sampling algorithm to escape local modes, to which expectation-maximization algorithms are prone (Bishop, 2006); and (iv) once we have an MCMC algorithm, a number of natural extensions are clear, like the marginal likelihood estimation methods we discuss next.

8.4 Model Comparison via Marginal Likelihood Estimation

The marginal likelihood is the probability of the data, $\boldsymbol{s}$, having integrated out the latent variables, $\boldsymbol{z}$ and $\boldsymbol{x}$, and the parameters, $\boldsymbol{\theta}$,

$$p(\boldsymbol{s}) = \int p(\boldsymbol{s} \mid \boldsymbol{z}, \boldsymbol{x}, \boldsymbol{\theta})\, p(\boldsymbol{z}, \boldsymbol{x}, \boldsymbol{\theta})\, \mathrm{d}\boldsymbol{z}\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{\theta}.$$

By integrating over the latent variables and parameters, the marginal likelihood captures a tradeoff between a model's complexity and its ability to explain the data. As such, it is a natural criterion for model comparison. In some cases, like linear Gaussian models with Gaussian observations, the marginal likelihood can be computed exactly. In these cases, marginal likelihood is often the gold-standard for model selection (Kass and Raftery, 1995; Grosse et al., 2015).

Unfortunately, seemingly small changes to the model can render the integration over parameters and latent variables intractable. For example, in linear Gaussian models with discrete observations, the marginal likelihood is no longer tractable. Instead, we must resort to approximate methods like annealed importance sampling (AIS) (Neal, 2001). AIS is based on sampling from a sequence of intermediate distributions that *anneal* between a tractable distribution and the intractable posterior. While AIS has proven highly effective for a variety of models (Grosse et al., 2015), the accuracy of the method hinges upon the efficiency of the Markov transition operators that target the intermediate distributions. Unfortunately, while the posterior distribution may admit efficient MCMC algorithms, the intermediate distributions may not. We show how the Pólya-gamma augmentation strategies above can

be extended to perform efficient annealed importance sampling in the class of switching linear dynamical systems models with count observations.

8.4.1 Annealed Importance Sampling

AIS starts with a sample from a tractable distribution with a computable normalization constant. The prior distribution often suffices. Given this initial sample, a sequence of Markov transition operators is applied. The stationary distributions of these transition operators interpolate between the tractable initial distribution and the intractable posterior. The posterior density is proportional to the joint density, and the normalizing constant is the marginal likelihood of interest. Formally, the annealing path is a sequence of distributions, $q_1(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x})$ to $q_M(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x}) = p(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x} \mid \boldsymbol{s})$, where

$$q_m(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x}) = \frac{f_m(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x})}{\mathcal{Z}_m}, \qquad f_M(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x}) = p(\theta, \boldsymbol{z}, \boldsymbol{x}, \boldsymbol{s}), \qquad \mathcal{Z}_M = p(\boldsymbol{s}).$$

Let $q_1(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x})$ be the normalized prior distribution such that $f_1(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x}) = p(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x})$ and $\mathcal{Z}_1 = 1$. Then, let $f_m(\boldsymbol{z}, \theta)$ be a geometric average of the prior and the joint:

$$\begin{aligned} f_m(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x}) &= \Big[p(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x})\Big]^{1-\beta_m} \Big[p(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x}, \boldsymbol{s})\Big]^{\beta_m} \\ &= p(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x})\, p(\boldsymbol{s} \mid \boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x})^{\beta_m}, \end{aligned}$$

with β_m monotonically increasing from $\beta_1 = 0$ to $\beta_M = 1$. As we anneal between $\beta = 0$ and $\beta = 1$, the intermediate distributions interpolate between the prior and the posterior. This geometric path is most common, but any path that starts with a tractable distribution and ends with the posterior will suffice (e.g. Grosse et al., 2013).

