Deep Generative Models: Hidden Markov Models

Fall Semester 2025

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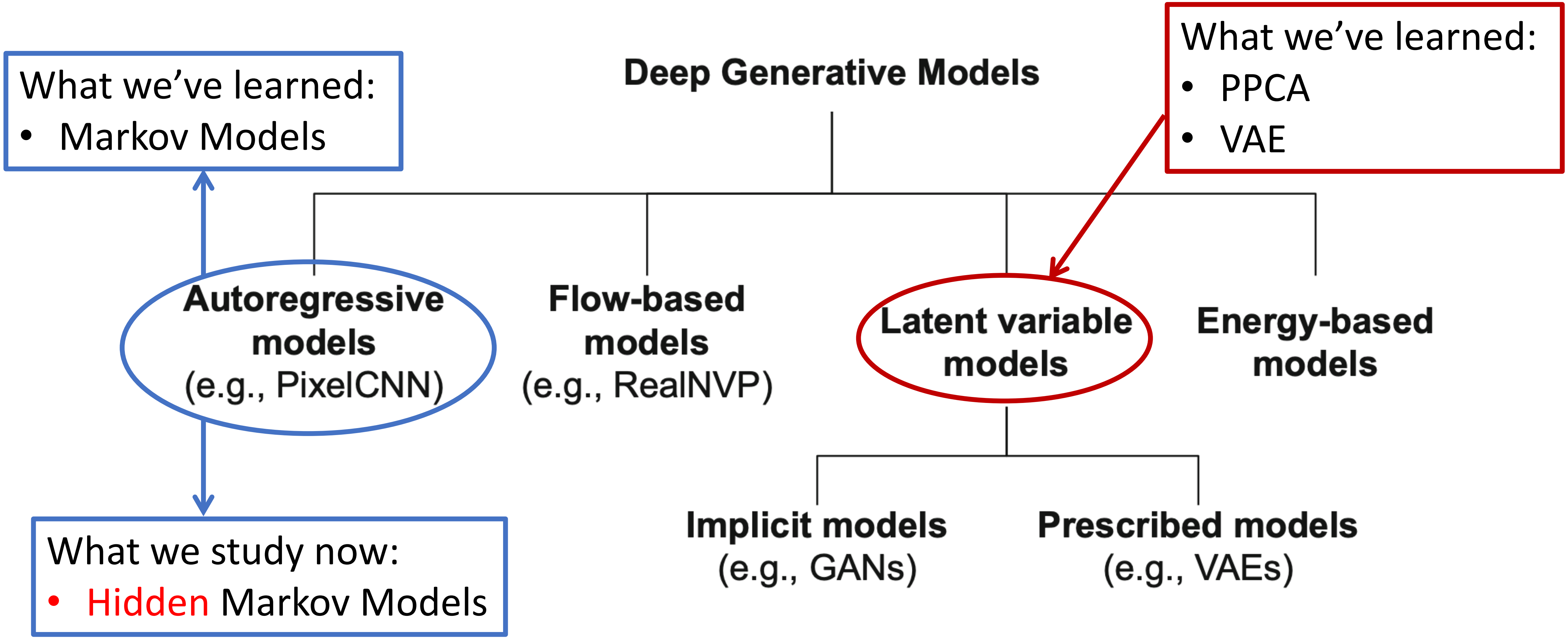
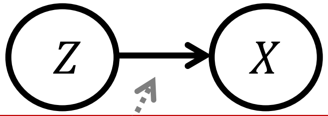
Taxonomy of Generative Models



Hidden Markov Models (Pictorial Definition)

Latent Variable Models

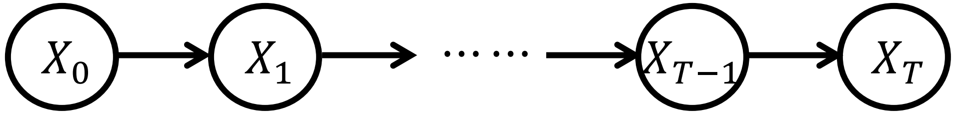
- Z: Latent variable
- X: Observation



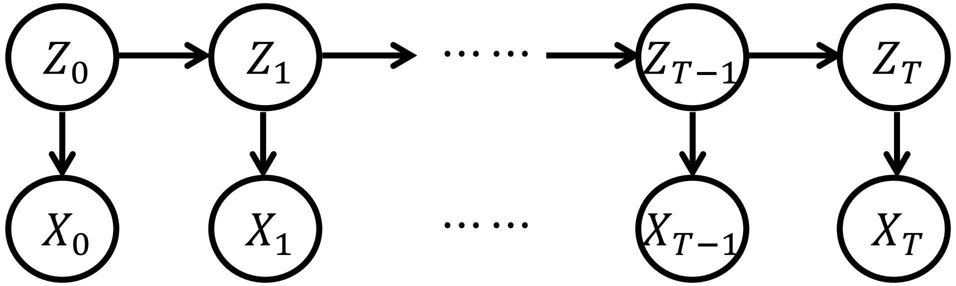
Read it: X depends on Z

Markov Models

- X_t: Observation (state)



