# Deep Generative Models: Hidden Markov Models

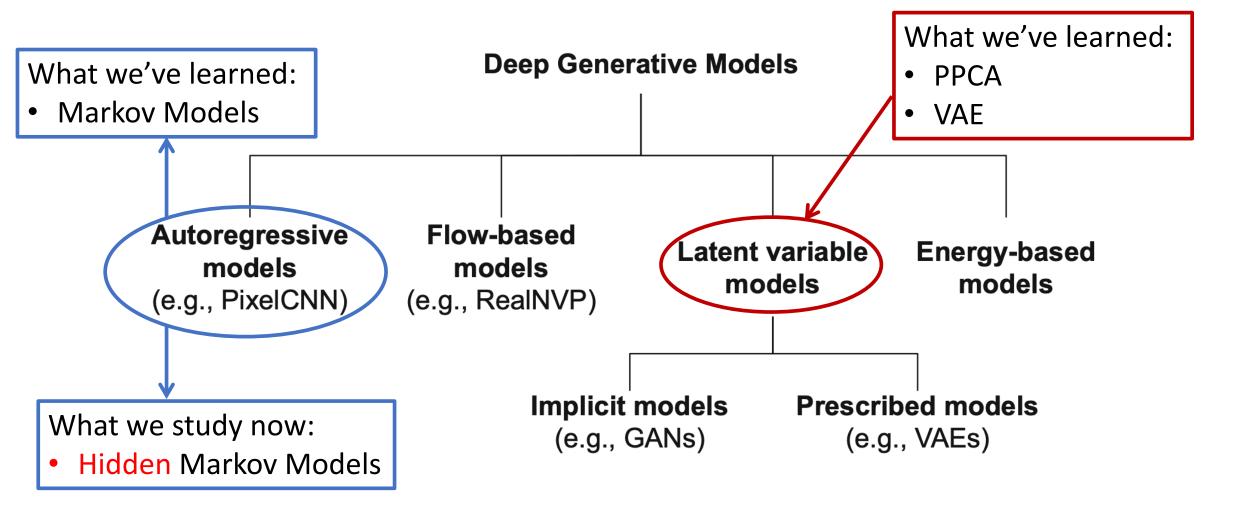
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## Taxonomy of Generative Models

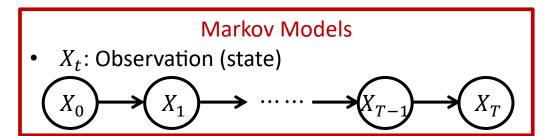


#### Hidden Markov Models (Pictorial Definition)

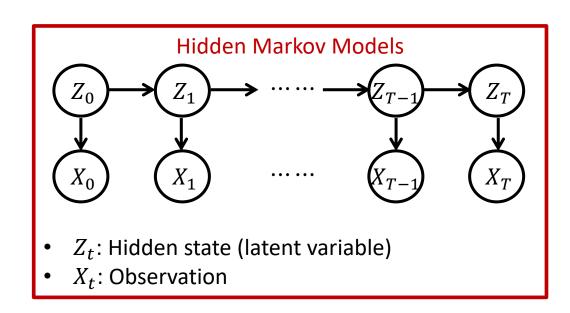
#### **Latent Variable Models**

- Z: Latent variable
- *X*: Observation

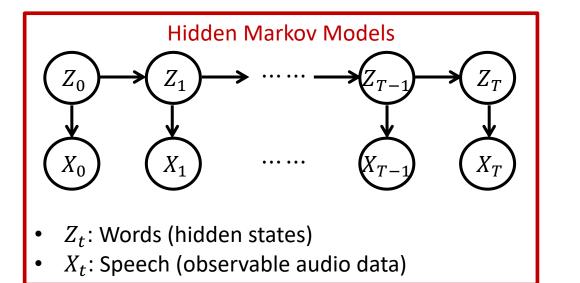




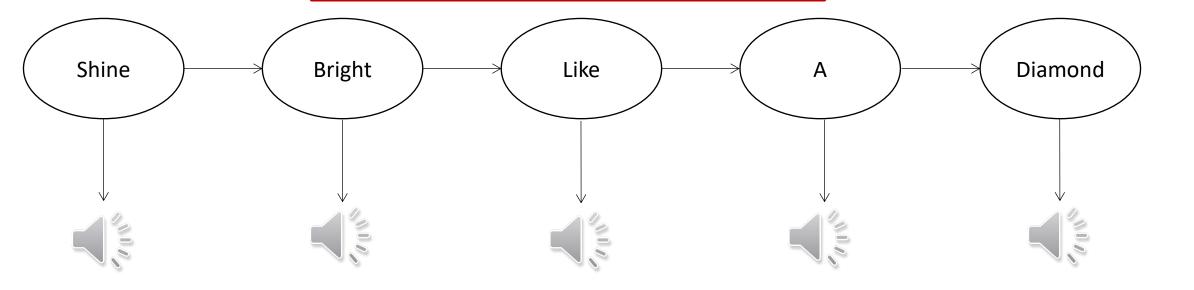
Read it: X depends on Z



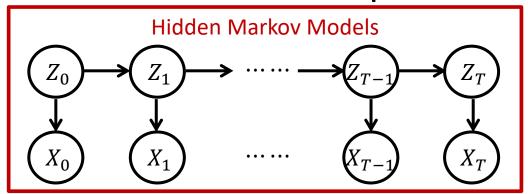
## Example: Speech Recognition



Goal: Given observations (audio), discover the hidden states (words)



#### State Space and Observation Space



- In Markov models, we had state space  $\Omega$  with K different states
  - So we labeled them as  $\Omega = \{1, ..., K\}$  without loss of generality
- In HMMs, we need to distinguish state space  $\Omega$  and observation space  $\Sigma$ 
  - So we define:

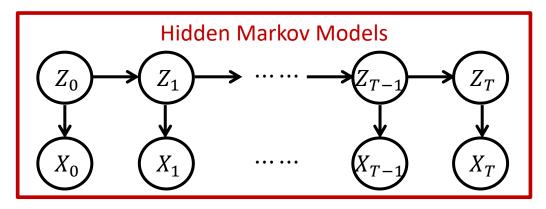
```
State Space \Omega = \{\omega_1, ..., \omega_K\}:
Each Z_t takes values in \Omega
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Observation Space  $\Sigma = \{\sigma_1, ..., \sigma_V\}$ : Each  $X_t$  takes values in  $\Sigma$ 

- But in words we might say:
  - "state i" for  $\omega_i$  (simpler than saying "state omega i")
  - "observation j" for  $\sigma_j$  (simpler than saying "observation sigma j")

#### Formal Definition of Hidden Markov Models

State Space  $\Omega = \{\omega_1, \dots, \omega_K\}$ : Each  $Z_t$  takes values in  $\Omega$ 



Observation Space  $\Sigma = \{\sigma_1, ..., \sigma_V\}$ : Each  $X_t$  takes values in  $\Sigma$ 

- Initial Probability:  $\pi_i = \mathbb{P}(Z_0 = \omega_i), i = 1, ..., K$ .
