SPR Day 18

Hidden Markov Models

Parameter Estimation and Likelihood Computation

Reading: Bishop PRML 13.2.1
13.2.2

Outline:
- Overview of EM for HMMs
- Defining $q(z)$ and computing expected log likelihood
- M step overview
- E step intro
  - FORWARD algorithm
  - BACKWARD algorithm
- Recap of E-step

Goal: Estimate parameters of an HMM using maximum likelihood method

$$\max_{\pi, A, \mu, \sigma} \log p(x_1, x_2, \cdots x_T | \pi, A, \mu, \sigma)$$

each $x_t \in \mathbb{R}$

Given: observed sequence $x_1, x_2, x_3, \cdots x_T$

Output: π initial probabilities
A transition probabilities
μ means
σ stddeviations

Notation

$\theta = \{\pi, A, \mu, \sigma\}$

All HMM parameters in one symbol θ

Challenges:
- how to compute this likelihood?

Complete is Easy: $p(x_{1:T}, z_{1:T} | \theta)$
(likelihood)

Incomplete is Hard: $p(x_{1:T} | \theta) = \sum_{z_{1:T} \in \Omega} p(x_{1:T}, z_{1:T} | \theta)$ (sum rule)
(likelihood)

Ω denotes all possible sequences of length T using symbols $\{1, 2, \cdots K\}$

Number of terms in sum is $|\mathcal{Z}| = K^T$

grows exponentially with T (#timesteps)

Not easy! What else can we do?

Big Idea:

(1) Let $q(z|s)$ be an "approximate" posterior, defining a valid distribution over the sequence $z = z_1, z_2, \dots z_T$

(2) Use the lower bound objective $\mathcal{L}$

$$\log p(x|\theta) \geq \mathop{\mathbb{E}}_{q(z|s)}\left[\log p(x,z|\theta) - \log q(z|s)\right] = \mathcal{L}(x, s, \theta)$$

(3) Iteratively optimize lower bound using coordinate ascent

Init: θ^0

for iteration $i = 1, 2, \dots$

E-step: $s_{1:T}^i \leftarrow \underset{s_{1:T}}{\text{argmax}}\ \mathcal{L}(x_{1:T}, s_{1:T}, \theta^{i-1})$

M-step: $\theta^i \leftarrow \underset{\theta}{\text{argmax}}\ \mathcal{L}(x_{1:T}, s_{1:T}^i, \theta)$

Punchline: Can do all key steps in affordable runtime $O(TK^2)$ or better

E-step, M-step, $\mathcal{L}$ calculation are all tractable

Idea: Define a tractable distribution

$q(z_{1:T} | S)$ over sequences $z_1, z_2, \cdots z_T$

with each $z_t \in \{1, 2, \cdots K\}$

If we want onehot notation, write vector ONEHOT(z_t)

How? Define joint probability of adjacent pair of timesteps: $(z_1, z_2), (z_2, z_3), \cdots (z_{T-1}, z_T)$

for $t = 1, 2, \cdots T-1$: $q(z_t = j, z_{t+1} = k) = S_{tjk}$

Requirements:

① each pairwise joint is valid PMF over $K \times K$ outcomes

S_t: $K \times K$ matrix

$\sum_j \sum_k S_{tjk} = 1$ for $t = 1, 2, \cdots T-1$

$S_{tjk} \geq 0$ for $t = 1, 2, \cdots T-1$, $j \in \{1, \cdots K\}$, $k \in \{1 \cdots K\}$

non-negative sums to 1

② neighboring pairs have consistent marginals

for all t,

$$q(z_t = k) = \sum_{j=1}^{K} q(z_{t-1} = j, z_t = k) = \sum_j S_{t-1,j,k}$$

$$= \sum_{l=1}^{K} q(z_t = k, z_{t+1} = l) = \sum_l S_{t,k,l}$$

Using this distribution, we can compute:

