## Hidden Markov Models

## Training - Selecting model parameters



## What we know

- The terminology and notation of hidden Markov models (HMMs)
- The forward- and backward-algorithms for determining the likelihood $p(\mathbf{X})$ of a sequence of observations, and computing the posterior decoding.
- The Viterbi-algorithm for finding the most likely underlying explanation (sequence of latent states) of a sequence of observation
- 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 ( $\mathbf{X}, \mathbf{Z}$ )'s, (or just a set of X's) ...


## Selecting "the right" parameters

Assume that (several) sequences of observations $\mathbf{X}=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}$ and corresponding latent states $\mathbf{Z}=\left\{\mathbf{z}_{1}, \ldots, \mathbf{z}_{n}\right\}$ are given $\ldots$


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

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How should we set the model parameters, i.e. transition $\mathbf{A}, \boldsymbol{\pi}$, and emission probabilities $\Phi$, to make the given (X,Z)'s most likely?

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

## Selecting "the right" transition probs


$A_{j k}$ is the probability of a transition from state $j$ to state $k$, and $\pi_{k}$ is the probability of starting in state $k \ldots$

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

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

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

## Selecting "the right" transition probs


$A_{j k}$ is the probability of a transition from state $j$ to state $k$, and $\pi_{k}$ is the probability of starting in state $k . .$.

How many times is the transition

$$
\begin{aligned}
A_{j k} & =\frac{\sum_{n=2}^{N} z_{n-1, j} z_{n k}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1, j} z_{n l}}= \\
\pi_{k} & =\frac{z_{1 k}}{\sum_{j=1}^{K} z_{1 j}}
\end{aligned}
$$ from state $j$ to state $k$ taken

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

## Selecting "the right" emission probs

 H H L L H


If we assume discrete observations, then $\Phi_{i k}$ is the probability of emitting symbol $i$ from state $k$...

How many times is symbol $i$

$$
\phi_{i k}=\frac{\sum_{n=1}^{N} z_{n k} x_{n i}}{\sum_{n=1}^{N} z_{n k}}=
$$ emitted from state $k$

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

## Selecting "the right" parameters

Assume that (several) sequences of observations $X=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$ and corresponding latent states $\mathbf{Z}=\left\{\mathbf{z}_{1}, \ldots, \mathbf{z}_{n}\right\}$ are given $\ldots$

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A_{j k}=\frac{\sum_{n=2}^{N} z_{n-1, j} z_{n k}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1, j} z_{n l}} \quad \pi_{k}=\frac{z_{1 k}}{\sum_{j=1}^{K} z_{1 j}} \quad \phi_{i k}=\frac{\sum_{n=1}^{N} z_{n k} x_{n i}}{\sum_{n=1}^{N} z_{n k}}
$$

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

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

This yield a maximum likelihood estimate (MLE) $\boldsymbol{\theta}^{*}$ of $p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$, which is what we mathematically want ...

$$
f_{\mathbf{X}, \mathbf{Z}}(\Theta)=p(\mathbf{X}, \mathbf{Z} \mid \Theta) \quad \Theta^{*}=\arg \max _{\Theta} f_{\mathbf{X}, \mathbf{Z}}(\Theta)
$$

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Assume that (several) sequences of observations $X=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$ and corresponding latent states $Z=\left\{\mathbf{z}_{1}, \ldots, \boldsymbol{z}_{n}\right\}$ are given ...

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## Any problems?

## Selecting "the right" parameters

Assume that (several) sequences of observations $\boldsymbol{X}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$ and corresponding latent states $\mathbf{Z}=\left\{\mathbf{z}_{1}, \ldots, \mathbf{z}_{n}\right\}$ are given $\ldots$

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> Any problems? What if e.g. the transition from state $j$ to $k$ is not observed, then probability $A_{j k}$ is set to 0 .

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

This yield a maximum likelihood estimate (MLE) $\boldsymbol{\theta}^{*}$ of $p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$, which is what we mathematically want ...

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

## Example



H H L L H


Without pseudocounts:

$$
\begin{array}{ll}
A_{H H}=1 / 2 & p(\text { sun } \mid H)=1 \\
A_{H L}=1 / 2 & p(\text { rain } \mid H)=0 \\
A_{L H}=1 / 2 & p(\text { sun } \mid L)=1 / 2 \\
A_{L L}=1 / 2 & p(\text { rain } \mid L)=1 / 2 \\
\Pi_{H}=1 & \\
\Pi_{L}=0 &
\end{array}
$$

## Example



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A_{L H}=1 / 2 & p(\text { sun } \mid L)=1 / 2 \\
A_{L L}=1 / 2 & p(\text { rain } \mid L)=1 / 2 \\
\Pi_{H}=1 & \\
\Pi_{L}=0 &
\end{array}
$$

## With pseudocounts:

$$
\begin{array}{ll}
A_{H H}=2 / 4 & p(\text { sun } \mid H)=4 / 5 \\
A_{H L}=2 / 4 & p(\text { rain } \mid H)=1 / 5 \\
A_{L H}=2 / 4 & p(\text { sun } \mid L)=2 / 4 \\
A_{L L}=2 / 4 & p(\text { rain } \mid L)=2 / 4 \\
\Pi_{H}=2 / 3 & \\
\Pi_{L}=1 / 3 &
\end{array}
$$

## Selecting "the right" parameters

What if only (several) sequences of observations $\mathbf{X}=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}$ is given, i.e the corresponding latent states $\mathbf{Z}=\left\{\mathbf{z}_{1}, \ldots, \mathbf{z}_{n}\right\}$ are unknown?


How should we set the model parameters, i.e. transitions A, $\boldsymbol{\pi}$, and emission probabilities $\boldsymbol{\Phi}$, to make the given X's most likely?