- Transition Probability:  $a_{ij} \coloneqq \mathbb{P}(Z_t = \omega_i \mid Z_{t-1} = \omega_i), i, j = 1, ... K.$
- Emission Probability:  $c_{jr}\coloneqq \mathbb{P}(X_t=\sigma_r\mid Z_t=\omega_j), j=1,\ldots,K, r=1,\ldots,V.$

Matrix Notation: Transition Matrix  $A \in \mathbb{R}^{K \times K}$ , Emission Matrix  $C \in \mathbb{R}^{K \times V}$ , Initial distribution  $\pi \in \mathbb{R}^K$ 

A hidden Markov model is fully specified by its parameters  $\theta := (\pi, A, C)$ 

#### **Notations**

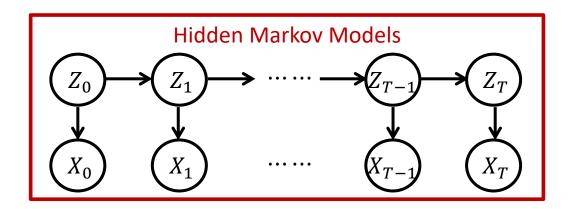
• Studying HMMs need a lot of notations. We review some of them here and spell out the convention that we follow

• 
$$\mathbf{x} := [x_0, \dots, x_T]^{\mathsf{T}}$$
 and similarly for  $\mathbf{z} := [z_0, \dots, z_T]^{\mathsf{T}}$ 

• 
$$n$$
-th observation  $\boldsymbol{x}^{(n)} := \left[x_0^{(n)}, \dots, x_T^{(n)}\right]^{\top}$ 

- $\mathbb{P}(Z_0=z_0,Z_1=z_1)$ : probability that  $Z_0=z_0$  and  $Z_1=z_1$ 
  - We might write  $p(z_0, z_1)$  or  $\mathbb{P}(z_0, Z_1 = z_1)$  for  $\mathbb{P}(Z_0 = z_0, Z_1 = z_1)$  when there is no confusion
  - $\mathbb{P}_{\theta}(Z_0 = z_0, Z_1 = z_1)$  or  $p_{\theta}(z_0, z_1)$  means the underlying probability distribution is parameterized by  $\theta$

#### Assumptions



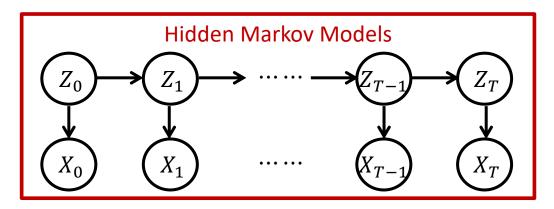
"Markov" Property:

$$p_{\theta}(z_t \mid z_0, ..., z_{t-1}) = p_{\theta}(z_t \mid z_{t-1})$$

Output Independence Assumption:

$$p_{\theta}(x_t \mid z_0, ..., z_T, x_0, ..., x_{t-1}) = p_{\theta}(x_t \mid z_t)$$

#### Consequences



- Emission Probability Factorization (proof: factorize w.r.t.  $x_0, ..., x_T$ ):
  - $p_{\theta}(x_0, ..., x_T \mid z_0, ..., z_T) = \prod_{t=0}^T p_{\theta}(x_t \mid z_t)$
- Transition Probability Factorization (proof: factorize w.r.t.  $z_0, \dots, z_T$ ):
  - $p_{\theta}(z_0, ..., z_T) = p_{\theta}(z_0) \prod_{t=1}^T p_{\theta}(z_t \mid z_{t-1})$
- Joint Probability Factorization (proof: use the above factorizations):

$$p_{\theta}(\mathbf{x}, \mathbf{z}) = p_{\theta}(\mathbf{x} \mid \mathbf{z}) \cdot p_{\theta}(\mathbf{z}) = \prod_{t=0}^{T} p_{\theta}(x_{t} \mid z_{t}) \ p_{\theta}(z_{0}) \prod_{t=1}^{T} p_{\theta}(z_{t} \mid z_{t-1})$$

## Inference, Decoding, and Learning

- Inference. Given  $\theta$ , compute the likelihood  $p_{\theta}(x)$  of observing x
- Decoding. Given observation x and parameters  $\theta$ , find best states:

$$\mathbf{z}^* \in \underset{\mathbf{z}}{\operatorname{argmax}} p_{\theta}(\mathbf{z} \mid \mathbf{x}) = \underset{\mathbf{z}}{\operatorname{argmax}} p_{\theta}(\mathbf{x}, \mathbf{z}) / p_{\theta}(\mathbf{x}) = \underset{\mathbf{z}}{\operatorname{argmax}} p_{\theta}(\mathbf{x}, \mathbf{z})$$

• Learning. Given N observations  $\{x^{(n)}\}_{n=1}^N$ , find best  $\theta$ :

$$\max_{\theta} \prod_{n=1}^{N} p_{\theta}(\boldsymbol{x}^{(n)})$$

- Example (Speech Recognition):
  - During training, we learn an HMM (i.e., parameter  $\theta$ ) from audio data  $x^{(1)}$ , ...,  $x^{(N)}$
  - At test time, we get an audio x. We need to use  $\theta$  and decode x into words  $z^*$  (states)

#### Decoding and Inference via "Brute-Force"

Exponential Time Complexity:  $O(K^{T+1})$ 

• Inference. Given  $\theta$ , x, compute  $p_{\theta}(x)$ :

$$p_{\theta}(\mathbf{x}) = \sum_{\mathbf{z}} p_{\theta}(\mathbf{x}, \mathbf{z}) = \sum_{\mathbf{z}} \prod_{t=0}^{T} p_{\theta}(x_t \mid z_t) \ p_{\theta}(z_0) \prod_{t=1}^{T} p_{\theta}(z_t \mid z_{t-1})$$

• Decoding. Given  $\theta$ , x, compute:

$$\mathbf{z}^* \in \operatorname*{argmax} p_{\theta}(\mathbf{x}, \mathbf{z})$$

- 1. For all possible states z, compute the likelihood  $p_{\theta}(x, z)$
- 2. Output the state that gives the maximum likelihood

State Space  $\Omega = \{\omega_1, ..., \omega_K\}$ : Each  $Z_t$  takes values in  $\Omega$ 

- Inference. Given  $\theta$ , x, compute  $p_{\theta}(x)$
- If T=0, then  $p_{\theta}(\textbf{\textit{x}})=\sum_{z_0}p_{\theta}(x_0,z_0)=\sum_{z_0}p_{\theta}(x_0\mid z_0)\cdot p_{\theta}(z_0)$ 
  - This is a sum of K terms, so we can compute  $p_{\theta}(x)$  in O(K) time
- If T=1, then  $p_{\theta}(x)=\sum_{z_0}\sum_{z_1}p_{\theta}(x_0,x_1,z_0,z_1)$ 
  - Update  $p_{\theta}(x_0, x_1, z_1)$  from  $p_{\theta}(x_0, z_0)$ :

$$p_{\theta}(x_0, x_1, z_1) = \sum_{z_0} p_{\theta}(x_0, x_1, z_1 \mid z_0) \cdot p_{\theta}(z_0)$$

$$= \sum_{z_0} p_{\theta}(x_1 \mid z_1) \cdot p_{\theta}(x_0 \mid z_0) \cdot p_{\theta}(z_0) \cdot p_{\theta}(z_1 \mid z_0)$$

$$= p_{\theta}(x_1 \mid z_1) \cdot \sum_{z_0} p_{\theta}(x_0, z_0) \cdot p_{\theta}(z_1 \mid z_0)$$

• We can compute  $p_{\theta}(x)$  in  $O(K^2)$  time (need to sum over all possible  $z_1$  and  $z_0$ ) Intuition. More generally, can we update  $p_{\theta}(x_0, ..., x_t, z_t)$  from  $p_{\theta}(x_0, ..., x_{t-1}, z_{t-1})$ ? If so, then we might be able to derive a faster algorithm for inference.

• Inference. Given  $\theta$ , x, compute  $p_{\theta}(x)$ 

Intuition. More generally, can we update  $p_{\theta}(x_0, ..., x_t, z_t)$  from  $p_{\theta}(x_0, ..., x_{t-1}, z_{t-1})$ ? If so, then we might be able to derive a faster algorithm for inference.

