COS 513: SEQUENCE MODELS I

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1. INTRODUCTION

In this lecture we consider how to model sequential data. Rather than assuming that the data are all independent of each other we assume they come in sequence $X_{1..T} = x_1, x_{2...}, x_T$. There are two types of sequential models that are quite similar to each other: *Hidden Markov Model (HMM)* and *Kalman Filter*. This lecture focuses on HMM which has many applications including genome modeling and action recognition.

HMMs are a generalization of the finite mixture model (MM) to sequences. In MM, the process of generating IID data involves choosing a



FIGURE 1. Diagram representing transitions between mixture components 1, 2, 3 and observed data. The probability of transition is shown on the edges. xs represent data points and x_1 and x_2 are indicated by the yellow and red x respectively.

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FIGURE 2. Graphical Model

component according to a distribution p(z), independent of choice of components in other steps, and choosing a data vector from the distribution, p(x|z). In HMM, the mixture component is chosen dependent on the previous component. Each component can be seen as a state, and we augment the basic MM to include a matrix of *transition probabilities*.

Figure 1 illustrates this difference. The *x*s are elements of the sequence. Let the *yellow x* represent x_1 and the *red x* represent x_2 . Then in MM, x_2 is approximately equally likely to belong to component 2 or 3. In HMM, x_2 is more likely to belong to component 2, since x_1 belongs to 1, and the probability of state transition from 1 to 2 is high.

2. GRAPHICAL MODEL FOR HMM

In Figure 2, each of the z_t is a multinomial random variable represented by a indicator vector of size K, whose component i is 1 if the cluster index i (for the clusters associated with data $x_{1:T}$) is indicated, and 0 if not. For a particular configuration $(z, y) = (z_1, z_2, ..., z_T, x_1, x_2, ...x_T)$ as shown in Figure 2, the joint probability is given by the product of local conditional probabilities as follows:

(1)
$$p(z_{1..T}, x_{1..T}) = p(z_1) \prod_{t=2}^{T} p(z_t | z_{t-1}) \prod_{t=1}^{T} p(x_t | z_t)$$

We assume above that the distribution $p(x_t|z_t)$ is independent of t.

2.1. Emission probabilities. For a given state k, there is a set of emission probabilities governing the distribution of y_t and we represent it by θ_k . For example, θ_k could be a parameter to a multivariate Gaussian or multinomial Poisson. Thus $p(x_t|z_t)$ can be written as:

(2)
$$p(x_t|z_t) = \prod_{k=1}^{K} p(x_t|\theta_k)^{z_t^k}$$

2.2. **Transition probabilities.** Define a *K* x *K* state transition matrix *A*, where each entry a_{ij} is the probability $p(z_t^j = 1 | z_{t-1}^i = 1)$. The probability of the next state z_t given the current z_{t-1} is given by:

(3)
$$p(z_t|z_{t-1}) = \prod_{k=1}^K \prod_{j=1}^K [a_{jk}]^{z_{t-1}^j z_t^k}$$

Since only one component of z_t or z_{t-1} is 1, there is only one factor on the right-hand side that is different from one.

2.3. **Initial distribution.** The first state node in the sequence has no parents. Thus we define π to be the distribution where $\pi_k = p(z_1^k = 1)$. A more formal definition is as follows:

(4)
$$p(z_1) = \prod_{k=1}^{K} \pi_k^{z_1^k}$$

2.4. Conditional independence. From the graphical model, and using Bayes ball, we can see that conditioning on z_{t-1} renders z_t and z_{t-2} independent. Thus the future is independent of the past, given the present. This is the *Markov property*. Note that this is not true when conditioned on the output node x_{t-1} instead of z_{t-1} .

3. ESTIMATING HMM PARAMETERS USING THE EM ALGORITHM

The parameters of an HMM include the emission probabilities $\hat{\theta}$, the transition matrix \hat{A} and the initial probability distribution $\hat{\pi}$. Given data $x_{1..T}$, we want to estimate these parameters. First we write down the expected complete log likelihood using equations 1 to 4 with respect to the posterior $p(z_{1..T}|x_{1..T})$:

(5)

$$\mathbb{E}[logp(x_{1..T}, z_{1..T})] = \mathbb{E}[log\{\prod_{k=1}^{K} \pi_k^{z_1^k} \prod_{t=2}^{T} \prod_{j=1}^{K} \prod_{k=1}^{K} [a_{jk}]^{z_{t-1}^j z_t^k} \prod_{t=1}^{T} \prod_{k=1}^{K} p(x_t | \theta_k)^{z_t^k}\}]$$

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$$= \sum_{k=1}^{K} \mathbb{E}[z_1^k] \log \pi_k + \sum_{t=2}^{T} \sum_{j=1}^{K} \sum_{k=1}^{K} \mathbb{E}[z_{t-1}^j z_t^k] \log[a_{jk}] + \sum_{t=1}^{T} \sum_{k=1}^{K} \mathbb{E}[z_t^k] \log[(x_t | \theta_k)]$$

E step. We need to compute the following conditional expectations. We will return to these expectations at the end of this section.