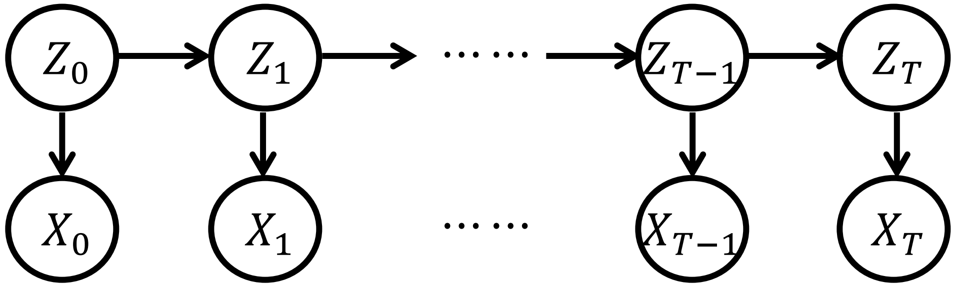
Hidden Markov Models



- Z_t: Hidden state (latent variable)
- X_t: Observation

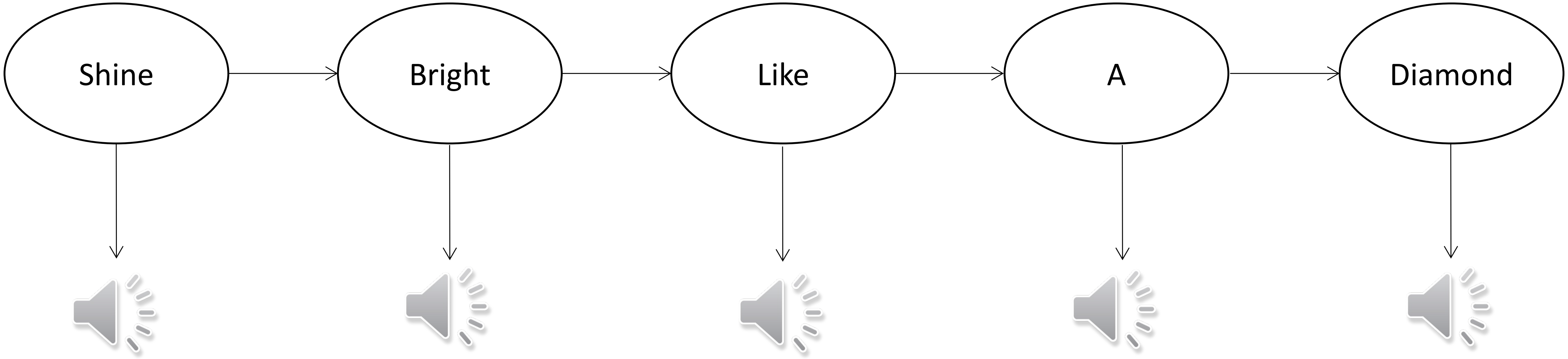
Example: Speech Recognition

Hidden Markov Models

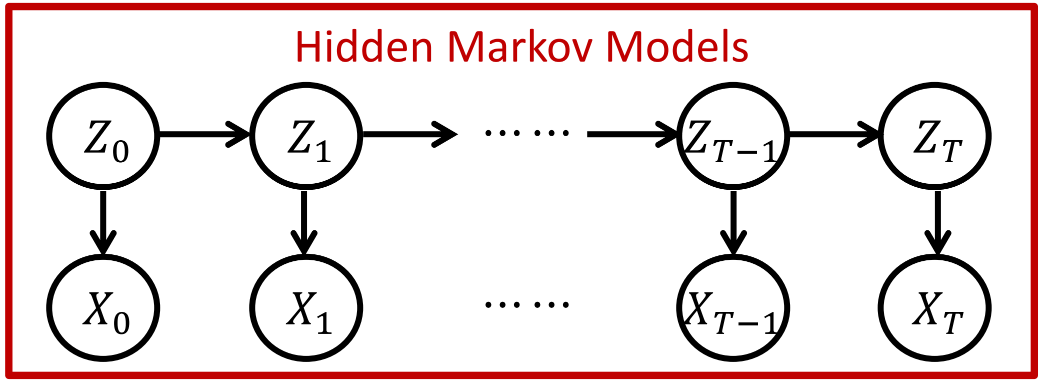


- Z_t: Words (hidden states)
- X_t: Speech (observable audio data)

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



State Space and Observation Space



- In Markov models, we had state space Ω with K different states
  - So we labeled them as $\Omega = \{1, \ldots, K\}$ without loss of generality

- In HMMs, we need to distinguish state space Ω and observation space Σ
  - So we define:

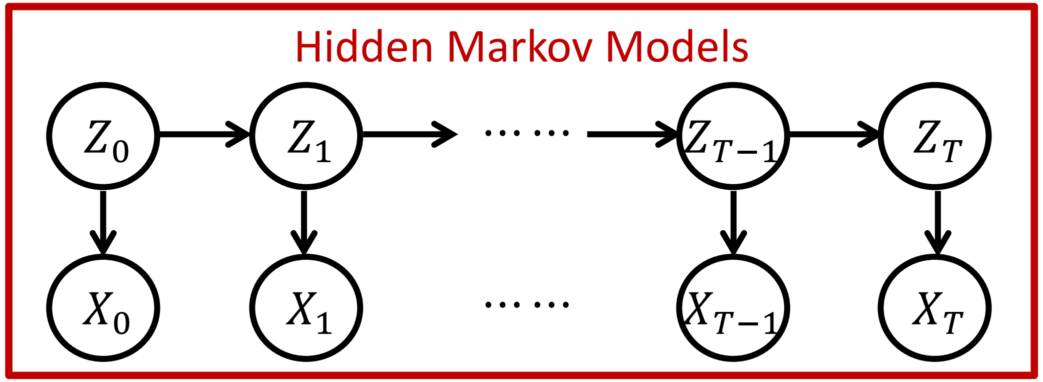
    State Space $\Omega = \{\omega_1, \ldots, \omega_K\}$:
    Each Z_t takes values in Ω

