Introduction to Probabilistic Graphical Models

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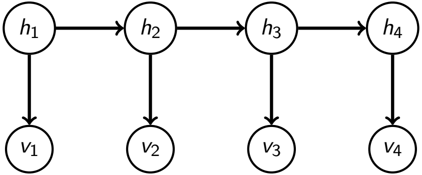
Inference in Hidden Markov Models

Hidden Markov Models

Reminder: a hidden Markov model (HMM) consists of

- a discrete Markov chain of hidden (or 'latent') variables $h_{1:T}$
- one observable (continous or discrete) variable v_i for each hidden variable h_i



$$p(h_{1:T}, v_{1:T}) = p(v_1|h_1)p(h_1)\prod_{t=2}^{T} p(v_t|h_t)p(h_t|h_{t-1})$$

We call the HMM stationary if

- the transition distribution $p(h_{t+1} = i'|h_t = i)$ and the emission distribution $p(v_t = j|h_t = i)$ do not depend on the position t, but only one the values i, i' and j

HMM parameters

Transition Distribution

For a stationary HMM the transition distribution $p(h_{t+1}|h_t)$ is defined by the $H \times H$ transition matrix

$$A_{i',i} = p(h_{t+1} = i'|h_t = i)$$

and an initial distribution

$$a_i = p(h_1 = i).$$

Emission Distribution

For a stationary HMM and emission distribution $p(v_t|h_t)$ with discrete states $v_t \in \{1, \dots, V\}$, we define a $V \times H$ emission matrix

$$B_{i,j} = p(v_t = i|h_t = j)$$

For continuous outputs, h_t selects one of H possible output distributions $p(v_t|h_t)$, $h_t \in \{1, \dots, H\}$.

The classical inference problems

Filtering	(Inferring the present)	$p(h_t \mid v_{1:t})$	
Prediction	(Inferring the future)	$p(h_t \mid v_{1:s})$	for $t > s$
	sometimes also	$p(v_t \mid v_{1:s})$	for $t > s$
Smoothing	(Inferring the past)	$p(h_t \mid v_{1:u})$	for $t < u$
Likelihood		$p(v_{1:T})$	
Most likely Hidden path	(Viterbi alignment)	$\text{argmax}\, h_{1:T}\, p(h_{1:T} \mid v_{1:T})$	
Learning	(Parameter estimation)	$\mathcal{D} \rightarrow A_{i,i'}, a_i, B_{i,j}$	

The Burglar Scenario

You're asleep upstairs in your house and awoken by noises from downstairs. You realise that a burglar is on the ground floor and attempt to understand where he his from listening to his movements.

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The HMM view

- You mentally partition the ground floor into a 5×5 grid.
- For each grid position you know the probability that if someone is in that position the floorboard will creak.
- Similarly you know for each position the probability that someone will bump into something in the dark.
- The floorboard creaking and bumping into objects can occur independently.
- In addition you assume that the burglar will move only one grid square – forwards, backwards, left or right in a single timestep.

Can you infer the burglar's position from the sounds?

The Burglar Scenario: Example

'creaks'

'bumps'

observations:

creaks	n	y	n	y	n	y	y	y	y	y
bumps	y	n	n	y	n	y	n	n	y	y

- latent variable $h_t \in \{1, \ldots, 25\}$ denotes the positions on 5×5 grid
  dark squares means probability 0.9, light means probability 0.1
- observed variables: $v_t = (c_t, b_t) \in \{(n, n), (n, y), (y, n), (y, y)\}$
- observed probability factorizes $p(v|h) = p(c|h)p(b|h)$

Burglar

Localising the burglar through time for 10 time steps

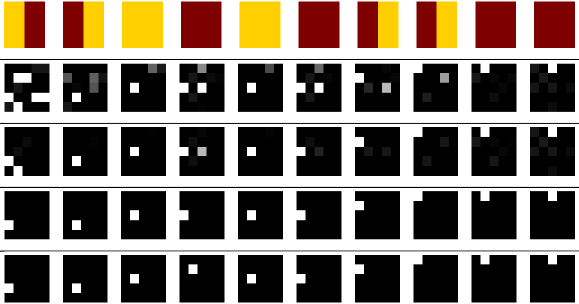
(a) Creaks and Bumps v_t

(b) Filtering $p(h_t|v_{1:t})$

(c) Smoothing $p(h_t|v_{1:T})$

(d) Viterbi $\text{argmax}_{h_{1:T}}\, p(h_{1:T}|v_{1:T})$

(e) True Burglar position $h^*_{1:T}$



Note:

- (b) is computed on-the-fly in every time step
- (c) and (d) are computed offline after all observations are available

Real-world example

https://www.youtube.com/watch?v=4Z3shNPOdQA

Filtering $p(h_t|v_{1:t})$

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$$
\begin{aligned}
p(h_t, v_{1:t}) &= \sum_{h_{t-1}} p(h_t, h_{t-1}, v_{1:t-1}, v_t) \\
&= \sum_{h_{t-1}} p(v_t|\cancel{v_{1:t-1}}, h_t, \cancel{h_{t-1}})p(h_t|\cancel{v_{1:t-1}}, h_{t-1})p(v_{1:t-1}, h_{t-1}) \\
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\end{aligned}
$$

Hence if we define $\alpha(h_t) \equiv p(h_t, v_{1:t})$ the above gives the α-recursion

$$
\alpha(h_t) = \overbrace{p(v_t|h_t)}^{\text{corrector}} \overbrace{\sum_{h_{t-1}} p(h_t|h_{t-1})\alpha(h_{t-1})}^{\text{predictor}}, \quad \text{with} \quad \alpha(h_1) = p(h_1, v_1) = p(v_1|h_1)p(h_1)
$$

Filtering $p(h_t|v_{1:t})$

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&= \sum_{h_{t-1}} p(v_t|h_t)p(h_t|h_{t-1})p(h_{t-1}, v_{1:t-1})
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Filtered posterior follows by normalization: $p(h_t|v_{1:t}) = \frac{p(h_t, v_{1:t})}{\sum_{\bar{h}_t} p(\bar{h}_t, v_{1:t})} = \frac{\alpha(h_t)}{\sum_{\bar{h}_t} \alpha(\bar{h}_t)}$

Likelihood $p(v_{1:T})$

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$$p(v_{1:T}) = \sum_{h_T} p(h_T, v_{1:T}) = \sum_{h_T} \alpha(h_T)$$

Smoothing $p(h_t|v_{1:T})$

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To compute the smoothed quantity we consider how h_t partitions the series into the past and future:

$$\begin{aligned} p(h_t, v_{1:T}) &= p(h_t, v_{1:t}, v_{t+1:T}) \\ &= \underbrace{p(h_t, v_{1:t})}_{\text{past}} \underbrace{p(v_{t+1:T}|h_t, v_{1:t})}_{\text{future}} = \alpha(h_t)\beta(h_t) \end{aligned}$$

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\end{aligned}
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Forward. The term $\alpha(h_t)$ is obtained from the 'forward' α recursion.

Backward. The term $\beta(h_t)$ we will obtain using a 'backward' β recursion as we show next.

Smoothing $p(h_t|v_{1:T})$

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Forward. The term $\alpha(h_t)$ is obtained from the 'forward' α recursion.

Backward. The term $\beta(h_t)$ we will obtain using a 'backward' β recursion as we show next.

The forward and backward recursions are independent and may therefore be run in parallel, with their results combined to obtain the smoothed posterior.

$$p(h_t|v_{1:T}) \equiv \gamma(h_t) = \frac{\alpha(h_t)\beta(h_t)}{\sum_{\bar{h}_t} \alpha(\bar{h}_t)\beta(\bar{h}_t)}$$

"Parallel Smoothing"

The β recursion

$$
\begin{aligned}
p(v_{t:T}|h_{t-1}) &= \sum_{h_t} p(v_t, v_{t+1:T}, h_t|h_{t-1}) \\
&= \sum_{h_t} p(v_t|\cancel{v_{t+1:T}}, h_t, \cancel{h_{t-1}})p(v_{t+1:T}, h_t|h_{t-1}) \\
&= \sum_{h_t} p(v_t|h_t)p(v_{t+1:T}|h_t, \cancel{h_{t-1}})p(h_t|h_{t-1})
\end{aligned}
$$

Defining $\beta(h_t) \equiv p(v_{t+1:T}|h_t)$ gives the β-recursion

$$
\beta(h_{t-1}) = \sum_{h_t} p(v_t|h_t)p(h_t|h_{t-1})\beta(h_t), \quad \text{for } 2 \leq t \leq T \quad \text{and} \quad \beta(h_T) = 1.
$$

Together the $\alpha - \beta$ recursions are called the Forward-Backward algorithm.

