Exact Inference for Hidden Markov Models

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Recap

- Assuming a factorisation / set of statistical independencies allowed us to efficiently represent the pdf or pmf of random variables
- Factorisation can be exploited for inference
  - by using the distributive law
  - by re-using already computed quantities
- Inference for general factor graphs (variable elimination)
- Inference for factor trees
- Sum-product and max-sum message passing

Program

1. Markov models
2. Inference by message passing

Program

1. Markov models
   - Markov chains
   - Transition distribution
   - Hidden Markov models (HMMs)
   - Emission distribution
   - Important instances of HMMs

2. Inference by message passing

Applications of (hidden) Markov models

Markov and hidden Markov models have many applications, e.g.

- speech modelling (speech recognition)
- text modelling (natural language processing)
- gene sequence modelling (bioinformatics)
- spike train modelling (neuroscience)
- object tracking (robotics)
- stock price prediction (finance)
- navigation systems (aerospace)
- ⋮

Markov chains

- First-order Markov chain: models that factorise as

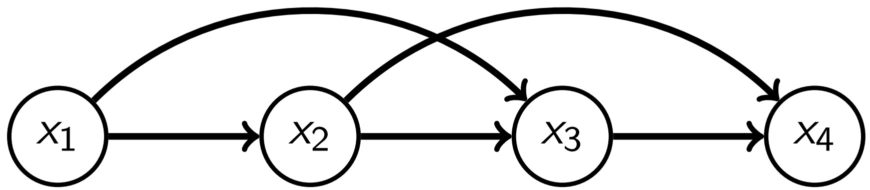
$$p(x_1, \ldots, x_d) = \prod_{i=1}^{d} p(x_i | x_{i-1})$$

- DAG (for d=4)

- $L-$th order Markov chain: models that factorise as

$$p(x_1, \ldots, x_d) = \prod_{i=1}^{d} p(x_i | x_{i-L}, \ldots, x_{i-1})$$

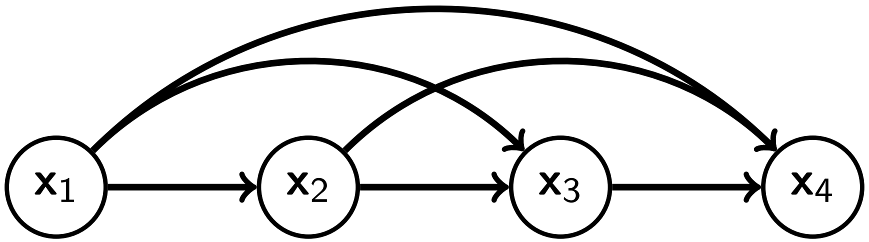
- DAG (L=2, d=4)



Vector-valued Markov chains

- While not explicitly discussed, the graphical models extend to vector-valued variables.
- Chain rule with ordering $\mathbf{x}_1, \ldots, \mathbf{x}_d$

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_d) = \prod_{i=1}^{d} p(\mathbf{x}_i | \mathbf{x}_1, \ldots, \mathbf{x}_{i-1})$$



- 1st order Markov chain:

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_d) = \prod_{i=1}^{d} p(\mathbf{x}_i | \mathbf{x}_{i-1})$$

Modelling time series

- Index i may refer to time t
- For example, 1st order Markov chain of length T:

$$p(x_1, \ldots, x_T) = \prod_{t=1}^{T} p(x_t | x_{t-1})$$

- Only the last time point x_{t-1} is relevant for x_t.

Transition distribution

(Consider 1st order Markov chain.)

- $p(x_i|x_{i-1})$ is called the transition distribution
- For discrete random variables, $p(x_i|x_{i-1})$ is defined by a transition matrix $\mathbf{A}^{(i)}$

$$p(x_i = k|x_{i-1} = k') = A^{(i)}_{k,k'} \qquad (A^{(i)}_{k',k} \text{ convention is also used})$$

- For continuous random variables, $p(x_i|x_{i-1})$ is a conditional pdf, e.g.

$$p(x_i|x_{i-1}) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{(x_i - f_i(x_{i-1}))^2}{2\sigma_i^2}\right)$$

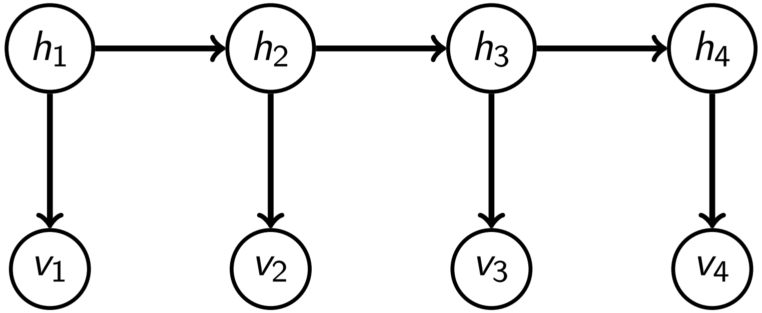
  for some (typically parameterised) function f_i
- Homogeneous Markov chain: $p(x_i|x_{i-1})$ does not depend on i, e.g.

$$\mathbf{A}^{(i)} = \mathbf{A} \quad \text{or} \qquad \sigma_i = \sigma, \quad f_i = f$$

- Inhomogeneous Markov chain: $p(x_i|x_{i-1})$ does depend on i

Hidden Markov models (HMMs)

DAG:



- 1st order Markov chain on hidden (latent) variables h_i.
- Each visible (observed) variable v_i only depends on the corresponding hidden variable h_i
- Factorisation

$$p(h_{1:d}, v_{1:d}) = p(v_1|h_1)p(h_1)\prod_{i=2}^{d} p(v_i|h_i)p(h_i|h_{i-1})$$

- The visibles are d-connected if hiddens are not observed
- Visibles are d-separated (independent) given the hiddens
- The h_is model/explain all dependencies between the v_is

Emission distribution

- $p(v_i|h_i)$ is called the emission distribution
- Discrete-valued v_i and h_i:
  $p(v_i|h_i)$ can be represented as a matrix
- Discrete-valued v_i and continuous-valued h_i:
  $p(v_i|h_i)$ is a conditional pmf.
- Continuous-valued v_i: $p(v_i|h_i)$ is a density
- As for the transition distribution, the emission distribution $p(v_i|h_i)$ may depend on i or not.
- If neither the transition nor the emission distribution depend on i, we have a stationary (or homogeneous) hidden Markov model.