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

  - But in words we might say:
    - "state i" for ω_i (simpler than saying "state omega i")
    - "observation j" for σ_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 Ω



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

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

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

  - $\boldsymbol{x} := [x_0, \dots, x_T]^\top$ and similarly for $\boldsymbol{z} := [z_0, \dots, z_T]^\top$

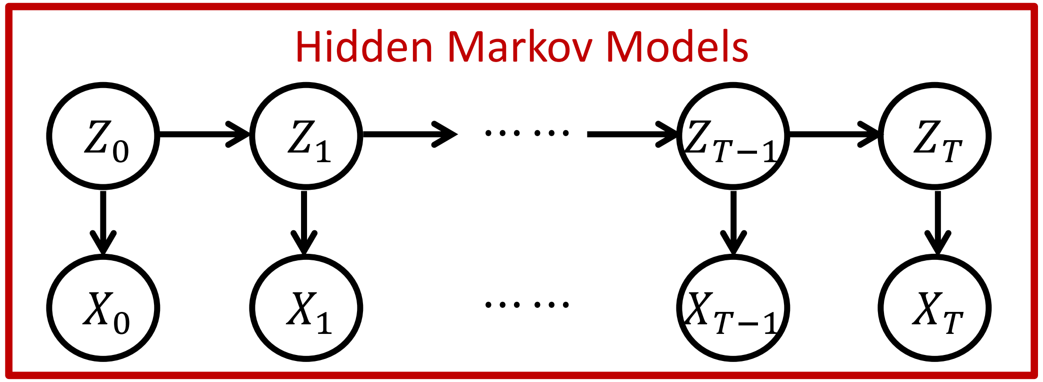
  - n-th observation $\boldsymbol{x}^{(n)} := \left[x_0^{(n)}, \dots, x_T^{(n)}\right]^\top$

  - $\mathbb{P}(Z_0 = z_0, Z_1 = z_1)$: 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 θ

Assumptions



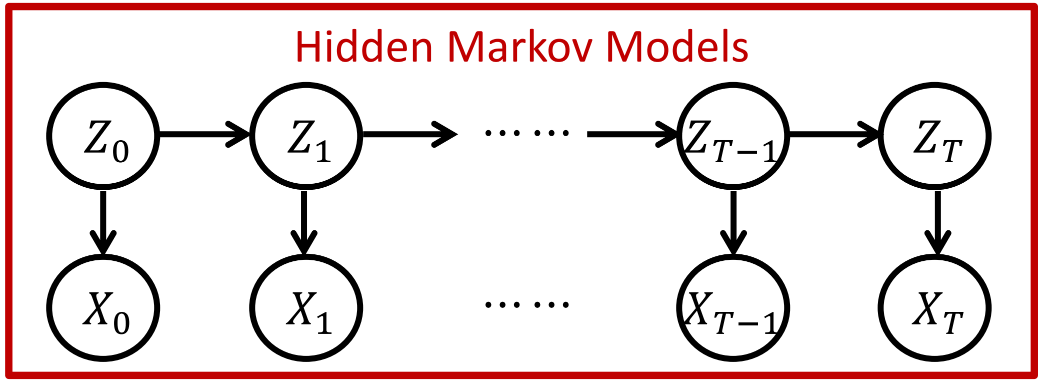
- Markov Property:

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

- Output Independence Assumption:

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

Consequences of The Assumptions



Assumptions

A1: $p_\theta(z_t \mid z_0, \dots, z_{t-1}) = p_\theta(z_t \mid z_{t-1})$

A2: $p_\theta(x_t \mid z_0, \dots, z_T, x_0, \dots, x_{t-1}) = p_\theta(x_t \mid z_t)$

- **Transition Probability Factorization** (proof: factorize w.r.t. $z_0, \dots, z_T$, use A1):
  - $p_\theta(z_0, \dots, z_T) = p_\theta(z_0) \prod_{t=1}^{T} p_\theta(z_t \mid z_{t-1})$

- **Emission Probability Factorization** (proof: factorize w.r.t. $x_0, \dots, x_T$, use A2):
  - $p_\theta(x_0, \dots, x_T \mid z_0, \dots, z_T) = \prod_{t=0}^{T} p_\theta(x_t \mid z_t)$

- **Joint Probability Factorization** (proof: use the above factorizations):

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

Inference, Decoding, and Learning

- Inference. Given θ, compute the likelihood $p_\theta(\boldsymbol{x})$ of observing $\boldsymbol{x}$

- Decoding. Given observation $\boldsymbol{x}$ and parameters θ, find best states:

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

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

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

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

Decoding and Inference via "Brute-Force"

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

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

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

- Decoding. Given $\theta, \boldsymbol{x}$, compute:

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

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

Faster Algorithms for Inference?