Smoothing $p(h_t|v_{1:T})$

"Correction Smoothing":

$$p(h_t|v_{1:T}) = \sum_{h_{t+1}} p(h_t, h_{t+1}|v_{1:T}) = \sum_{h_{t+1}} p(h_t|h_{t+1}, v_{1:t}, \cancel{v_{t+1:T}})p(h_{t+1}|v_{1:T})$$

This gives a recursion for $\gamma(h_t) \equiv p(h_t|v_{1:T})$:

$$\gamma(h_t) = \sum_{h_{t+1}} p(h_t|h_{t+1}, v_{1:t})\gamma(h_{t+1})$$

with $\gamma(h_T) \propto \alpha(h_T)$. The term $p(h_t|h_{t+1}, v_{1:t})$ may be computed using the filtered results $p(h_t|v_{1:t})$:

$$p(h_t|h_{t+1}, v_{1:t}) \propto p(h_{t+1}, h_t|v_{1:t}) \propto p(h_{t+1}|h_t)p(h_t|v_{1:t})$$

where the proportionality constant is found by normalisation. This is sequential since we need to first complete the α recursions, after which the γ recursion may begin. This 'corrects' the filtered result. Interestingly, once filtering has been carried out, the evidential states $v_{1:T}$ are not needed during the subsequent γ recursion.

Computing the pairwise marginal $p(h_t, h_{t+1}|v_{1:T})$

To implement the EM algorithm for learning, we require terms such as $p(h_t, h_{t+1}|v_{1:T})$.

$$\begin{aligned} p(h_t, h_{t+1}|v_{1:T}) &\propto p(v_{1:t}, v_{t+1}, v_{t+2:T}, h_{t+1}, h_t) \\ &= p(v_{t+2:T}|\cancel{v_{1:t}, v_{t+1}, h_t}, h_{t+1})p(v_{1:t}, v_{t+1}, h_{t+1}, h_t) \\ &= p(v_{t+2:T}|h_{t+1})p(v_{t+1}|\cancel{v_{1:t}, h_t}, h_{t+1})p(v_{1:t}, h_{t+1}, h_t) \\ &= p(v_{t+2:T}|h_{t+1})p(v_{t+1}|h_{t+1})p(h_{t+1}|\cancel{v_{1:t}}, h_t)p(v_{1:t}, h_t) \end{aligned}$$

After rearranging:

$$p(h_t, h_{t+1}|v_{1:T}) \propto \alpha(h_t)p(v_{t+1}|h_{t+1})p(h_{t+1}|h_t)\beta(h_{t+1})$$

Prediction

Predicting the future hidden variable:

$$p(h_{t+1}|v_{1:t}) =$$

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Predicting the future hidden variable:

$$p(h_{t+1}|v_{1:t}) = \sum_{h_t} p(h_{t+1}|h_t) \underbrace{p(h_t|v_{1:t})}_{\textit{filtering}}$$

Prediction

Predicting the future hidden variable:

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Predicting the future observation The one-step ahead predictive distribution is given by

$$p(v_{t+1}|v_{1:t}) =$$

Prediction

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Most likely joint state

The most likely path $h_{1:T}$ of $p(h_{1:T}|v_{1:T})$ is the same as the most likely state of

$$p(h_{1:T}, v_{1:T}) = \prod_t p(v_t|h_t)p(h_t|h_{t-1}) \qquad \text{with } h_0 = \emptyset$$

Consider

$$\max_{h_T} \prod_{t=1}^{T} p(v_t|h_t)p(h_t|h_{t-1})$$
$$= \left\{ \prod_{t=1}^{T-1} p(v_t|h_t)p(h_t|h_{t-1}) \right\} \underbrace{\max_{h_T} p(v_T|h_T)p(h_T|h_{T-1})}_{\mu(h_{T-1})}$$

The "message" $\mu(h_{T-1})$ conveys information from the end of the chain to the penultimate timestep.