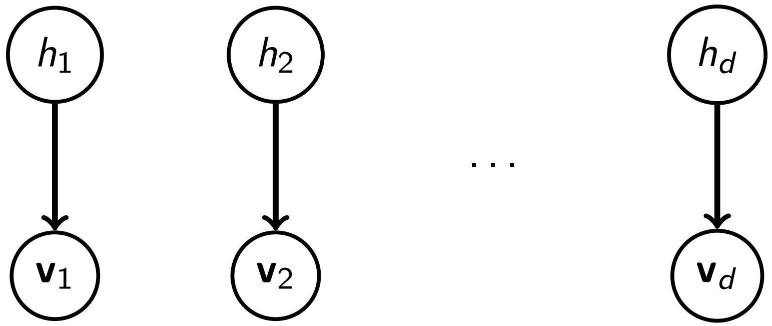
Gaussian emission model with discrete-valued latents

- Special case: $h_i \perp\!\!\!\perp h_{i-1}$, and $\mathbf{v}_i \in \mathbb{R}^m$, $h_i \in \{1, \ldots, K\}$

$$p(h = k) = p_k$$

$$p(\mathbf{v}|h = k) = \frac{1}{|\det 2\pi \boldsymbol{\Sigma}_k|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{v} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1}(\mathbf{v} - \boldsymbol{\mu}_k)\right)$$

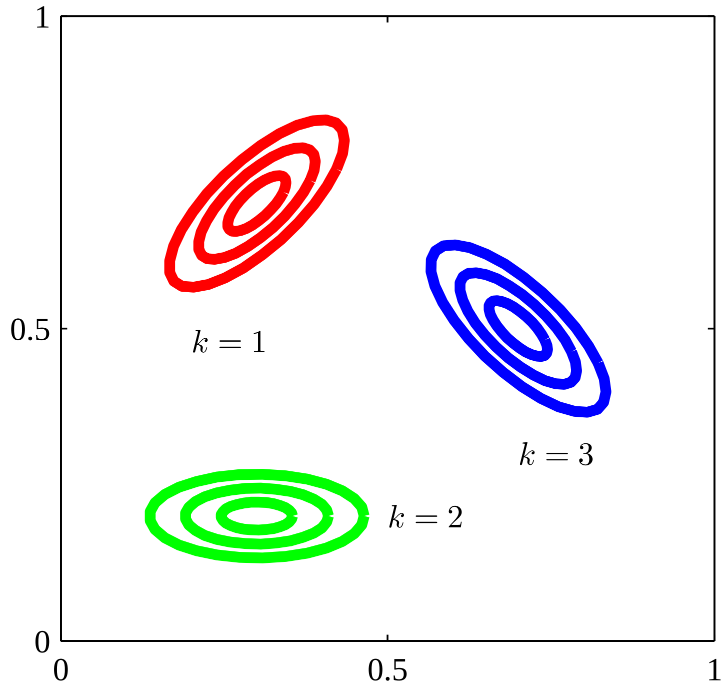
  for all h_i and $\mathbf{v}_i$.
- DAG

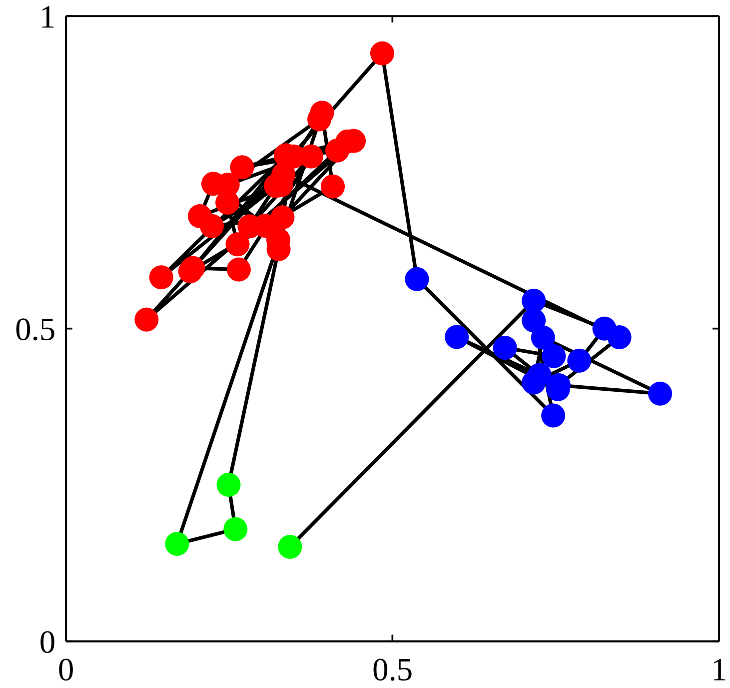


- Corresponds to d iid draws from a Gaussian mixture model with K mixture components
  - Mean $\mathbb{E}[\mathbf{v}|h = k] = \boldsymbol{\mu}_k$
  - Covariance matrix $\mathbb{V}[\mathbf{v}|h = k] = \boldsymbol{\Sigma}_k$

Gaussian emission model with discrete-valued latents

The HMM is a generalisation of the Gaussian mixture model where cluster membership at "time" i (the value of h_i) generally depends on cluster membership at "time" $i-1$ (the value of h_{i-1}).