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

- Inference. Given $\theta, \boldsymbol{x}$, compute $p_\theta(\boldsymbol{x})$
- If $T = 0$, then $p_\theta(\boldsymbol{x}) = \sum_{z_0} p_\theta(x_0, z_0) = \sum_{z_0} p_\theta(\, x_0 \mid z_0 \,) \cdot p_\theta(z_0)$
  - We can compute $p_\theta(\boldsymbol{x})$ in $O(K)$ time (we need to sum over K possible values of z_0)
- If $T = 1$, then $p_\theta(\boldsymbol{x}) = \sum_{z_0} \sum_{z_1} p_\theta(x_0, x_1, z_0, z_1)$
  - Therefore, $p_\theta(\boldsymbol{x}) = \sum_{z_0} \sum_{z_1} p_\theta(x_1 \mid z_1) \cdot p_\theta(x_0 \mid z_0) \cdot p_\theta(z_1 \mid z_0) \cdot p_\theta(z_0)$
  - We can compute $p_\theta(\boldsymbol{x})$ in $O(K^2)$ time (need to sum over all possible z_1 and z_0)

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

Formalize the Intuition

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

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

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

- Forward Probability:

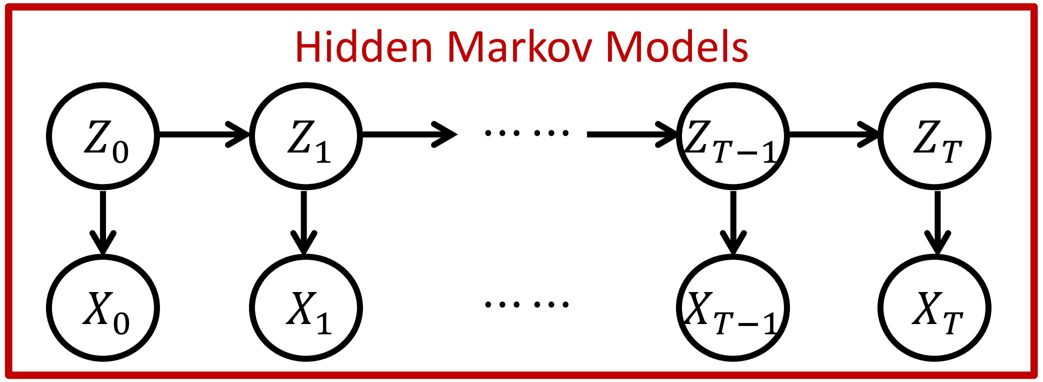
$$\alpha_j(t) := \mathbb{P}_\theta(x_0, \dots, x_t, Z_t = \omega_j)$$

- By definition, we have

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

- It remains to derive an update formula for $\alpha_j(t)$ for $t = 0, \dots, T$

Formalize the Intuition



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

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

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

- Forward Probability:

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

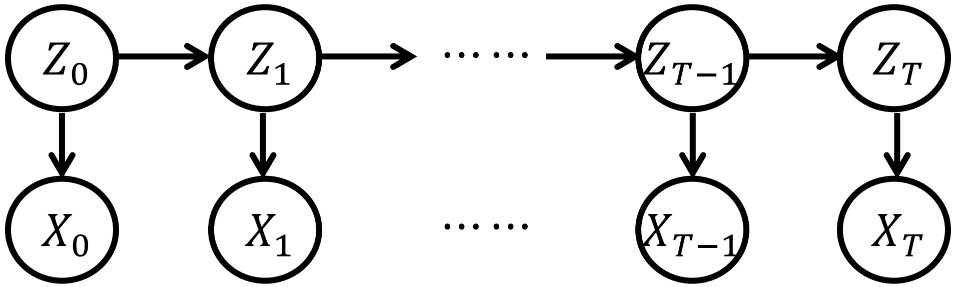
- Recurrence Relation:

$$\alpha_j(t) = \mathbb{P}_\theta(\, x_t \mid x_0, \dots, x_{t-1}, Z_t = \omega_j \,) \cdot \mathbb{P}_\theta(x_0, \dots, x_{t-1}, Z_t = \omega_j)$$
$$= \mathbb{P}_\theta(\, x_t \mid Z_t = \omega_j \,) \textstyle\sum_{i=1,\dots,K} \mathbb{P}_\theta(x_0, \dots, x_{t-1}, Z_t = \omega_j, Z_{t-1} = \omega_i)$$
$$= c_j(x_t) \textstyle\sum_{i=1}^{K} \mathbb{P}_\theta(x_0, \dots, x_{t-1}, Z_{t-1} = \omega_i) \cdot \mathbb{P}_\theta(Z_t = \omega_j \mid x_0, \dots, x_{t-1}, Z_{t-1} = \omega_i)$$
$$= c_j(x_t) \textstyle\sum_{i=1}^{K} \alpha_i(t-1) \cdot a_{ij}$$

Faster Algorithm for Inference

Time Complexity: $O(TK^2)$

Hidden Markov Models



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

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

- **Inference**. Given $\theta, \boldsymbol{x}$, compute $p_\theta(\boldsymbol{x})$
- **Forward Probability**: $\alpha_j(t) \coloneqq \mathbb{P}_\theta(x_0, \ldots, x_t, Z_t = \omega_j)$
- **Recurrence Relation**: $\alpha_j(t) = c_j(x_t) \sum_{i=1}^{K} \alpha_i(t-1) \cdot a_{ij}$
- **Algorithm**:
  - Initialization: $\alpha_j(0) = \pi_j \cdot c_j(x_0)$ $\quad \forall j = 1, \ldots, K$
  - Recursion: $\alpha_j(t) = c_j(x_t) \sum_{i=1}^{K} \alpha_i(t-1) \cdot a_{ij}$ $\quad \forall j = 1, \ldots, K, \forall t = 1, \ldots, T$
  - Termination: Output $\sum_{j=1}^{K} \alpha_j(T)$

What About Decoding?