Most likely joint state

We can continue in this manner, defining the recursion

$$\mu(h_{t-1}) = \max_{h_t} p(v_t|h_t)p(h_t|h_{t-1})\mu(h_t), \quad \text{for } 2 \leq t \leq T \quad \text{and} \quad \mu(h_T) = 1.$$

The effect of maximising over $h_2, \ldots, h_T$ is compressed into a message $\mu(h_1)$
$\rightarrow$ the first entry most likely state, h_1^*, is given by

$$h_1^* = \operatorname*{argmax}_{h_1} p(v_1|h_1)p(h_1)\mu(h_1)$$

Once computed, backtracking gives the remaining entries:

$$h_t^* = \operatorname*{argmax}_{h_t} p(v_t|h_t)p(h_t|h_{t-1}^*)\mu(h_t)$$

Learning Hidden Markov Models

Learning HMMs

Setting:

- given: data $\mathcal{V} = \{\mathbf{v}^1, \dots, \mathbf{v}^N\}$ of N sequences, each sequence $\mathbf{v}^N = v^N_{1:T_N}$ is of length T_n
- goal: maximum-likelihood of HMM parameters $\theta = (\mathbf{A}, \mathbf{B}, \mathbf{a})$, where
  - $\mathbf{A}$ is the HMM transition matrix, $p(h_{t+1}|h_t)$
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- assumption: the sequences are i.i.d. (within sequences, data are still dependent, of course)
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Find θ that maximizes

$$p(\mathbf{v}^1, \dots, \mathbf{v}^N; \theta) = \sum_{\mathbf{h}^1, \dots, \mathbf{h}^N} p(\mathbf{v}^1, \dots, \mathbf{v}^N, \mathbf{h}^1, \dots, \mathbf{h}^N; \theta) = \prod_{n=1}^{N} \sum_{\mathbf{h}^n} p(\mathbf{v}^n, \mathbf{h}^n; \theta)$$

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How?

Learning HMMs

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How? EM-algorithm (for HMMs called Baum-Welch algorithm for historic reasons)

Learning HMMs

Like for GMM, construct a lower bound using a distribution $q(\mathbf{h}^1, \dots, \mathbf{h}^N)$

$$\log p(\mathbf{v}^1, \dots, \mathbf{v}^N; \theta) = \log \sum_{\mathbf{h}^1, \dots, \mathbf{h}^N} p(\mathbf{v}^1, \dots, \mathbf{v}^N, \mathbf{h}^1, \dots, \mathbf{h}^N; \theta)$$

$$\leq \mathop{\mathbb{E}}_{(\mathbf{h}^1, \dots, \mathbf{h}^N) \sim q} \log p(\mathbf{v}^1, \dots, \mathbf{v}^N, \mathbf{h}^1, \dots, \mathbf{h}^N; \theta) - \mathop{\mathbb{E}}_{(\mathbf{h}^1, \dots, \mathbf{h}^N) \sim q} \log q(\mathbf{h}^1, \dots, \mathbf{h}^N)$$

EM algorithm:

initialize θ^0
for $t = 1, 2, \dots,$ until convergence **do**
$q^t \leftarrow \text{argmax}_q \; G(\theta^{t-1}, q)$ // E-step
$\theta^t \leftarrow \text{argmax}_\theta \; G(\theta, q^t)$ // M-step
end for

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E-step, Part 1

$$q \leftarrow \underset{q}{\operatorname{argmax}} \; G(\theta^{t-1}, q)$$

- as for GMMs:

$$q^t \leftarrow p(\mathbf{h}^1, \dots, \mathbf{h}^N | \mathbf{v}^1, \dots, \mathbf{v}^N; \theta^{t-1}) \overset{i.i.d.}{=} \prod_{n=1}^{N} p(\mathbf{h}^n | \mathbf{v}^n; \theta^{t-1})$$

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later more...