$$\mathbb{E}_{q(z|S)}\left[\text{ONEHOT}(z_t)_k\right] = \sum_{l=1}^{K} S_{tkl} \quad \text{for } t = 1, 2, \cdots T$$

$$\mathbb{E}_{q(z|S)}\left[\text{ONEHOT}(z_{t-1})_j \cdot \text{ONEHOT}(z_t)_k\right] = S_{tjk} \quad \text{for } t = 1, 2, \cdots T-1$$

scalar • scalar

If we know z: complete log likelihood for HMM

$$\log p(z_{1:T}, x_{1:T} | \theta) = \log p(z_{1:T}|\theta) + \log p(x_{1:T}|z_{1:T}, \theta)$$

$$= \log \text{CatPMF}(z_1 | \pi) + \sum_{t=1}^{T-1} \log \text{CatPMF}(z_{t+1} | \text{ONEHOT}(z_t)^T A) + \sum_{t=1}^{T} \sum_{k=1}^{K} \text{ONEHOT}(z_t)_k \log \text{Norm}(x_n | \mu_k, \sigma_k^2)$$

$$= \sum_{k=1}^{K} \text{ONEHOT}(z_t)_k \log \pi_k + \sum_{t=1}^{T-1} \sum_{j=1}^{K} \sum_{k=1}^{K} \text{ONEHOT}(z_t)_j \, \text{ONEHOT}(z_{t+1})_k \log A_{jk} + \sum_{t=1}^{T} \sum_{k=1}^{K} \text{ONEHOT}(z_t)_k \log \text{Norm}(x_n | \mu_k, \sigma_k^2)$$

If we only know $q(z)$, replace above with expectation

$$\mathbb{E}_{q(z|s)}[\log p(x, z)] = \sum_{k=1}^{K} r_{1k}(s) \log \pi_k + \sum_{t=1}^{T-1} \sum_{j=1}^{K} \sum_{k=1}^{K} s_{tjk} \log A_{jk} + \sum_{t=1}^{T} \sum_{k} r_{tk}(s) \log \text{Norm}(x_t | \mu_k, \sigma_k^2)$$

We have defined useful notation for marginals at each time t

$$q(z_t = k) = r_{tk} = r_{tk}(s) = \begin{cases} \sum_{l=1}^{K} s_{tkl} & \text{for } t \in 1, 2, \ldots T-1 \\ \sum_{j=1}^{K} s_{t-1,jk} & \text{for } t = T \end{cases}$$

M-Step for HMMs

Using simplified expression for expected complete likelihood, can see M-step takes as input:

- r_{tk} probability of assigning timestep t to cluster k (deterministic given s, $r_{tk} = \sum_\ell s_{tk\ell}$)
- s_{tjk} probability of assigning z_t to j and z_{t+1} to k

Given r, s, we can see how M-step is simplified

$$\pi^* \leftarrow \underset{\pi \in \Delta^K}{\operatorname{argmax}} \sum_k r_{1k} \log \pi_k \qquad \boxed{\pi_k^* = \frac{r_{1k}}{1}}$$

$$A_{j\cdot}^* \leftarrow \underset{A_j \in \Delta^K}{\operatorname{argmax}} \sum_t \sum_k s_{tjk} \log A_{jk} \qquad \boxed{A_{jk}^* = \frac{\sum_t s_{tjk}}{\sum_t \sum_k s_{tjk}}}$$

$$\mu_k^*, \Sigma_k^* \leftarrow \underset{\mu_k, \Sigma_k}{\operatorname{argmax}} \sum_t r_{tk} \log \mathrm{Norm}(x_t | \mu_k, \Sigma_k)$$

μ_k^*, Σ_k^*: same as GMM Mstep using $r = r(s)$

Note: likely want to use Penalty or MAP for Σ and π, maybe also A

How to do the E-step?