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How should we set the model parameters, i.e. transitions A, $\boldsymbol{\pi}$, and emission probabilities $\Phi$, to make the given X's most likely?

Maximize $p(\mathbf{X} \mid \Theta)=\sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} \mid \Theta)$ w.r.t. $\boldsymbol{\theta} \ldots$

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What if only (several) sequences of observations $\mathbf{X}=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}$ is given, i.e the corresponding latent states $\mathbf{Z}=\left\{\mathbf{z}_{1}, \ldots, \mathbf{z}_{n}\right\}$ are unknown?

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

$$
p(\mathbf{X} \mid \Theta)=\sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} \mid \Theta)
$$

How should we set the model parameters, i.e. transitions $\mathbf{A}, \boldsymbol{\pi}$, and emission probabilities $\Phi$, to make the given X's most likely?

Maximize $p(\mathbf{X} \mid \Theta)=\sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} \mid \Theta)$ w.r.t. $\boldsymbol{\theta} \ldots$

## Practical Solution - Viterbi training

A more "practical" thing to do is Viterbi Training:
1.Decide on some initial parameter $\boldsymbol{\theta}^{0}$
2. Find the most likely sequence of states $\mathbf{Z}^{*}$ explaining $\mathbf{X}$ using the the Viterbi Algorithm and the current parameters $\boldsymbol{\theta}^{\mathbf{i}}$
3. Update parameters to $\boldsymbol{\theta}^{\mathbf{i + 1}}$ by "counting" (with pseudo counts) according to ( $\mathbf{X}, \mathbf{Z}^{*}$ ).
4.Repeat 2-3 until $P\left(\mathbf{X}, \mathbf{Z}^{*} \mid \boldsymbol{\theta}^{i}\right)$ is satisfactory (or the Viterbi sequence of states does not change).

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Finds a (local) maximum of:

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

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

## Summary: Training-by-Counting

Training-by-Counting: We are given a sequence of observations $\mathbf{X}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$ and the corresponding latent states $\mathbf{Z}=\left\{\mathbf{z}_{1}, \ldots, \boldsymbol{z}_{n}\right\}$. We want to find a model:

$$
\Theta_{\mathrm{TbC}}^{*}=\arg \max _{\Theta} p(\mathbf{X}, \mathbf{Z} \mid \Theta)=\arg \max _{\Theta} \log p(\mathbf{X}, \mathbf{Z} \mid \Theta)
$$

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

If only $X=\left\{x_{1}, \ldots, x_{n}\right\}$ is given, then we want to find a model:

$$
\Theta_{\mathbf{X}}^{*}=\arg \max _{\Theta} p(\mathbf{X} \mid \Theta)=\arg \max _{\Theta} \log p(\mathbf{X} \mid \Theta)
$$

## Summary: Viterbi Training

Viterbi Training: We are given a sequence of observations $\mathbf{X}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$. Pick an initial set of parameters $\boldsymbol{\theta}_{\text {vit }}^{0}$ and compute the best explanation of $\mathbf{X}$ under assumption of these parameters using the Viterbi algorithm:

$$
\mathbf{Z}_{\mathrm{Vit}}^{0}=\arg \max _{\mathbf{Z}} p\left(\mathbf{X}, \mathbf{Z} \mid \Theta_{\mathrm{Vit}}^{0}\right)=\arg \max _{\mathbf{Z}} \log p\left(\mathbf{X}, \mathbf{Z} \mid \Theta_{\mathrm{Vit}}^{0}\right)
$$

Compute $\boldsymbol{\theta}^{1}{ }_{\text {vit }}$ from $\boldsymbol{\theta}_{\text {vit }}^{0}$ and $\mathbf{Z}^{0}{ }_{\text {vit }}$ using TbC and iterate:

$$
\begin{aligned}
& \Theta_{\mathrm{Vit}}^{1}=\arg \max _{\Theta} p\left(\mathbf{X}, \mathbf{Z}_{\mathrm{Vit}}^{0} \mid \Theta\right)=\arg \max _{\Theta} \log p\left(\mathbf{X}, \mathbf{Z}_{\mathrm{Vit}}^{0} \mid \Theta\right) \\
& \mathbf{Z}_{\mathrm{Vit}}^{1}=\arg \max _{\mathbf{Z}} p\left(\mathbf{X}, \mathbf{Z} \mid \Theta_{\mathrm{Vit}}^{1}\right)=\arg \max _{\mathbf{Z}} \log p\left(\mathbf{X}, \mathbf{Z} \mid \Theta_{\mathrm{Vit}}^{1}\right)
\end{aligned}
$$

$p\left(\mathbf{X} \mid \Theta_{\mathrm{V} \text { it }}^{i}\right)$ is usually close to $p\left(\mathbf{X} \mid \Theta_{\mathbf{X}}^{*}\right)$, but no guarantees

## Expectation Maximization

EM Training: We are given a sequence of observations $\mathbf{X}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$. Pick an initial set of parameters $\boldsymbol{\theta}^{0}{ }_{E M}$ and consider the expectation of $\log p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$ over $\mathbf{Z}$ (given $\mathbf{X}$ and $\boldsymbol{\theta}_{\text {EM }}{ }^{\circ}$ ) as a function of $\boldsymbol{\theta}$ :

$$
E M_{\mathbf{X}, \Theta_{\mathrm{EM}}^{0}}(\Theta)=\mathrm{E}_{\mathbf{Z} \mid \mathbf{X}, \Theta_{\mathrm{EM}}^{0}}(\log p(\mathbf{X}, \mathbf{Z} \mid \Theta))=\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta_{\mathrm{EM}}^{0}\right) \log p(\mathbf{X}, \mathbf{Z} \mid \Theta)
$$

For HMMs, we can find $\boldsymbol{\theta}^{1}$ EM analytically, and iterate to get $\boldsymbol{\theta}_{\mathrm{EM}}^{\boldsymbol{e}}$ :