M-step

M-step

$$\mathop{\mathbb{E}}_{(\mathbf{h}^1,\dots,\mathbf{h}^N)\sim q} \log p(\mathbf{v}^1,\dots,\mathbf{v}^N,\mathbf{h}^1,\dots,\mathbf{h}^N;\theta)$$

$$\overset{i.i.d.}{=} \mathop{\mathbb{E}}_{(\mathbf{h}^1,\dots,\mathbf{h}^n\sim q} \sum_{n=1}^{N} \log p(\mathbf{v}^n,\mathbf{h}^n;\theta) = \sum_{n=1}^{N} \mathop{\mathbb{E}}_{\mathbf{h}\sim q^n} \log p(v^n_{1:T^n}, h_{1:T^n};\theta)$$

$$\overset{\text{HMM graph}}{=} \sum_{n=1}^{N} \mathop{\mathbb{E}}_{\mathbf{h}\sim q^n} \log \left[p(h_1;a) \prod_{t=2}^{T^n} p(h_t|h_{t-1};A) \prod_{t=1}^{T^n} p(v^n_t|h_t;B) \right]$$

$$= \underbrace{\sum_{n=1}^{N} \mathop{\mathbb{E}}_{\mathbf{h}\sim q^n} \log p(h_1;a)}_{\mathcal{L}_{\text{initial}}(a)} + \underbrace{\sum_{n=1}^{N}\sum_{t=2}^{T^n} \mathop{\mathbb{E}}_{\mathbf{h}\sim q^n} \log p(h_t|h_{t-1};A)}_{\mathcal{L}_{\text{transition}}(A)} + \underbrace{\sum_{n=1}^{N}\sum_{t=1}^{T^n} \mathop{\mathbb{E}}_{\mathbf{h}\sim q^n} \log p(v^n_t|h_t;B)}_{\mathcal{L}_{\text{emission}}(B)}$$

sum of independent terms $\rightarrow$ we can optimize for a, A and B separately

$$\mathcal{L}_{\text{initial}}(a) = \sum_{n=1}^{N} \mathop{\mathbb{E}}_{h_{1:T_n} \sim q^n} \log p(h_1; a) = \sum_{n=1}^{N} \mathop{\mathbb{E}}_{h_1 \sim q^n} \log a_{h_1}$$

a is a discrete probability distribution over H states, *i.e.* $\sum_i a_i = 1$. Use Langragian:

$$\mathfrak{L}(a, \lambda) = \mathcal{L}_{\text{initial}}(a) - \lambda\Big(\sum_i a_i - 1\Big)$$

$$\frac{d\mathcal{L}_{\text{initial}}(a)}{da_i}(a) = \frac{d}{da_i} \sum_{n=1}^{N} \mathop{\mathbb{E}}_{h_1 \sim q^n} \sum_{i'=1}^{H} [\![h_1 = i']\!] \log a_{i'} = \sum_{n=1}^{N} \mathop{\mathbb{E}}_{h_1 \sim q^n} [\![h_1 = i]\!] \frac{1}{a_i} = \frac{1}{a_i} \sum_{n=1}^{N} q^n(h_1)$$

$$0 = \frac{d\mathfrak{L}(a, \lambda)}{da_i}(\hat{a}, \hat{\lambda}) = \frac{1}{\hat{a}_i} \sum_{n=1}^{N} q^n(h_1 = i) - \lambda \quad \rightarrow \quad \hat{a}_i = \frac{1}{\hat{\lambda}} \sum_{n=1}^{N} q^n(h_1)$$

$$0 = \frac{d\mathfrak{L}(a, \lambda)}{d\lambda}(\hat{a}, \hat{\lambda}) = -1 + \sum_{i=1}^{H} \frac{1}{\hat{\lambda}} \sum_{n=1}^{N} q^n(h_1 = i) = -1 + \sum_{i=1}^{H} \frac{1}{\hat{\lambda}} \quad \rightarrow \quad \hat{\lambda} = n$$

$$\mathcal{L}_{\text{transition}}(A) = \sum_{n=1}^{N}\sum_{t=2}^{T^n} \mathop{\mathbb{E}}_{\mathbf{h}\sim q^n} \log p(h_t | h_{t-1}; A)$$
$$= \sum_{n=1}^{N}\sum_{t=2}^{T^n} \mathop{\mathbb{E}}_{h_{1:T^n}\sim q^n} \sum_{i,i'=1}^{H} [\![h_t = i \wedge h_{t-1} = i']\!] \log A_{i,i'}$$
$$= \sum_{n=1}^{N}\sum_{t=2}^{T^n} \sum_{i,i'=1}^{H} q^n(h_t = i, h_{t-1} = i') \log A_{i,i'}$$

