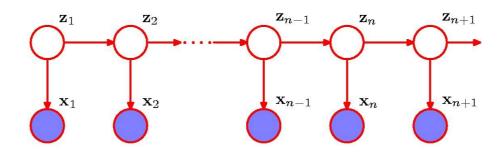
Hidden Markov Models Training – Selecting model parameters



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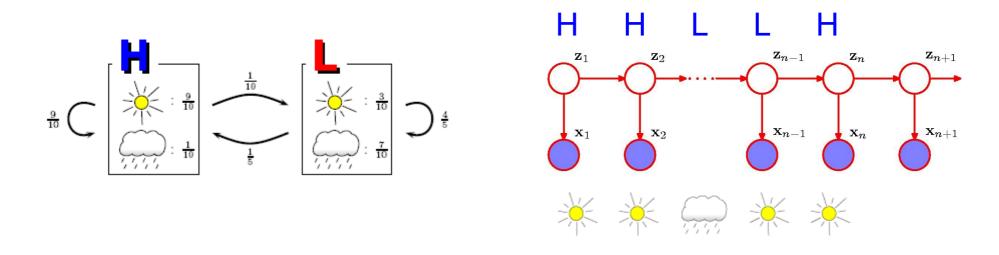
What we know

- The terminology and notation of hidden Markov models (HMMs)
- The forward- and backward-algorithms for determining the likelihood p(X) of a sequence of observations, and computing the posterior decoding.
- The Viterbi-algorithm for finding the most likely explanation (sequence of latent states) of a sequence of observations.
- How to implement the Viterbi-algorithm using log-transform (and the forward- and backward-algorithms using scaling).

Now

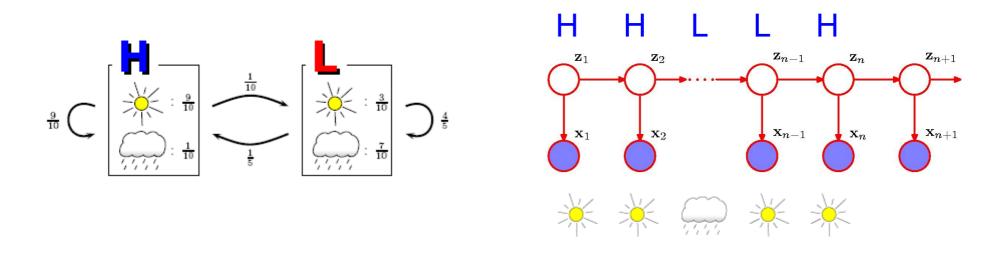
Training, or how to select model parameters (transition and emission probabilities) to reflect either a set of corresponding (X,Z)'s, (or just a set of X's) ...

Assume that (several) sequences of observations $X = \{x_1, ..., x_N\}$ and corresponding latent states $Z = \{z_1, ..., z_N\}$ are given ...



How should we set the model parameters, i.e. transition A, π , and emission probabilities Φ , to make the given (X,Z)'s most likely?

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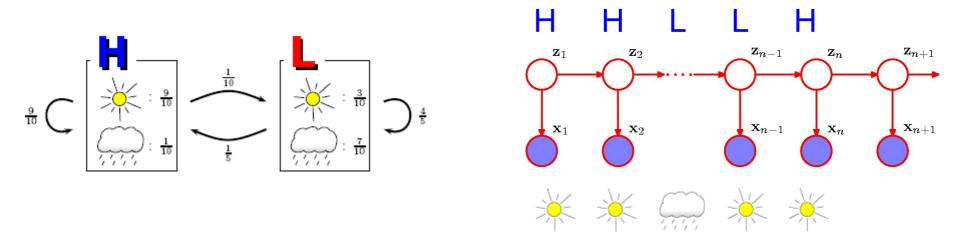


How should we set the model parameters, i.e. transition A, π , and emission probabilities Φ , to make the given (X,Z)'s most likely?

Intuition: The parameters should reflect what we have seen ...

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Selecting "the right" transition probs



 A_{jk} is the probability of a transition from state *j* to state *k*, and π_k is the probability of starting in state *k*...

How many times is the transition from state *j* to state *k* taken

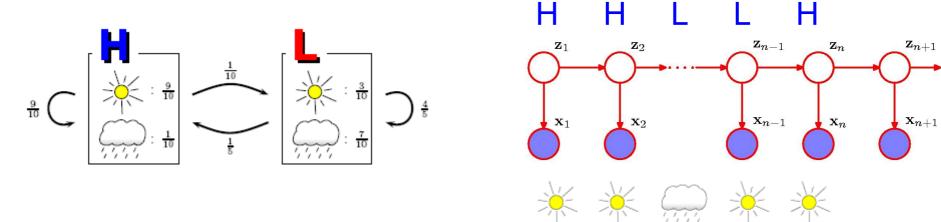
$$A_{jk} = \frac{\sum_{n=2}^{N} z_{n-1,j} z_{nk}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1,j} z_{nl}} =$$

 $\longrightarrow \lambda t$

How many times is a transition from state *j* to any state taken

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Selecting "the right" transition probs



 A_{ik} is the probability of a transition from state *j* to state *k*, and π_k is the probability of starting in state k...