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

$p\left(\mathbf{X} \mid \Theta_{\mathrm{EM}}^{i}\right)$ converges towards a (local) maximum of $p\left(\mathbf{X} \mid \Theta_{\mathbf{X}}^{*}\right)$

## Expectation Maximization

E-Step: Define the Q-function:

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

i.e. the expectation of $\log p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$ over $\mathbf{Z}$ (given $\mathbf{X}$ and $\boldsymbol{\theta}^{\text {old }}$ ) as a function of $\boldsymbol{\theta}$

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

$$
\begin{gathered}
\operatorname{EM}_{\mathbf{X}, \Theta^{\text {old }}}(\Theta)=E_{\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}}[\log p(\mathbf{X}, \mathbf{Z} \mid \Theta)]=\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{X}, \mathbf{Z} \mid \Theta) \\
\Theta^{*}=\arg \max _{\Theta} \operatorname{EM}_{\mathbf{X}, \Theta^{\text {old }}}(\Theta)
\end{gathered}
$$

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

## Maximizing the likelihood

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

$$
p(\mathbf{X} \mid \Theta)=\sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} \mid \Theta) \quad p(\mathbf{X} \mid \Theta)=\frac{p(\mathbf{X}, \mathbf{Z} \mid \Theta)}{p(\mathbf{Z} \mid \mathbf{X}, \Theta)}
$$

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

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

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$$

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$$
\begin{aligned}
\log p(\mathbf{X} \mid \Theta) & =\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{X} \mid \Theta) \\
& =\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right)(\log p(\mathbf{X}, \mathbf{Z} \mid \Theta)-\log p(\mathbf{Z} \mid \mathbf{X}, \Theta)) \\
& =\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{X}, \mathbf{Z} \mid \Theta)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{Z} \mid \mathbf{X}, \Theta)
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\end{aligned}
$$

The expectation (under $\boldsymbol{\theta}^{\text {old }}$ ) of the log-likelihood of the complete data (i.e. observations $\mathbf{X}$ and underlying states $\mathbf{Z}$ ) as a function of $\boldsymbol{\theta}$

## Maximizing the likelihood

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$$

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

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\begin{aligned}
\log p(\mathbf{X} \mid \Theta) & =\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{X} \mid \Theta) \\
& =\sum_{\mathbf{Z}}^{\text {old }} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right)(\log p(\mathbf{X}, \mathbf{Z} \mid \Theta)-\log p(\mathbf{Z} \mid \mathbf{X}, \Theta)) \\
& =\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{X}, \mathbf{Z} \mid \Theta) \\
& =Q\left(\Theta, \Theta^{\text {old }}\right)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{Z} \mid \mathbf{X}, \Theta)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{Z} \mid \mathbf{X}, \Theta)
\end{aligned}
$$

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

$$
\begin{aligned}
\log p(\mathbf{X} \mid \Theta) & =Q\left(\Theta, \Theta^{\text {old }}\right)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{Z} \mid \mathbf{X}, \Theta) \\
\log p\left(\mathbf{X} \mid \Theta^{\text {old }}\right) & =Q\left(\Theta^{\text {old }}, \Theta^{\text {old }}\right)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right)
\end{aligned}
$$

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

$$
\begin{aligned}
\log p(\mathbf{X} \mid \Theta)- & \log p\left(\mathbf{X} \mid \Theta^{\mathrm{old}}\right)= \\
& Q\left(\Theta, \Theta^{\mathrm{old}}\right)-Q\left(\Theta^{\mathrm{old}}, \Theta^{\mathrm{old}}\right)+\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\mathrm{old}}\right) \log \frac{p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\mathrm{old}}\right)}{p(\mathbf{Z} \mid \mathbf{X}, \Theta)}
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Assume that we have valid set of parameters $\boldsymbol{\theta}^{\text {old }}$, and that we want to estimate a set $\boldsymbol{\theta}$ which yields a better likelihood. We have:

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\begin{aligned}
\log p(\mathbf{X} \mid \Theta) & =Q\left(\Theta, \Theta^{\mathrm{old}}\right)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\mathrm{old}}\right) \log p(\mathbf{Z} \mid \mathbf{X}, \Theta) \\
\log p\left(\mathbf{X} \mid \Theta^{\mathrm{old}}\right) & =Q\left(\Theta^{\mathrm{old}}, \Theta^{\mathrm{old}}\right)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\mathrm{old}}\right) \log p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\mathrm{old}}\right)
\end{aligned}
$$

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

$$
\log p(\mathbf{X} \mid \Theta)-\log p\left(\mathbf{X} \mid \Theta^{\text {old }}\right)=
$$

$$
Q\left(\Theta, \Theta^{\text {old }}\right)-Q\left(\Theta^{\text {old }}, \Theta^{\text {old }}\right)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log \frac{p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right)}{p(\mathbf{Z} \mid \mathbf{X}, \Theta)}
$$

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

## Maximizing the likelihood

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

$$
\begin{aligned}
\log p(\mathbf{X} \mid \Theta) & =Q\left(\Theta, \Theta^{\text {old }}\right)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p(\mathbf{Z} \mid \mathbf{X}, \Theta) \\
\log p\left(\mathbf{X} \mid \Theta^{\text {old }}\right) & =Q\left(\Theta^{\text {old }}, \Theta^{\text {old }}\right)-\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right) \log p\left(\mathbf{Z} \mid \mathbf{X}, \Theta^{\text {old }}\right)
\end{aligned}
$$

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

$$
\log p(\mathbf{X} \mid \Theta)-\log p\left(\mathbf{X} \mid \Theta^{\mathrm{old}}\right) \geq Q\left(\Theta, \Theta^{\mathrm{old}}\right)-Q\left(\Theta^{\mathrm{old}}, \Theta^{\mathrm{old}}\right)
$$

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

## EM for HMMs

E-Step: Define the Q-function:

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

i.e. the expectation of $\log p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$ over $\mathbf{Z}$ (given $\mathbf{X}$ and $\boldsymbol{\theta}^{\text {old }}$ ) as a function of $\boldsymbol{\theta}$

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

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 $p(\mathbf{X} \mid \boldsymbol{\theta})$ converges to a (local) maximum

## EM for HMMs

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 $p(\mathbf{X} \mid \boldsymbol{\theta})$, 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.

