

osl-dynamics: HMM Cost Function

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Abstract

We describe the calculation of the cost function used to update the observation model parameters (state means and covariances) in the `osl-dynamics` implementation of a Hidden Markov Model (HMM). We also describe the calculation of the variational free energy for this model.

1 Variational Free Energy

In variational Bayesian inference we learn a posterior distribution for model parameters, $q(\cdot)$, by minimising the *variational free energy*, \mathcal{F} , given some data we have observed, x_t . For the HMM, our model parameters are:

- The hidden state at each time point, s_t .
- The state transition probability at each time point, π_t , which depends on s_{t-1} .
- The initial state probability, π_1 .
- The observation model parameters, θ_{obs} .

If we were being Bayesian on all of these model parameters, we would minimise the following variational free energy¹ [1]

$$\mathcal{F} = \iiint q(s_{1:T})q(\pi_t)q(\pi_1)q(\theta_{\text{obs}}) \log \left[\frac{q(s_{1:T})q(\pi_t)q(\pi_1)q(\theta_{\text{obs}})}{p(x_{1:T}, s_{1:T}, \pi_t, \pi_1, \theta_{\text{obs}})} \right] ds_{1:T}d\pi_t d\pi_1 d\theta_{\text{obs}}, \quad (1)$$

where $s_{1:T}$ and $x_{1:T}$ denote s_1, \dots, s_T and x_1, \dots, x_T respectively. However, in the `osl-dynamics` implementation of an HMM, we will only be Bayesian on the hidden states, $s_{1:T}$. We will learn point estimates for all the other parameters: θ_{obs} , π_t and π_1 . We learn all of our model parameters by minimising the following variational free energy,

$$\mathcal{F} = \int q(s_{1:T}) \log \left[\frac{q(s_{1:T})}{p(x_{1:T}, s_{1:T})} \right] ds_{1:T}. \quad (2)$$

We will show that Eq. (2) implicitly depends on the point estimates for θ_{obs} below.

¹We have used the mean field approximation.

2 Generative Model

The denominator in the log function, $p(\cdot)$, is determined by our generative model. For the HMM, if we were being fully Bayesian this would be [1]

$$p(x_{1:T}, s_{1:T}, \pi_t, \pi_1, \theta_{\text{obs}}) = p(x_1|s_1, \theta_{\text{obs}})p(s_1|\pi_1)p(\pi_1)p(\theta_{\text{obs}}) \prod_{t=2}^T p(x_t|s_t, \theta_{\text{obs}})p(s_t|s_{t-1}, \pi_t)p(\pi_t). \quad (3)$$

However, because we are learning point estimates for most of these parameters ($\theta_{\text{obs}}, \pi_t, \pi_0$) their prior distributions disappear. We will use the following generative model,

$$p(x_{1:T}, s_{1:T}) = p(x_1|s_1, \theta_{\text{obs}})p(s_1) \prod_{t=2}^T p(x_t|s_t, \theta_{\text{obs}})p(s_t|s_{t-1}), \quad (4)$$

where θ_{obs} is a point estimate. We assume a multivariate normal distribution for the observed data,

$$p(x_t|s_t = k, \theta_{\text{obs}}) = \mathcal{N}(m_k, C_k), \quad (5)$$

where m_k and C_k are the mean and covariance for state k respectively. Our observation model parameters θ_{obs} are the set of state means and covariances, $\theta_{\text{obs}} = \{m_k, C_k\}$.

3 Cost Function for Learning $\theta_{\text{obs}} = \{m_k, C_k\}$

We update our point estimate for θ_{obs} by minimising Eq. (2). We separate Eq. (2) into the following terms²

$$\mathcal{F} = - \int q(s_{1:T}) \log [p(x_{1:T}, s_{1:T})] ds_{1:T} + \int q(s_{1:T}) \log [q(s_{1:T})] ds_{1:T}. \quad (6)$$

Only the first term depends on θ_{obs} so the second term can be ignored. Substituting Eq. (4) into the first term, we have

$$\mathcal{F} \propto - \int q(s_{1:T}) \log \left[p(x_1|s_1, \theta_{\text{obs}})p(s_1) \prod_{t=2}^T p(x_t|s_t, \theta_{\text{obs}})p(s_t|s_{t-1}) \right] ds_{1:T}. \quad (7)$$

Again, only retaining the factors that depend on θ_{obs} , we have

$$\begin{aligned} \mathcal{F} &\propto - \int q(s_{1:T}) \log \left[\prod_{t=1}^T p(x_t|s_t, \theta_{\text{obs}}) \right] ds_{1:T} \\ &\propto - \sum_{t=1}^T \int q(s_{1:T}) \log [p(x_t|s_t, \theta_{\text{obs}})] ds_{1:T} \\ &\propto - \sum_{t=1}^T \int \dots \int q(s_1) \dots q(s_T) \log [p(x_t|s_t, \theta_{\text{obs}})] ds_1 \dots ds_T \\ &\propto - \sum_{t=1}^T \int q(s_t) \log [p(x_t|s_t, \theta_{\text{obs}})] ds_t = \mathcal{L}. \end{aligned} \quad (8)$$

Here, we have defined the negative log-likelihood loss, \mathcal{L} , which is minimised via stochastic gradient descent to learn the parameters θ_{obs} . $q(s_t)$ is the marginal posterior calculated using

²We have used $\int q(\xi) d\xi = 1$ to evaluate some of the integrals.