 $A_{jk} = \frac{\sum_{n=2}^{K} z_{n-1,j} z_{nk}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1,j} z_{nl}} =$ z_{1k} π_k

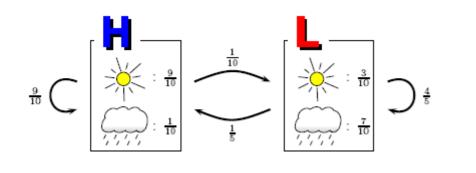
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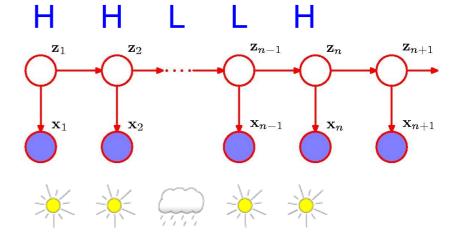
How many times is a transition from state *j* to any state taken

 \mathbf{z}_{n+1}

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Selecting "the right" emission probs





If we assume discrete observations, then Φ_{ik} is the probability of emitting symbol *i* from state *k* ...

$$\phi_{ik} = \frac{\sum_{n=1}^{N} z_{nk} x_{ni}}{\sum_{n=1}^{N} z_{nk}} =$$

How many times is symbol *i* emitted from state *k*

How many times is a symbol emitted from state *k*

Assume that (several) sequences of observations $X = \{x_1, ..., x_N\}$ and corresponding latent states $Z = \{z_1, ..., z_N\}$ are given ...

$$A_{jk} = \frac{\sum_{n=2}^{N} z_{n-1,j} z_{nk}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1,j} z_{nl}} \qquad \pi_k = \frac{z_{1k}}{\sum_{j=1}^{K} z_{1j}} \qquad \phi_{ik} = \frac{\sum_{n=1}^{N} z_{nk} x_{ni}}{\sum_{n=1}^{N} z_{nk}}$$

We simply count how many times each outcome of the multinomial variables (a transition or emission) is observed ...

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This yield a maximum likelihood estimate (MLE) θ^* of $p(X, Z | \theta)$, which is what we mathematically want ...

$$f_{\mathbf{X},\mathbf{Z}}(\Theta) = p(\mathbf{X},\mathbf{Z}|\Theta) \qquad \Theta^* = \arg\max_{\Theta} f_{\mathbf{X},\mathbf{Z}}(\Theta)$$

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Any problems? What if e.g. the transition from state *j* to *k* is *not* observed, then probability A_{jk} is set to 0. <u>Practical solution</u>: Assume that every transition and emission is seen once (pseudocount) ...

L

 \mathbf{z}_{n+1}

 \mathbf{x}_{n+1}

Η

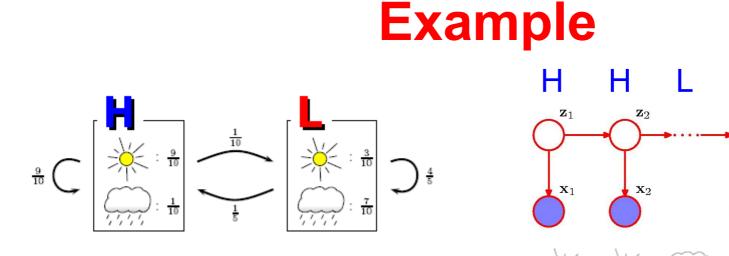
 \mathbf{z}_n

 \mathbf{x}_n

L

 \mathbf{z}_{n-1}

 \mathbf{x}_{n-1}

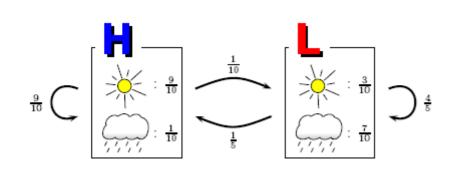


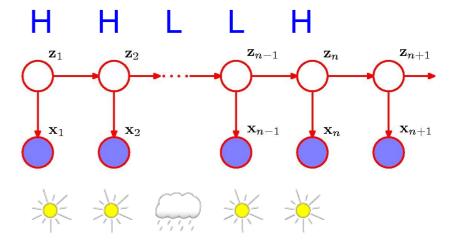
** *

Without pseudocounts:

A _{HH} = 1/2	p(sun H) = 1
$A_{HL} = 1/2$	p(rain H) = 0
$A_{IH} = 1/2$	p(sun L) = 1/2
$A_{LL}^{-1} = 1/2$	p(rain L) = 1/2
π _н = 1	
$\pi_{1} = 0$	







Without pseudocounts:

 $A_{HH} = 1/2$ $A_{HL} = 1/2$ $A_{LH} = 1/2$ $A_{LL} = 1/2$ $\pi_{H} = 1$ $\pi_{L} = 0$ p(sun|H) = 1p(rain|H) = 0p(sun|L) = 1/2p(rain|L) = 1/2

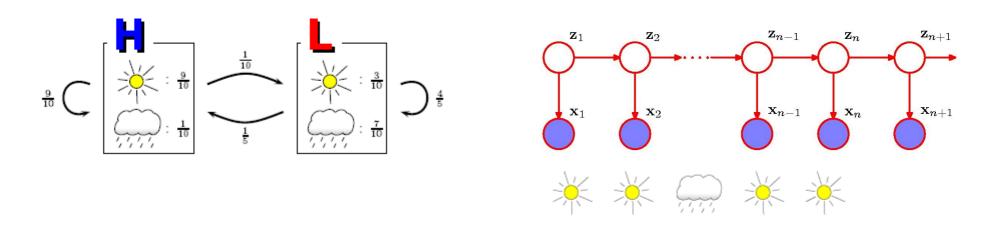
With pseudocounts:

$$A_{HH} = 2/4$$

 $A_{HL} = 2/4$
 $A_{LH} = 2/4$
 $A_{LL} = 2/4$
 $\pi_{H} = 2/3$
 $\pi_{L} = 1/3$

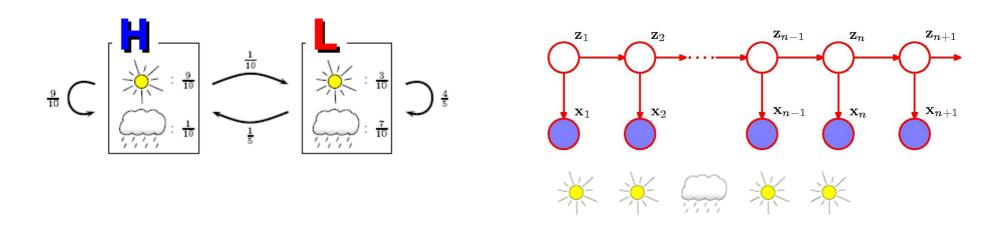
p(sun|H) = 4/5p(rain|H) = 1/5p(sun|L) = 2/4p(rain|L) = 2/4

What if only (several) sequences of observations $X = \{x_1, ..., x_N\}$ is given, i.e the corresponding latent states $Z = \{z_1, ..., z_N\}$ are unknown?