(7)
$$\mathbb{E}[z_t^k] = p(z_t = k | x_{1..T})$$

(8)
$$\mathbb{E}[z_{t-1}^{j} z_{t}^{k}] = p(z_{t-1} = j, z_{t} = k | x_{1..T})$$

M step. In the M step, the parameters are adjusted using a process that is equivalent to assuming that the latent variables have been observed. Holding the above expectations fixed, we optimize the parameters to try to eventually converge to a maximum likelihood estimate. An estimate for the prior probability of state z_1 , π_k is given by:

(9)
$$\pi_k = \mathbb{E}[z_1^k] / \sum_{j=1}^k \mathbb{E}[z_1^j]$$

We then estimate the probability of moving from j^{th} state to k^{th} state. In equation 10, the numerator is the number of transitions from j^{th} to k^{th} state and the denominator the total number of transitions from j^{th} state.

(10)
$$a_{jk} = \sum_{t=2}^{T} \mathbb{E}[z_{t-1}^{j} z_{t}^{k}] / \sum_{t=2}^{T} \sum_{l=1}^{k} \mathbb{E}[z_{t-1}^{j} z_{t}^{l}]$$

 θ_k is estimated as the weighted maximum likelihood estimate with weights given by $\mathbb{E}[z_t^k]$. For example, in the Gaussian case, μ_k , the cluster center, is estimated as follows:

(11)
$$\mu_k = \sum_{t=1}^T \mathbb{E}[z_t^k] x_t / \sum_{t=1}^T \mathbb{E}[z_t^k]$$

Each term in the numerator in equation 11 is the probability of x_t being in cluster k multiplied by x_t , and the denominator is the expected number

(6)

of data points in cluster k. The multinomial case where each x_t has exactly one of D fixed, finite outcomes, is as follows:

(12)
$$p(x_t|\theta_k) = \prod_{i=1}^D \theta_{k,i}^{x_t^i}$$

(13)
$$\theta_{k,i} = \sum_{t=1}^{T} \mathbb{E}[z_t^k] x_t^i / \sum_{t=1}^{T} \mathbb{E}[z_t^k]$$

Now, let us consider how to compute $\mathbb{E}(z_t|x_{1..T})$ and $\mathbb{E}[z_{t-1}, z_t|x_{1..T}]$ in the E step. Define $\alpha(z_t)$, $\beta(z_t)$ as follows using a simple application of the Bayes rule, chain rule and conditional independence.

$$\mathbb{E}[z_t|x_{1..T}] = p(z_t|x_{1..T})$$

= $p(z_t, x_{1..T})/p(x_{1..T})$
= $p(x_{1..t}, z_t) \cdot p(x_{t+1..T}|z_t)/p(x_{1..T})$
= $\alpha(z_t) \cdot \beta(z_t)/p(x_{1..T})$

 $\alpha(z_t)$ is the probability of emitting a sequence of outputs $x_{1..t}$ and ending up in state z_t . $\beta(z_t)$ is the probability of emitting a sequence of outputs $x_{t+1..T}$ starting from state z_t .

$$\mathbb{E}[z_{t-1}, z_t | x_{1..T}] = p(z_{t-1}, z_t | x_{1..T})$$

$$= p(x_{1..T}, z_{t-1}, z_t)/p(x_{1..T})$$

$$= p(x_{1..t-1}, z_{t-1}) \cdot p(x_{t..T}, z_t | x_{1..t-1}, z_{t-1})/p(x_{1..T})$$

$$= p(x_{1..t-1}, z_{t-1}) \cdot p(z_t | z_{t-1}) \cdot p(x_{t..T} | z_t, z_{t-1})/p(x_{1..T})$$

$$= p(x_{1..t-1}, z_{t-1}) \cdot p(z_t | z_{t-1}) \cdot p(x_t | z_t, z_{t-1}) \cdot p(x_{t+1..T} | z_t, z_{t-1})/p(x_{1..T})$$

$$= p(x_{1..t-1}, z_{t-1}) \cdot p(z_t | z_{t-1}) \cdot p(x_t | z_t) \cdot p(x_{t+1..T} | z_t)/p(x_{1..T})$$

$$= \alpha(z_{t-1}) \cdot p(z_t | z_{t-1}) \cdot p(x_t | z_t) \cdot \beta(z_t)/p(x_{1..T})$$

(14)

In the above sequence of equations, step 3 follows from splitting the sequence $x_{1..T}$ into $x_{1..t-1}$ and $x_{t..T}$, and applying Bayes rule. In step 4, we use the independence of z_t from $x_{1..t-1}$ given z_{t-1} , and the independence of $x_{t..T}$ from $x_{1..t-1}$ given z_t . Steps 5 and 6 use the independence of x_t from z_{t-1} and $x_{t+1..T}$ from z_{t-1} , and from each other, given z_t . Note that $p(z_t|z_{t-1})$ is given by $a_{z_t,z_{t-1}}$. In the next lecture, we will consider algorithms to compute $\alpha(z_t)$ and $\beta(z_t)$.