- Decoding. Given $\theta, \boldsymbol{x}$, compute:

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

- 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 $\sum_{\boldsymbol{z}} p_\theta(\boldsymbol{x}, \boldsymbol{z})$

- Two differences from inference:
  - Need to calculate the maximum of $p_\theta(\boldsymbol{x}, \boldsymbol{z})$ over $\boldsymbol{z}$ rather than sum

  - Need to find states $\boldsymbol{z}^*$ attaining the maximum

Inference Versus Decoding

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

- **Inference**. Given $\theta, \boldsymbol{x}$, compute:

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

- **Recurrence Term**:

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

- **Marginalization**:

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

- **Recurrence Relation**:

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

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

- **Decoding**. Given $\theta, \boldsymbol{x}$, compute:

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

- **Recurrence Term**:

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

- **Maximization**:

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

- **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 $v_j(t)$ is indeed obtained by replacing sum with max

Inference Versus Decoding

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

- Inference. Given $\theta, \boldsymbol{x}$, compute:

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

- Initialization: $(\forall j = 1, \dots, K)$

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

- Recursion: $(\forall j = 1, \dots, K, \forall t = 1, \dots, T)$

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

- Output:

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

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

- Decoding. Given $\theta, \boldsymbol{x}$, compute:

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

- Initialization: $(\forall j = 1, \dots, K)$

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

- Recursion: $(\forall j = 1, \dots, K, \forall t = 1, \dots, T)$

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

- Output:

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

One more step needed: find $\boldsymbol{z}^*$ that attains the optimum
Solution: “backtracking” (next page)

Backtracking for Decoding

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

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

- 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 $(\forall t = T, \dots, 1)$:

$$i^*(t-1) = prev_{i^*(t)}(t)$$

Algorithm (Viterbi)

- Initialization: $(\forall j = 1, \dots, K)$

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

- Recursion: $(\forall j = 1, \dots, K, \forall t = 1, \dots, T)$

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

$$prev_j(t) = \operatorname*{argmax}_{i=1,\dots,K} \{v_i(t-1) \cdot a_{ij}\}$$

- Output:

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

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

- Backtracking: $(\forall t = T, \dots, 1)$

$$i^*(t-1) = prev_{i^*(t)}(t)$$

Remark. The final algorithm is known as *the Viterbi algorithm*. It is an instance of *dynamic programming*.

Inference, Decoding, and Learning

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

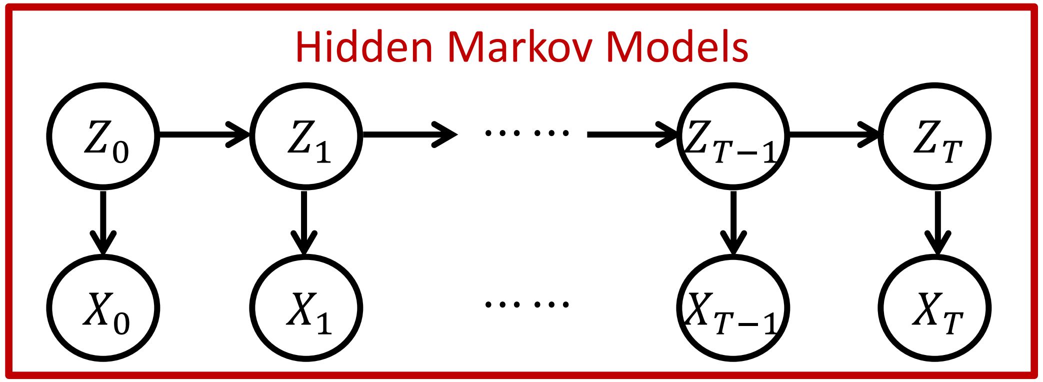
$$\boldsymbol{z}^* \in \operatorname*{argmax}_{\boldsymbol{z}} p_\theta(\boldsymbol{x}, \boldsymbol{z})$$

- Learning. Given N observations $\left\{\boldsymbol{x}^{(n)}\right\}_{n=1}^{N}$, find best θ:

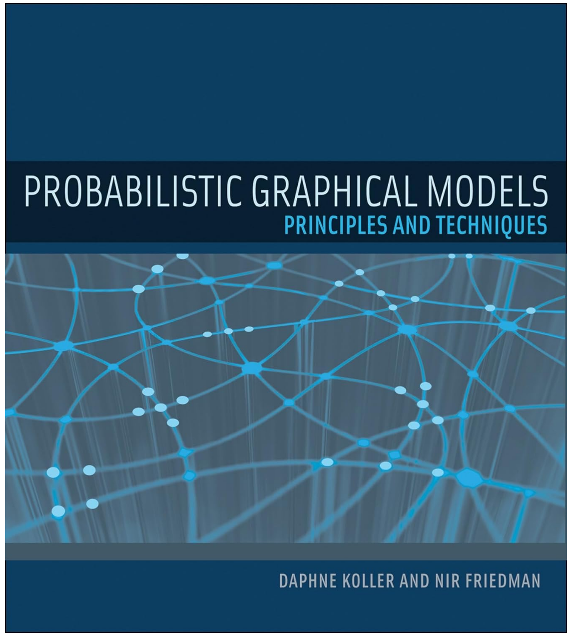
$$\max_\theta \prod_{n=1}^{N} p_\theta(\boldsymbol{x}^{(n)})$$