How should we set the model parameters, i.e. transitions A, π , and emission probabilities Φ , to make the given X's most likely?

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How should we set the model parameters, i.e. transitions **A**, π , and emission probabilities Φ , to make the given **X**'s most likely?

$$\label{eq:maximize} \mbox{Maximize} \ p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\Theta) \ \mbox{w.r.t.} \ \mathbf{\theta} \dots$$

What if only (several) sequences of observations $X = \{x_1, ..., x_N\}$ is given, i.e the corresponding latent states $Z = \{z_1, ..., z_N\}$ are unknown?

Direct maximization of the likelihood (or log-likelihood) is hard ...

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Practical Solution - Viterbi training

A more "practical" thing to do is Viterbi Training:

- 1. Decide on some initial parameter θ^{0}
- 2. Find the most likely sequence of states Z^* explaining X using the the Viterbi Algorithm and the current parameters θ^i
- 3.Update parameters to θ^{i+1} by "counting" (with pseudo counts) according to (X,Z*).

4.Repeat 2-3 until P(**X**,**Z*** | θⁱ) is satisfactory (or the Viterbi sequence of states does not change).

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- 3.Update parameters to θ^{i+1} by "counting" (with pseudo counts) according to (X,Z*).
- Repeat 2-3 until P(X,Z* | θⁱ) is satisfactory (or the Viterbi sequence of states does not change).

Finds a (local) maximum of:

$$\operatorname{VIT}_{\mathbf{X}}(\Theta) = \max_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \Theta)$$

The identified parameters θ^* is not a MLE of $p(\mathbf{X} | \theta)$, but works "ok"

Summary: Training-by-Counting

Training-by-Counting: We are given a sequence of observations $X = \{x_1, ..., x_N\}$ and the corresponding latent states $Z = \{z_1, ..., z_N\}$. We want to find a model:

$$\Theta^*_{\text{TbC}} = \arg\max_{\Theta} p(\mathbf{X}, \mathbf{Z}|\Theta) = \arg\max_{\Theta} \log p(\mathbf{X}, \mathbf{Z}|\Theta)$$

This can be done analytically by counting the frequency by which each transition and emission occur in the training data (**X**, **Z**).

If only $X = \{x_1, \dots, x_n\}$ is given, then we want to find a model:

$$\Theta_{\mathbf{X}}^* = \arg\max_{\Theta} p(\mathbf{X}|\Theta) = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta)$$

Summary: Viterbi Training

Viterbi Training: We are given a sequence of observations $X = \{x_1, ..., x_N\}$. Pick an initial set of parameters θ_{vit}^0 and compute the best explanation of X under assumption of these parameters using the Viterbi algorithm:

$$\begin{aligned} \mathbf{Z}_{\mathrm{Vit}}^{0} &= \arg\max_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \Theta_{\mathrm{Vit}}^{0}) = \arg\max_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z} | \Theta_{\mathrm{Vit}}^{0}) \\ \end{aligned}$$

$$\begin{aligned} & \mathsf{Compute} \ \mathbf{\theta}_{\mathsf{vit}}^{1} \text{ from } \mathbf{\theta}_{\mathsf{vit}}^{0} \text{ and } \mathbf{Z}_{\mathsf{vit}}^{0} \text{ using TbC and iterate:} \\ & \Theta_{\mathrm{Vit}}^{1} = \arg\max_{\Theta} p(\mathbf{X}, \mathbf{Z}_{\mathrm{Vit}}^{0} | \Theta) = \arg\max_{\Theta} \log p(\mathbf{X}, \mathbf{Z}_{\mathrm{Vit}}^{0} | \Theta) \\ & \mathbf{Z}_{\mathrm{Vit}}^{1} = \arg\max_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \Theta_{\mathrm{Vit}}^{1}) = \arg\max_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z} | \Theta_{\mathrm{Vit}}^{1}) \end{aligned}$$

 $p(\mathbf{X}|\Theta^i_{\mathrm{Vit}})$ is usually close to $~p(\mathbf{X}|\Theta^*_{\mathbf{X}})~$, but no guarantees

Expectation Maximization

EM Training: We are given a sequence of observations $X = \{x_1, \dots, x_N\}$. Pick an initial set of parameters θ_{EM}^0 and consider the expectation of log $p(X, Z | \theta)$ over Z (given X and θ_{EM}^0) as a function of θ :

$$EM_{\mathbf{X},\Theta_{\rm EM}^{0}}(\Theta) = E_{\mathbf{Z}|\mathbf{X},\Theta_{\rm EM}^{0}}(\log p(\mathbf{X},\mathbf{Z}|\Theta)) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta_{\rm EM}^{0})\log p(\mathbf{X},\mathbf{Z}|\Theta)$$

For HMMs, we can find θ_{EM}^1 analytically, and iterate to get θ_{EM}^i :

$$\Theta_{EM}^{1} = \arg\max_{\Theta} \mathrm{EM}_{\mathbf{X},\Theta_{\mathrm{EM}}^{0}}(\Theta)$$

 $p(\mathbf{X}|\Theta_{\mathrm{EM}}^{i})$ converges towards a (local) maximum of $p(\mathbf{X}|\Theta)$

Expectation Maximization

E-Step: Define the Q-function:

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z} | \mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z} | \Theta)$$

e. the expectation of log p(**X**, **Z** | **\Theta**) over **Z** (given **X** and **D**^{old}) as a function of **\Theta**

M-Step: Maximize $Q(\theta, \theta^{old})$ w.r.t. θ

$$\begin{split} \mathrm{EM}_{\mathbf{X},\Theta^{\mathrm{old}}}(\Theta) &= E_{\mathbf{Z}|\mathbf{X},\Theta^{\mathrm{old}}}[\log p(\mathbf{X},\mathbf{Z}|\Theta)] = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta^{\mathrm{old}})\log p(\mathbf{X},\mathbf{Z}|\Theta) \\ \\ \Theta^* &= \arg\max_{\Theta} \mathrm{EM}_{\mathbf{X},\Theta^{\mathrm{old}}}(\Theta) \end{split}$$