In addition to a annealing path, we also need a sequence of MCMC transition operators that leave the intermediate distributions q_m invariant,

$$\mathcal{T}_m(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x} \to \boldsymbol{\theta}', \boldsymbol{z}', \boldsymbol{x}').$$

Starting with a sample from the prior and applying these transition operators for $m = 1, \ldots, M$ yields a sample that is closer in distribution to the posterior. AIS uses

this procedure as a proposal distribution for importance sampling. The importance weights are given by a product of ratios between f_m and f_{m-1}. Since the target density is the unnormalized posterior density, the importance weights will be unbiased estimates of the normalization constant, namely the marginal likelihood, $\mathcal{Z}_M = p(\boldsymbol{s})$. The annealed importance sampling algorithm is summarized in Algorithm 8.3.

for $\ell = 1$ to L **do**
  $w^{(\ell)} \leftarrow \mathcal{Z}_1$
  Sample $\boldsymbol{\theta}^{(1)}, \boldsymbol{z}^{(1)}, \boldsymbol{x}^{(1)} \sim q_1(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x})$
  for $m = 2$ to M **do**
    $w^{(\ell)} \leftarrow w^{(\ell)} \times \frac{f_m(\boldsymbol{\theta}^{(m-1)}, \boldsymbol{z}^{(m-1)}, \boldsymbol{x}^{(m-1)})}{f_{m-1}(\boldsymbol{\theta}^{(m-1)}, \boldsymbol{z}^{(m-1)}, \boldsymbol{x}^{(m-1)})}$
    Sample $\boldsymbol{\theta}^{(m)}, \boldsymbol{z}^{(m)}, \boldsymbol{x}^{(m)} \sim \mathcal{T}_m(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x} \leftarrow \boldsymbol{\theta}^{(m-1)}, \boldsymbol{z}^{(m-1)}, \boldsymbol{x}^{(m-1)})$
  end for
end for
return $\widehat{\mathcal{Z}}_M = \frac{1}{L} \sum_{\ell=1}^{L} w^{(\ell)}$

Algorithm 8.3: Annealed Importance Sampling (AIS). Adapted from (Grosse et al., 2015).

How can we reduce the variance of this estimator? First, we can increase the number of intermediate distributions; second, we can design rapidly mixing transition operators, $\mathcal{T}_m$. In this section, we develop transition operators that are both computationally efficient, allowing us to run more transitions in a fixed amount of time, and more effective, in that they reach the equilibrium distribution more quickly.

With a geometric annealing path, the intermediate distributions of the switching LDS are given by,

$$f_m(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x}) = p(\boldsymbol{\theta}, \boldsymbol{z}, \boldsymbol{x}) \prod_{t=1}^{T} \prod_{n=1}^{N} c(s_{t,n}, \nu_n)^{\beta_m} \frac{(e^{\psi_{t,n}})^{a(s_{t,n},\nu_n)\cdot\beta_m}}{(1+e^{\psi_{t,n}})^{b(s_{t,n},\nu_n)\cdot\beta_m}}. \tag{8.8}$$

where, again, ν_n is a parameter in $\boldsymbol{\theta}$, and $\psi_{t,n}$ is a function of $\boldsymbol{x}$ and $\boldsymbol{\theta}$. Raising the likelihood to the power β_m does change its functional form; it only changes the power in the exponent. Most importantly, it is still amenable to Pólya-gamma augmentation! Thus, the Gibbs sweep defined in Algorithm 8.2 can be used as a transition operator, $\mathcal{T}_m$. The only

differences in targeting f_m are that,

$$\kappa(s_{t,n}, \nu_n) = \left(a(s_{t,n}, \nu) - \frac{1}{2} b(s_{t,n}, \nu_n)\right) \cdot \beta_m,$$

and

$$p(\omega_{t,n} \mid \psi_{t,n}, s_{t,n}, \nu_n) \propto p_{\mathrm{PG}}(\omega_{t,n} \mid \underbrace{b(s_{t,n}, \nu_n) \cdot \beta_m}_{\text{often } <1}, \psi_{t,n}).$$

This provides some intuition into how AIS works. When β_m approaches zero, the intermediate distribution reduces to the prior. This is equivalent to setting κ and ω to zero. As $b \to 0$, the density Pólya-gamma density, $\mathrm{PG}(\omega \mid b, \psi)$, approaches a delta function at zero.

