`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).

1 Variational Free Energy

In variational Bayesian inference we infer a posterior distribution for model parameters, $q(.)$, 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 is dependent on s_{t-1}.
- The initial state probability, π_0.
- The observation model parameters, θ_{obs}.

Therefore, we infer our model parameters by minimising the following variational free energy[1] [1]

$$\mathcal{F} = \iiiint q(s_{1:T})q(\pi_t)q(\pi_0)q(\theta_{\text{obs}}) \log \left[\frac{q(s_{1:T})q(\pi_t)q(\pi_0)q(\theta_{\text{obs}})}{p(x_{1:T}, s_{1:T}, \pi_t, \pi_0, \theta_{\text{obs}})} \right] ds_{1:T} d\pi_t d\pi_0 d\theta_{\text{obs}}, \tag{1}$$

where $s_{1:T}$ and $x_{1:T}$ denote $s_1, ..., s_T$ and $x_1, ..., x_T$ respectively. However, in the `osl-dynamics` implementation of an HMM, we will not be Bayesian on θ_{obs}, instead of learning $q(\theta_{\text{obs}})$ we will learn point estimates for θ_{obs}. We will learn the posterior distributions $q(s_{1:T})$, $q(\pi_t)$, $q(\pi_0)$ and point estimates for θ_{obs} by minimising the following variational free energy,

$$\mathcal{F} = \iiint q(s_{1:T})q(\pi_t)q(\pi_0) \log \left[\frac{q(s_{1:T})q(\pi_t)q(\pi_0)}{p(x_{1:T}, s_{1:T}, \pi_t, \pi_0)} \right] ds_{1:T} d\pi_t d\pi_0. \tag{2}$$

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

2 Generative Model

The term $p(x_{1:T}, s_{1:T}, \pi_t, \pi_0)$ is determined by our generative model. For the HMM, if we were being fully Bayesian this would be [1]

$$p(x_{1:T}, s_{1:T}, \pi_t, \pi_0, \theta_{\text{obs}}) = p(s_0|\pi_0)p(\pi_0) \prod_{t=1}^{T} p(x_t|s_t, \theta_{\text{obs}}) p(s_t|s_{t-1}, \pi_t) p(\pi_t) p(\theta_{\text{obs}}). \tag{3}$$

[1]We have used the mean field approximation.

However, because we are learning point estimates for θ_{obs} we do not have the prior $p(\theta_{\text{obs}})$. We will use the following generative model,

$$p(x_{1:T}, s_{1:T}, \pi_t, \pi_0) = p(s_0|\pi_0)p(\pi_0) \prod_{t=1}^{T} p(x_t|s_t, \theta_{\text{obs}}) p(s_t|s_{t-1}, \pi_t) p(\pi_t), \tag{4}$$

where θ_{obs} are point estimates.

We assume a multivariate normal distribution for the observed data,

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

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 terms[2]

$$\begin{aligned}
\mathcal{F} &= -\iiint q(s_{1:T})q(\pi_t)q(\pi_0) \log\left[p(x_{1:T}, s_{1:T}, \pi_t, \pi_0)\right] ds_{1:T} d\pi_t d\pi_0 \\
&\quad + \iiint q(s_{1:T})q(\pi_t)q(\pi_0) \log\left[q(s_{1:T})q(\pi_t)q(\pi_0)\right] ds_{1:T} d\pi_t d\pi_0 \\
\mathcal{F} &= -\iiint q(s_{1:T})q(\pi_t)q(\pi_0) \log\left[p(x_{1:T}, s_{1:T}, \pi_t, \pi_0)\right] ds_{1:T} d\pi_t d\pi_0 \\
&\quad + \int q(s_{1:T}) \log\left[q(s_{1:T})\right] ds_{1:T} + \int q(\pi_t) \log\left[q(\pi_t)\right] d\pi_t + \int q(\pi_0) \log\left[q(\pi_0)\right] d\pi_0
\end{aligned} \tag{6}$$

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

$$\begin{aligned}
\mathcal{F} &\propto -\iiint q(s_{1:T})q(\pi_t)q(\pi_0) \log\left[p(x_{1:T}, s_{1:T}, \pi_t, \pi_0)\right] ds_{1:T} d\pi_t d\pi_0 \\
&\propto -\iiint q(s_{1:T})q(\pi_t)q(\pi_0) \log\left[p(s_0|\pi_0)p(\pi_0) \prod_{t=1}^{T} p(x_t|s_t, \theta_{\text{obs}}) p(s_t|s_{t-1}, \pi_t) p(\pi_t)\right] ds_{1:T} d\pi_t d\pi_0.
\end{aligned} \tag{7}$$

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

$$\begin{aligned}
\mathcal{F} &\propto -\iint q(s_{1:T})q(\pi_t) \log\left[\prod_{t=1}^{T} p(x_t|s_t, \theta_{\text{obs}}) p(s_t|s_{t-1}, \pi_t) p(\pi_t)\right] ds_{1:T} d\pi_t \\
&\propto -\sum_{t=1}^{T} \iint q(s_{1:T})q(\pi_t) \log\left[p(x_t|s_t, \theta_{\text{obs}}) p(s_t|s_{t-1}, \pi_t) p(\pi_t)\right] ds_{1:T} d\pi_t \\
&\propto -\sum_{t=1}^{T} \iint q(s_{1:T})q(\pi_t) \left\{\log\left[p(x_t|s_t, \theta_{\text{obs}})\right] + \log\left[p(s_t|s_{t-1}, \pi_t) p(\pi_t)\right]\right\} ds_{1:T} d\pi_t
\end{aligned} \tag{8}$$

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

Only retaining the term that depends on θ_{obs}, we have

$$\begin{aligned}
\mathcal{F} &\propto -\sum_{t=1}^{T} \iint q(s_{1:T}) q(\pi_t) \log\left[p(x_t|s_t, \theta_{\text{obs}})\right] ds_{1:T} d\pi_t \\
&\propto -\sum_{t=1}^{T} \int q(s_{1:T}) \log\left[p(x_t|s_t, \theta_{\text{obs}})\right] ds_{1:T} \\
&\propto -\sum_{t=1}^{T} \int ... \int q(s_1)...q(s_T) \log\left[p(x_t|s_t, \theta_{\text{obs}})\right] ds_1...ds_T \\
&\propto -\sum_{t=1}^{T} \int q(s_t) \log\left[p(x_t|s_t, \theta_{\text{obs}})\right] ds_t = \mathcal{L}.
\end{aligned} \tag{9}$$

Here, we have defined the negative log-likelihood loss, $\mathcal{L}$, which is minimised via stochastic gradient descent to learn the parameters θ_{obs}. As $q(s_t)$ is a discrete probability distribution for the state, we can evaluate the integral as

$$\begin{aligned}
\mathcal{L} &= -\sum_{t=1}^{T} \sum_{k=1}^{K} q(s_t = k) \log\left[p(x_t|s_t = k, \theta_{\text{obs}})\right] \\
&= -\sum_{t=1}^{T} \sum_{k=1}^{K} \gamma_{kt} \log\left[p(x_t|s_t = k, \theta_{\text{obs}})\right],
\end{aligned} \tag{10}$$

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

$$\mathcal{L} = -\sum_{t=1}^{T} \sum_{k=1}^{K} \gamma_{kt} \log\left[\mathcal{N}(m_k, C_k)\right], \tag{11}$$

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

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).