# Hidden Markov Models

## STATS 305C: Applied Statistics

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# Gaussian Mixture Models

Recall the basic Gaussian mixture model,

$$z_t \overset{\text{iid}}{\sim} \mathrm{Cat}(\pi) \tag{1}$$
$$x_t \mid z_t \sim \mathcal{N}(\boldsymbol{\mu}_{z_t}, \boldsymbol{\Sigma}_{z_t}) \tag{2}$$

where

- $z_t \in \{1, \ldots, K\}$ is a **latent mixture assignment**
- $x_t \in \mathbb{R}^D$ is an **observed data point**
- $\pi \in \Delta_K$, $\boldsymbol{\mu}_k \in \mathbb{R}^D$, and $\boldsymbol{\Sigma}_k \in \mathbb{R}_{\succeq 0}^{D \times D}$ are parameters

(Here we've switched to indexing data points by $t$ rather than $n$.)

Let $\boldsymbol{\Theta}$ denote the set of parameters. We can be Bayesian and put a prior on $\boldsymbol{\Theta}$ and run Gibbs or VI, or we can point estimate $\boldsymbol{\Theta}$ with EM, etc.

# Gaussian Mixture Models II

**Draw the graphical model.**

# Gaussian Mixture Models III

Recall the EM algorithm for mixture models,

- **E step:** Compute the posterior distribution

$$q(\boldsymbol{z}_{1:T}) = p(\boldsymbol{z}_{1:T} \mid \boldsymbol{x}_{1:T}; \boldsymbol{\Theta}) \tag{3}$$

$$= \prod_{t=1}^{T} p(z_t \mid \boldsymbol{x}_t; \boldsymbol{\Theta}) \tag{4}$$

$$= \prod_{t=1}^{T} q_t(z_t) \tag{5}$$

- **M step:** Maximize the ELBO wrt $\boldsymbol{\Theta}$,

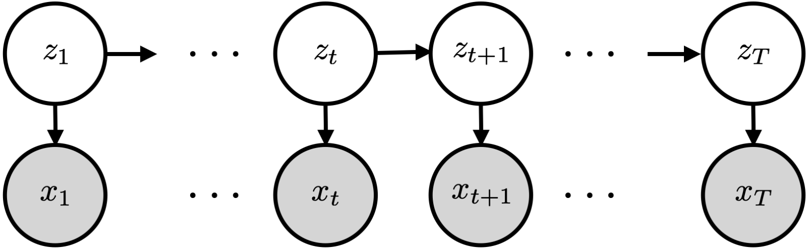
$$\mathscr{L}(\boldsymbol{\Theta}) = \mathbb{E}_{q(\boldsymbol{z}_{1:T})}\left[\log p(\boldsymbol{x}_{1:T}, \boldsymbol{z}_{1:T}; \boldsymbol{\Theta}) - \log q(\boldsymbol{z}_{1:T})\right] \tag{6}$$

$$= \mathbb{E}_{q(\boldsymbol{z}_{1:T})}\left[\log p(\boldsymbol{x}_{1:T}, \boldsymbol{z}_{1:T}; \boldsymbol{\Theta})\right] + c. \tag{7}$$

For exponential family mixture models, the M-step only requires expected sufficient statistics.

# Hidden Markov Models

Hidden Markov Models (HMMs) are like mixture models with temporal dependencies between the mixture assignments.




This graphical model says that the joint distribution factors as,

$$p(z_{1:T}, \boldsymbol{x}_{1:T}) = p(z_1) \prod_{t=2}^{T} p(z_t \mid z_{t-1}) \prod_{t=1}^{T} p(\boldsymbol{x}_t \mid z_t). \tag{8}$$

We call this an HMM because the *hidden* states follow a Markov chain, $p(z_1) \prod_{t=2}^{T} p(z_t \mid z_{t-1})$.