## EM for HMMs

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

$$
\begin{aligned}
p(\mathbf{X}, \mathbf{Z} \mid \Theta) & =p\left(\mathbf{z}_{1} \mid \pi\right) \prod_{n=2}^{N} p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}, \mathbf{A}\right) \prod_{n=1}^{N} p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}, \phi\right) \\
& =\prod_{k=1}^{K} \pi_{k}^{z_{1 k}} \prod_{n=2}^{N} \prod_{j=1}^{K} \prod_{k=1}^{K} A_{j k}^{z_{n-1, j} z_{n k}} \prod_{n=1}^{N} \prod_{k=1}^{K} p\left(\mathbf{x}_{n} \mid \phi_{k}\right)^{z_{n k}}
\end{aligned}
$$

## EM for HMMs

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

$$
\begin{aligned}
p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\Theta}) & =p\left(\mathbf{z}_{1} \mid \pi\right) \prod_{n=2}^{N} p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}, \mathbf{A}\right) \prod_{n=1}^{N} p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}, \phi\right) \\
& =\prod_{k=1}^{K} \pi_{k}^{z_{1 k}} \prod_{n=2}^{N} \prod_{j=1}^{K} \prod_{k=1}^{K} A_{j k}^{z_{n-1, j} z_{n k}} \prod_{n=1}^{N} \prod_{k=1}^{K} p\left(\mathbf{x}_{n} \mid \phi_{k}\right)^{z_{n k}}
\end{aligned}
$$

$$
\begin{gathered}
p\left(\mathbf{z}_{1} \mid \pi\right)=\prod_{k=1}^{K} \pi_{k}^{z_{1 k}} \quad p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}, \mathbf{A}\right)=\prod_{k=1}^{K} \prod_{j=1}^{K} A_{j k}^{z_{n-1, j} z_{n k}} \\
p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}, \phi\right)=\prod_{k=1}^{K} p\left(\mathbf{x}_{n} \mid \phi_{k}\right)^{z_{n k}}
\end{gathered}
$$

## EM for HMMs

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

$$
\begin{aligned}
p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\Theta}) & =p\left(\mathbf{z}_{1} \mid \pi\right) \prod_{n=2}^{N} p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}, \mathbf{A}\right) \prod_{n=1}^{N} p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}, \phi\right) \\
& =\prod_{k=1}^{K} \pi_{k}^{z_{1 k}} \prod_{n=2}^{N} \prod_{j=1}^{K} \prod_{k=1}^{K} A_{j k}^{z_{n-1, j} z_{n k}} \prod_{n=1}^{N} \prod_{k=1}^{K} p\left(\mathbf{x}_{n} \mid \phi_{k}\right)^{z_{n k}}
\end{aligned}
$$

Taking the log yields:
$\log p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\Theta})=\sum_{k=1}^{K} z_{1 k} \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} z_{n-1, j} z_{n k} \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} z_{n k} \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)$

## EM for HMMs

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

$$
\begin{aligned}
p(\mathbf{X}, \mathbf{Z} \mid \Theta) & =p\left(\mathbf{z}_{1} \mid \pi\right) \prod_{n=2}^{N} p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}, \mathbf{A}\right) \prod_{n=1}^{N} p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}, \phi\right) \\
& =\prod_{k=1}^{K} \pi_{k}^{z_{1 k}} \prod_{n=2}^{N} \prod_{j=1}^{K} \prod_{k=1}^{K} A_{j k}^{z_{n-1, j} z_{n k}} \prod_{n=1}^{N} \prod_{k=1}^{K} p\left(\mathbf{x}_{n} \mid \phi_{k}\right)^{z_{n k}}
\end{aligned}
$$

Taking the log yields:
$\log p(\mathbf{X}, \mathbf{Z} \mid \mathbf{\Theta})=\sum_{k=1}^{K} z_{1 k} \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} z_{n-1, j} z_{n k} \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} z_{n k} \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)$
Taking the expectation (under $\boldsymbol{\theta}^{\text {old }}$ and $\mathbf{X}$ ) over $\mathbf{Z}$ yields $Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text {old }}\right)$, i.e:
$Q\left(\Theta, \Theta^{\text {old }}\right)=\sum_{k=1}^{K} E\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} E\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} E\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)$

## EM for HMMs

$$
Q\left(\Theta, \Theta^{\text {old }}\right)=\sum_{k=1}^{K} E\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} E\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} E\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)
$$

E-Step: To calculate $Q$, we must compute the expectations $E\left(z_{1 k}\right)$, $\mathrm{E}\left(z_{n k}\right)$, and $\mathrm{E}\left(z_{n-1, j} z_{n k}\right)$. Consider the probabilities:

$$
\gamma\left(\mathbf{z}_{n}\right)=p\left(\mathbf{z}_{n} \mid \mathbf{X}, \Theta^{\mathrm{old}}\right)
$$

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

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

## EM for HMMs

$$
Q\left(\Theta, \Theta^{\mathrm{old}}\right)=\sum_{k=1}^{K} E\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} E\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} E\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)
$$

E-Step: To calculate $Q$, we must compute the expectations $E\left(z_{1 k}\right)$, $\mathrm{E}\left(z_{n k}\right)$, and $\mathrm{E}\left(z_{n-1, j} z_{n k}\right)$. Consider the probabilities:

$$
\gamma\left(\mathbf{z}_{n}\right)=p\left(\mathbf{z}_{n} \mid \mathbf{X}, \Theta^{\mathrm{old}}\right)
$$

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

## binary variables

A KxK-table wherc is the prob $\xi\left(z_{n-1, j} z_{n k}\right)$ 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 $p(z=1) \ldots$...