Recall: $\log p(x|\theta) \geq \mathcal{L}(x, s, \theta) + KL\left(q(z|s) \,\middle|\, p(z|x,\theta)\right)$

lower bound objective — KL term ≥ 0

Best possible E step update would make $KL = 0$

and thus $\log p(x|\theta) = \mathcal{L}(x, s, \theta)$ [bound is tight]

This is achieved by finding s such that

$$q(z|s) = p(z|x, \theta)$$

In words, we match our learned distribution q to the hiddens-given-data posterior $p(z|x,\theta)$

While we could, instead derive the optimal update by solving

$$s^* = \underset{s \text{ that meet sum to one and neighbor consistency constraints}}{\operatorname{argmax}} \mathcal{L}(x, s, \theta)$$

we would find the same optimal s^*, "matching the posterior" will be simpler.

Procedure: Analyse the posterior $p(z|x,\theta)$, specifically its moments for marginals (t): $p(z_t|x_{1:T})$ and pairwise joints (t, t+1): $p(z_t, z_{t+1}|x_{1:T})$

We'll see both can be computed exactly via dynamic programming

Single Timestep Marginal Posterior

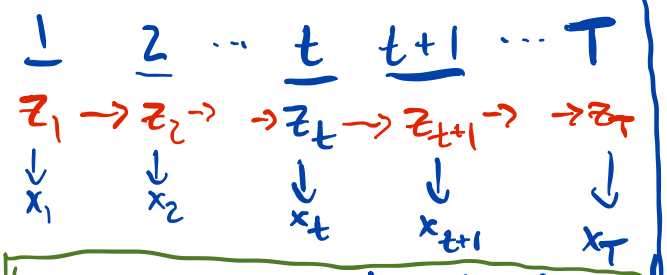
For each timestep t, we have:

$$p(z_t | x_{1:T}) = \frac{p(x_{1:T}, z_t)}{p(x_{1:T})}$$ by Bayes rule

z_t: which of K states at time t

$x_{1:T}$: given all data from start to end of sequence

$$= \frac{p(x_{1:t}, z_t)\, p(x_{t+1:T} | x_{1:t}, z_t)}{p(x_{1:T})}$$ product rule



x_{t+1} is conditionally indep of x_t given z_t

$$= \frac{p(x_{1:t}, z_t)\, p(x_{t+1:T} | z_t)}{p(x_{1:T})}$$ via HMM conditional independence assumption

$$= \frac{p(x_{1:t})\, p(z_t | x_{1:t})\, p(x_{t+1:T} | z_t)}{p(x_{1:T})}$$

$p(x_{1:t})$: const; $p(x_{1:T})$: const

Path forward: Suppose we can compute

$$\alpha_{tk} = p(z_t = k | x_{1:t}) \quad \text{for } t = 1, 2, \dots T,\ k = 1, 2, \dots K$$

$$\beta_{tk} = p(x_{t+1:T} | z_t = k) \quad \text{for } t = 1, 2, \dots T,\ k = 1, 2, \dots K$$

Then, we can compute single timestep posterior marginal as:

$$p(z_t = k | x_{1:T}) = \frac{\alpha_{tk} \beta_{tk}}{\sum_l \alpha_{tl} \beta_{tl}}$$

Adjacent Timestep Joint Posterior

For each timestep t in $1, 2, \ldots T-1$ we have

$$p(z_t, z_{t+1} | x_{1:T}) = \frac{p(z_t, z_{t+1}, x_{1:T})}{p(x_{1:T})}$$

$$= \frac{1}{p(x_{1:T})} p(z_t, z_{t+1}, x_{1:t+1}) p(x_{t+2:T} | z_{t+1})$$ product rule & x_{t+2} indep of $x_{1:t+1}$ given z_{t+1}

$$= \frac{1}{p(x_{1:T})} p(z_t, x_{1:t}) p(z_{t+1} | z_t, \cancel{x_{1:t}}) p(x_{t+1} | z_{t+1}, \cancel{z_t}, \cancel{x_{1:t}}) p(x_{t+2:T} | z_{t+1})$$ product rule

$$= \underbrace{\frac{1}{p(x_{1:T})}}_{\text{Const wrt } z} \underbrace{\frac{p(z_t | x_{1:t})}{\frac{1}{p(x_{1:t})}}}_{\alpha_t} p(z_{t+1} | z_t) p(x_{t+1} | z_{t+1}) \underbrace{p(x_{t+2:T} | z_{t+1})}_{\beta_{t+1}}$$ conditional independence assumptions