When iterated, the likelihood $p(\mathbf{X}|\boldsymbol{\theta})$ converges to a (local) maximum

Direct maximization of the likelihood (or log-likelihood) is hard ...

$$p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) \qquad \qquad p(\mathbf{X}|\Theta) = \frac{p(\mathbf{X}, \mathbf{Z}|\Theta)}{p(\mathbf{Z}|\mathbf{X}, \Theta)}$$

$$\log p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}|\Theta)$$

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$$\operatorname{This \ sums \ to \ 1} \dots$$
$$\log p(\mathbf{X}|\Theta) = \left(\sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\mathrm{old}}) \log p(\mathbf{X}|\Theta)\right)$$

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$$\log p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}|\Theta)$$

$$= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) (\log p(\mathbf{X}, \mathbf{Z}|\Theta) - \log p(\mathbf{Z}|\mathbf{X}, \Theta))$$

$$= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\Theta) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{Z}|\mathbf{X}, \Theta)$$

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Assume that we have valid set of parameters θ^{old} , and that we want to estimate a set θ which yields a better likelihood. We can write:

$$\log p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\Theta)$$

$$= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) (\log p(\mathbf{X}, \mathbf{Z}|\Theta) - \log p(\mathbf{Z}|\mathbf{X}, \Theta))$$

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The expectation (under θ^{old}) of the log-likelihood of the complete data (i.e. observations **X** and underlying states **Z**) as a function of θ

Direct maximization of the likelihood (or log-likelihood) is hard ...

$$p(\mathbf{X}|\Theta) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\Theta) \qquad \qquad p(\mathbf{X}|\Theta) = \frac{p(\mathbf{X}, \mathbf{Z}|\Theta)}{p(\mathbf{Z}|\mathbf{X}, \Theta)}$$

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$$= Q(\Theta, \Theta^{\text{old}}) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{Z}|\mathbf{X}, \Theta)$$

Assume that we have valid set of parameters θ^{old} , and that we want to estimate a set θ which yields a better likelihood. We have:

$$\log p(\mathbf{X}|\Theta) = Q(\Theta, \Theta^{\text{old}}) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{Z}|\mathbf{X}, \Theta)$$
$$\log p(\mathbf{X}|\Theta^{\text{old}}) = Q(\Theta^{\text{old}}, \Theta^{\text{old}}) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}})$$

The increase of the log-likelihood can thus be written as:

 $\log p(\mathbf{X}|\Theta) - \log p(\mathbf{X}|\Theta^{\text{old}}) = Q(\Theta, \Theta^{\text{old}}) - Q(\Theta^{\text{old}}, \Theta^{\text{old}}) + \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log \frac{p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}})}{p(\mathbf{Z}|\mathbf{X}, \Theta)}$

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The relative entropy of $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$ relative to $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta})$, i.e. ≥ 0

Assume that we have valid set of parameters θ^{old} , and that we want to estimate a set θ which yields a better likelihood. We have:

$$\log p(\mathbf{X}|\Theta) = Q(\Theta, \Theta^{\text{old}}) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{Z}|\mathbf{X}, \Theta)$$
$$\log p(\mathbf{X}|\Theta^{\text{old}}) = Q(\Theta^{\text{old}}, \Theta^{\text{old}}) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}})$$

The increase of the log-likelihood can thus be written as:

$$\log p(\mathbf{X}|\Theta) - \log p(\mathbf{X}|\Theta^{\text{old}}) \ge Q(\Theta, \Theta^{\text{old}}) - Q(\Theta^{\text{old}}, \Theta^{\text{old}})$$

By maximizing the expectation $Q(\theta, \theta^{old})$ w.r.t. θ , we do not decrease the likelihood, hence name *expectation maximization* ...

E-Step: Define the Q-function:

$$\begin{aligned} Q(\Theta,\Theta^{\text{old}}) &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta^{\text{old}}) \log p(\mathbf{X},\mathbf{Z}|\Theta) \\ \text{.e. the expectation of log } p(\mathbf{X},\mathbf{Z} \mid \mathbf{\theta}) \text{ over } \mathbf{Z} \text{ (given } \mathbf{X} \text{ and } \mathbf{\theta}) \\ \mathbf{\theta}^{\text{old}} \text{) as a function of } \mathbf{\theta} \end{aligned}$$

M-Step: Maximize $Q(\theta, \theta^{old})$ w.r.t. θ

For HMMs Q has a closed form and maximization can be performed explicitly. Iterate until no or little increase in likelihood is observed, or some maximum number of iterations is reached ...

When iterated, the likelihood $p(\mathbf{X}|\boldsymbol{\theta})$ converges to a (local) maximum

- Init: Pick "suitable" parameters (transition and emission probabilities). Observe that if a parameter is initialized to zero, it remains zero ...
- **E-Step:** 1) Run the forward- and backward-algorithms with the current choice of parameters (to get the params of Q-func).
- **Stop?:** 2) Compute the likelihood $p(\mathbf{X}|\boldsymbol{\theta})$, if sufficient (or another stopping criteria is meet) then stop.
- M-Step: 3) Compute new parameters using the values stored by the forward- and backward-algorithms. Repeat 1-3.