## EM for HMMs

$$
Q\left(\Theta, \Theta^{\mathrm{old}}\right)=\sum_{k=1}^{K} E\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} E\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} E\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)
$$

$$
\begin{aligned}
& \mathrm{E}-\text { Step: To calculate } \mathrm{Q}, \mathrm{w} \\
& \mathrm{E}\left(z_{n k}\right), \text { and } \mathrm{E}\left(z_{n-1, j}, \mathrm{z}_{n k}\right) . \mathrm{Co} \\
& \mathrm{E}\left(z_{n-1, j} z_{n k}\right)=\xi\left(z_{n-1, j}\right)=\gamma\left(z_{n k}\right)
\end{aligned}
$$

$$
\gamma\left(\mathbf{z}_{n}\right)=p\left(\mathbf{z}_{n} \mid \mathbf{X}, \Theta^{\text {old }}\right) \quad \text { prob } \gamma\left(\mathbf{z}_{n k}\right) \text { of being in state } \mathrm{k} \text { in }
$$ the n'th step ...

## binary variables

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

## EM for HMMs

$$
Q\left(\Theta, \Theta^{\mathrm{old}}\right)=\sum_{k=1}^{K} \gamma\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} \gamma\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)
$$

M-Step: If we assume discrete observables $x_{i}$, then maximizing the above w.r.t. $\theta$, i.e. $A, \pi$, and $\Phi$, yields:

## EM for HMMs

$$
Q\left(\Theta, \Theta^{\text {old }}\right)=\sum_{k=1}^{K} \gamma\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} \gamma\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)
$$

M-Step: If we assume discrete observables $x_{i}$, then maximizing the above w.r.t. $\boldsymbol{\theta}$, i.e. $A, \pi$, and $\boldsymbol{\Phi}$, yields:

$$
A_{j k}=\frac{\sum_{n=2}^{N} \xi\left(z_{n-1, j} z_{n k}\right)}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi\left(z_{n-1, j} z_{n l}\right)}=
$$

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

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

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

## EM for HMMs

$$
Q\left(\Theta, \Theta^{\text {old }}\right)=\sum_{k=1}^{K} \gamma\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} \gamma\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)
$$

M-Step: If we assume discrete observables $x_{i}$, then maximizing the above w.r.t. $\boldsymbol{\theta}$, i.e. $A, \pi$, and $\Phi$, yields:

## Expected number of times

$$
\phi_{i k}=\frac{\sum_{n=1}^{N} \gamma\left(z_{n k}\right) x_{n i}}{\sum_{n=1}^{N} \gamma\left(z_{n k}\right)}=\frac{\text { symbol } i \text { is emitted from state } k}{\begin{array}{l}
\text { Expected number of times a } \\
\text { symbol is emitted from state } k
\end{array}}
$$

## EM for HMMs

$$
Q\left(\Theta, \Theta^{\text {old }}\right)=\sum_{k=1}^{K} \gamma\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} \gamma\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)
$$

M-Step: If we assume discrete observables $x_{i}$, then maximizing the above w.r.t. $\boldsymbol{\theta}$, i.e. $A, \pi$, and $\Phi$, yields:

$$
A_{j k}=\frac{\sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n k}\right)}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n l}\right)} \quad \pi_{k}=\frac{\gamma\left(z_{1 k}\right)}{\sum_{j=1}^{K} \gamma\left(z_{1 j}\right)} \quad \phi_{i k}=\frac{\sum_{n=1}^{N} \gamma\left(z_{n k}\right) x_{n i}}{\sum_{n=1}^{N} \gamma\left(z_{n k}\right)}
$$

## EM for HMMs

$$
Q\left(\Theta, \Theta^{\text {old }}\right)=\sum_{k=1}^{K} \gamma\left(z_{1 k}\right) \log \pi_{k}+\sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \xi\left(z_{n-1, j} z_{n k}\right) \log A_{j k}+\sum_{n=1}^{N} \sum_{k=1}^{K} \gamma\left(z_{n k}\right) \log p\left(\mathbf{x}_{n} \mid \phi_{k}\right)
$$

M-Step: If we assume discrete observables $x_{i}$, then maximizing the above w.r.t. $\theta$, i.e. $A, \pi$, and $\Phi$, yields:

$$
A_{j k}=\frac{\sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n k}\right)}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n l}\right)} \quad \pi_{k}=\frac{\gamma\left(z_{1 k}\right)}{\sum_{j=1}^{K} \gamma\left(z_{1 j}\right)} \quad \phi_{i k}=\frac{\sum_{n=1}^{N} \gamma\left(z_{n k}\right) x_{n i}}{\sum_{n=1}^{N} \gamma\left(z_{n k}\right)}
$$

Compare this to the formulas when $\mathbf{X}$ and $\mathbf{Z}$ where given:

$$
A_{j k}=\frac{\sum_{n=2}^{N} z_{n-1, j} z_{n k}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1, j} z_{n l}} \quad \pi_{k}=\frac{z_{1 k}}{\sum_{j=1}^{K} z_{1 j}} \quad \phi_{i k}=\frac{\sum_{n=1}^{N} z_{n k} x_{n i}}{\sum_{n=1}^{N} z_{n k}}
$$