- Const wrt z
- easy given θ
- using α, β defined on prev page

$p(z_{t+1} | z_t) = A_{z_t, z_{t+1}}$

$p(x_{t+1} | z_{t+1}) = \text{NormPDF}(x_{t+1} | \mu_{z_{t+1}}, \sigma_{z_{t+1}})$

Thus, we can compute the adjacent timestep posterior if we have precomputed $\{\alpha_t, \beta_t\}_{t=1}^T$ as:

$$p(z_t = j, z_{t+1} = k | x_{1:T}) = \frac{\alpha_{tj} A_{jk} L_{t+1,k} \beta_{t+1,k}}{\sum_{l=1}^{K} \sum_{m=1}^{K} \alpha_{tl} A_{lm} L_{t+1,m} \beta_{t+1,m}}$$ for $t = 1, 2, \ldots T-1$

where $L_{tk} = p(x_t | z_t = k, \theta) = \text{NormPDF}(x_t | \mu_k, \sigma_k^2)$ when emission model is Gaussian

Computing Forward Messages α via Dynamic Programming (FORWARD alg.)

Definition: $\alpha_{tk} = p(z_t = k \mid x_{1:t})$ for $t = 1, 2, \cdots T$

Procedure: Dynamic Program, with base case $t=1$ and recurrence relation that computes $\alpha_{t+1,:}$ from $\alpha_{t,:}$

$$\alpha_{t+1,:} = f(\alpha_{t,:})$$

$$\alpha_{t+1,k} = p(z_{t+1}=k \mid x_{1:t+1}) = \sum_j p(z_t=j, z_{t+1}=k \mid x_{1:t+1})$$

multiply by $\frac{p(x_{t+1} \mid x_{1:t})}{p(x_{t+1} \mid x_{1:t})}$

$$= \frac{1}{p(x_{t+1} \mid x_{1:t})} \sum_j p(z_t=j, z_{t+1}=k, x_{t+1} \mid x_{1:t})$$

product rule

$$= \frac{1}{p(x_{t+1} \mid x_{1:t})} \sum_j p(z_t=j \mid x_{1:t}) p(z_{t+1}=k \mid z_t=j, \cancel{x_{1:t}}) p(x_{t+1} \mid z_{t+1}=k, \cancel{z_t}, \cancel{x_{1:t}})$$

cond indep. / cond. indep.

Recursive update:

$$\alpha_{t+1,k} = \frac{\sum_{j=1}^{K} \alpha_{tj} A_{jk} L_{t+1,k}}{\sum_l \sum_j \alpha_{tj} A_{jl} L_{t+1,l}}$$

alpha_update(α_t, A, L_{t+1})
"Forward" update from α_t to α_{t+1}
Input: α_t: length K vector, sums to 1
A: K×K transition proba matrix
L_{t+1}: length K vector "likelihood" $L_{t+1,k} = p(x_{t+1} \mid z_t = k)$

FORWARD algorithm

Base Case $t=1$: $\alpha_{1k} = \frac{\pi_k L_{1k}}{\sum_l \pi_l L_{1l}}$

for $t = 2, 3, 4, \cdots T$:

$\alpha_{tk} = \text{alpha\_update}(\alpha_{t-1}, A, L_t)$

return $\{\alpha_t\}_{t=1}^T$

Runtime
linear in T
quadratic in K

Using Forward Messages to compute incomplete log likelihood.