We want a closed form for $Q(\Theta, \Theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\Theta)$

$$p(\mathbf{X}, \mathbf{Z} | \mathbf{\Theta}) = p(\mathbf{z}_1 | \pi) \prod_{n=2}^{N} p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}) \prod_{n=1}^{N} p(\mathbf{x}_n | \mathbf{z}_n, \phi)$$

$$= \prod_{k=1}^{K} \pi_k^{z_{1k}} \prod_{n=2}^{N} \prod_{j=1}^{K} \prod_{k=1}^{K} A_{jk}^{z_{n-1,j} z_{nk}} \prod_{n=1}^{N} \prod_{k=1}^{K} p(\mathbf{x}_n | \phi_k)^{z_{nk}}$$

We want a closed form for $Q(\Theta, \Theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\Theta)$

$$p(\mathbf{X}, \mathbf{Z} | \mathbf{\Theta}) = p(\mathbf{z}_1 | \pi) \prod_{n=2}^{N} p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}) \prod_{n=1}^{N} p(\mathbf{x}_n | \mathbf{z}_n, \phi)$$

$$= \prod_{k=1}^{K} \pi_k^{z_{1k}} \prod_{n=2}^{N} \prod_{j=1}^{K} \prod_{k=1}^{K} A_{jk}^{z_{n-1,j} z_{nk}} \prod_{n=1}^{N} \prod_{k=1}^{K} p(\mathbf{x}_n | \phi_k)^{z_{nk}}$$

$$p(\mathbf{z}_{1}|\pi) = \prod_{k=1}^{K} \pi_{k}^{z_{1k}} \qquad p(\mathbf{z}_{n}|\mathbf{z}_{n-1}, \mathbf{A}) = \prod_{k=1}^{K} \prod_{j=1}^{K} A_{jk}^{z_{n-1,j}z_{nk}}$$
$$p(\mathbf{x}_{n}|\mathbf{z}_{n}, \phi) = \prod_{k=1}^{K} p(\mathbf{x}_{n}|\phi_{k})^{z_{nk}}$$

We want a closed form for $Q(\Theta, \Theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\Theta)$

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$$= \prod_{k=1}^{K} \pi_k^{z_{1k}} \prod_{n=2}^{N} \prod_{j=1}^{K} \prod_{k=1}^{K} A_{jk}^{z_{n-1,j} z_{nk}} \prod_{n=1}^{N} \prod_{k=1}^{K} p(\mathbf{x}_n | \phi_k)^{z_{nk}}$$

Taking the log yields:

$$\log p(\mathbf{X}, \mathbf{Z} | \mathbf{\Theta}) = \sum_{k=1}^{K} z_{1k} \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} z_{n-1,j} z_{nk} \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \log p(\mathbf{x}_n | \phi_k)$$

We want a closed form for $Q(\Theta, \Theta^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \Theta^{\text{old}}) \log p(\mathbf{X}, \mathbf{Z}|\Theta)$

$$p(\mathbf{X}, \mathbf{Z} | \mathbf{\Theta}) = p(\mathbf{z}_1 | \pi) \prod_{n=2}^{N} p(\mathbf{z}_n | \mathbf{z}_{n-1}, \mathbf{A}) \prod_{n=1}^{N} p(\mathbf{x}_n | \mathbf{z}_n, \phi)$$

$$= \prod_{k=1}^{K} \pi_k^{z_{1k}} \prod_{n=2}^{N} \prod_{j=1}^{K} \prod_{k=1}^{K} A_{jk}^{z_{n-1,j} z_{nk}} \prod_{n=1}^{N} \prod_{k=1}^{K} p(\mathbf{x}_n | \phi_k)^{z_{nk}}$$

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$$\log p(\mathbf{X}, \mathbf{Z} | \mathbf{\Theta}) = \sum_{k=1}^{K} z_{1k} \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} z_{n-1,j} z_{nk} \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \log p(\mathbf{x}_n | \phi_k)$$

Taking the expectation (under θ^{old} and **X**) over **Z** yields Q(θ , θ^{old}), i.e.

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{k=1}^{K} E(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} E(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} E(z_{nk}) \log p(\mathbf{x}_n | \phi_k)$$

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{k=1}^{K} E(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} E(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} E(z_{nk}) \log p(\mathbf{x}_n | \phi_k)$$

E-Step: To calculate *Q*, we must compute the expectations $E(z_{1k})$, $E(z_{nk})$, and $E(z_{n-1,i}z_{nk})$. Consider the probabilities:

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n | \mathbf{X}, \Theta^{\text{old}})$$

A *K*-vector where entry *k* is the prob $\gamma(z_{nk})$ of being in state k in the n'th step ...

$$\xi(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X}, \Theta^{\text{old}})$$

A *KxK*-table where entry (j,k)is the prob $\xi(z_{n-1,j}, z_{nk})$ of being in state *j* and *k* in the (n-1)'th and n'th step ...

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{k=1}^{K} E(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} E(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} E(z_{nk}) \log p(\mathbf{x}_n | \phi_k)$$

E-Step: To calculate Q, we must compute the expectations $E(z_{1k})$, $E(z_{nk})$, and $E(z_{n-1,i}z_{nk})$. Consider the probabilities:

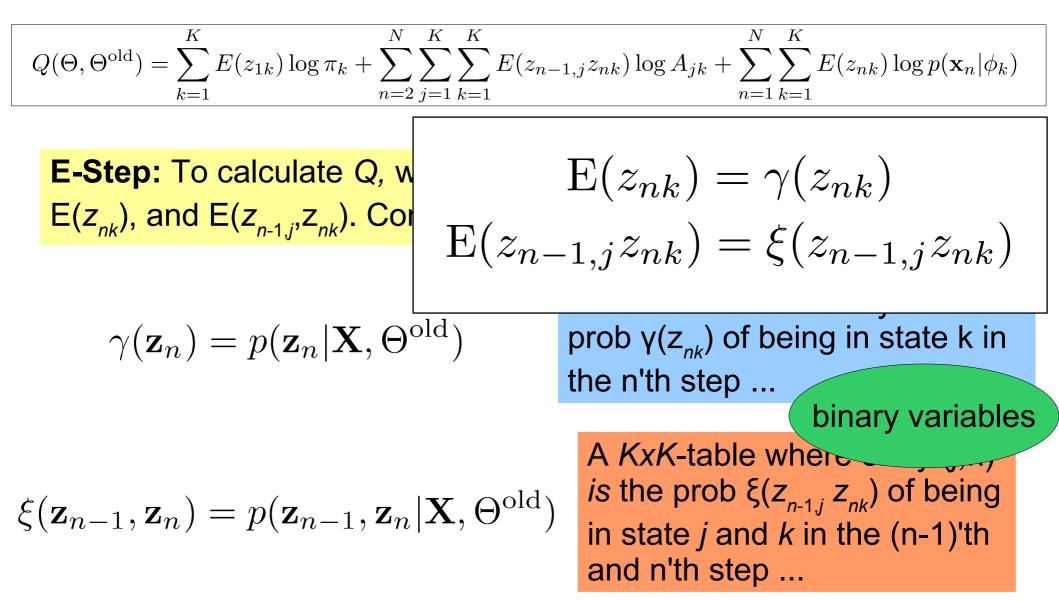
$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n | \mathbf{X}, \Theta^{\text{old}})$$

$$\xi(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X}, \Theta^{\text{old}})$$