## Computing $y$ and $\xi$

$$
\begin{aligned}
\gamma\left(\mathbf{z}_{n}\right) & =p\left(\mathbf{z}_{n} \mid \mathbf{X}\right) \\
& =\frac{p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}, \mathbf{z}_{n}\right) p\left(\mathbf{x}_{n+1}, \ldots, \mathbf{x}_{N} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})} \\
& =\frac{\alpha\left(\mathbf{z}_{n}\right) \beta\left(\mathbf{z}_{n}\right)}{p(\mathbf{X})}
\end{aligned}
$$

$$
\begin{aligned}
\xi\left(\mathbf{z}_{n-1}, \mathbf{z}_{n}\right) & =p\left(\mathbf{z}_{n-1}, \mathbf{z}_{n} \mid \mathbf{X}\right) \\
& =\frac{p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{n-1}, \mathbf{z}_{n-1}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right) p\left(\mathbf{x}_{n+1}, \ldots, \mathbf{x}_{N} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})} \\
& =\frac{\alpha\left(\mathbf{z}_{n-1}\right) \beta\left(\mathbf{z}_{n}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})}
\end{aligned}
$$

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

## Computing the new parameters

$$
\begin{aligned}
& \pi_{k}=\frac{\gamma\left(z_{1 k}\right)}{\sum_{j=1}^{K} \gamma\left(z_{1 j}\right)}=\frac{\alpha\left(z_{1 k}\right) \beta\left(z_{1 k}\right) / p(\mathbf{X})}{\sum_{j=1}^{K} \alpha\left(z_{1 j}\right) \beta\left(z_{1 j}\right) / p(\mathbf{X})}=\frac{\alpha\left(z_{1 k}\right) \beta\left(z_{1 k}\right)}{\sum_{j=1}^{K} \alpha\left(z_{1 j}\right) \beta\left(z_{1 j}\right)} \\
& A_{j k}=\frac{\sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n k}\right)}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n l}\right)}=\frac{\sum_{n=2}^{N} \alpha\left(z_{n-1, j}\right) \beta\left(z_{n k}\right) p\left(\mathbf{x}_{n} \mid \phi_{k}\right) A_{j k}}{\sum_{l=1}^{K} \sum_{n=2}^{N} \alpha\left(z_{n-1, j}\right) \beta\left(z_{n l}\right) p\left(\mathbf{x}_{n} \mid \phi_{l}\right) A_{j l}}
\end{aligned}
$$

$$
\phi_{i k}=\frac{\sum_{n=1}^{N} \alpha\left(z_{n k}\right) \beta\left(z_{n k}\right) x_{n i}}{\sum_{n=1}^{N} \alpha\left(z_{n k}\right) \beta\left(z_{n k}\right)}
$$

$$
\gamma\left(\mathbf{z}_{n}\right)=\frac{\alpha\left(\mathbf{z}_{n}\right) \beta\left(\mathbf{z}_{n}\right)}{p(\mathbf{X})}
$$

$$
\xi\left(\mathbf{z}_{n-1}, \mathbf{z}_{n}\right)=\frac{\alpha\left(\mathbf{z}_{n-1}\right) \beta\left(\mathbf{z}_{n}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})}
$$



## Computing the new parameters

$\pi_{k}=\frac{\gamma\left(z_{1 k}\right)}{\sum_{j=1}^{K} \gamma\left(z_{1 j}\right)}=\frac{\alpha\left(z_{1 k}\right) \beta\left(z_{1 k}\right) / p(\mathbf{X})}{\sum_{j=1}^{K} \alpha\left(z_{1 j}\right) \beta\left(z_{1 j}\right) / p(\mathbf{X})}=\frac{\alpha\left(z_{1 k}\right) \beta\left(z_{1 k}\right)}{\sum_{\text {The old parameters }}^{K}}$
$A_{j k}=\frac{\sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n k}\right)}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n l}\right)}=\frac{\left.\sum_{n=2}^{N} \alpha\left(z_{n-1, j}\right) \beta\left(z_{n k}\right)\right)\left(\mathbf{x}_{n} \mid \phi_{k}\right) A_{j k}}{\sum_{l=1}^{K} \sum_{n=2}^{N} \alpha\left(z_{n-1, j}\right) \beta\left(z_{n l}\right) p\left(\mathbf{x}_{n} \mid \phi_{l}\right) A_{j l}}$
$\phi_{i k}=\frac{\sum_{n=1}^{N} \alpha\left(z_{n k}\right) \beta\left(z_{n k}\right) x_{n i}}{\sum_{n=1}^{N} \alpha\left(z_{n k}\right) \beta\left(z_{n k}\right)}$

The new parameters

$n$

## 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 $p(\mathbf{X} \mid \boldsymbol{\theta})$, 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:

$\mathrm{O}\left(K^{2} N+K K+K^{2} N K+K D N\right)$, where $D$ is number of observable symbols By using memorization in 3), we can improve it to $\mathrm{O}\left(K^{2} N+K D N\right)$

## Using the scaled values in EM

$$
\begin{aligned}
\gamma\left(\mathbf{z}_{n}\right) & =p\left(\mathbf{z}_{n} \mid \mathbf{X}\right) \\
& =\frac{p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}, \mathbf{z}_{n}\right) p\left(\mathbf{x}_{n+1}, \ldots, \mathbf{x}_{N} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})} \\
& =\frac{\alpha\left(\mathbf{z}_{n}\right) \beta\left(\mathbf{z}_{n}\right)}{p(\mathbf{X})} \\
& =\hat{\alpha}\left(\mathbf{z}_{n}\right) \hat{\beta}\left(\mathbf{z}_{n}\right)
\end{aligned}
$$

$$
\xi\left(\mathbf{z}_{n-1}, \mathbf{z}_{n}\right)=p\left(\mathbf{z}_{n-1}, \mathbf{z}_{n} \mid \mathbf{X}\right)
$$

$$
=\frac{p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{n-1}, \mathbf{z}_{n-1}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right) p\left(\mathbf{x}_{n+1}, \ldots, \mathbf{x}_{N} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})}
$$

$$
=\frac{\alpha\left(\mathbf{z}_{n-1}\right) \beta\left(\mathbf{z}_{n}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})}
$$

$$
=\hat{\alpha}\left(\mathbf{z}_{n-1}\right) \hat{\beta}\left(\mathbf{z}_{n}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right) / c_{n}
$$