Example for $\mathbf{v}_i \in \mathbb{R}^2$, $h_i \in \{1, 2, 3\}$. Left: $p(\mathbf{v}|h = k)$. Right: samples

(Bishop, Figure 13.8)

Gaussian emission model with Gaussian latents

- HMMs with Gaussian emission and transition distributions correspond to linear dynamical systems.
- Transition model:

$$p(\mathbf{h}_i|\mathbf{h}_{i-1}) = \mathcal{N}(\mathbf{h}_i; \mathbf{A}\mathbf{h}_{i-1}, \mathbf{\Sigma}^h) \tag{1}$$

$$\mathbf{h}_i = \mathbf{A}\mathbf{h}_{i-1} + \mathbf{n}_i^h, \quad \mathbf{n}_i^h \sim \mathcal{N}(\mathbf{n}_i^h; 0, \mathbf{\Sigma}^h) \tag{2}$$

- Emission model:

$$p(\mathbf{v}_i|\mathbf{h}_{i-1}) = \mathcal{N}(\mathbf{v}_i; \mathbf{C}\mathbf{h}_{i-1}, \mathbf{\Sigma}^v) \tag{3}$$

$$\mathbf{v}_i = \mathbf{C}\mathbf{h}_{i-1} + \mathbf{n}_i^v, \quad \mathbf{n}_i^h \sim \mathcal{N}(\mathbf{n}_i^v; 0, \mathbf{\Sigma}^v) \tag{4}$$

- If $p(\mathbf{h}_1)$ is Gaussian, the whole model is jointly Gaussian
- Computation of $p(\mathbf{h}_t|\mathbf{v}_{1:t})$ is the filtering problem: for the model above, this was solved by Kalman (1960) and is now called Kalman filtering.
- Very widely used, e.g. in location and navigation systems.

Program

1. Markov models
   - Markov chains
   - Transition distribution
   - Hidden Markov models (HMMs)
   - Emission distribution
   - Important instances of HMMs
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Program

1. Markov models
2. Inference by message passing
   - Inference: filtering, prediction, smoothing, Viterbi
   - Filtering: Sum-product message passing yields the α-recursion
   - Smoothing: Sum-product message passing yields the α-β recursion

The classical inference problems

(Considering the index i to refer to time t)

Filtering	(Inferring the present)	$p(h_t \| v_{1:t})$	
Smoothing	(Inferring the past)	$p(h_t \| v_{1:u})$	$t < u$
Prediction	(Inferring the future)	$p(h_t \| v_{1:u})$	$t > u$
		$p(v_t \| v_{1:u})$	$t > u$
Most likely hidden path	(Viterbi algorithm)	$\mathrm{argmax}_{h_{1:t}} p(h_{1:t} \| v_{1:t})$	
Posterior sampling	(Forward filtering backward sampling)	$h_{1:t} \sim p(h_{1:t} \| v_{1:t})$	

For the HMM, all tasks can be solved via message passing (sum-product or max-sum algorithm).

The classical inference problems

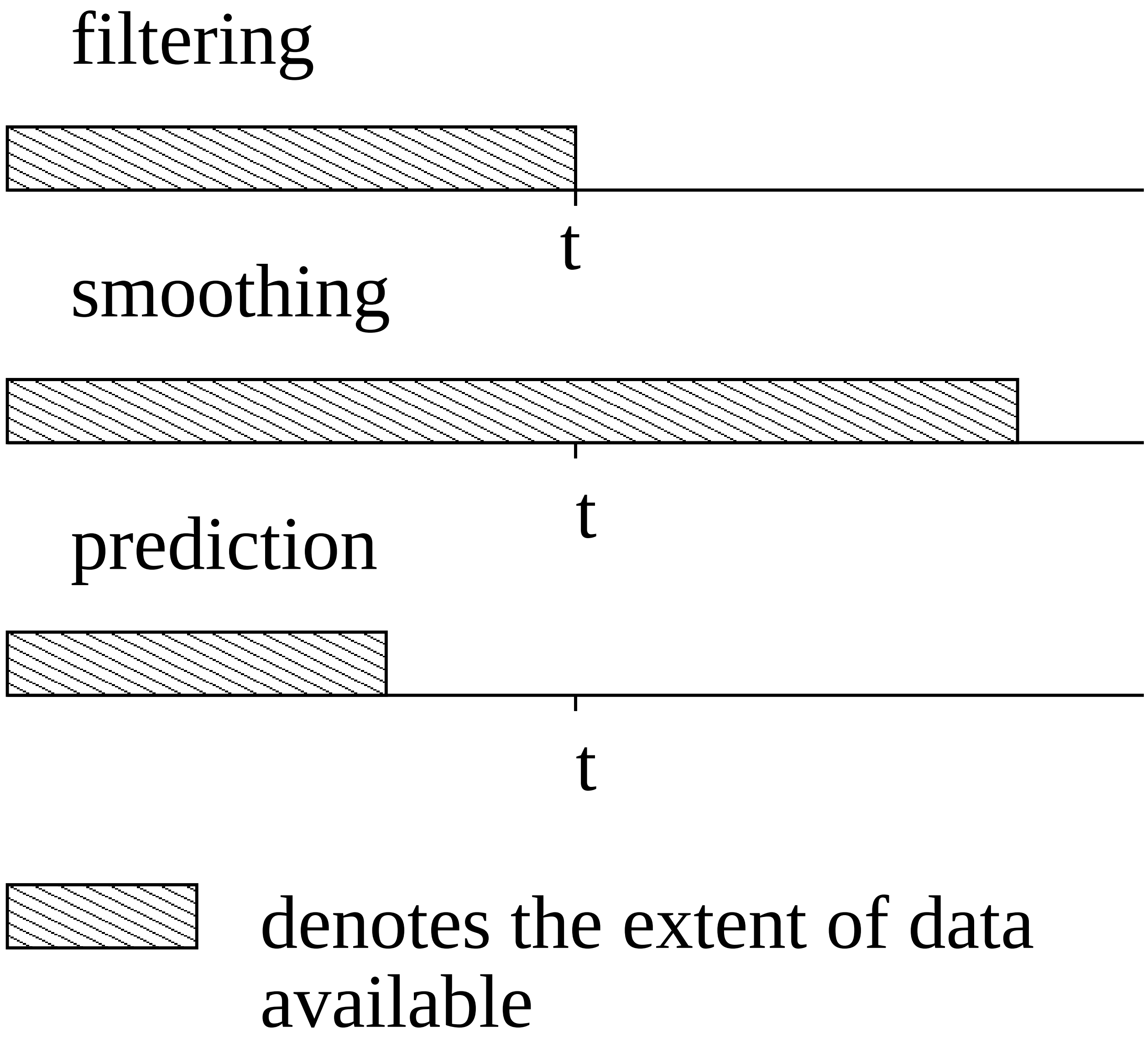
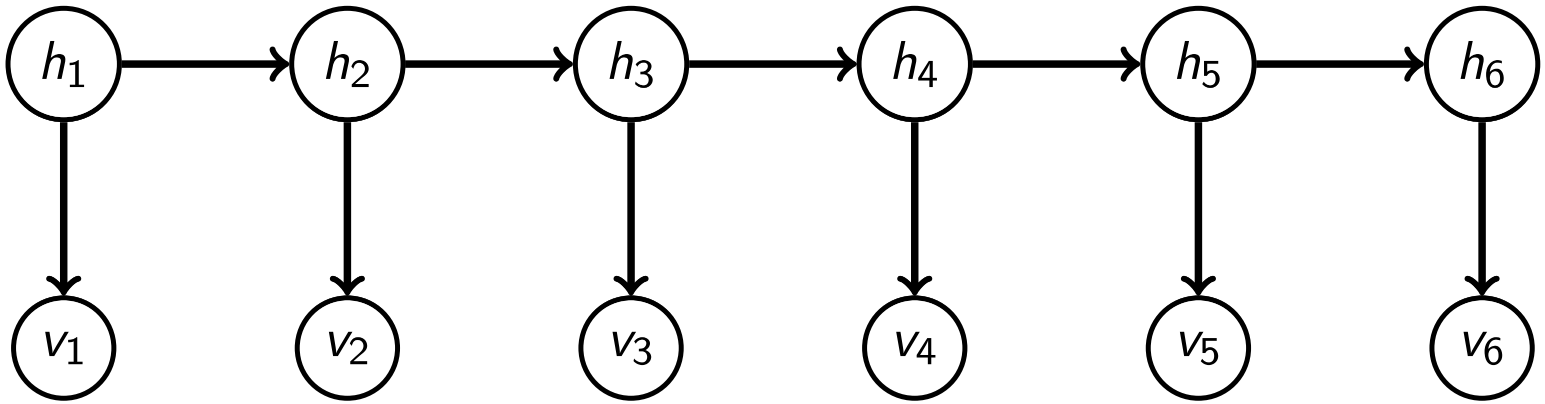