Each column of A is a (conditional) distribution over the rows, *i.e.* $\sum_i A_{i,i'} = 1$ for any $i' \in \{1, \ldots, H\}$. We can optimize for any fixed i' independently:

$$\mathfrak{L}(A, \lambda) = \mathcal{L}_{\text{transition}}(A) - \lambda\Big(\sum_i A_{i,i'} - 1\Big)$$

$$\hat{A}_{i,i'} \propto \sum_{n=1}^{n}\sum_{t=2}^{T_n} q^n(h_t = i, h_{t-1} = i') \quad \text{with normalization to make } \hat{A}_{i,i'} = 1 \text{ for each } i'$$

$$\mathcal{L}_{\text{emission}}(A) = \sum_{n=1}^{N}\sum_{t=1}^{T^n} \mathop{\mathbb{E}}_{\mathbf{h}\sim q^n} \log p(v_t^n | h_t; B) = \sum_{n=1}^{N}\sum_{t=1}^{T^n}\sum_{j=1}^{V} [\![v_t^n = j]\!] \mathop{\mathbb{E}}_{h_{1:T^n}\sim q^n} \sum_{i=1}^{H} [\![h_t = i]\!] \log B_{j,i}$$

$$= \sum_{n=1}^{N}\sum_{t=1}^{T^n}\sum_{j=1}^{V} [\![v_t^n = j]\!] \sum_{i=1}^{H} q^n(h_t = i) \log B_{j,i}$$

Each column of B is a (conditional) distribution over the rows, *i.e.* $\sum_j B_{j,i} = 1$ for any $j \in \{1, \ldots, V\}$. We can optimize for any fixed i independently:

$$\mathfrak{L}(B, \lambda) = \mathcal{L}_{\text{emission}}(B) - \lambda\left(\sum_j B_{j,i} - 1\right)$$

$$\hat{B}_{j,i} \propto \sum_{n=1}^{n}\sum_{t=1}^{T_n} [\![v_t^n = j]\!] q^n(h_t = i) \quad \text{with normalization to make } \hat{B}_{j,i} = 1 \text{ for each } i$$

E-step, Part 2

For the M-step we compute:

$$\hat{a}_i \propto \sum_{n=1}^{N} q^n(h_1) \qquad \hat{A}_{i,i'} \propto \sum_{n=1}^{n} \sum_{t=2}^{T_n} q^n(h_t = i, h_{t-1} = i') \qquad \hat{B}_{j,i} \propto \sum_{n=1}^{n} \sum_{t=1}^{T_n} [\![v_t^n = j]\!] q^n(h_t = i)$$

Of $q^n(\mathbf{h}) = p(\mathbf{h}|\mathbf{v}^n; \theta)$ we really only need:

- $q^n(h_1) = p(h_1|v^n_{1:T^n}; \theta)$ for a
- $q^n(h_t, h_{t-1}) = p(h_t, h_{t-1}|v^n_{1:T^n}; \theta)$ for A
- $q^n(h_t) = p(h_t|v^n_{1:T^n}; \theta)$ for B

For computing all of these we have derived efficient ways in the previous section.

EM for HMMs: Initialization

EM algorithm:

initialize θ^0
for $t = 1, 2, \ldots,$ until convergence **do**
$q^t \leftarrow \text{argmax}_q \; G(\theta^{t-1}, q)$ // E-step
$\theta^t \leftarrow \text{argmax}_\theta \; G(\theta, q^t)$ // M-step
end for

Parameter initialisation

- EM algorithm converges to a local maximum of the likelihood,
- in general, there is no guarantee that the algorithm will find the global maximum
- often, the initialization determined how good the found solution is
- practical strategy:
  - first, train non-temporal mixture model for $p(v) = \sum_h p(v|h)p(h)$
  - initialize a and B from this, and assume independence for A

HMM with Continuous observations

For an HMM with continuous observation $\mathbf{v}_t$, we need a model of $p(\mathbf{v}_t|h_t)$, i.e. a continuous distribution for each state of h_t.

Inference

- filtering, smoothing, etc. remain largely unchanged, as everything is conditioned on $\mathbf{v}_{1:T}$

Learning

- learning requires computing normalization constants w.r.t. v
- depending on the model, this might or might not be tractable