- We've seen how to perform inference and decoding in $O(TK^2)$ time
  - sum vs. max, dynamic programming, backtracking
- 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

$$\boldsymbol{x}^{(n)} := \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$
$$\boldsymbol{z} := (z_0, \dots, z_T)$$

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

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

- EM Algorithm. Initialize θ^0 and alternate: (k = iteration counter)

E-step:
$$q^k\left(\boldsymbol{z} \mid \boldsymbol{x}^{(n)}\right) = p_{\theta^k}\left(\boldsymbol{z} \mid \boldsymbol{x}^{(n)}\right)$$

M-step:
$$\theta^{k+1} = \mathrm{argmax}_\theta \sum_{n=1}^{N} \sum_{\boldsymbol{z}} q^k\left(\boldsymbol{z} \mid \boldsymbol{x}^{(n)}\right) \log p_\theta\left(\boldsymbol{x}^{(n)}, \boldsymbol{z}\right)$$

Substitute E-step into M-step

$$\theta^{k+1} = \mathrm{argmax}_\theta \sum_{n=1}^{N} \sum_{\boldsymbol{z}} p_{\theta^k}\left(\boldsymbol{z} \mid \boldsymbol{x}^{(n)}\right) \cdot \log p_\theta\left(\boldsymbol{x}^{(n)}, \boldsymbol{z}\right)$$

- 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:

$$p^* = \text{argmax}_p \sum_{i=1}^{K} s_i \log(p_i) \qquad \text{subject to} \qquad p_1 + \cdots + p_K = 1$$

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

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

- 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

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

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

$$p_\theta\left(\boldsymbol{x}^{(n)}, \boldsymbol{z}\right) := \prod_{t=0}^{T} p_C(x_t^{(n)}|z_t)\, p_\pi(z_0) \prod_{t=1}^{T} p_A(z_t|z_{t-1})$$

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

The objective function is separable

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

$$C^{k+1} = \text{argmax}_C \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{\boldsymbol{z}} p_{\theta^k}(\boldsymbol{z} \,|\boldsymbol{x}^{(n)}) \log p_C\left(x_t^{(n)} \middle| z_t\right)$$

$$A^{k+1} = \text{argmax}_A \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{\boldsymbol{z}} p_{\theta^k}(\boldsymbol{z} \,|\boldsymbol{x}^{(n)}) \log p_A(z_t|z_{t-1})$$

Instantiate EM for HMMs

$$\boldsymbol{x}^{(n)} := \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$
$$\boldsymbol{z} := (z_0, \dots, z_T)$$

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

$$C^{k+1} = \operatorname{argmax}_C \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{\boldsymbol{z}} p_{\theta^k}(\boldsymbol{z}\,|\boldsymbol{x}^{(n)}) \log p_C\left(x_t^{(n)} \middle| z_t\right)$$

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

Observation. The summation over $\boldsymbol{z}$ in the above can be simplified, e.g.,

- In the update of π^{k+1},
  - $\log p_\pi(z_0)$ depends only on z_0
  - $p_{\theta^k}(\boldsymbol{z}\,|\boldsymbol{x}^{(n)})$ depends on $\boldsymbol{z} := (z_0, \dots, z_T)$
- So we have

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

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

Instantiate EM for HMMs

$$\boldsymbol{x}^{(n)} := \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$
$$\boldsymbol{z} := (z_0, \dots, z_T)$$

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

$$C^{k+1} = \operatorname{argmax}_C \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{\boldsymbol{z}} p_{\theta^k}(\boldsymbol{z} \,|\boldsymbol{x}^{(n)}) \log p_C\left(x_t^{(n)} \middle| z_t\right)$$

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

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

$$C^{k+1} = \operatorname{argmax}_C \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{z_t} p_{\theta^k}(z_t \,|\boldsymbol{x}^{(n)}) \log p_C\left(x_t^{(n)} \middle| z_t\right)$$

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

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

Updating π^{k+1}

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

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

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

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

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

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?

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

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

Updating A^{k+1}

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

$\boldsymbol{x}^{(n)} \coloneqq \left(x_0^{(n)}, \ldots, x_T^{(n)}\right)$

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

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

$$A^{k+1} = \text{argmax}_A \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{j=1}^{K} \sum_{i=1}^{K} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j, Z_{t-1} = \omega_i \middle| \boldsymbol{x}^{(n)}\right) \log a_{ij} \qquad \text{subject to} \sum_{j=1}^{K} a_{ij} = 1 \ (\forall i)$$

The objective function and constraints are separable

$$(a_{i1}^{k+1}, \ldots, a_{iK}^{k+1}) = \text{argmax}_A \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{j=1}^{K} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j, Z_{t-1} = \omega_i \middle| \boldsymbol{x}^{(n)}\right) \log a_{ij} \qquad \text{subject to} \sum_{j=1}^{K} a_{ij} = 1$$

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?