Recall $\log p(x_{1:T} | \theta)$ is useful to know

difficult to compute by naively summing out $z_{1:T}$

Studying the recurrence relation in alpha_update, we focus on the denominator and see

$$p(x_{t+1} | x_{1:t}) = \sum_{j=1}^{K} \sum_{k=1}^{K} \alpha_{tj} A_{jk} L_{t+1,k}$$

$$= \text{mat\_mult}(\alpha_t, A) \cdot L_{t+1}$$

↑ dot product or inner product

Insight: Compute

$$\log p(x_{1:T}) = \log \underbrace{p(x_1)}_{\text{use denominator in base case } (t=1) \text{ of FORWARD alg.}} + \sum_{t=2}^{T} \log \underbrace{p(x_t | x_{1:t-1})}_{\text{use denominator in step } t \text{ of FORWARD alg.}}$$

Computing backward messages β_t via dynamic programming (BACKWARD alg.)

Definition: $\beta_{tk} = p(x_{t+1:T} \mid z_t = k)$, for $t = 1, 2, \ldots T$

special case: $\beta_{Tk} = 1 \quad \forall k$

because T is final timestep. x_{T+1} does not exist

Procedure: Dynamic Programming

Need to fill in table β: $K \times T$

Start with $\beta_{T:} = 1$

Work back in time using recurrance relation

$\beta_{t-1} = f(\beta_t)$ for $t = T, T-1, \ldots 3, 2, 1$

BACKWARD

Init: $\beta_{T:} = 1$

for $T-1, T-2, \ldots 1$:

$\beta_{tk} = \text{beta\_update}(\beta_{t+1}, L_{t+1}, A)$

Relation

$$\beta_{t-1,k} = p(x_{t:T} \mid z_{t-1} = k) = \sum_{l=1}^{K} p(x_{t:T}, z_t = l \mid z_{t-1} = k) \quad \text{sum rule}$$

$$= \sum_{l=1}^{K} p(x_t, x_{t+1:T} \mid z_t = l, z_{t-1} = k)\, p(z_t = l \mid z_{t-1} = k)$$

$$= \sum_{l=1}^{K} p(x_{t+1:T} \mid z_t = l)\, p(x_t \mid z_t = l)\, p(z_t = l \mid z_{t-1} = k)$$

β

x_{t+1} indep of prev x or $z_{1:t-1}$ given z_t

x_t indep of all else given z_t

L_{tl}

A_{kl}

beta_update

Input: β_t K-len vector

L_t K-len vector of likelihoods

A $K \times K$ trans. proba

$$\beta_{t-1,k} = \sum_{l=1}^{K} \beta_{tl} L_{tl} A_{kl}$$

Recap: E Step

Goal: Update s parameters of $q(z|s)$ to optimal values

Procedure:

Input: π, A, μ, σ (HMM params)

Step 1: Calc likelihood $L = \{L_{tk}\}$

$L_{tk} = \text{NormPDF}(x_t | \mu_k, \sigma_k^2)$

Step 2: Calc forward messages $\alpha = \{\alpha_{tk}\}$

$\log p(x|\theta), \alpha = \text{FORWARD}(\pi, A, L)$ $O(TK^2)$

Calc backward messages $\beta = \{\beta_{tk}\}$

$\beta = \text{BACKWARD}(A, L)$ $O(TK^2)$

Can compute $\log p(x|\theta)$ in FORWARD easily

Step 3: Update s_t to match adjacent timestep joint posterior

for $t = 1, 2, \dots T-1$:

$$s_{tjk} = p(z_t = j, z_{t+1} = k \mid x_{1:T}) \quad \text{for } j,k \text{ in } 1 \dots K$$
$$\propto \alpha_{tj} A_{jk} L_{t+1,k} \beta_{t+1,k}$$

Step 4: Update $r = \{r_{tk}\}$ to match single timestep posterior

for $t = 1, 2, \dots T$

$$r_{tk} \propto \alpha_{tk} \beta_{tk}$$

Remember: $r = r(s)$ We can deterministically calculate r from s. Just useful to have direct expression.

return $\log p(x_{1:T}|\theta), s, r$