# Hidden Markov Models II

An HMM consists of three components:

1. **Initial distribution:** $z_1 \sim \mathrm{Cat}(\pi_0)$
2. **Transition matrix:** $z_t \sim \mathrm{Cat}(\boldsymbol{P}_{z_{t-1}})$ where $\boldsymbol{P} \in [0,1]^{K \times K}$ is a *row-stochastic* transition matrix with rows $\boldsymbol{P}_k$.
3. **Emission distribution:** $\boldsymbol{x}_t \sim p(\cdot \mid \boldsymbol{\theta}_{z_t})$

# Hidden Markov Models III

We are interested in questions like:

- What are the *predictive distributions* of $p(z_{t+1} \mid \boldsymbol{x}_{1:t})$?
- What is the *posterior marginal* distribution $p(z_t \mid \boldsymbol{x}_{1:T})$?
- What is the *posterior pairwise marginal* distribution $p(z_t, z_{t+1} \mid \boldsymbol{x}_{1:T})$?
- What is the *posterior mode* $z^\star_{1:T} = \arg\max p(z_{1:T} \mid \boldsymbol{x}_{1:T})$?
- How can we *sample the posterior* $p(\boldsymbol{z}_{1:T} \mid \boldsymbol{x}_{1:T})$ of an HMM?
- What is the *marginal likelihood* $p(\boldsymbol{x}_{1:T})$?
- How can we *learn the parameters* of an HMM?

**Question:** Why might these sound like hard problems?

# Computing the predictive distributions

The predictive distributions give the probability of the latent state $z_{t+1}$ given observations *up to but not including* time $t+1$. Let,

$$\begin{aligned}
\alpha_{t+1}(z_{t+1}) &\triangleq p(z_{t+1}, \boldsymbol{x}_{1:t}) && (9)\\
&= \sum_{z_1=1}^{K} \cdots \sum_{z_t=1}^{K} p(z_1) \prod_{s=1}^{t} p(\boldsymbol{x}_s \mid z_s)\, p(z_{s+1} \mid z_s) && (10)\\
&= \sum_{z_t=1}^{K} \left[ \left( \sum_{z_1=1}^{K} \cdots \sum_{z_{t-1}=1}^{K} p(z_1) \prod_{s=1}^{t-1} p(\boldsymbol{x}_s \mid z_s)\, p(z_{s+1} \mid z_s) \right) p(\boldsymbol{x}_t \mid z_t)\, p(z_{t+1} \mid z_t) \right] && (11)\\
&= \sum_{z_t=1}^{K} \alpha_t(z_t)\, p(\boldsymbol{x}_t \mid z_t)\, p(z_{t+1} \mid z_t). && (12)
\end{aligned}$$

We call $\alpha_t(z_t)$ the *forward messages*. We can compute them recursively! The base case is $p(z_1 \mid \varnothing) \triangleq p(z_1)$.

# Computing the predictive distributions II

We can also write these recursions in a vectorized form. Let

$$\boldsymbol{\alpha}_t = \begin{bmatrix} \alpha_t(z_t = 1) \\ \vdots \\ \alpha_t(z_t = K) \end{bmatrix} = \begin{bmatrix} p(z_t = 1, \boldsymbol{x}_{1:t-1}) \\ \vdots \\ p(z_t = K, \boldsymbol{x}_{1:t-1}) \end{bmatrix} \quad \text{and} \quad \boldsymbol{l}_t = \begin{bmatrix} p(\boldsymbol{x}_t \mid z_t = 1) \\ \vdots \\ p(\boldsymbol{x}_t \mid z_t = K) \end{bmatrix} \tag{13}$$

both be vectors in $\mathbb{R}_+^K$. Then,

$$\boldsymbol{\alpha}_{t+1} = \boldsymbol{P}^\top (\boldsymbol{\alpha}_t \odot \boldsymbol{l}_t) \tag{14}$$

where $\odot$ denotes the Hadamard (elementwise) product and $\boldsymbol{P}$ is the transition matrix.