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

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

Updating C^{k+1}

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

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

$$\boldsymbol{x}^{(n)} := \left(x_0^{(n)}, \dots, x_T^{(n)}\right)$$

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

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

$$\begin{aligned} C^{k+1} &= \operatorname{argmax}_C \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{j=1}^{K} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,|\boldsymbol{x}^{(n)}\right) \log p_C\left(x_t^{(n)} \middle| Z_t = \omega_j\right) \\ &= \operatorname{argmax}_C \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{j=1}^{K} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,|\boldsymbol{x}^{(n)}\right) \sum_{r=1}^{V} \mathbb{I}\left(x_t^{(n)} = \sigma_r\right) \log c_{jr} \end{aligned} \qquad \text{s.t. } \sum_{r=1}^{V} c_{jr} = 1 \ (\forall j)$$

The objective function and constraints are separable

$$(c_{j1}^{k+1}, \dots, c_{jV}^{k+1}) = \operatorname{argmax}_C \sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{r=1}^{V} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,|\boldsymbol{x}^{(n)}\right) \mathbb{I}\left(x_t^{(n)} = \sigma_r\right) \log c_{jr} \qquad \text{s.t. } \sum_{r=1}^{V} c_{jr} = 1$$

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?

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,|\boldsymbol{x}^{(n)}\right) \mathbb{I}\left(x_t^{(n)} = \sigma_r\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \sum_{r=1}^{V} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,|\boldsymbol{x}^{(n)}\right) \mathbb{I}\left(x_t^{(n)} = \sigma_r\right)} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,|\boldsymbol{x}^{(n)}\right) \mathbb{I}\left(x_t^{(n)} = \sigma_r\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,|\boldsymbol{x}^{(n)}\right)} \quad (\forall j, r)$$

Remark. We will calculate $\mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,|\boldsymbol{x}^{(n)}\right)$ later

Updating π^{k+1}, A^{k+1}, C^{k+1}

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

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

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^k}(Z_t = \omega_j \mid \boldsymbol{x}^{(n)}) \mathbb{I}\left(x_t^{(n)} = \sigma_r\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \mathbb{P}_{\theta^k}(Z_t = \omega_j \mid \boldsymbol{x}^{(n)})} \qquad (\forall j, r)$$

- 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:

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

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

Updating $\pi^{k+1}, A^{k+1}, C^{k+1}$

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

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

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

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

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

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

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_j^k(t, n) \mathbb{I}\left(x_t^{(n)} = \sigma_r\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_j^k(t, n)} \quad (\forall j, r)$$

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

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

Updating $\pi^{k+1}, A^{k+1}, C^{k+1}$

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

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

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_j^k(t,n) \mathbb{I}\left(x_t^{(n)} = \sigma_r\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_j^k(t,n)} \qquad (\forall j,r)$$

- $\xi_{ij}^k(t,n) \coloneqq \mathbb{P}_{\theta^k}\left(Z_t = \omega_j, Z_{t-1} = \omega_i \mid \boldsymbol{x}^{(n)}\right)$ $(\forall t > 0)$
- $\gamma_j^k(t,n) \coloneqq \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \mid \boldsymbol{x}^{(n)}\right)$ $(\forall t \geq 0)$

- 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

Updating $\pi^{k+1}, A^{k+1}, C^{k+1}$

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

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

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_j^k(t,n)\mathbb{I}\left(x_t^{(n)} = \sigma_r\right)}{\sum_{n=1}^{N} \sum_{t=0}^{T} \gamma_j^k(t,n)} \qquad (\forall j,r)$$

- $\xi_{ij}^k(t,n) \coloneqq \mathbb{P}_{\theta^k}\left(Z_t = \omega_j, Z_{t-1} = \omega_i \,\middle|\, \boldsymbol{x}^{(n)}\right)$ $(\forall t > 0)$
- $\gamma_j^k(t,n) \coloneqq \mathbb{P}_{\theta^k}\left(Z_t = \omega_j \,\middle|\, \boldsymbol{x}^{(n)}\right)$ $(\forall t \geq 0)$

- Dropping indices n, k for clarity, we can reformulate our goal (**E-step**) as follows:

E-step. Given $\boldsymbol{y} = (x_1, \dots, x_T)$ and θ, compute $(\forall i,j)$

- $\xi_{ij}(t) = \mathbb{P}_\theta\left(Z_t = \omega_j, Z_{t-1} = \omega_i \,\middle|\, x_0, \dots, x_T\right)$ $\qquad (t > 0)$
- $\gamma_j(t) = \mathbb{P}_\theta\left(Z_t = \omega_j \,\middle|\, x_0, \dots, x_T\right)$ $\qquad (t \geq 0)$

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 $\boldsymbol{x} = (x_1, \dots, x_T)$ and θ, compute $(\forall i, j)$
- $\xi_{ij}(t) = \mathbb{P}_\theta\left(Z_t = \omega_j, Z_{t-1} = \omega_i \,\middle|\, x_0, \dots, x_T\right) \qquad (t > 0)$
- $\gamma_j(t) = \mathbb{P}_\theta\left(Z_t = \omega_j \,\middle|\, x_0, \dots, x_T\right) \qquad (t \geq 0)$