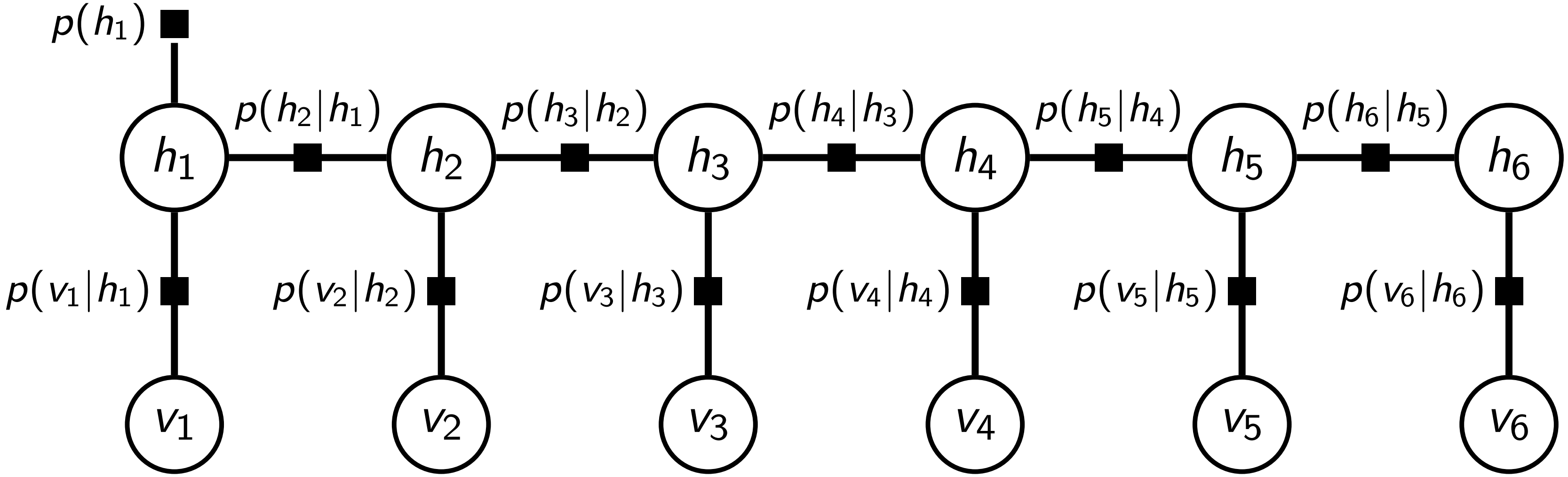
Figure based on Fig. 1.0-1 of Gelb et al (1974)

Factor graph for hidden Markov model

DAG:



Factor graph:

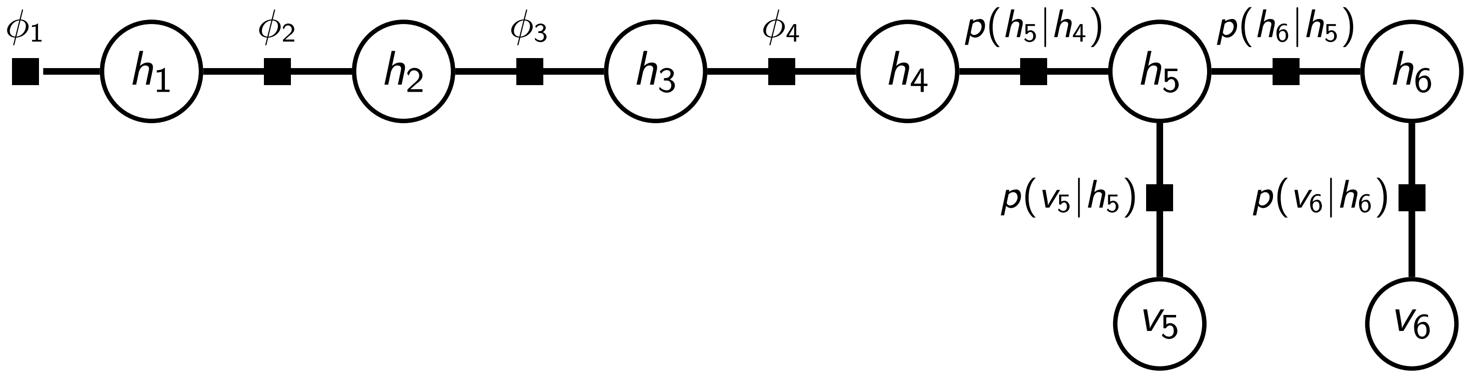


Filtering $p(h_t|v_{1:t})$: factor graph

- When computing $p(h_t|v_{1:t})$, the $v_{1:t} = (v_1, \ldots, v_t)$ are assumed known and are kept fixed (e.g. $t = 4$)
- For $s = 1, \ldots, t$, the factors $p(v_s|h_s)$ depend only on h_s. Combine them with $p(h_s|h_{s-1})$ and form new factors ϕ_s