A *K*-vector where entry *k* is the prob $\gamma(z_{nk})$ of being in state k in the n'th step ... binary variables A *KxK*-table where is the prob $\xi(z_{n-1,j}, z_{nk})$ of being in state *j* and *k* in the (n-1)'th

and n'th step ...

Fact: The expectation of a binary variable *z* is just p(z=1) ...



Fact: The expectation of a binary variable *z* is just p(z=1) ...

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{k=1}^{K} \gamma(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log p(\mathbf{x}_n | \phi_k)$$

M-Step: If we assume discrete observables x_i , then maximizing the above w.r.t. θ , i.e. A, π , and Φ , yields:

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{k=1}^{K} \gamma(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log p(\mathbf{x}_n | \phi_k)$$

M-Step: If we assume discrete observables x_i , then maximizing the above w.r.t. θ , i.e. A, π , and Φ , yields:

$$A_{jk} = \frac{\sum_{n=2}^{N} \xi(z_{n-1,j} z_{nk})}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j} z_{nl})}$$

Expected number of transitions from state *j* to state *k*

Expected number of transitions from state *j* to any state

$$\pi_k = \frac{\gamma(z_{1k})}{\sum_{j=1}^K \gamma(z_{1j})}$$

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{k=1}^{K} \gamma(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log p(\mathbf{x}_n | \phi_k)$$

M-Step: If we assume discrete observables x_i , then maximizing the above w.r.t. θ , i.e. A, π , and Φ , yields:

Expected number of times symbol *i* is emitted from state *k*

$$\phi_{ik} = \frac{\sum_{n=1}^{N} \gamma(z_{nk}) x_{ni}}{\sum_{n=1}^{N} \gamma(z_{nk})} =$$

Expected number of times a symbol is emitted from state *k*

$$Q(\Theta, \Theta^{\text{old}}) = \sum_{k=1}^{K} \gamma(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log p(\mathbf{x}_n | \phi_k)$$

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$$Q(\Theta, \Theta^{\text{old}}) = \sum_{k=1}^{K} \gamma(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \log p(\mathbf{x}_n | \phi_k)$$

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Compare this to the formulas when **X** and **Z** where given:

$$A_{jk} = \frac{\sum_{n=2}^{N} z_{n-1,j} z_{nk}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1,j} z_{nl}} \qquad \pi_k = \frac{z_{1k}}{\sum_{j=1}^{K} z_{1j}} \qquad \phi_{ik} = \frac{\sum_{n=1}^{N} z_{nk} x_{ni}}{\sum_{n=1}^{N} z_{nk}}$$

Computing γ and ξ

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n | \mathbf{X})$$

$$= \frac{p(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{z}_n) p(\mathbf{x}_{n+1}, \dots, \mathbf{x}_N | \mathbf{z}_n)}{p(\mathbf{X})}$$

$$= \frac{\alpha(\mathbf{z}_n) \beta(\mathbf{z}_n)}{p(\mathbf{X})}$$

$$\begin{aligned} \xi(\mathbf{z}_{n-1}, \mathbf{z}_n) &= p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X}) \\ &= \frac{p(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{z}_{n-1}) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n) p(\mathbf{x}_{n+1}, \dots, \mathbf{x}_N | \mathbf{z}_n)}{p(\mathbf{X})} \\ &= \frac{\alpha(\mathbf{z}_{n-1}) \beta(\mathbf{z}_n) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n)}{p(\mathbf{X})} \end{aligned}$$

Can be computed efficiently using the forward- and backward-algorithm

Computing the new parameters

$$\pi_k = \frac{\gamma(z_{1k})}{\sum_{j=1}^K \gamma(z_{1j})} = \frac{\alpha(z_{1k})\beta(z_{1k})/p(\mathbf{X})}{\sum_{j=1}^K \alpha(z_{1j})\beta(z_{1j})/p(\mathbf{X})} = \frac{\alpha(z_{1k})\beta(z_{1k})}{\sum_{j=1}^K \alpha(z_{1j})\beta(z_{1j})}$$

$$A_{jk} = \frac{\sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nl})} = \frac{\sum_{n=2}^{N} \alpha(z_{n-1,j}) \beta(z_{nk}) p(\mathbf{x}_n | \phi_k) A_{jk}}{\sum_{l=1}^{K} \sum_{n=2}^{N} \alpha(z_{n-1,j}) \beta(z_{nl}) p(\mathbf{x}_n | \phi_l) A_{jl}}$$

Computing the new parameters

$$\pi_{k} = \frac{\gamma(z_{1k})}{\sum_{j=1}^{K} \gamma(z_{1j})} = \frac{\alpha(z_{1k})\beta(z_{1k})/p(\mathbf{X})}{\sum_{j=1}^{K} \alpha(z_{1j})\beta(z_{1j})/p(\mathbf{X})} = \frac{\alpha(z_{1k})\beta(z_{1k})}{\sum_{k=1}^{K} \gamma(z_{1k})}$$
The old parameters
$$A_{jk} = \frac{\sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})}{\sum_{k=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})} = \frac{\sum_{n=2}^{N} \alpha(z_{n-1,j})\beta(z_{nk})p(\mathbf{x}_{n}|\phi_{k})A_{jk}}{\sum_{k=1}^{K} \sum_{n=2}^{N} \alpha(z_{n-1,j})\beta(z_{nk})p(\mathbf{x}_{n}|\phi_{k})A_{jl}}$$