Note, however, that in order to implement $\mathcal{T}_m$ efficiently, we must be able to sample from the Pólya-gamma conditional distribution in the regime where $b(s_{t,n}, \nu_n) \cdot \beta_m < 1$. For Bernoulli observations, $b(s_{t,n}, \nu_n) \equiv 1$, so we will be in this regime for all $\beta_m \in [0, 1)$. While efficient samplers exist for Pólya-gamma distributed variables when $b(s_{t,n}, \nu_n) \cdot \beta_m \geq 1$ (Windle et al., 2014), the default method for this "small shape" regime is to approximate a Pólya-gamma sample with a truncated sum of gamma random variates (Polson et al., 2013). As the number of random variates in the sum approaches infinity, the approximate sample converges to a true draw from the Pólya-gamma distribution. To get a reasonably accurate draw, we typically need to sample around 200 gamma random variates per Pólya-gamma sample. With TN auxiliary variables, this quickly becomes prohibitively expensive. Next, we develop a novel sampling algorithm that makes these conditional updates very efficient, and renders AIS with Pólya-gamma augmented transitions highly effective.

8.5 A Novel Sampling Algorithm for the Pólya-gamma Distribution

The Pólya-gamma distribution, $\mathrm{PG}(b, \psi)$, is closely related to the Jacobi distribution, $J^*(b, \psi)$, surveyed by Biane et al. (2001) and elaborated upon in Windle et al. (2014).

Specifically,

$$Y \sim J^*(b, \tfrac{\psi}{2}) \implies \frac{1}{4}Y \sim \mathrm{PG}(b, \psi).$$

Thus, to develop a sampler for the Pólya-gamma distribution, it is sufficient to be able to sample the Jacobi distribution.

As derived by Windle et al. (2014), the density of $J^*(b, \psi)$ can be written as an infinite alternating sum,

$$p_{J^*}(\omega \mid b, \psi) = \cosh^b(\psi) e^{-\omega\psi^2/2} \frac{2^b}{\Gamma(b)} \sum_{n=0}^{\infty} (-1)^n \frac{\Gamma(n+b)}{\Gamma(n+1)} \frac{(2n+b)}{\sqrt{2\pi\omega^3}} \exp\left\{-\frac{(2n+b)^2}{2\omega}\right\}. \quad (8.9)$$

Windle et al. (2014) developed a number of methods for sampling this distribution. Most rely on finding tractable upper bounds on the density that can serve as a proposal distribution. Given a sample from the proposal, it is possible to accept or reject using the *alternating series method* (Devroye, 1986). We will go into more detail on this shortly.

We take the same basic approach, but we present a novel means of finding an upper bound on the Jacobi density. Massaging terms in (8.9), we can factor it into the product of three terms:

$$p_{J^*}(\omega \mid b, \psi) = \alpha^{-1}(b, \psi)\, p_{\mathrm{IG}}\left(\omega \,\middle|\, \frac{b}{|\psi|},\, b^2\right) \Phi(\omega \mid b). \quad (8.10)$$

The first term, $\alpha^{-1}(b, \psi)$, is a scaling constant greater than one,

$$\alpha^{-1}(b, \psi) = 2^b \cosh^b(\psi)\, e^{-b|\psi|} = \left(1 + e^{-2|\psi|}\right)^b \geq 1.$$

The second is an inverse Gaussian density,

$$p_{\mathrm{IG}}\left(\omega \,\middle|\, \frac{b}{|\psi|},\, b^2\right) = \frac{b}{\sqrt{2\pi\omega^3}} \exp\left\{-\frac{\psi^2}{2\omega}\left(\omega - \frac{b}{|\psi|}\right)^2\right\}.$$

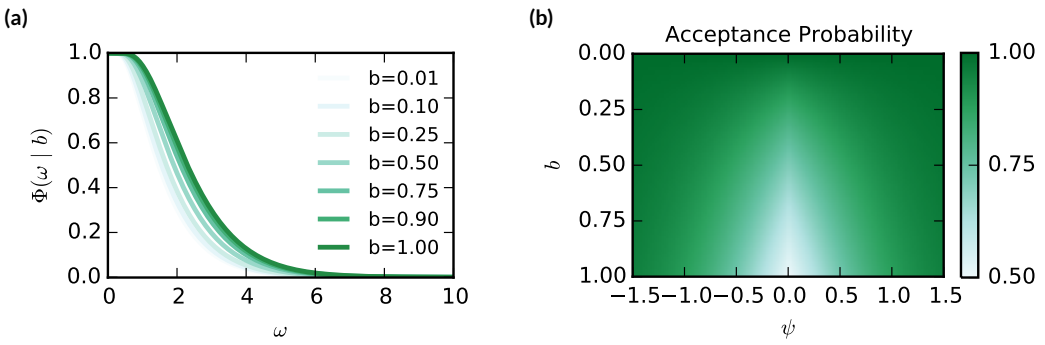

Figure 8.2: **(a)** Plot of $\Phi(\omega \mid b)$, the conditional acceptance probability for a proposed value of ω, for a range of $b \in (0, 1]$. In all cases, this function is monotonically decreasing from 1 to 0 as a function of ω, and thus defines a cumulative distribution function. **(b)** Acceptance probability, $\alpha(b, \psi)$, as a function of b and ψ.