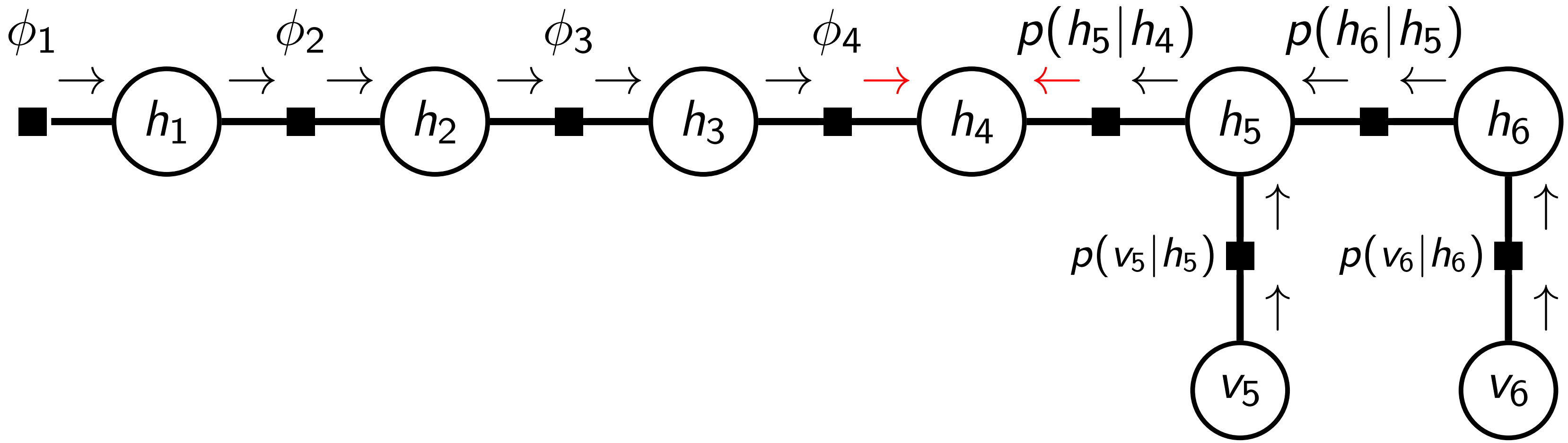
$$\phi_1(h_1) = p(v_1|h_1)p(h_1), \quad \phi_s(h_{s-1}, h_s) = p(v_s|h_s)p(h_s|h_{s-1})$$

- Factor graph



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

Messages needed to compute $p(h_4|v_{1:4})$: $(t = 4)$



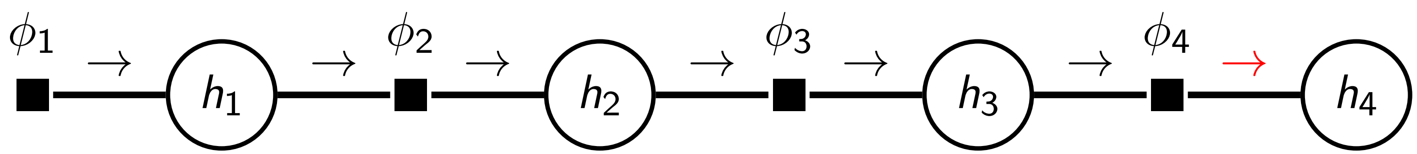
There is a simplification:

- The message from $p(h_5|h_4)$ to h_4 equals 1!
- Follows from message passing starting at leaves v_5 and v_6 since the factors $p(.|.)$ are conditionals and sum to one, e.g.

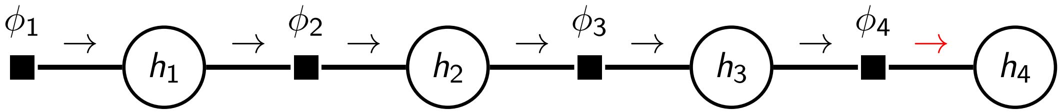
$$\sum_{v_6} p(v_6|h_6) = 1 \qquad \sum_{h_6} p(h_6|h_5) = 1$$

Filtering $p(h_t|v_{1:t})$: reduce to inference on chain

- A message is an effective factor obtained by summing out all variables downstream from where the message is coming from.
- This means that we can replace the factor sub-graph to the right of the last observed variable v_t and latent h_t (here v_4 and h_4) with the effective factor.
- Effective factor is 1, so that we can just remove the sub-graph.
- Also can be seen by "marginalising out" the unobserved future
- Reduces problem to message passing on a chain.