- 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 $\gamma_j(t)$ gives

$$\gamma_j(t) = \frac{\mathbb{P}_\theta(x_0,\dots,x_T, Z_t=\omega_j)}{\mathbb{P}_\theta(x_0,\dots,x_T)} = \frac{\mathbb{P}_\theta(x_0,\dots,x_t,Z_t=\omega_j) \cdot \mathbb{P}_\theta(x_{t+1},\dots,x_T \mid x_0,\dots,x_t,Z_t=\omega_j)}{\mathbb{P}_\theta(x_0,\dots,x_T)}$$

$$= \frac{\mathbb{P}_\theta(x_0,\dots,x_t,Z_t=\omega_j) \cdot \mathbb{P}_\theta(x_{t+1},\dots,x_T \mid Z_t=\omega_j)}{\mathbb{P}_\theta(x_0,\dots,x_T)} = \frac{\alpha_j(t) \cdot \mathbb{P}_\theta(x_{t+1},\dots,x_T \mid Z_t=\omega_j)}{\sum_{i=1}^K \alpha_i(t) \cdot \mathbb{P}_\theta(x_{t+1},\dots,x_T \mid Z_t=\omega_i)} = \frac{\alpha_j(t)\beta_j(t)}{\sum_{i=1}^K \alpha_i(t)\beta_i(t)}$$

  - $\beta_j(t)$ 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 $\boldsymbol{x} = (x_1, \dots, x_T)$ and θ, compute $(\forall i, j)$

- $\xi_{ij}(t) = \mathbb{P}_\theta\left(Z_t = \omega_j, Z_{t-1} = \omega_i \,\middle|\, x_0, \dots, x_T\right)$ $\quad (t > 0)$
- $\gamma_j(t) = \mathbb{P}_\theta\left(Z_t = \omega_j \,\middle|\, x_0, \dots, x_T\right)$ $\quad (t \geq 0)$

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

- $\gamma_j(t) = \dfrac{\mathbb{P}_\theta(x_0,\dots,x_T, Z_t = \omega_j)}{\mathbb{P}_\theta(x_0,\dots,x_T)} = \dfrac{\boxed{\alpha_j(t)}\beta_j(t)}{\sum_{i=1}^K \alpha_i(t)\beta_i(t)}$

Remark. Recall the recursion:
$\boxed{\alpha_j(t)} = \boxed{c_j(y_t) \cdot \sum_{i=1}^K a_{ij} \cdot \alpha_i(t-1)}$

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

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

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

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

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

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

E-step. Given $\boldsymbol{x} = (x_1, \dots, x_T)$ and θ, compute $(\forall i, j)$

- $\xi_{ij}(t) = \mathbb{P}_\theta\left(Z_t = \omega_j, Z_{t-1} = \omega_i \,\middle|\, x_0, \dots, x_T\right) \qquad (t > 0)$
- $\gamma_j(t) = \mathbb{P}_\theta\left(Z_t = \omega_j \,\middle|\, x_0, \dots, x_T\right) \qquad (t \geq 0)$

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

Remark.

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

Updating $\alpha_j(t)$ and $\beta_j(t)$

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

$c_j(x_t) := \mathbb{P}_\theta\left(x_t \middle| Z_t = \omega_j\right)$

- Compute forward probability $\alpha_j(t)$:
  - Initialization: $\alpha_j(0) = \pi_j \cdot c_j(y_0)$ $\quad \forall j = 1, \dots, K$
  - Recursion: $\alpha_j(t) = c_j(x_t) \sum_{i=1}^{K} \alpha_i(t-1) \cdot a_{ij}$ $\quad \forall j = 1, \dots, K, \forall t = 1, \dots, T$

- Compute backward probability $\beta_j(t)$: (details omitted, please verify)
  - Initialization: $\beta_j(T) = 1$ $\quad \forall j = 1, \dots, K$
  - Recursion: $\beta_j(t-1) = \sum_{i=1}^{K} c_i(x_t) \cdot \beta_i(t) \cdot a_{ji}$ $\quad \forall j = 1, \dots, K, \forall t = T, \dots, 1$

Summary of the EM Algorithm

1. We derived the formula of the EM algorithm for updating π^{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

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

Indices n, k added back

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

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

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

Implement EM (Iteration k)

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

$$\alpha_j^k(t,n) \coloneqq \mathbb{P}_{\theta^k}\left(x_0^{(n)},\ldots,x_t^{(n)},Z_t=\omega_j\right)$$

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

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

1. Compute forward probability $\alpha_j^k(t,n)$ and backward probability $\beta_j^k(t,n)$ $(\forall n)$:

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 $(\forall j,t)$

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

$$\beta_j^k(t-1,n) = \sum_{i=1}^K c_i^k\left(x_t^{(n)}\right)\cdot\beta_i^k(t,n)\cdot a_{ji}^k$$

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

$$\gamma_j^k(t,n) = \frac{\alpha_j^k(t,n)\beta_j^k(t,n)}{\sum_{i=1}^K \alpha_i^k(t,n)\beta_i^k(t,n)}$$

$$\xi_{ij}^k(t,n) = \frac{c_j^k\left(x_t^{(n)}\right)\cdot a_{ij}^k \cdot \alpha_i^k(t-1,n)\beta_j^k(t,n)}{\sum_{i=1}^K \alpha_i^k(t,n)\beta_i^k(t,n)}$$

3. M-Step: Compute parameters π^{k+1}, A^{k+1}, C^{k+1}

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

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

$$c_{jr}^{k+1} = \frac{\sum_{n=1}^N\sum_{t=0}^T \gamma_j^k(t,n)\mathbb{I}\left(x_t^{(n)}=\sigma_r\right)}{\sum_{n=1}^N\sum_{t=0}^T \gamma_j^k(t,n)} \qquad (\forall j,r)$$

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