# Computing the predictive distributions III

Finally, to get the predictive distributions we just have to normalize,

$$p(z_{t+1} \mid \boldsymbol{x}_{1:t}) \propto p(z_{t+1}, \boldsymbol{x}_{1:t}) = \alpha_{t+1}(z_{t+1}). \tag{15}$$

**Question:** What does the normalizing constant tell us?

# Computing the posterior marginal distributions

The posterior marginal distributions give the probability of the latent state $z_t$ given *all the observations* up to time $T$.

$$p(z_t \mid \boldsymbol{x}_{1:T}) = \sum_{z_1=1}^{K} \cdots \sum_{z_{t-1}=1}^{K} \sum_{z_{t+1}=1}^{K} \cdots \sum_{z_T=1}^{K} p(\boldsymbol{z}_{1:T}, \boldsymbol{x}_{1:T}) \tag{16}$$

$$\begin{aligned} &= \left[ \sum_{z_t=1}^{K} \cdots \sum_{z_{t-1}=1}^{K} p(z_1) \prod_{s=1}^{t-1} p(\boldsymbol{x}_s \mid z_s)\, p(z_{s+1} \mid z_s) \right] \times p(\boldsymbol{x}_t \mid z_t) \\ &\quad \times \left[ \sum_{z_{t+1}=1}^{K} \cdots \sum_{z_T=1}^{K} \prod_{u=t+1}^{T} p(z_u \mid z_{u-1})\, p(\boldsymbol{x}_u \mid z_u) \right] \end{aligned} \tag{17}$$

$$= \alpha_t(z_t) \times p(\boldsymbol{x}_t \mid z_t) \times \beta_t(z_t) \tag{18}$$

where we have introduced the *backward messages* $\beta_t(z_t)$.

# Computing the backward messages

The backward messages can be computed recursively too,

$$\beta_t(z_t) \triangleq \sum_{z_{t+1}=1}^{K} \cdots \sum_{z_T=1}^{K} \prod_{u=t+1}^{T} p(z_u \mid z_{u-1})\, p(\boldsymbol{x}_u \mid z_u) \tag{19}$$

$$= \sum_{z_{t+1}=1}^{K} p(z_{t+1} \mid z_t)\, p(\boldsymbol{x}_{t_1} \mid z_{t+1}) \left( \sum_{z_{t+2}=1}^{K} \cdots \sum_{z_T=1}^{K} \prod_{u=t+2}^{T} p(z_u \mid z_{u-1})\, p(\boldsymbol{x}_u \mid z_u) \right) \tag{20}$$

$$= \sum_{z_{t+1}=1}^{K} p(z_{t+1} \mid z_t)\, p(\boldsymbol{x}_{t_1} \mid z_{t+1})\, \beta_{t+1}(z_{t+1}). \tag{21}$$

For the base case, let $\beta_T(z_T) = 1$.

# Computing the backward messages (vectorized)

Let

$$\boldsymbol{\beta}_t = \begin{bmatrix} \beta_t(z_t = 1) \\ \vdots \\ \beta_t(z_t = K) \end{bmatrix} \tag{22}$$

be a vector in $\mathbb{R}_+^K$. Then,

$$\boldsymbol{\beta}_t = \boldsymbol{P}(\boldsymbol{\beta}_{t+1} \odot \boldsymbol{l}_{t+1}). \tag{23}$$

Let $\boldsymbol{\beta}_T = \mathbf{1}_K$.

Now we have everything we need to compute the posterior marginal,

$$p(z_t = k \mid \boldsymbol{x}_{1:T}) = \frac{\alpha_{t,k}\, l_{t,k}\, \beta_{t,k}}{\sum_{j=1}^K \alpha_{t,j} l_{t,j} \beta_{t,j}}. \tag{24}$$

We just derived the **forward-backward algorithm** for HMMs [Rabiner and Juang, 1986].