Filtering $p(h_t|v_{1:t})$: message passing on the chain



- Initialisation: $\mu_{\phi_1 \to h_1}(h_1) = \phi_1(h_1)$
- Variable node h_1 copies the message:

$$\mu_{h_1 \to \phi_2}(h_1) = \mu_{\phi_1 \to h_1}(h_1)$$

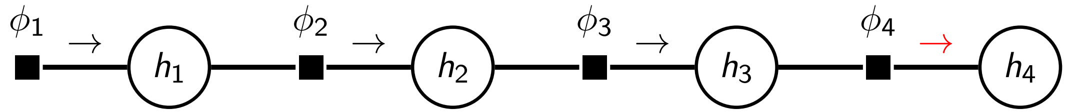
- Same for other variable nodes. Let us write the algorithm in terms of $\mu_{\phi_i \to h_i}(h_i)$ messages only.
- Message from ϕ_2 to h_2:

$$\mu_{\phi_2 \to h_2}(h_2) = \sum_{h_1} \phi_2(h_1, h_2)\mu_{\phi_1 \to h_1}(h_1)$$

- Message from ϕ_s to h_s, for $s = 2, \ldots, t$:

$$\mu_{\phi_s \to h_s}(h_s) = \sum_{h_{s-1}} \phi_s(h_{s-1}, h_s)\mu_{\phi_{s-1} \to h_{s-1}}(h_{s-1})$$

Filtering $p(h_t|v_{1:t})$: message passing on the chain



- The messages $\mu_{\phi_s \to h_s}(h_s)$ are traditionally denoted by $\alpha(h_s)$.
- Message passing for filtering becomes:
  - Init: $\alpha(h_1) = \phi_1(h_1) = p(v_1|h_1)p(h_1)$
  - Update rule for $s = 2, \ldots t$:

$$\begin{aligned}\alpha(h_s) &= \sum_{h_{s-1}} \phi_s(h_{s-1}, h_s)\alpha(h_{s-1}) \\ &= p(v_s|h_s) \sum_{h_{s-1}} p(h_s|h_{s-1})\alpha(h_{s-1})\end{aligned}$$

- Algorithm known as “alpha-recursion”.
- Desired probability:

$$p(h_t|v_{1:t}) = \frac{1}{Z_t}\alpha(h_t) \qquad\qquad Z_t = \sum_{h_t} \alpha(h_t)$$

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

- Joint model for $h_{1:t}$ and $v_{1:t}$

$$p(h_{1:t}, v_{1:t}) = p(v_1|h_1)p(h_1)\prod_{i=2}^{t} p(v_i|h_i)p(h_i|h_{i-1})$$

- Conditional $p(h_{1:t}|v_{1:t})$ is *proportional* to the joint

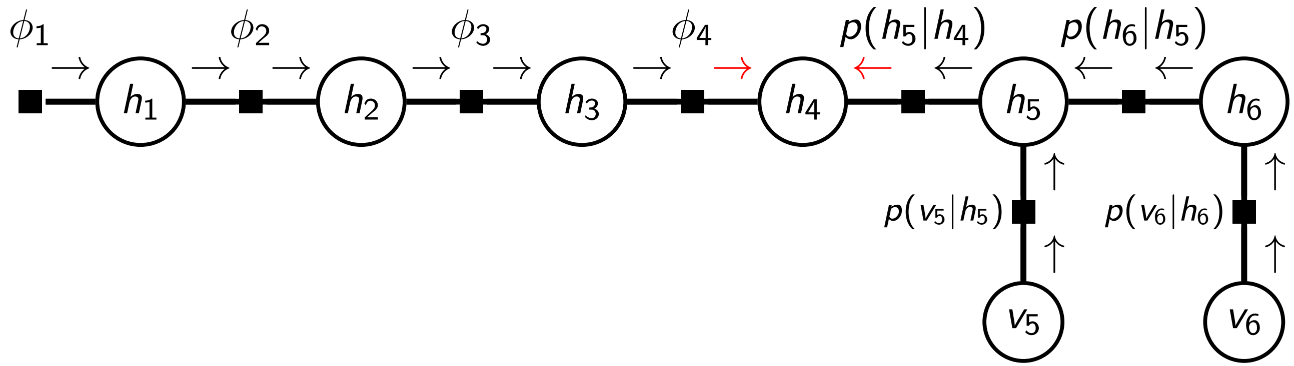
$$p(h_{1:t}|v_{1:t}) \propto p(v_1|h_1)p(h_1)\prod_{i=2}^{t} p(v_i|h_i)p(h_i|h_{i-1})$$

- Normalising constant for the equation above is the likelihood/marginal $p(v_{1:t})$
- From results on message passing: Z_t that normalises the posterior marginal $p(h_t|v_{1:t})$ is also the normaliser of $p(h_{1:t}|v_{1:t})$, i.e. $p(v_{1:t})$:

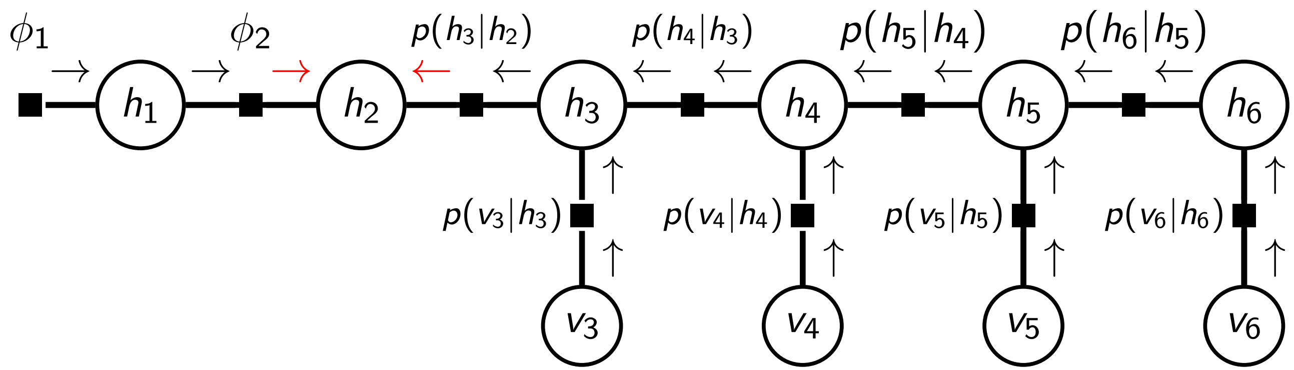
$$Z_t = \sum_{h_t} \alpha(h_t) = p(v_{1:t})$$

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

- We have seen that $p(h_t|v_{1:t}) \propto \alpha(h_t)$.



- Consider $p(h_s|v_{1:s})$ with $s < t$ (e.g. $s = 2$ and $t = 4$)



- Messages to the left of h_s are the same as for $p(h_t|v_{1:t})$.
- Messages to the right of h_s are all equal to one.