Forward Probability:

$$\alpha_j(t) \coloneqq \mathbb{P}_{\theta}(x_0, ..., x_t, Z_t = \omega_j)$$

• By definition, we have

$$p_{\theta}(x_0, ..., x_T) = \sum_{j=1}^K \mathbb{P}_{\theta}(x_0, ..., x_T, Z_T = \omega_j) = \sum_{j=1}^K \alpha_j(T)$$

• It remains to derive an update formula for  $\alpha_i(t)$  for t=0,...,T

#### Formalize the Intuition

State Space  $\Omega = \{\omega_1, ..., \omega_K\}$ : Each  $Z_t$  takes values in  $\Omega$ 

$$c_j(x_t) \coloneqq \mathbb{P}_{\theta}\big(x_t \big| Z_t = \omega_j\big)$$

- Inference. Given  $\theta$ , x, compute  $p_{\theta}(x)$
- Forward Probability:

$$\alpha_j(t) \coloneqq \mathbb{P}_{\theta}(x_0, ..., x_t, Z_t = \omega_j)$$

Recurrence Relation:

$$\alpha_{j}(t) = \mathbb{P}_{\theta}(x_{t} \mid x_{0}, ..., x_{t-1}, Z_{t} = \omega_{j}) \cdot \mathbb{P}_{\theta}(x_{0}, ..., x_{t-1}, Z_{t} = \omega_{j})$$

$$= \mathbb{P}_{\theta}(x_{t} \mid Z_{t} = \omega_{j}) \sum_{i=1,...,K} \mathbb{P}_{\theta}(x_{0}, ..., x_{t-1}, Z_{t} = \omega_{j}, Z_{t-1} = \omega_{i})$$

$$= c_{j}(x_{t}) \sum_{i=1}^{K} \mathbb{P}_{\theta}(x_{0}, ..., x_{t-1}, Z_{t-1} = \omega_{i}) \cdot \mathbb{P}_{\theta}(Z_{t} = \omega_{j} \mid x_{0}, ..., x_{t-1}, Z_{t-1} = \omega_{i})$$

$$= c_{j}(x_{t}) \sum_{i=1}^{K} \alpha_{i}(t-1) \cdot \alpha_{ij}$$

## Faster Algorithm for Inference

State Space  $\Omega = \{\omega_1, ..., \omega_K\}$ : Each  $Z_t$  takes values in  $\Omega$ 

Each 
$$Z_t$$
 takes values in  $\Omega$ 

$$c_j(x_t) \coloneqq \mathbb{P}_{\theta}\big(x_t \big| Z_t = \omega_j\big)$$

Time Complexity:  $O(TK^2)$ 

- Inference. Given  $\theta$ , x, compute  $p_{\theta}(x)$
- Forward Probability:  $\alpha_i(t) \coloneqq \mathbb{P}_{\theta}(x_0, ..., x_t, Z_t = \omega_i)$
- Recurrence Relation:  $\alpha_i(t) = c_i(x_t) \sum_{i=1}^K \alpha_i(t-1) \cdot a_{ij}$

- Algorithm:
  - Initialization:  $\alpha_j(0) = \pi_j \cdot c_j(x_0)$

$$\forall j = 1, ..., K$$

• Recursion:  $\alpha_j(t) = c_j(x_t) \sum_{i=1}^K \alpha_i(t-1) \cdot a_{ij}$ 

$$\forall j = 1, ..., K, \forall t = 1, ..., T$$

• Termination: Output  $\sum_{j=1}^{K} \alpha_j(T)$ 

#### What About Decoding?

• Decoding. Given  $\theta$ , x, compute:

$$z^* \in \underset{z}{\operatorname{argmax}} p_{\theta}(x, z)$$

• We know how to decode in  $O(K^{T+1})$  time

- Can we do it in  $O(TK^2)$  time (similarly to inference)?
  - During inference, we need to calculate  $\sum_{\mathbf{z}} p_{\theta}(\mathbf{x}, \mathbf{z})$
- Two differences from inference:
  - Need to calculate the maximum of  $p_{\theta}(x, z)$  over z rather than sum
  - Need to find states  $z^*$  attaining the maximum

## Inference Versus Decoding

State Space  $\Omega = \{\omega_1, ..., \omega_K\}$ : Each  $Z_t$  takes values in  $\Omega$ 

• Inference. Given  $\theta$ , x, compute:

$$p_{\theta}(\mathbf{x}) = \sum_{\mathbf{z}} p_{\theta}(\mathbf{x}, \mathbf{z})$$

• Decoding. Given  $\theta$ , x, compute:

$$\mathbf{z}^* \in \operatorname*{argmax} p_{\theta}(\mathbf{x}, \mathbf{z})$$

Recurrence Term:

$$\alpha_j(t) \coloneqq \mathbb{P}_{\theta}(x_0, \dots, x_t, Z_t = \omega_j)$$

• Recurrence Term:

$$\nu_j(t) \coloneqq \max_{z_0,\dots,z_{t-1} \in \Omega} \mathbb{P}_{\theta}(x_0,\dots,x_t,z_0,\dots,z_{t-1},Z_t = \omega_j)$$

• Decomposition:

$$p_{\theta}(x_0, \dots, x_T) = \sum_{j=1}^K \alpha_j(T)$$

• Decomposition:

$$\max_{z_0, \dots, z_T \in \Omega} p_{\theta}(x_0, \dots, x_T, z_0, \dots, z_T) = \max_{j=1, \dots, K} \nu_j(T)$$

Recurrence Relation:

$$\alpha_j(t) = c_j(x_t) \cdot \sum_{i=1}^K \alpha_i(t-1) \cdot a_{ij}$$

Recurrence Relation: (proof omitted)

$$v_j(t) = c_j(x_t) \cdot \max_{i=1,\dots,K} v_i(t-1) \cdot a_{ij}$$

Intuition. For decoding, just replace sum of inference with max

• Summation over  $z_0, \dots, z_{t-1}$  is implicit in the definition of  $\alpha_j(t)$ , and  $\nu_j(t)$  is indeed obtained by replacing sum with max

$$c_j(x_t) \coloneqq \mathbb{P}_{\theta}(x_t \mid Z_t = \omega_j)$$

• Inference. Given  $\theta$ , x, compute:

$$p_{\theta}(\mathbf{x}) = \sum_{\mathbf{z}} p_{\theta}(\mathbf{x}, \mathbf{z})$$

• Initialization: 
$$(\forall j = 1, ..., K)$$
  
 $\alpha_j(0) = \pi_j \cdot c_j(x_0)$ 

• Recursion:  $(\forall j = 1, ..., K, \forall t = 1, ..., T)$  $\alpha_j(t) = c_j(x_t) \cdot \sum_{i=1}^K \alpha_i(t-1) \cdot a_{ij}$ 

• Output:

optimal value = 
$$\sum_{j=1}^{K} \alpha_j(T)$$

$$c_j(x_t) \coloneqq \mathbb{P}_{\theta}(x_t \mid Z_t = \omega_j)$$

• Decoding. Given  $\theta$ , x, compute:  $z^* \in \operatorname{argmax} p_{\theta}(x, z)$ 

• Initialization:  $(\forall j = 1, ..., K)$  $v_i(0) = \pi_i \cdot c_i(x_0)$ 

• Recursion:  $(\forall j = 1, ..., K, \forall t = 1, ..., T)$  $v_j(t) = c_j(x_t) \cdot \max_{i=1,...,K} v_i(t-1) \cdot a_{ij}$ 

Output:

optimal value = 
$$\max_{j=1,...,K} v_j(T)$$

One more step needed: find  $z^*$  that attains the optimum Solution: "backtracking" (next page)

- Understanding Backtracking:
  - $i^*(T)$ : optimal state index at time T
  - $prev_j(t)$ : "optimal" state index at time t-1 to arrive at state j at time t
  - Question: What is  $prev_{i^*(T)}(T)$ ?