$$\phi_{ik} = \frac{\sum_{n=1}^{N} \alpha(z_{nk})\beta(z_{nk})x_{ni}}{\sum_{n=1}^{N} \alpha(z_{nk})\beta(z_{nk})}$$

$$\alpha(z_{nk}) \text{ or } \beta(z_{nk})$$
The new parameters
$$k$$

EM for HMMs - Summary

- Init: Pick "suitable" parameters (transition and emission probabilities). Observe that if a parameter is initialized to zero, it remains zero ...
- **E-Step:** 1) Run the forward- and backward-algorithms with the current choice of parameters (to get t.he params of Q-func).
- **Stop?:** 2) Compute the likelihood $p(\mathbf{X}|\boldsymbol{\theta})$, if sufficient (or another stopping criteria is meet) then stop.
- M-Step: 3) Compute new parameters using the values stored by the forward- and backward-algorithms. Repeat 1-3.

Running time per iteration:

 $O(K^2N + KK + K^2NK + KDN)$, where D is number of observable symbols

By using memorization in 3), we can improve it to $O(K^2N + KDN)$

Using the scaled values in EM

$$\begin{aligned} \gamma(\mathbf{z}_n) &= p(\mathbf{z}_n | \mathbf{X}) \\ &= \frac{p(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{z}_n) p(\mathbf{x}_{n+1}, \dots, \mathbf{x}_N | \mathbf{z}_n)}{p(\mathbf{X})} \\ &= \frac{\alpha(\mathbf{z}_n) \beta(\mathbf{z}_n)}{p(\mathbf{X})} \\ &= \hat{\alpha}(\mathbf{z}_n) \hat{\beta}(\mathbf{z}_n) \end{aligned}$$

$$\begin{aligned} \xi(\mathbf{z}_{n-1}, \mathbf{z}_n) &= p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X}) \\ &= \frac{p(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{z}_{n-1}) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n) p(\mathbf{x}_{n+1}, \dots, \mathbf{x}_N | \mathbf{z}_n)}{p(\mathbf{X})} \\ &= \frac{\alpha(\mathbf{z}_{n-1}) \beta(\mathbf{z}_n) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n)}{p(\mathbf{X})} \\ &= \hat{\alpha}(\mathbf{z}_{n-1}) \hat{\beta}(\mathbf{z}_n) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n) / c_n \end{aligned}$$

Can be computed using the modified forward- and backward-algorithm

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$$\begin{aligned} \xi(\mathbf{z}_{n-1}, \mathbf{z}_n) &= p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X}) \\ &= \frac{p(\mathbf{x}_1, \dots, \mathbf{x}_{n-1}, \mathbf{z}_{n-1}) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n) p(\mathbf{x}_{n+1}, \dots, \mathbf{x}_N | \mathbf{z}_n)}{p(\mathbf{X})} \\ &= \frac{\alpha(\mathbf{z}_{n-1}) \beta(\mathbf{z}_n) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n)}{p(\mathbf{X})} \\ &= \hat{\alpha}(\mathbf{z}_{n-1}) \hat{\beta}(\mathbf{z}_n) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n) / c_n \end{aligned}$$
Error in book

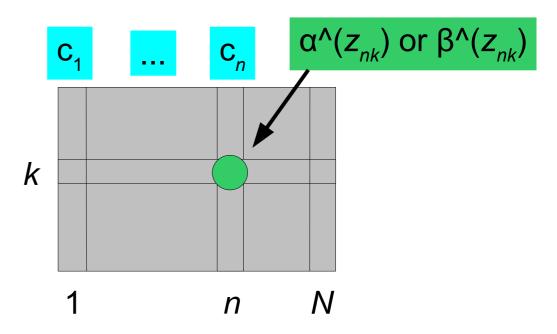
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Computing the new parameters

$$\pi_k = \frac{\gamma(z_{1k})}{\sum_{j=1}^K \gamma(z_{1j})} = \frac{\hat{\alpha}(z_{1k})\hat{\beta}(z_{1k})}{\sum_{j=1}^K \hat{\alpha}(z_{1j})\hat{\beta}(z_{1j})}$$

$$A_{jk} = \frac{\sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nl})} = \frac{\sum_{n=2}^{N} \hat{\alpha}(z_{n-1,j}) \hat{\beta}(z_{nk}) p(\mathbf{x}_n | \phi_k) A_{jk} / c_n}{\sum_{l=1}^{K} \sum_{n=2}^{N} \hat{\alpha}(z_{n-1,j}) \hat{\beta}(z_{nl}) p(\mathbf{x}_n | \phi_l) A_{jl} / c_n}$$

$$\phi_{ik} = \frac{\sum_{n=1}^{N} \hat{\alpha}(z_{nk}) \hat{\beta}(z_{nk}) x_{ni}}{\sum_{n=1}^{N} \hat{\alpha}(z_{nk}) \hat{\beta}(z_{nk})}$$



Summary

- Selecting parameters by counting to reflect a set of (X,Z)'s, i.e. if full information about observables and corresponding latent values is given.
- Selecting parameters by Viterbi Training or Expectation Maximization to reflect a set of X's, i.e. if only information about observables is given.

Summary

- Selecting parameters by counting to reflect a set of (X,Z)'s i.e. if full information about observables and corresponding latent values is given.
- Selecting parameters by Viterbi Training or Expectation Maximization to reflect a set of X's, i.e. if only information about observables is given.

How to deal with multiple "training sequences"?

When multiple (X, Z)'s are given ...