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

Using the scaled val

$$
\begin{aligned}
\gamma\left(\mathbf{z}_{n}\right) & =p\left(\mathbf{z}_{n} \mid \mathbf{X}\right) \\
& =\frac{p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}, \mathbf{z}_{n}\right) p\left(\mathbf{x}_{n+1}, \ldots, \mathbf{x}\right.}{p(\mathbf{X})}
\end{aligned}
$$

$$
=\frac{\alpha\left(\mathbf{z}_{n}\right) \beta\left(\mathbf{z}_{n}\right)}{p(\mathbf{X})}
$$

$$
\begin{aligned}
& \alpha\left(\mathbf{z}_{n}\right)=\left(\prod_{m=1}^{n} c_{m}\right) \hat{\alpha}\left(\mathbf{z}_{n}\right) \\
& \beta\left(\mathbf{z}_{n}\right)=\left(\prod_{m=n+1}^{N} c_{m}\right) \hat{\beta}\left(\mathbf{z}_{n}\right)
\end{aligned}
$$

$$
=\hat{\alpha}\left(\mathbf{z}_{n}\right) \hat{\beta}\left(\mathbf{z}_{n}\right)
$$

$$
\xi\left(\mathbf{z}_{n-1}, \mathbf{z}_{n}\right)=p\left(\mathbf{z}_{n-1}, \mathbf{z}_{n} \mid \mathbf{X}\right)
$$

$$
=\frac{p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{n-1}, \mathbf{z}_{n-1}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right) p\left(\mathbf{x}_{n+1}, \ldots, \mathbf{x}_{N} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})}
$$

$$
=\frac{\alpha\left(\mathbf{z}_{n-1}\right) \beta\left(\mathbf{z}_{n}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right)}{p(\mathbf{X})}
$$

$$
=\hat{\alpha}\left(\mathbf{z}_{n-1}\right) \hat{\beta}\left(\mathbf{z}_{n}\right) p\left(\mathbf{z}_{n} \mid \mathbf{z}_{n-1}\right) p\left(\mathbf{x}_{n} \mid \mathbf{z}_{n}\right) / c_{n}
$$

## Error in book

## Computing the new parameters

$$
\begin{aligned}
& \pi_{k}=\frac{\gamma\left(z_{1 k}\right)}{\sum_{j=1}^{K} \gamma\left(z_{1 j}\right)}=\frac{\hat{\alpha}\left(z_{1 k}\right) \hat{\beta}\left(z_{1 k}\right)}{\sum_{j-1}^{K} \hat{\alpha}\left(z_{1 k}\right) \hat{\beta}\left(z_{1 k}\right)} \\
& A_{j k}=\frac{\sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n k}\right)}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n l}\right)}=\frac{\sum_{n=2}^{N} \hat{\alpha}\left(z_{n-1, j}\right) \hat{\beta}\left(z_{n k}\right) p\left(\mathbf{x}_{n} \mid \phi_{k}\right) A_{j k} / c_{n}}{\sum_{l=1}^{K} \sum_{n=2}^{N} \hat{\alpha}\left(z_{n-1, j}\right) \hat{\beta}\left(z_{n l}\right) p\left(\mathbf{x}_{n} \mid \phi_{l}\right) A_{j l} / c_{n}} \\
& \phi_{i k}=\frac{\sum_{n=1}^{N} \hat{\alpha}\left(z_{n k}\right) \hat{\beta}\left(z_{n k}\right) x_{n i}}{\sum_{n=1}^{N} \hat{\alpha}\left(z_{n k}\right) \hat{\beta}\left(z_{n k}\right)} \\
& c_{1} \ldots \\
& c_{n} \alpha^{\wedge}\left(z_{n k}\right) \text { or } \beta^{\wedge}\left(z_{n k}\right) \\
& 1
\end{aligned}
$$

## 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.


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

Assume that (several) sequences of observations $\mathbf{X}=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}$ and corresponding latent states $\mathbf{Z}=\left\{\mathbf{z}_{1}, \ldots, \mathbf{z}_{n}\right\}$ are given $\ldots$

$$
A_{j k}=\frac{\sum_{n=2}^{N} z_{n-1, j} z_{n k}}{\sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1, j} z_{n l}} \quad \pi_{k}=\frac{z_{1 k}}{\sum_{j=1}^{K} z_{1 j}} \quad \phi_{i k}=\frac{\sum_{n=1}^{N} z_{n k} x_{n i}}{\sum_{n=1}^{N} z_{n k}}
$$

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

$$
\begin{gathered}
A_{j k}=\frac{\sum_{(\mathbf{X}, \mathbf{Z})} \sum_{n=2}^{N} z_{n-1, j} z_{n k}}{\sum_{(\mathbf{X}, \mathbf{Z})} \sum_{l=1}^{K} \sum_{n=2}^{N} z_{n-1, j} z_{n l}} \pi_{k}=\frac{\sum_{(\mathbf{X}, \mathbf{Z})} z_{1 k}}{\sum_{(\mathbf{X}, \mathbf{Z})} \sum_{j=1}^{K} z_{1 j}} \\
\phi_{i k}=\frac{\sum_{(\mathbf{X}, \mathbf{Z})} \sum_{n=1}^{N} z_{n k} x_{n i}}{\sum_{(\mathbf{X}, \mathbf{Z})} \sum_{n=1}^{N} z_{n k}}
\end{gathered}
$$