  - Answer:
    - it is the optimal state index at time T-1
    - thus, we assign it to  $i^*(T-1)$
  - Therefore  $(\forall t = T, ..., 1)$ :  $i^*(t-1) = prev_{i^*(t)}(t)$

#### Algorithm (Viterbi)

• Initialization:  $(\forall j = 1, ..., K)$ 

$$v_j(0) = \pi_j \cdot c_j(x_0)$$

- Recursion:  $(\forall j = 1, ..., K, \forall t = 1, ..., T)$   $v_{j}(t) = c_{j}(x_{t}) \cdot \max_{i=1,...,K} \{v_{i}(t-1) \cdot a_{ij}\}$   $prev_{j}(t) = \underset{i=1,...,K}{\operatorname{argmax}} \{v_{i}(t-1) \cdot a_{ij}\}$
- Output:

optimal value = 
$$\max_{j=1,...,K} v_j(T)$$

$$i^*(T) = \underset{j=1,\dots,K}{\operatorname{argmax}} v_j(T)$$

• Backtracking:  $(\forall t = T, ..., 1)$  $i^*(t-1) = prev_{i^*(t)}(t)$ 

## Inference, Decoding, and Learning

- Inference. Given  $\theta$ , x, compute  $p_{\theta}(x)$
- Decoding. Given  $\theta$ , x, compute:

$$\mathbf{z}^* \in \operatorname*{argmax} p_{\theta}(\mathbf{x}, \mathbf{z})$$

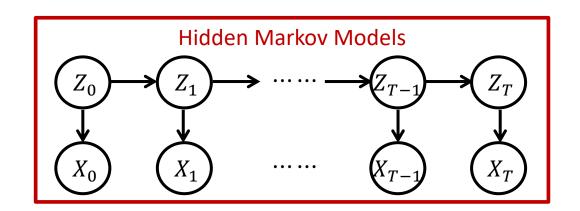
• Learning. Given N observations  $\{x^{(n)}\}_{n=1}^{N}$ , find best  $\theta$ :

$$\max_{\theta} \prod_{n=1}^{N} p_{\theta}(\boldsymbol{x}^{(n)})$$

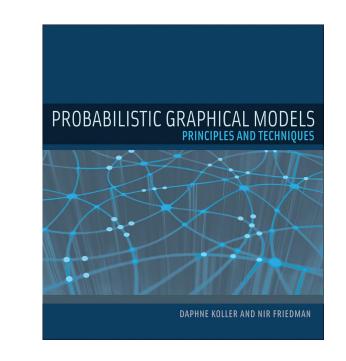
- We've seen how to perform inference and decoding in  $O(TK^2)$  time
  - sum vs. max, dynamic programming, backtracing
- We can perform learning via the EM algorithm
  - derivations are algebraically involved and are given at the end of the slides.

#### Conclusion

- We have studied HMMs
  - Inference, Decoding, and Learning
  - Viterbi algorithm for decoding



- Further Study: Probabilistic Graphical Models (PGMs)
  - Graph can model more complicated dependency:
    - nodes denote random variables
    - edges denote the dependency between random variables
  - HMMs are examples of PGMs
  - We can extend the notions of inference and learning for PGMs



## Appendix (Optional)

• In the subsequent slides, we derive EM for learning the parameters of HMMs.

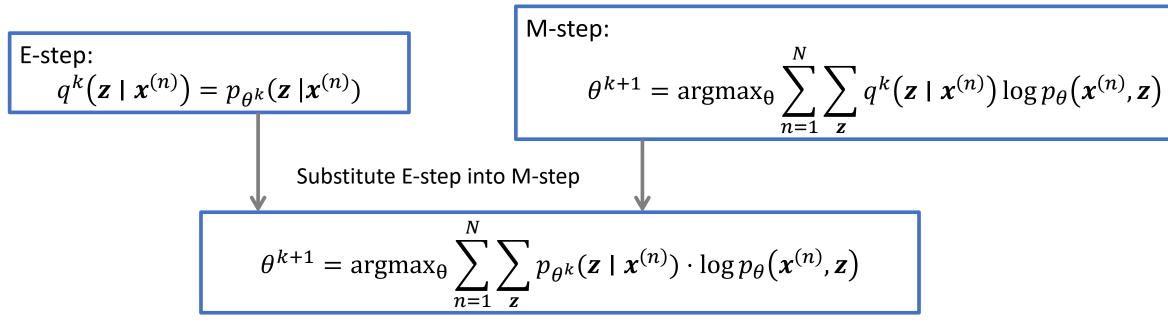
#### Learning Hidden Markov Models

$$\mathbf{x}^{(n)} \coloneqq \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$
 $\mathbf{z} \coloneqq \left(z_0, \dots, z_T\right)$ 

• Learning. Given N observations  $\{x^{(n)}\}_{n=1}^{N}$ , find best  $\theta$ :

$$\max_{\theta} \prod_{n=1}^{N} p_{\theta}(\boldsymbol{x}^{(n)})$$

• EM Algorithm. Initialize  $\theta^0$  and alternate: (k= iteration counter)



- We next instantiate the EM algorithm based on the hidden Markov model
  - Caution: This involves multiple pages of derivations

#### EM for Mixture Models: A Basic Fact

To proceed, we recall a basic fact we've seen multiple times

Fact. Consider the following optimization problem:

$$p^* = \operatorname{argmax}_p \sum_{i=1}^K s_i \log(p_i)$$

subject to 
$$p_1 + \dots + p_K = 1$$

This problem admits a closed-form solution for  $p^* = [p_1^*, ..., p_K^*]$ :

$$p_i^* = \frac{s_i}{\sum_{i=1}^K s_i}$$

• In the sequel, we will use this fact often. When we use it, we write (concisely):

Fact:  $\sum_{i=1}^{K} s_i \log(p_i)$  is maximized at  $p_i = s_i / (\sum_{i=1}^{K} s_i)$ 

#### Instantiate EM for HMMs

$$\mathbf{x}^{(n)} \coloneqq \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$
 $\mathbf{z} \coloneqq \left(z_0, \dots, z_T\right)$ 

$$\theta^{k+1} = \operatorname{argmax}_{\theta} \sum_{n=1}^{N} \sum_{\mathbf{z}} p_{\theta^{k}}(\mathbf{z} | \mathbf{x}^{(n)}) \cdot \log p_{\theta}(\mathbf{x}^{(n)}, \mathbf{z})$$

$$p_{\theta}(\mathbf{x}^{(n)}, \mathbf{z}) := \prod_{t=0}^{T} p_{C}(x_{t}^{(n)} | z_{t}) p_{\pi}(z_{0}) \prod_{t=1}^{T} p_{A}(z_{t} | z_{t-1})$$

$$(\pi^{k+1}, A^{k+1}, C^{k+1}) = \operatorname{argmax}_{\pi, A, C} \sum_{n=1}^{N} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \,|\, \mathbf{x}^{(n)}) \left( \log p_{\pi}(z_0) + \sum_{t=0}^{T} \log p_{C} \left( x_t^{(n)} \,|\, z_t \right) + \sum_{t=1}^{T} \log p_{A}(z_t | z_{t-1}) \right)$$

The objective function is separable

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{n=1}^{N} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0)$$

$$C^{k+1} = \operatorname{argmax}_{C} \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)}) \log p_{C}\left(x_t^{(n)} \mid z_t\right)$$

$$A^{k+1} = \operatorname{argmax}_{A} \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{\mathbf{z}} p_{\theta^{k}}(\mathbf{z} | \mathbf{x}^{(n)}) \log p_{A}(z_{t} | z_{t-1})$$

#### Instantiate EM for HMMs

$$\mathbf{x}^{(n)} \coloneqq \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$
 $\mathbf{z} \coloneqq \left(z_0, \dots, z_T\right)$ 

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{n=1}^{N} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0)$$

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{n=1}^{N} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0) \qquad C^{k+1} = \operatorname{argmax}_{C} \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)}) \log p_{C}\left(x_t^{(n)} \mid z_t\right)$$

$$A^{k+1} = \operatorname{argmax}_{A} \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{\mathbf{z}} p_{\theta^{k}}(\mathbf{z} | \mathbf{x}^{(n)}) \log p_{A}(z_{t} | z_{t-1})$$

#### Observation. The summation over z in the above can be simplified, e.g.,

- In the update of  $\pi^{k+1}$ ,
  - $\log p_{\pi}(z_0)$  depends only on  $z_0$
  - $p_{Ak}(\mathbf{z} | \mathbf{x}^{(n)})$  depends on  $\mathbf{z} \coloneqq (z_0, ..., z_T)$
- So we have

$$\sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \,|\, \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0) = \sum_{z_0, \dots, z_T} p_{\theta^k}(\mathbf{z} \,|\, \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0) = \sum_{z_0} p_{\theta^k}(\mathbf{z}_0 \,|\, \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0)$$

• Similarly we can simplify the updates of  $A^{k+1}$  and  $C^{k+1}$ 

#### Instantiate EM for HMMs

$$\mathbf{x}^{(n)} \coloneqq \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$
 $\mathbf{z} \coloneqq \left(z_0, \dots, z_T\right)$ 

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{n=1}^{N} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0)$$