When $\psi = 0$, the inverse Gaussian density reduces to an inverse gamma density,

$$p_{\text{IGa}}(\omega \mid \tfrac{1}{2}, \tfrac{b^2}{2}) = \frac{b}{\sqrt{2\pi\omega^3}} \exp\left\{-\frac{b^2}{2\omega}\right\}.$$

Finally, the third term we have called $\Phi(\omega \mid b)$,

$$\begin{aligned}\Phi(\omega \mid b) &= \sum_{n=0}^{\infty} (-1)^n \phi_n(\omega \mid b) \\ \phi_n(\omega \mid b) &= \frac{\Gamma(n+b)}{\Gamma(n+1)} \frac{2n+b}{\Gamma(b+1)} \exp\left\{-\frac{2n(n+b)}{\omega}\right\},\end{aligned}$$

where each term, $\phi_n(\omega \mid b)$, is nonnegative, and $\phi_0(\omega \mid b) = 1$.

Figure 8.2a plots $\Phi(\omega \mid b)$ for various values of b. In all cases, it appears that $\Phi(\omega \mid b)$ is monotonically decreasing and its range is $[0, 1]$. We have not proven this, but our numerical experiments suggest that it is true. We formalize this as a conjecture:

Conjecture 1. *For all $b > 0$, $\Phi(\omega \mid b)$ is a monotonically decreasing function of ω with,*

$$\lim_{0 \leftarrow \omega} \Phi(\omega \mid b) = 1,$$
$$\textit{and,} \quad \lim_{\omega \to \infty} \Phi(\omega \mid b) = 0.$$

Assuming this conjecture is true, as our plots suggest, all three terms in (8.10) are

nonnegative. With $\Phi(\omega \mid b) \leq 1$, the product $\alpha^{-1}(b, \psi)\, p_{\text{IG}}(\omega \mid \frac{b}{|\psi|}, b^2)$ must dominate $p_{J^*}(\omega \mid b, \psi)$. Thus, the inverse Gaussian is a natural proposal distribution for a rejection sampling algorithm. To determine whether a proposed value of ω is accepted, we must sample $u \sim \text{Unif}(0, 1)$, and check whether $u < \Phi(\omega \mid b)$.

The acceptance probability is $\alpha(b, \psi)$, the inverse of the scaling constant. It is bounded between $[\frac{1}{2}, 1]$ when $b \leq 1$. The lower bound (worst case) is achieved when $\psi = 0$ and $b = 1$. The upper bound (best case) is approached as b goes to zero or $|\psi|$ goes to infinity. This is illustrated in Figure 8.2b for a range of b and ψ. In fact, this rejection sampling algorithm works for $b \geq 1$ as well, but as b increases, the acceptance probability goes to zero. For this regime, the existing approaches of Windle et al. (2014) are a better choice.

Determining acceptance In order to determine whether to accept or reject a proposed value of ω, we need to compare against $\Phi(\omega \mid b)$. This function is not analytically tractable; however, it is still possible to determine whether or not to accept with finite computation. To do so, we use a slight modification of the alternating series method (Devroye, 1986). We exploit the fact that $\Phi(\omega \mid b)$ is an alternating sum, and the terms, $\phi_n(\omega \mid b)$, are eventually monotonically decreasing as a function of the index n for all fixed values of ω and b. We formalize this with the following lemma,

Lemma 1. *For all fixed values of ω and b,*

$$\exists m : \forall n \geq m : \phi_{n+1}(\omega \mid b) < \phi_n(\omega \mid b).$$

Proof. We show that the ratio of ϕ_{n+1} to ϕ_n is a decreasing function whose limit is zero.