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

- This means that the intermediate $\alpha(h_s)$ that we compute when computing $p(h_t|v_{1:t})$ are unnormalised posteriors themselves:

$$\alpha(h_s) \propto p(h_s|v_{1:s})$$

  Note that we condition on $v_{1:s}$ and not $v_{1:t}$.
- Moreover $p(v_{1:s}) = \sum_{h(s)} \alpha(h_s)$.
- Hence, the alpha-recursion gives us posteriors $p(h_s|v_{1:s})$ and likelihoods $p(v_{1:s})$ for $s = 1, \ldots, t$.

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

- Proof by induction shows that $\alpha(h_s) = p(h_s, v_{1:s})$.
- Base case holds by definition: $\alpha(h_1) = p(h_1)p(v_1|h_1)$.
- Assume it holds for $\alpha(h_{s-1})$. Then:

$$
\begin{aligned}
\alpha(h_s) &= \sum_{h_{s-1}} p(v_s|h_s)p(h_s|h_{s-1})\alpha(h_{s-1}) \\
&\overset{\text{(induction hyp)}}{=} \sum_{h_{s-1}} p(v_s|h_s)p(h_s|h_{s-1})p(h_{s-1}, v_{1:s-1}) \\
&\overset{\text{(Markov prop)}}{=} \sum_{h_{s-1}} p(v_s|h_s, h_{s-1}, v_{1:s-1})p(h_s|h_{s-1}, v_{1:s-1})p(h_{s-1}, v_{1:s-1}) \\
&\overset{\text{(product rule)}}{=} \sum_{h_{s-1}} p(v_s|h_s, h_{s-1}, v_{1:s-1})p(h_s, h_{s-1}, v_{1:s-1}) \\
&\overset{\text{(product rule)}}{=} \sum_{h_{s-1}} p(v_s, h_s, h_{s-1}, v_{1:s-1}) \\
&\overset{\text{(marginalise)}}{=} p(v_s, h_s, v_{1:s-1}) \\
&= p(h_s, v_{1:s})
\end{aligned}
$$

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

- Update rule as prediction-correction algorithm:

$$
\begin{aligned}
\alpha(h_s) &\overset{\text{(prev slide)}}{=} p(h_s, v_{1:s}) \\
&\overset{\text{(product rule)}}{=} p(v_s|h_s, v_{1:s-1})p(h_s, v_{1:s-1}) \\
&\overset{\text{(Markov prop)}}{=} p(v_s|h_s)p(h_s, v_{1:s-1}) \\
&\propto \underbrace{p(v_s|h_s)}_{\text{correction}}\underbrace{p(h_s|v_{1:s-1})}_{\text{prediction}}
\end{aligned}
$$

- The correction term updates the predictive distribution $p(h_s|v_{1:s-1})$ to include the new data v_s.

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

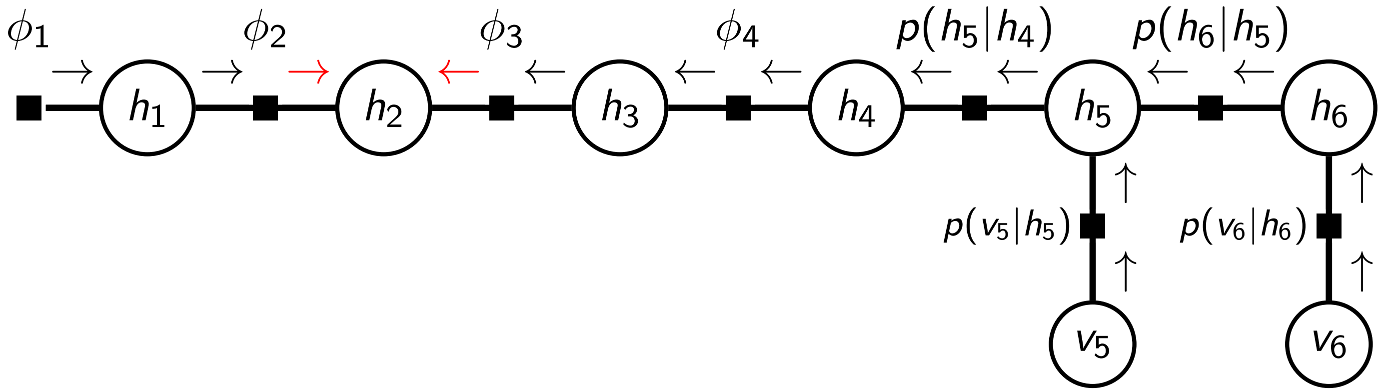
- Conditioning reduces the factor graph for the HMM to a chain.
- Message passing for filtering:
  - Init: $\alpha(h_1) = p(v_1|h_1)p(h_1)$
  - Update rule for $s = 2, \ldots t$:

$$\alpha(h_s) = p(v_s|h_s)\sum_{h_{s-1}} p(h_s|h_{s-1})\alpha(h_{s-1})$$

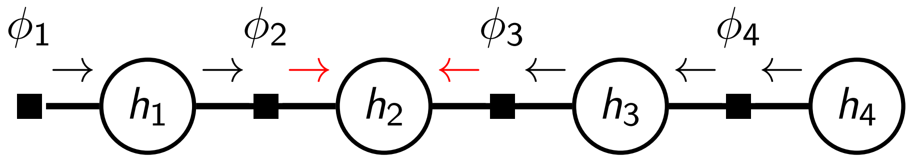
    which involves prediction of h_s given $v_{1:s-1}$ and correction using new datum v_s.
- $\alpha(h_s) = p(h_s, v_{1:s}) \propto p(h_s|v_{1:s})$ and $p(v_{1:s}) = \sum_{h_s} \alpha(h_s)$, for $s = 1, \ldots, t$

Smoothing $p(h_t|v_{1:u})$, $t < u$: reduce to inference on chain

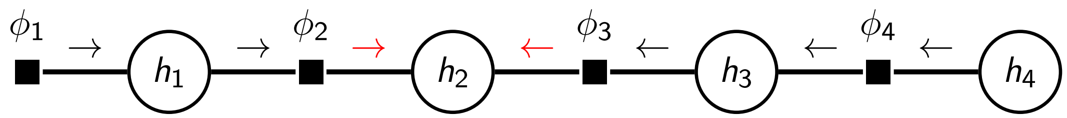
- Unlike in filtering where we predict h_t from data up to time t, in smoothing we have observations from later time points.
- Messages needed to compute $p(h_t|v_{1:u})$ (e.g. $t = 2$, $u = 4$)