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{n=1}^{N} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0) \qquad C^{k+1} = \operatorname{argmax}_{C} \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{\mathbf{z}} p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)}) \log p_{C}\left(x_t^{(n)} \mid z_t\right)$$

$$A^{k+1} = \operatorname{argmax}_{A} \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{\mathbf{z}} p_{\theta^{k}}(\mathbf{z} | \mathbf{x}^{(n)}) \log p_{A}(z_{t} | z_{t-1})$$

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{n=1}^{N} \sum_{z_0} p_{\theta^k}(z_0 | \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0)$$

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{n=1}^{N} \sum_{z_0} p_{\theta^k}(z_0 \mid \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0) \qquad C^{k+1} = \operatorname{argmax}_{C} \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{z_t} p_{\theta^k}(z_t \mid \mathbf{x}^{(n)}) \log p_{C} \left( x_t^{(n)} \mid z_t \right)$$

$$A^{k+1} = \operatorname{argmax}_{A} \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{z_{t}, z_{t-1}} p_{\theta^{k}}(z_{t}, z_{t-1} | \boldsymbol{x}^{(n)}) \log p_{A}(z_{t} | z_{t-1})$$

We will next handle the update of  $\pi^{k+1}$ ,  $A^{k+1}$ , and  $C^{k+1}$  in succession

State Space  $\Omega = \{\omega_1, ..., \omega_K\}$ :

Each  $Z_t$  takes values in  $\Omega$ 

 $\boldsymbol{x}^{(n)} \coloneqq \left(\boldsymbol{x}_0^{(n)}, \dots, \boldsymbol{x}_T^{(n)}\right)$ 

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{n=1}^{N} \sum_{z_0} p_{\theta^k}(z_0 | \mathbf{x}^{(n)}) \cdot \log p_{\pi}(z_0)$$

Rewrite the objective using the definition of  $\pi_i$  and add the constraints  $\pi_1 + \cdots + \pi_K = 1$ 

$$\pi^{k+1} = \operatorname{argmax}_{\pi} \sum_{i=1}^{K} \sum_{i=1}^{K} \mathbb{P}_{\theta^k}(Z_0 = \omega_i \mid \boldsymbol{x}^{(n)}) \log(\pi_i) \quad \text{subject to} \quad \pi_1 + \dots + \pi_K = 1$$

Fact:  $\sum_{i=1}^{K} s_i \log(p_i)$  is maximized at  $p_i = s_i / (\sum_{i=1}^{K} s_i)$ . But what is  $s_i$ ?

$$\pi_i^{k+1} = \frac{\sum_{n=1}^{N} \mathbb{P}_{\theta^k}(Z_0 = \omega_i \mid \boldsymbol{x}^{(n)})}{\sum_{n=1}^{N} \sum_{i=1}^{K} \mathbb{P}_{\theta^k}(Z_0 = \omega_i \mid \boldsymbol{x}^{(n)})} = \frac{\sum_{n=1}^{N} \mathbb{P}_{\theta^k}(Z_0 = \omega_i \mid \boldsymbol{x}^{(n)})}{N}, \qquad \forall i = 1, ..., K$$

Remark. We will calculate  $\mathbb{P}_{\theta^k}(Z_0 = \omega_i \mid \boldsymbol{x}^{(n)})$  later

## Updating $A^{k+1}$

State Space  $\Omega = \{\omega_1, ..., \omega_K\}$ :

Each  $Z_t$  takes values in  $\Omega$ 

 $\mathbf{x}^{(n)} \coloneqq \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$ 

$$A^{k+1} = \operatorname{argmax}_{A} \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{z_{t}, z_{t-1}} p_{\theta^{k}}(z_{t}, z_{t-1} | \boldsymbol{x}^{(n)}) \log p_{A}(z_{t} | z_{t-1})$$

Rewrite the objective using the definition of  $a_{ij}$  and add the constraints  $\sum_{j=1}^{K} a_{ij} = 1 \ (\forall i)$ 

$$A^{k+1} = \operatorname{argmax}_{A} \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{j=1}^{K} \sum_{i=1}^{K} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j}, Z_{t-1} = \omega_{i} | \mathbf{x}^{(n)}) \log a_{ij} \qquad \text{subject to } \sum_{j=1}^{K} a_{ij} = 1 \ (\forall i)$$

↓ The objective function and constraints are separable

$$(a_{i1}^{k+1}, \dots, a_{iK}^{k+1}) = \operatorname{argmax}_{A} \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{j=1}^{K} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j}, Z_{t-1} = \omega_{i} | \mathbf{x}^{(n)}) \log a_{ij} \qquad \text{subject to } \sum_{j=1}^{K} a_{ij} = 1$$

Fact:  $\sum_{j=1}^{K} s_j \log(p_j)$  is maximized at  $p_j = s_j / (\sum_{j=1}^{K} s_j)$ . But what is  $s_j$ ?

$$a_{ij}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j}, Z_{t-1} = \omega_{i} | \boldsymbol{x}^{(n)})}{\sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{j=1}^{K} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j}, Z_{t-1} = \omega_{i} | \boldsymbol{x}^{(n)})} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j}, Z_{t-1} = \omega_{i} | \boldsymbol{x}^{(n)})}{\sum_{n=1}^{N} \sum_{t=1}^{T} \mathbb{P}_{\theta^{k}} (Z_{t-1} = \omega_{i} | \boldsymbol{x}^{(n)})}$$
 (\forall i, j)

Remark. We will calculate  $\mathbb{P}_{\theta^k}(Z_t = \omega_i, Z_{t-1} = \omega_i | \mathbf{x}^{(n)})$  and  $\mathbb{P}_{\theta^k}(Z_{t-1} = \omega_i | \mathbf{x}^{(n)})$  later

## Updating $C^{k+1}$

State Space  $\Omega = \{\omega_1, ..., \omega_K\}$ :

Each  $Z_t$  takes values in  $\Omega$ 

Observation Space  $\Sigma = \{\sigma_1, ..., \sigma_V\}$ :

Each 
$$X_t$$
 takes values in  $\Sigma$ 

$$C^{k+1} = \operatorname{argmax}_{C} \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{z_{t}} \mathbb{P}_{\theta^{k}}(z_{t} | \boldsymbol{x}^{(n)}) \log p_{C}\left(\boldsymbol{x}_{t}^{(n)} \middle| z_{t}\right)$$

$$\mathbf{x}^{(n)} \coloneqq \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$

Rewrite the objective using the definition of  $b_{jr}$ , indicator function  $\mathbb{I}(\cdot)$ , and add the constraints  $\sum_{r=1}^{V} c_{jr} = 1 \ (\forall j)$ 

$$C^{k+1} = \operatorname{argmax}_{C} \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{j=1}^{K} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j} | \boldsymbol{x}^{(n)}) \log p_{C} \left( \boldsymbol{x}_{t}^{(n)} | Z_{t} = \omega_{j} \right)$$

$$= \operatorname{argmax}_{C} \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{j=1}^{K} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j} | \boldsymbol{x}^{(n)}) \sum_{r=1}^{V} \mathbb{I} \left( \boldsymbol{x}_{t}^{(n)} = \sigma_{r} \right) \log c_{jr}$$
s.t.  $\sum_{r=1}^{V} c_{jr} = 1 \ (\forall j)$ 

$$(c_{j1}^{k+1}, \dots, c_{jV}^{k+1}) = \operatorname{argmax}_{C} \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{r=1}^{V} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j} \mid \mathbf{x}^{(n)}) \mathbb{I} \left( \mathbf{x}_{t}^{(n)} = \sigma_{r} \right) \log c_{jr} \quad \text{s.t. } \sum_{r=1}^{V} c_{jr} = 1$$

Fact:  $\sum_{r=1}^{V} s_r \log(p_r)$  is maximized at  $p_r = s_r / (\sum_{r=1}^{V} s_r)$ . But what is  $s_r$ ?