Assume that (several) sequences of observations $X = \{x_1, ..., x_N\}$ and corresponding latent states $Z = \{z_1, ..., z_N\}$ are given ...

$$A_{jk} = \frac{\sum_{n=2}^{N} z_{n-1,j} z_{nk}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1,j} z_{nl}} \qquad \pi_k = \frac{z_{1k}}{\sum_{j=1}^{K} z_{1j}} \qquad \phi_{ik} = \frac{\sum_{n=1}^{N} z_{nk} x_{ni}}{\sum_{n=1}^{N} z_{nk}}$$

... just sum each nominator and denominator over all (X,Z)'s, i.e. we divide total counts ...

$$A_{jk} = \frac{\sum_{(\mathbf{X},\mathbf{Z})} \sum_{n=2}^{N} z_{n-1,j} z_{nk}}{\sum_{(\mathbf{X},\mathbf{Z})} \sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1,j} z_{nl}} \qquad \pi_k = \frac{\sum_{(\mathbf{X},\mathbf{Z})} \sum_{j=1}^{K} z_{nk} z_{nj}}{\sum_{(\mathbf{X},\mathbf{Z})} \sum_{j=1}^{K} z_{nk} z_{nk}}$$
$$\phi_{ik} = \frac{\sum_{(\mathbf{X},\mathbf{Z})} \sum_{n=1}^{N} z_{nk} z_{nk}}{\sum_{(\mathbf{X},\mathbf{Z})} \sum_{n=1}^{N} z_{nk}}$$

 z_{1j}

When multiple X's are given ...

Assume that a set sequences of observations $X = \{x_1, ..., x_N\}$ is given

$$A_{jk} = \frac{\sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nl})} \quad \pi_k = \frac{\gamma(z_{1k})}{\sum_{j=1}^{K} \gamma(z_{1j})} \quad \phi_{ik} = \frac{\sum_{n=1}^{N} \gamma(z_{nk}) x_{ni}}{\sum_{n=1}^{N} \gamma(z_{nk})}$$

... just sum each nominator and denominator over all X's, i.e. we divide total expectation, and we must run the forward- and backward algorithms for each training sequence X ...

$$A_{jk} = \frac{\sum_{\mathbf{X}} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})}{\sum_{\mathbf{X}} \sum_{l=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nl})} \qquad \pi_k = \frac{\sum_{\mathbf{X}} \gamma(z_{1k})}{\sum_{\mathbf{X}} \sum_{j=1}^{K} \gamma(z_{1j})}$$
$$\phi_{ik} = \frac{\sum_{\mathbf{X}} \sum_{n=1}^{N} \gamma(z_{nk}) x_{ni}}{\sum_{\mathbf{X}} \sum_{n=1}^{N} \gamma(z_{nk})}$$

Summary: Training-by-Counting

Training-by-Counting: We are given a sequence of observations $X = \{x_1, ..., x_N\}$ and the corresponding latent states $Z = \{z_1, ..., z_N\}$. We want to find a model:

$$\Theta^*_{\text{TbC}} = \arg\max_{\Theta} p(\mathbf{X}, \mathbf{Z}|\Theta) = \arg\max_{\Theta} \log p(\mathbf{X}, \mathbf{Z}|\Theta)$$

This can be done analytically by counting the frequency by which each transition and emission occur in the training data (**X**, **Z**).

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This can be done analytically by counting the frequency by which each transition and emission occur in the training data (**X**, **Z**).

If only $X = \{x_1, \dots, x_n\}$ is given, then we want to find a model:

$$\Theta_{\mathbf{X}}^* = \arg\max_{\Theta} p(\mathbf{X}|\Theta) = \arg\max_{\Theta} \log p(\mathbf{X}|\Theta)$$

Finding θ_{x}^{*} is hard. We have seen two approaches.

Summary: Viterbi Training

Viterbi Training: We are given a sequence of observations $X = \{x_1, ..., x_N\}$. Pick an initial set of parameters θ_{vit}^0 and compute the best explanation of X under assumption of these parameters using the Viterbi algorithm:

$$\begin{aligned} \mathbf{Z}_{\mathrm{Vit}}^{0} &= \arg\max_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \Theta_{\mathrm{Vit}}^{0}) = \arg\max_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z} | \Theta_{\mathrm{Vit}}^{0}) \\ \end{aligned}$$

$$\begin{aligned} & \mathsf{Compute} \ \mathbf{\theta}_{\mathsf{vit}}^{1} \text{ from } \mathbf{\theta}_{\mathsf{vit}}^{0} \text{ and } \mathbf{Z}_{\mathsf{vit}}^{0} \text{ using TbC and iterate:} \\ & \Theta_{\mathrm{Vit}}^{1} = \arg\max_{\Theta} p(\mathbf{X}, \mathbf{Z}_{\mathrm{Vit}}^{0} | \Theta) = \arg\max_{\Theta} \log p(\mathbf{X}, \mathbf{Z}_{\mathrm{Vit}}^{0} | \Theta) \\ & \mathbf{Z}_{\mathrm{Vit}}^{1} = \arg\max_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} | \Theta_{\mathrm{Vit}}^{1}) = \arg\max_{\mathbf{Z}} \log p(\mathbf{X}, \mathbf{Z} | \Theta_{\mathrm{Vit}}^{1}) \end{aligned}$$

 $p(\mathbf{X}|\Theta^i_{\mathrm{Vit}})$ is usually close to $~p(\mathbf{X}|\Theta^*_{\mathbf{X}})~$, but no guarantees

Summary: Expectation Maximization

EM Training: We are given a sequence of observations $X = \{x_1, ..., x_N\}$. Pick an initial set of parameters θ_{EM}^0 and consider the expectation of log $p(X, Z | \theta)$ over Z (given X and θ_{EM}^0) as a function of θ :

$$EM_{\mathbf{X},\Theta_{\rm EM}^{0}}(\Theta) = E_{\mathbf{Z}|\mathbf{X},\Theta_{\rm EM}^{0}}(\log p(\mathbf{X},\mathbf{Z}|\Theta)) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\Theta_{\rm EM}^{0})\log p(\mathbf{X},\mathbf{Z}|\Theta)$$

For HMMs, we can find θ_{EM}^1 analytically, and iterate to get θ_{EM}^i :

$$\Theta_{EM}^{1} = \arg\max_{\Theta} \mathrm{EM}_{\mathbf{X},\Theta_{\mathrm{EM}}^{0}}(\Theta)$$

 $p(\mathbf{X}|\Theta_{\mathrm{EM}}^{i})$ converges towards a (local) maximum of $p(\mathbf{X}|\Theta)$