the Baum-Welch algorithm, commonly denoted using the symbol γ . As $q(s_t)$ is a discrete probability distribution for the state, we can evaluate the integral as

$$\begin{aligned}\mathcal{L} &= - \sum_{t=1}^T \sum_{k=1}^K q(s_t = k) \log [p(x_t | s_t = k, \theta_{\text{obs}})] \\ &= - \sum_{t=1}^T \sum_{k=1}^K \gamma_{kt} \log [p(x_t | s_t = k, \theta_{\text{obs}})],\end{aligned}\tag{9}$$

where K is the number of states and $q(s_t = k) = \gamma_{kt}$ is the probability of state k at time t . Substituting Eq. (5) into this we have

$$\mathcal{L} = - \sum_{t=1}^T \sum_{k=1}^K \gamma_{kt} \log [\mathcal{N}(x_t | m_k, C_k)],\tag{10}$$

which is the log-likelihood loss function implemented in `osl-dynamics` for inferring the point estimates for the observation model parameters $\theta_{\text{obs}} = \{m_k, C_k\}$.

4 Calculation of the Variational Free Energy

Once we have trained an HMM we may want to evaluate the variational free energy, i.e. Eq.(2). This can be done with the `free_energy` method of the `hmm.Model` class. The method calculates Eq. (2) by first splitting it into three terms:

$$\begin{aligned}\mathcal{F} &= \int q(s_{1:T}) \log \left[\frac{q(s_{1:T})}{p(x_{1:T}, s_{1:T})} \right] ds_{1:T}, \\ &= \int q(s_{1:T}) \log \left[\frac{q(s_{1:T})}{p(x_1 | s_1) p(s_1) \prod_{t=2}^T p(x_t | s_t) p(s_t | s_{t-1})} \right] ds_{1:T}, \\ &= - \int q(s_{1:T}) \log \left[\prod_{t=1}^T p(x_t | s_t) \right] ds_{1:T} + \int q(s_{1:T}) \log \left[\frac{q(s_{1:T})}{p(s_1) \prod_{t=2}^T p(s_t | s_{t-1})} \right] ds_{1:T}, \\ &= - \int q(s_{1:T}) \log \left[\prod_{t=1}^T p(x_t | s_t) \right] ds_{1:T} + \int q(s_{1:T}) \log [q(s_{1:T})] ds_{1:T} \\ &\quad - \int q(s_{1:T}) \log \left[p(s_1) \prod_{t=2}^T p(s_t | s_{t-1}) \right] ds_{1:T}, \\ &= -LL + E - P,\end{aligned}\tag{11}$$

where LL is the posterior expected log-likelihood (same as Eq. (10)), E is the posterior entropy and P is the posterior expected prior probability. To evaluate the terms in the above equation we factorise the posterior as

$$q(s_{1:T}) = q(s_1) \prod_{t=2}^T q(s_t | s_{t-1}) = q(s_1) \prod_{t=2}^T \frac{q(s_{t-1}, s_t)}{q(s_{t-1})} = q(s_1) \prod_{t=1}^{T-1} \frac{q(s_t, s_{t+1})}{q(s_t)}.\tag{12}$$

The above factorisation is an assumption of the Baum-Welch algorithm. Let's first look at the entropy term,

$$\begin{aligned}
E &= \int q(s_{1:T}) \log [q(s_{1:T})] ds_{1:T}, \\
&= \int q(s_{1:T}) \log \left[q(s_1) \prod_{t=1}^{T-1} \frac{q(s_t, s_{t+1})}{q(s_t)} \right] ds_{1:T}, \\
&= \sum_{t=1}^{T-1} \int q(s_t, s_{t+1}) \log q(s_t, s_{t+1}) ds_t ds_{t+1} - \sum_{t=2}^{T-1} \int q(s_t) \log q(s_t) ds_t.
\end{aligned} \tag{13}$$

This can be calculated using the marginal posterior, $\gamma(t) = q(s_t)$, and joint posterior, $\xi(t) = q(s_t, s_{t+1})$, provided by the Baum-Welch algorithm:

$$E = \sum_{t=1}^{T-1} \sum_{i,j=1}^K \xi_{ij}(t) \log \xi_{ij}(t) - \sum_{t=2}^{T-1} \sum_{i=1}^K \gamma_i \log \gamma_i(t). \tag{14}$$

Finally, we calculate the posterior expected prior probability as

$$\begin{aligned}
P &= \int q(s_{1:T}) \log \left[p(s_1) \prod_{t=2}^T p(s_t | s_{t-1}) \right] ds_{1:T}, \\
&= \int q(s_1) \prod_{t=1}^{T-1} \frac{q(s_t, s_{t+1})}{q(s_t)} \log \left[p(s_1) \prod_{t=2}^T p(s_t | s_{t-1}) \right] ds_{1:T}, \\
&= \int q(s_1) \log p(s_1) ds_1 + \sum_{t=1}^{T-1} \int q(s_t, s_{t+1}) \log p(s_{t+1} | s_t) ds_t ds_{t+1}.
\end{aligned} \tag{15}$$

Using the marginal and joint posterior provided by the Baum-Welch algorithm and the point estimates for the initial probabilities, π_1 and transition probability matrix, π_t , this is evaluated as

$$P = \sum_{i=1}^K \gamma_i(1) \log \pi_{1,i} + \sum_{t=1}^{T-1} \sum_{i,j=1}^K \xi_{ij}(t) \log \pi_{t,ij}. \tag{16}$$

References

- [1] I. Rezek and S. Roberts, Ensemble hidden Markov models with extended observation densities for biosignal analysis. Probabilistic modeling in bioinformatics and medical informatics. Springer, London, 419-450 (2005).