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j} \mid \boldsymbol{x}^{(n)}) \mathbb{I} \left( \boldsymbol{x}_{t}^{(n)} = \sigma_{r} \right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{r=1}^{V} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j} \mid \boldsymbol{x}^{(n)}) \mathbb{I} \left( \boldsymbol{x}_{t}^{(n)} = \sigma_{r} \right)} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j} \mid \boldsymbol{x}^{(n)}) \mathbb{I} \left( \boldsymbol{x}_{t}^{(n)} = \sigma_{r} \right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^{k}} (Z_{t} = \omega_{j} \mid \boldsymbol{x}^{(n)})} \quad (\forall j, r)$$

Remark. We will calculate  $\mathbb{P}_{\theta^k}(Z_t = \omega_i | \mathbf{x}^{(n)})$  later

$$\pi_{i}^{k+1} = \frac{\sum_{n=1}^{N} \mathbb{P}_{\theta^{k}}(Z_{0} = \omega_{i} \mid \boldsymbol{x}^{(n)})}{N}$$

$$a_{ij}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \mathbb{P}_{\theta^{k}}(Z_{t} = \omega_{j}, Z_{t-1} = \omega_{i} \mid \boldsymbol{x}^{(n)})}{\sum_{n=1}^{N} \sum_{t=1}^{T} \mathbb{P}_{\theta^{k}}(Z_{t-1} = \omega_{i} \mid \boldsymbol{x}^{(n)})}$$

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^{k}}(Z_{t} = \omega_{j} \mid \boldsymbol{x}^{(n)}) \mathbb{I}\left(\boldsymbol{x}_{t}^{(n)} = \sigma_{r}\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^{k}}(Z_{t} = \omega_{j} \mid \boldsymbol{x}^{(n)})}$$

$$(\forall i, j)$$

$$(\forall i, j)$$

$$(\forall j, r)$$

- Question: How to understand and interpret the above update formulas?
- Hint: Probability is expectation of indicator function, that is

$$\sum_{n=1}^{N} \mathbb{P}_{\theta^k}(Z_0 = \omega_i \mid \boldsymbol{x}^{(n)}) = \sum_{n=1}^{N} \mathbb{E}_{\theta^k}[\mathbb{I}(Z_0 = \omega_i) \mid \boldsymbol{x}^{(n)}]$$

Answer:

$$\pi_i^{k+1} = \frac{\text{Expected number of times that } Z_0 = \omega_i \text{ takes place, given } \left\{x^{(n)}\right\}_{n=1}^N \text{ and } \theta^k}{N}$$

We can interpret  $a_{ij}^{k+1}$  and  $c_{jr}^{k+1}$  similarly (how?)

$$\pi_{i}^{k+1} = \frac{\sum_{n=1}^{N} \mathbb{P}_{\theta^{k}}(Z_{0} = \omega_{i} \mid \boldsymbol{x}^{(n)})}{N}$$

$$\alpha_{ij}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \mathbb{P}_{\theta^{k}}(Z_{t} = \omega_{j}, Z_{t-1} = \omega_{i} \mid \boldsymbol{x}^{(n)})}{\sum_{n=1}^{N} \sum_{t=1}^{T} \mathbb{P}_{\theta^{k}}(Z_{t-1} = \omega_{i} \mid \boldsymbol{x}^{(n)})}$$

$$C_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^{k}}(Z_{t} = \omega_{j} \mid \boldsymbol{x}^{(n)}) \mathbb{I}\left(\boldsymbol{x}_{t}^{(n)} = \sigma_{r}\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^{k}}(Z_{t} = \omega_{j} \mid \boldsymbol{x}^{(n)})}$$

$$(\forall i, j)$$

$$(\forall i, j)$$

$$(\forall j, r)$$

- To proceed, it suffices to calculate the following "posteriors"  $(\forall i, j)$ :
  - $\xi_{ij}^k(t,n) \coloneqq \mathbb{P}_{\theta^k}(Z_t = \omega_j, Z_{t-1} = \omega_i \mid \mathbf{x}^{(n)}) \ (\forall t > 0)$
  - $\gamma_j^k(t,n) \coloneqq \mathbb{P}_{\theta^k}(Z_t = \omega_j \mid \boldsymbol{x}^{(n)}) \ (\forall t \ge 0)$
- Indeed, we have:

Remark. Computing  $\xi_{ij}^k(t,n)$  and  $\gamma_i^k(t,n)$  is the **E-step!** 

- In general, the E-step requires computing the posterior  $p_{\theta^k}(\mathbf{z} \mid \mathbf{x}^{(n)})$  for all possible  $\mathbf{z}$ .
- For HMMs, computing  $\xi_{ij}^k(t,n)$  and  $\gamma_i^k(t,n)$  is enough

$$\pi_{i}^{k+1} = \frac{\sum_{n=1}^{N} \gamma_{i}^{k}(0, n)}{N}$$

$$\alpha_{ij}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \xi_{ij}^{k}(t, n)}{\sum_{n=1}^{N} \sum_{t=1}^{T} \gamma_{i}^{k}(t-1, n)}$$

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_{j}^{k}(t, n) \mathbb{I}\left(x_{t}^{(n)} = \sigma_{r}\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_{j}^{k}(t, n)}$$

$$(\forall i, j)$$

$$(\forall i, j)$$

$$(\forall j, r)$$

$$\pi_{i}^{k+1} = \frac{\sum_{n=1}^{N} \gamma_{i}^{k}(0, n)}{N}$$

$$a_{ij}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \xi_{ij}^{k}(t, n)}{\sum_{n=1}^{N} \sum_{t=1}^{T} \gamma_{i}^{k}(t-1, n)}$$

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_{j}^{k}(t, n) \mathbb{I}\left(x_{t}^{(n)} = \sigma_{r}\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_{j}^{k}(t, n)}$$

$$(\forall i, j)$$

$$(\forall i, j)$$

$$(\forall i, j)$$

$$(\forall j, r)$$

- $\xi_{ij}^k(t,n) \coloneqq \mathbb{P}_{\theta^k}(Z_t = \omega_j, Z_{t-1} = \omega_i \mid \mathbf{x}^{(n)}) \ (\forall t > 0)$
- $\gamma_j^k(t,n) \coloneqq \mathbb{P}_{\theta^k}(Z_t = \omega_j \mid \mathbf{x}^{(n)}) \ (\forall t \ge 0)$
- Question. Wouldn't it be enough to compute  $\xi_{ij}^k(t,n)$  only, as we obviously have

$$\gamma_{j}^{k}(t-1,n) = \sum_{i=1}^{K} \xi_{ij}^{k}(t,n)$$
?