## When multiple $X$ 's are given ...

Assume that a set sequences of observations $\mathbf{X}=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right\}$ is given

$$
A_{j k}=\frac{\sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n k}\right)}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n l}\right)} \quad \pi_{k}=\frac{\gamma\left(z_{1 k}\right)}{\sum_{j=1}^{K} \gamma\left(z_{1 j}\right)} \quad \phi_{i k}=\frac{\sum_{n=1}^{N} \gamma\left(z_{n k}\right) x_{n i}}{\sum_{n=1}^{N} \gamma\left(z_{n k}\right)}
$$

... 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 $\mathbf{X}$...

$$
\begin{gathered}
A_{j k}=\frac{\sum_{\mathbf{X}} \sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n k}\right)}{\sum_{\mathbf{X}} \sum_{l=1}^{K} \sum_{n=2}^{N} \xi\left(z_{n-1, j}, z_{n l}\right)} \quad \pi_{k}=\frac{\sum_{\mathbf{x}} \gamma\left(z_{1 k}\right)}{\sum_{\mathbf{X}} \sum_{j=1}^{K} \gamma\left(z_{1 j}\right)} \\
\phi_{i k}=\frac{\sum_{\mathbf{x}} \sum_{n=1}^{N} \gamma\left(z_{n k}\right) x_{n i}}{\sum_{\mathbf{X}} \sum_{n=1}^{N} \gamma\left(z_{n k}\right)}
\end{gathered}
$$

## Summary: Training-by-Counting

Training-by-Counting: We are given a sequence of observations $\mathbf{X}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$ and the corresponding latent states $\mathbf{Z}=\left\{\mathbf{z}_{1}, \ldots, \boldsymbol{z}_{n}\right\}$. We want to find a model:

$$
\Theta_{\mathrm{TbC}}^{*}=\arg \max _{\Theta} p(\mathbf{X}, \mathbf{Z} \mid \Theta)=\arg \max _{\Theta} \log p(\mathbf{X}, \mathbf{Z} \mid \Theta)
$$

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

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$$

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

If only $X=\left\{x_{1}, \ldots, x_{n}\right\}$ is given, then we want to find a model:

$$
\Theta_{\mathbf{X}}^{*}=\arg \max _{\Theta} p(\mathbf{X} \mid \Theta)=\arg \max _{\Theta} \log p(\mathbf{X} \mid \Theta)
$$

Finding $\boldsymbol{\theta}^{*}{ }_{x}$ is hard. We have seen two approaches.

## Summary: Viterbi Training

Viterbi Training: We are given a sequence of observations $\mathbf{X}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$. Pick an initial set of parameters $\boldsymbol{\theta}_{\text {vit }}^{0}$ and compute the best explanation of $\mathbf{X}$ under assumption of these parameters using the Viterbi algorithm:

$$
\mathbf{Z}_{\mathrm{Vit}}^{0}=\arg \max _{\mathbf{Z}} p\left(\mathbf{X}, \mathbf{Z} \mid \Theta_{\mathrm{Vit}}^{0}\right)=\arg \max _{\mathbf{Z}} \log p\left(\mathbf{X}, \mathbf{Z} \mid \Theta_{\mathrm{Vit}}^{0}\right)
$$

Compute $\boldsymbol{\theta}^{1}{ }_{\text {vit }}$ from $\boldsymbol{\theta}_{\text {vit }}^{0}$ and $\mathbf{Z}^{0}{ }_{\text {vit }}$ using TbC and iterate:

$$
\begin{aligned}
& \Theta_{\mathrm{Vit}}^{1}=\arg \max _{\Theta} p\left(\mathbf{X}, \mathbf{Z}_{\mathrm{Vit}}^{0} \mid \Theta\right)=\arg \max _{\Theta} \log p\left(\mathbf{X}, \mathbf{Z}_{\mathrm{Vit}}^{0} \mid \Theta\right) \\
& \mathbf{Z}_{\mathrm{Vit}}^{1}=\arg \max _{\mathbf{Z}} p\left(\mathbf{X}, \mathbf{Z} \mid \Theta_{\mathrm{Vit}}^{1}\right)=\arg \max _{\mathbf{Z}} \log p\left(\mathbf{X}, \mathbf{Z} \mid \Theta_{\mathrm{Vit}}^{1}\right)
\end{aligned}
$$

$p\left(\mathbf{X} \mid \Theta_{\mathrm{V} \text { it }}^{i}\right)$ is usually close to $p\left(\mathbf{X} \mid \Theta_{\mathbf{X}}^{*}\right)$, but no guarantees

## Summary: Expectation Maximization

EM Training: We are given a sequence of observations $\mathbf{X}=\left\{\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{n}\right\}$. Pick an initial set of parameters $\boldsymbol{\theta}^{0}{ }_{E M}$ and consider the expectation of $\log p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$ over $\mathbf{Z}$ (given $\mathbf{X}$ and $\boldsymbol{\theta}^{\boldsymbol{0}}{ }_{\text {EM }}$ ) as a function of $\boldsymbol{\theta}$ :

$$
E M_{\mathbf{X}, \Theta_{\mathrm{EM}}^{0}}(\Theta)=\mathrm{E}_{\mathbf{Z} \mid \mathbf{X}, \Theta_{\mathrm{EM}}^{0}}(\log p(\mathbf{X}, \mathbf{Z} \mid \Theta))=\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \Theta_{\mathrm{EM}}^{0}\right) \log p(\mathbf{X}, \mathbf{Z} \mid \Theta)
$$

For HMMs, we can find $\boldsymbol{\theta}^{\mathbf{E}}$, analytically, and iterate to get $\boldsymbol{\theta}_{\mathrm{EM}}{ }^{\text {: }}$ :

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

$p\left(\mathbf{X} \mid \Theta_{\mathrm{EM}}^{i}\right)$ converges towards a (local) maximum of $p\left(\mathbf{X} \mid \Theta_{\mathbf{X}}^{*}\right)$