- As in filtering, we can simplify to a chain



Smoothing $p(h_t|v_{1:u})$, $t < u$: message passing on chain

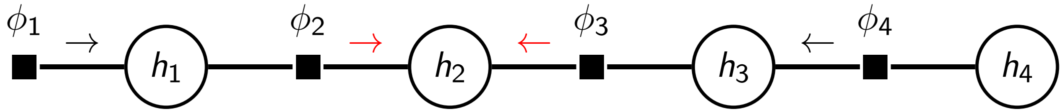


- Messages $\rightarrow$ from factor leaf ϕ_1 to h_t same as in filtering.
- Messages $\leftarrow$ from variable leaf h_u to h_t via message passing.
- Init: $\mu_{h_u \rightarrow \phi_u}(h_u) = 1$
- Next message $\mu_{\phi_u \rightarrow h_{u-1}}(h_{u-1}) = \sum_{h_u} \phi_u(h_{u-1}, h_u)$
- Variable nodes just copy the incoming message. Write the algorithm in terms of $\beta(h_s) = \mu_{\phi_{s+1} \rightarrow h_s}(h_s)$ only:

$$\begin{aligned}\beta(h_{s-1}) &= \sum_{h_s} \phi_s(h_{s-1}, h_s)\beta(h_s) \\ &= \sum_{h_s} p(v_s|h_s)p(h_s|h_{s-1})\beta(h_s)\end{aligned}$$

- Gives "alpha-beta recursion" for smoothing.

Smoothing $p(h_t | v_{1:u})$, $t < u$: message passing on chain



- $\rightarrow$ Forwards via alpha-recursion
  - Init: $\alpha(h_1) = p(v_1|h_1)p(h_1)$
  - Update rule for $s = 2, \ldots t$:

$$\alpha(h_s) = p(v_s|h_s) \sum_{h_{s-1}} p(h_s|h_{s-1})\alpha(h_{s-1})$$

- $\leftarrow$ Backwards via beta-recursion
  - Init: $\beta(h_u) = 1$
  - Update rule for $s = u, \ldots t+1$:

$$\beta(h_{s-1}) = \sum_{h_s} p(v_s|h_s)p(h_s|h_{s-1})\beta(h_s)$$

- Desired probability:

$$p(h_t|v_{1:u}) = \frac{1}{Z_t^u}\alpha(h_t)\beta(h_t) \qquad Z_t^u = \sum_{h_t} \alpha(h_t)\beta(h_t)$$

Smoothing $p(h_t|v_{1:u})$, $t < u$: interpretation

- We now show that $\beta(h_s)$ equals the probability of the upstream observations given h_s,

$$\beta(h_s) = p(v_{s+1:u}|h_s) \quad \text{for all } s < u$$

- First consider $\beta(h_{u-1})$:

$$\beta(h_{u-1}) = \sum_{h_u} p(v_u|h_u)p(h_u|h_{u-1}) \underbrace{\beta(h_u)}_{1}$$

$$\stackrel{\text{(Markov prop)}}{=} \sum_{h_u} p(v_u|h_u, h_{u-1})p(h_u|h_{u-1})$$

$$\stackrel{\text{(product rule)}}{=} \sum_{h_u} p(v_u, h_u|h_{u-1})$$

$$\stackrel{\text{(marginalise)}}{=} p(v_u|h_{u-1})$$

- Hence $\beta(h_s) = p(v_{s+1:u}|h_s)$ holds for $s = u - 1$. Provides the base case for a proof by induction.

Smoothing $p(h_t|v_{1:u}), t < u$: interpretation

Assume $\beta(h_s) = p(v_{s+1:u}|h_s)$ holds. Then:

$$
\begin{aligned}
\beta(h_{s-1}) &= \sum_{h_s} p(v_s|h_s)p(h_s|h_{s-1})\beta(h_s) \\
&\overset{\text{(induction hyp)}}{=} \sum_{h_s} p(v_s|h_s)p(h_s|h_{s-1})p(v_{s+1:u}|h_s) \\
&\overset{\text{(Markov prop)}}{=} \sum_{h_s} p(v_s|h_s)p(h_s|h_{s-1})p(v_{s+1:u}|h_s, v_s) \\
&\overset{\text{(product rule)}}{=} \sum_{h_s} p(v_{s:u}|h_s)p(h_s|h_{s-1}) \\
&\overset{\text{(Markov prop)}}{=} \sum_{h_s} p(v_{s:u}|h_s, h_{s-1})p(h_s|h_{s-1}) \\
&\overset{\text{(product rule)}}{=} \sum_{h_s} p(v_{s:u}, h_s|h_{s-1}) \\
&\overset{\text{(marginalise)}}{=} p(v_{s:u}|h_{s-1})
\end{aligned}
$$

By induction, $\beta(h_s) = p(v_{s+1:u}|h_s)$ for all $s < u$.

Doing more with the $\alpha(h_s), \beta(h_s)$

- Due to link to message passing: Knowing all $\alpha(h_s), \beta(h_s) \Longrightarrow$ knowing all marginals *and* all joints of neighbouring latents given the observed data, which will be needed when estimating the parameters of HMMs (see later).
- We can use the $\alpha(h_s)$ for predictions (see exercises).
- We can use the $\alpha(h_s)$ for sampling posterior trajectories, i.e. to sample from $p(h_1, \ldots h_t | v_1, \ldots, v_t)$ (see exercises).
- Algorithms extend to the case of continuous random variables: replace sums with integrals.

Program recap

1. Markov models
   - Markov chains
   - Transition distribution
   - Hidden Markov models (HMMs)
   - Emission distribution
   - Important instances of HMMs

2. Inference by message passing
   - Inference: filtering, prediction, smoothing, Viterbi
   - Filtering: Sum-product message passing yields the α-recursion
   - Smoothing: Sum-product message passing yields the α-β recursion