- Answer.
  - $\xi_{ij}^k(t,n)$  and  $\gamma_j^k(t,n)$  are widely used notations elsewhere: Not possible to uproot them

$$\pi_{i}^{k+1} = \frac{\sum_{n=1}^{N} \gamma_{i}^{k}(0, n)}{N}$$

$$\alpha_{ij}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \xi_{ij}^{k}(t, n)}{\sum_{n=1}^{N} \sum_{t=1}^{T} \gamma_{i}^{k}(t-1, n)}$$

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_{j}^{k}(t, n) \mathbb{I}\left(x_{t}^{(n)} = \sigma_{r}\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_{j}^{k}(t, n)}$$

$$(\forall i, j)$$

$$(\forall i, j)$$

$$(\forall j, r)$$

- $\xi_{ij}^{k}(t,n) \coloneqq \mathbb{P}_{\theta^{k}}(Z_{t} = \omega_{i}, Z_{t-1} = \omega_{i} \mid \boldsymbol{x}^{(n)}) \ (\forall t > 0)$
- $\gamma_i^k(t,n) \coloneqq \mathbb{P}_{\theta^k}(Z_t = \omega_i \mid \mathbf{x}^{(n)}) \ (\forall t \ge 0)$
- Dropping indices n, k for clarity, we can reformulate our goal (**E-step**) as follows:

**E-step.** Given 
$$\mathbf{y} = (x_1, ..., x_T)$$
 and  $\theta$ , compute  $(\forall i, j)$   
•  $\xi_{ij}(t) = \mathbb{P}_{\theta}(Z_t = \omega_i, Z_{t-1} = \omega_i \mid x_0, ..., x_T)$  ( $t$ 

- (t > 0)
- $\gamma_i(t) = \mathbb{P}_{\theta}(Z_t = \omega_i \mid x_0, ..., x_T)$

# Computing $\xi_{ij}(t)$ and $\gamma_j(t)$

$$\begin{aligned} & \alpha_j(t) \coloneqq \mathbb{P}_{\theta}(x_0, \dots, x_t, Z_t = \omega_j) \\ & \beta_j(t) \coloneqq \mathbb{P}_{\theta}(x_{t+1}, \dots, x_T \mid Z_t = \omega_j) \end{aligned}$$

- **E-step.** Given  $\mathbf{x} = (x_1, ..., x_T)$  and  $\theta$ , compute  $(\forall i, j)$
- $\xi_{ij}(t) = \mathbb{P}_{\theta}(Z_t = \omega_j, Z_{t-1} = \omega_i \mid x_0, ..., x_T)$  (t > 0)
- $\gamma_j(t) = \mathbb{P}_{\theta}(Z_t = \omega_j \mid x_0, \dots, x_T)$   $(t \ge 0)$
- Intuition:  $\xi_{ij}(t)$  and  $\gamma_j(t)$  are "posteriors"
  - To compute them, we need to convert them into likelihood via Bayes rule
- Applying the Bayes rule to  $\gamma_i(t)$  gives

$$\gamma_{j}(t) = \frac{\mathbb{P}_{\theta}(x_{0},\dots,x_{T},Z_{t}=\omega_{j})}{\mathbb{P}_{\theta}(x_{0},\dots,x_{T})} = \frac{\mathbb{P}_{\theta}(x_{0},\dots,x_{t},Z_{t}=\omega_{j}) \cdot \mathbb{P}_{\theta}(x_{t+1},\dots,x_{T} \mid x_{0},\dots,x_{t},Z_{t}=\omega_{j})}{\mathbb{P}_{\theta}(x_{0},\dots,x_{T})}$$

$$= \frac{\mathbb{P}_{\theta}(x_{0},\dots,x_{t},Z_{t}=\omega_{j}) \cdot \mathbb{P}_{\theta}(x_{t+1},\dots,x_{T} \mid Z_{t}=\omega_{j})}{\mathbb{P}_{\theta}(x_{0},\dots,x_{T})} = \frac{\alpha_{j}(t) \cdot \mathbb{P}_{\theta}(x_{t+1},\dots,x_{T} \mid Z_{t}=\omega_{j})}{\sum_{i=1}^{K} \alpha_{i}(t) \cdot \mathbb{P}_{\theta}(x_{t+1},\dots,x_{T} \mid Z_{t}=\omega_{i})} = \frac{\alpha_{j}(t)\beta_{j}(t)}{\sum_{i=1}^{K} \alpha_{i}(t)\beta_{i}(t)}$$

- $\beta_i(t)$  is called "backward probability"
- To update  $\gamma_j(t)$ , it suffices to recursively update  $\alpha_j(t)$  and  $\beta_j(t)$

# Computing $\xi_{ij}(t)$ and $\gamma_j(t)$

 $\alpha_{j}(t) \coloneqq \mathbb{P}_{\theta}(x_{0}, \dots, x_{t}, Z_{t} = \omega_{j})$  $\beta_{j}(t) \coloneqq \mathbb{P}_{\theta}(x_{t+1}, \dots, x_{T} \mid Z_{t} = \omega_{j})$ 

**E-step.** Given 
$$\mathbf{x} = (x_1, ..., x_T)$$
 and  $\theta$ , compute  $(\forall i, j)$ 

• 
$$\xi_{ij}(t) = \mathbb{P}_{\theta}(Z_t = \omega_i, Z_{t-1} = \omega_i \mid x_0, \dots, x_T)$$
  $(t > 0)$ 

• 
$$\gamma_i(t) = \mathbb{P}_{\theta}(Z_t = \omega_i \mid x_0, \dots, x_T)$$
  $(t \ge 0)$ 

$$c_j(x_t) \coloneqq \mathbb{P}_{\theta}(x_t | Z_t = \omega_j)$$

• 
$$\gamma_j(t) = \frac{\mathbb{P}_{\theta}(x_0,...,x_T,Z_t=\omega_j)}{\mathbb{P}_{\theta}(x_0,...,x_T)} = \frac{\alpha_j(t)\beta_j(t)}{\sum_{i=1}^K \alpha_i(t)\beta_i(t)}$$

• Similarly, applying the Bayes rule to  $\xi_{ij}(t)$  gives: (details omitted, please verify)

$$\xi_{ij}(t) = \frac{\mathbb{P}_{\theta}(x_0, \dots, x_T, Z_t = \omega_j, Z_{t-1} = \omega_i)}{\mathbb{P}_{\theta}(x_0, \dots, x_T)} = \dots = \frac{\underbrace{c_j(y_t) \cdot a_{ij} \cdot \alpha_i(t-1)\beta_j(t)}}{\sum_{i=1}^K \alpha_i(t)\beta_i(t)}$$

Remark.  $\gamma_j(t)$  and  $\xi_{ij}(t)$  have the same denominator.