$$\begin{aligned}
\frac{\phi_{n+1}(\omega \mid b)}{\phi_n(\omega \mid b)} &= \frac{\Gamma(n+1)\Gamma(n+1+b)(2n+2+b)\exp\left\{-\frac{2(n+1)(n+1+b)}{\omega}\right\}}{\Gamma(n+2)\Gamma(n+b)(2n+b)\exp\left\{-\frac{2n(n+b)}{\omega}\right\}} \\
&= \frac{(n+b)(2n+b+2)}{(n+1)(2n+b)}\exp\left\{-\frac{4n+2b+2}{\omega}\right\} \\
&= \ell(n)r(n),
\end{aligned}$$

where

$$\begin{aligned}\ell(n) &= \frac{2n^2 + nb + 2n + b + 2(n+1)b + b^2}{2n^2 + nb + 2n + b} \\ &= 1 + \mathcal{O}\left(\tfrac{1}{n}\right), \\ r(n) &= \exp\left\{-\frac{4n + 2b + 2}{\omega}\right\}.\end{aligned}$$

Observe that $\ell(n)$ is monotonically decreasing toward one as n approaches infinity. The rate of convergence is inverse polynomial in n. In contrast, $r(n)$ decreases to zero exponentially quickly as n approaches infinity. Thus, there exists a threshold m such that this ratio is less than one for all $n \geq m$. Equivalently,

$$\forall\, n \geq m :\ \phi_{n+1}(\omega \mid b) \leq \phi_n(\omega \mid b).$$

□

Lemma 1 guarantees that once we have computed the increasing terms, all subsequent partial sums for even n are upper bounds, and all subsequent partial sums for odd n are lower bounds on $\Phi(\omega \mid b)$. To determine acceptance of u, we evaluate until we find an upper bound less than u, at which point we reject, or a lower bound greater than u, at which point we accept. In practice, determining acceptance takes only a small number of iterations.

Algorithm 8.4 provides pseudocode for the final rejection sampling algorithm.

Require: $b > 0, \psi \in \mathbb{R}$
  accept $\leftarrow$ False
  while not accept **do**
    $\omega \sim \mathrm{IG}\left(\frac{b}{|\psi/2|}, b^2\right)$ ▷ Inv. Gaussian proposal
    $u \sim \mathrm{Unif}(0, 1)$ ▷ Sample acceptance variable
    $\Phi = 1$ ▷ Initialize partial sum with first term
    for $n = 1$ to ∞ **do**
      $\Phi \leftarrow \Phi + (-1)^n \phi_n(\omega \mid b)$ ▷ Update partial sum
      if $\phi_n(\omega \mid b) < \phi_{n-1}(\omega \mid b)$ **then** ▷ Check if terms are decreasing
        if n odd **and** $u \leq \Phi$ **then** ▷ Compare to lower bound
          accept $\leftarrow$ True ▷ Accept and return
          break
        end if
        if n even **and** $u > \Phi$ **then** ▷ Compare to upper bound
          break ▷ Reject and make new proposal
        end if
      end if
    end for
  end while
  return $\frac{1}{4}\omega$

Algorithm 8.4: A rejection sampling algorithm for the Pólya-gamma distribution that is most efficient in the "small-shape" ($b < 1$) regime.

8.6 Conclusion

This chapter has explored various facets of modeling neural spike trains with switching linear dynamical systems models. This powerful model for nonlinear dynamical systems contains a number of simpler models as special cases. We have shown how a simple MCMC inference algorithm based on the Pólya-gamma augmentation provides a unified means of performing inference for the SLDS and its special cases.

As we consider hierarchical models like these — models constructed out of layers of latent structure — we must turn our attention to the important question of model selection. How should we justify our modeling choices? Marginal likelihood estimates provide one answer to this question. We have shown how the same Pólya-gamma augmentations can be

applied inside annealed importance sampling algorithms, one of the most successful means of approximating marginal likelihoods. In order to make these methods work in practice, however, we needed to improve the efficiency of sampling the Pólya-gamma distribution in the "small shape" regime. By leveraging a particular decomposition of the related Jacobi density, we derived a novel rejection sampling algorithm with acceptance probability of at least one half.

Next, we turn our attention to another important question. For all their structure, what can these models teach us about neural computation? The next chapter provides some initial attempts to connect the methods we have developed thus far to more abstract theoretical models of neural computation.

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