# What do the backward messages represent?

**Question:** If the forward messages represent the predictive probabilities $\alpha_{t+1}(z_{t+1}) = p(z_{t+1}, \boldsymbol{x}_{1:t})$, what do the backward messages represent?

# Computing the posterior pairwise marginals

**Exercise:** Use the forward and backward messages to compute the posterior pairwise marginals $p(z_t, z_{t+1} \mid \boldsymbol{x}_{1:T})$.

# Normalizing the messages for numerical stability

If you're working with long time series, especially if you're working with 32-bit floating point, you need to be careful.

The messages involve products of probabilities, which can quickly overflow.

There's a simple fix though: after each step, re-normalize the messages so that they sum to one. I.e replace

$$\boldsymbol{\alpha}_{t+1} = \boldsymbol{P}^\top (\boldsymbol{\alpha}_t \odot \boldsymbol{l}_t) \tag{25}$$

with

$$\widetilde{\boldsymbol{\alpha}}_{t+1} = \frac{1}{A_t} \boldsymbol{P}^\top (\widetilde{\boldsymbol{\alpha}}_t \odot \boldsymbol{l}_t) \tag{26}$$

$$A_t = \sum_{k=1}^{K} \sum_{j=1}^{K} P_{jk} \widetilde{\alpha}_{t,j} l_{t,j} \equiv \sum_{j=1}^{K} \widetilde{\alpha}_{t,j} l_{t,j} \quad \text{(since } \boldsymbol{P} \text{ is row-stochastic).} \tag{27}$$

This leads to a nice interpretation: The normalized messages are predictive likelihoods $\widetilde{\alpha}_{t+1,k} = p(z_{t+1} = k \mid \boldsymbol{x}_{1:t})$, and the normalizing constants are $A_t = p(\boldsymbol{x}_t \mid \boldsymbol{x}_{1:t-1})$.

## EM for Hidden Markov Models

Now we can put it all together. To perform EM in an HMM,

- **E step:** Compute the posterior distribution

$$q(\boldsymbol{z}_{1:T}) = p(\boldsymbol{z}_{1:T} \mid \boldsymbol{x}_{1:T}; \boldsymbol{\Theta}). \tag{28}$$

  (Really, run the **forward-backward algorithm** to get posterior marginals and pairwise marginals.)

- **M step:** Maximize the ELBO wrt $\boldsymbol{\Theta}$,

$$\mathscr{L}(\boldsymbol{\Theta}) = \mathbb{E}_{q(\boldsymbol{z}_{1:T})}\left[\log p(\boldsymbol{x}_{1:T}, \boldsymbol{z}_{1:T}; \boldsymbol{\Theta})\right] + c \tag{29}$$

$$= \mathbb{E}_{q(\boldsymbol{z}_{1:T})}\left[\sum_{k=1}^{K} \mathbb{I}[z_1 = k] \log \pi_{0,k}\right] + \mathbb{E}_{q(\boldsymbol{z}_{1:T})}\left[\sum_{t=1}^{T-1}\sum_{i=1}^{K}\sum_{j=1}^{K} \mathbb{I}[z_t = i, z_{t+1} = j] \log P_{i,j}\right]$$
$$+ \mathbb{E}_{q(\boldsymbol{z}_{1:T})}\left[\sum_{t=1}^{T}\sum_{k=1}^{K} \mathbb{I}[z_t = k] \log p(\boldsymbol{x}_t; \theta_k)\right] \tag{30}$$

For exponential family observations, the M-step only requires expected sufficient statistics.

# What else?

- How can we sample the posterior?
- How can we find the posterior mode?
- How can we choose the number of states?
- What if my transition matrix is sparse?

# References I

Lawrence Rabiner and Biinghwang Juang. An introduction to hidden Markov models. *ieee assp magazine*, 3(1):4–16, 1986.