## Computing $\xi_{ij}(t)$ and $\gamma_j(t)$

**E-step.** Given  $x = (x_1, ..., x_T)$  and  $\theta$ , compute  $(\forall i, j)$ 

• 
$$\xi_{ij}(t) = \mathbb{P}_{\theta}(Z_t = \omega_i, Z_{t-1} = \omega_i \mid x_0, \dots, x_T)$$
  $(t > 0)$ 

• 
$$\gamma_i(t) = \mathbb{P}_{\theta}(Z_t = \omega_i \mid x_0, \dots, x_T)$$
  $(t \ge 0)$ 

• 
$$\gamma_j(t) = \frac{\mathbb{P}_{\theta}(x_0,...,x_T,Z_t=\omega_j)}{\mathbb{P}_{\theta}(x_0,...,x_T)} = \frac{\alpha_j(t)\beta_j(t)}{\sum_{i=1}^K \alpha_i(t)\beta_i(t)}$$

• 
$$\xi_{ij}(t) = \frac{\mathbb{P}_{\theta}(x_0,\dots,x_T,Z_t=\omega_j,Z_{t-1}=\omega_i)}{\mathbb{P}_{\theta}(x_0,\dots,x_T)} = \dots = \frac{c_j(y_t)\cdot a_{ij}\cdot \alpha_i(t-1)\beta_j(t)}{\sum_{i=1}^K \alpha_i(t)\beta_i(t)}$$

$$\alpha_{j}(t) := \mathbb{P}_{\theta}(x_{0}, \dots, x_{t}, Z_{t} = \omega_{j})$$
  
$$\beta_{j}(t) := \mathbb{P}_{\theta}(x_{t+1}, \dots, x_{T} \mid Z_{t} = \omega_{j})$$

$$c_j(x_t) \coloneqq \mathbb{P}_{\theta}\big(x_t \big| Z_t = \omega_j\big)$$

#### Remark.

- Now we only need to compute  $\alpha_i(t)$  and  $\beta_i(t)$ 
  - We've seen how to update  $\alpha_i(t)$  via the recursion  $\alpha_i(t) = c_i(y_t) \cdot \sum_{i=1}^K a_{ij} \cdot \alpha_i(t-1)$

Updating 
$$\alpha_i(t)$$
 and  $\beta_i(t)$ 

$$\alpha_{j}(t) \coloneqq \mathbb{P}_{\theta}(x_{0}, \dots, x_{t}, Z_{t} = \omega_{j})$$
$$\beta_{j}(t) \coloneqq \mathbb{P}_{\theta}(x_{t+1}, \dots, x_{T} \mid Z_{t} = \omega_{j})$$

$$c_j(x_t) \coloneqq \mathbb{P}_{\theta}\big(x_t \big| Z_t = \omega_j\big)$$

• Compute forward probability  $\alpha_i(t)$ :

• Initialization: 
$$\alpha_i(0) = \pi_i \cdot c_i(y_0)$$

• Recursion: 
$$\alpha_j(t) = c_j(x_t) \sum_{i=1}^K \alpha_i(t-1) \cdot a_{ij}$$

$$\forall j = 1, ..., K$$

$$\forall i = 1, ..., K, \forall t = 1, ..., T$$

• Compute backward probability  $\beta_i(t)$ : (details omitted, please verify)

- Initialization:  $\beta_i(T) = 1$
- Recursion:  $\beta_j(t-1) = \sum_{i=1}^K c_i(x_t) \cdot \beta_i(t) \cdot a_{ji}$

$$\forall j = 1, ..., K$$

$$\forall j = 1, \dots, K, \forall t = T, \dots, 1$$

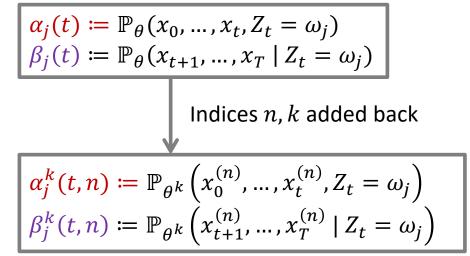
#### Summary of the EM Algorithm

- 1. We derived the formula of the EM algorithm for updating  $\pi^{k+1}$ ,  $A^{k+1}$ ,  $C^{k+1}$  and showed that their updates depend on posteriors  $\xi_{ij}^k(t,n)$  and  $\gamma_j^k(t,n)$
- 2. We dropped indices n, k and defined  $\xi_{ij}(t)$  and  $\gamma_j(t)$

3. We showed that  $\xi_{ij}(t)$  and  $\gamma_j(t)$  depend on the forward probability and backward probability,  $\alpha_j(t)$  and  $\beta_j(t)$ , which can be updated recursively

Remark. To implement the EM algorithm, we need to **go backwards**:

- 1. Compute  $\alpha_i^k(t, n)$  and  $\beta_i^k(t, n)$  (indices n, k added back)
- **2. E-Step**: Compute  $\xi_{ij}^k(t,n)$  and  $\gamma_j^k(t,n)$
- 3. M-Step: Compute  $\pi^{k+1}$ ,  $A^{k+1}$ ,  $C^{k+1}$



## Implement EM (Iteration k)

- 1. Compute  $\alpha_i^k(t,n)$  and  $\beta_i^k(t,n)$  (indices added back)
- **2. E-Step**: Compute  $\xi_{ij}^k(t,n)$  and  $\gamma_j^k(t,n)$
- **3. M-Step**: Compute  $\pi^{k+1}$ ,  $A^{k+1}$ ,  $C^{k+1}$

$$\alpha_j^k(t,n) \coloneqq \mathbb{P}_{\theta^k} \left( x_0^{(n)}, \dots, x_t^{(n)}, Z_t = \omega_j \right)$$
$$\beta_j^k(t,n) \coloneqq \mathbb{P}_{\theta^k} \left( x_{t+1}^{(n)}, \dots, x_T^{(n)} \mid Z_t = \omega_j \right)$$

$$c_j^k\left(x_t^{(n)}\right) \coloneqq \mathbb{P}_{\theta^k}\left(x_t^{(n)} \middle| Z_t = \omega_j\right)$$

**1.** Compute forward probability  $\alpha_i^k(t,n)$  and backward probability  $\beta_i^k(t,n)$  ( $\forall n$ ):

**1.1.** Initialization 
$$(\forall j)$$

$$\alpha_j^k(0,n) = \pi_j^k \cdot c_j^k \left(x_0^{(n)}\right), \qquad \beta_j^k(T,n) = 1$$

#### **1.2.** Recursion $(\forall j, t)$

$$\alpha_{j}^{k}(t,n) = c_{j}^{k} \left(x_{t}^{(n)}\right) \sum_{i=1}^{K} \alpha_{i}^{k}(t-1,n) \cdot \alpha_{ij}^{k}$$

$$\beta_{j}^{k}(t-1,n) = \sum_{i=1}^{K} c_{i}^{k} \left(x_{t}^{(n)}\right) \cdot \beta_{i}^{k}(t,n) \cdot \alpha_{ji}^{k}$$

**2. E-Step:** Compute posteriors  $\xi_{ij}^k(t,n)$  and  $\gamma_j^k(t,n)$ 

$$\gamma_{j}^{k}(t,n) = \frac{\alpha_{j}^{k}(t,n)\beta_{j}^{k}(t,n)}{\sum_{i=1}^{K} \alpha_{i}^{k}(t,n)\beta_{i}^{k}(t,n)}$$

$$\xi_{ij}^{k}(t,n) = \frac{c_{j}^{k}(x_{t}^{(n)}) \cdot a_{ij}^{k} \cdot \alpha_{i}^{k}(t-1,n)\beta_{j}^{k}(t,n)}{\sum_{i=1}^{K} \alpha_{i}^{k}(t,n)\beta_{i}^{k}(t,n)}$$

Congrats! You have derived the "Baum-Welch algorithm" (Google search it)

**3. M-Step:** Compute parameters  $\pi^{k+1}$ ,  $A^{k+1}$ ,  $C^{k+1}$ 

$$\pi_i^{k+1} = \frac{\sum_{n=1}^{N} \gamma_i^k(0, n)}{N}$$
 (\forall i)

$$a_{ij}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=1}^{T} \xi_{ij}^{k}(t,n)}{\sum_{n=1}^{N} \sum_{t=1}^{T} \gamma_{i}^{k}(t-1,n)}$$
 (\forall i,j)

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_{j}^{k}(t, n) \mathbb{I}\left(x_{t}^{(n)} = \sigma_{r}\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_{j}^{k}(t, n)} \tag{\forall j, r}$$