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-product message passing

Program

1. Markov models
2. Inference by message passing

Program

1. Markov models
   - Markov chains
   - Transition distribution
   - Hidden Markov models
   - Emission distribution
   - Mixture of Gaussians as special case
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)

Markov chains

- Chain rule with ordering $x_1, \dots, x_d$

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

- If p satisfies ordered Markov property, the number of variables in the conditioning set can be reduced to a subset $\pi_i \subseteq \{x_1, \dots, x_{i-1}\}$
- Not all predecessors but only subset π_i is "relevant" for x_i.
- L-th order Markov chain: $\pi_i = \{x_{i-L}, \dots, x_{i-1}\}$

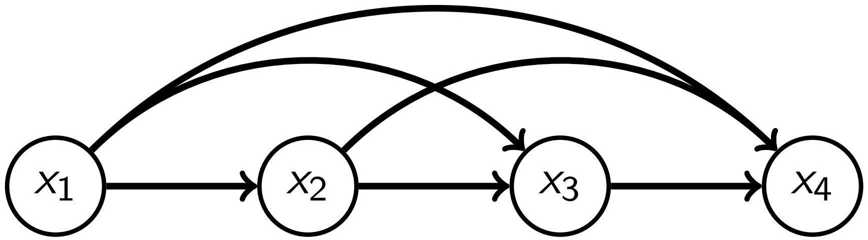
$$p(x_1, \dots, x_d) = \prod_{i=1}^{d} p(x_i | x_{i-L}, \dots, x_{i-1})$$

- 1st order Markov chain: $\pi_i = \{x_{i-1}\}$

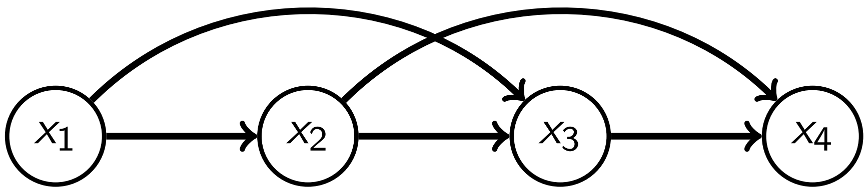
$$p(x_1, \dots, x_d) = \prod_{i=1}^{d} p(x_i | x_{i-1})$$

Markov chain — DAGs

Chain rule



Second-order Markov chain

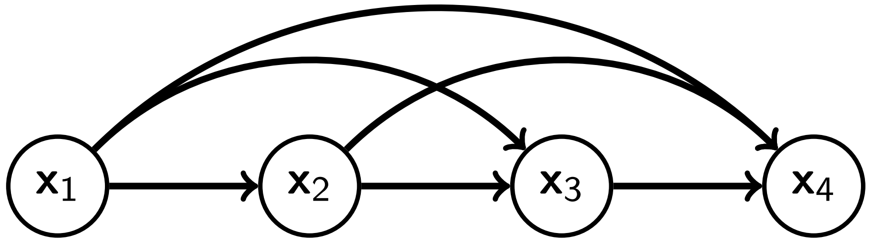


First-order Markov chain

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
- L-th order Markov chain of length T:

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

  Only the recent past of L time points $x_{t-L}, \ldots, x_{t-1}$ is relevant for x_t
- 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 $\mathbf{A}^i$

$$p(x_i = k|x_{i-1} = k') = A^i_{k,k'}$$

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

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

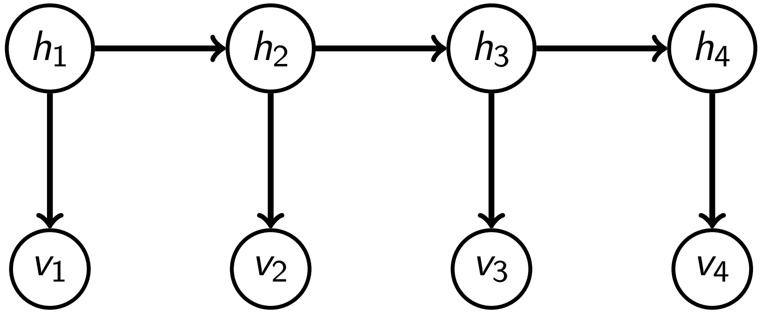
  for some function f_i
- Homogeneous Markov chain: $p(x_i|x_{i-1})$ does not depend on i, e.g.

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

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

Hidden Markov model

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_i model/explain all dependencies between the v_i

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.

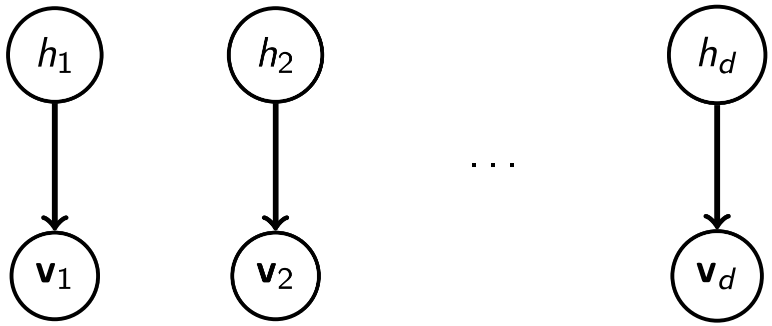
Gaussian emission model with discrete-valued latents

- 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 $\mathbf{v}_i$.

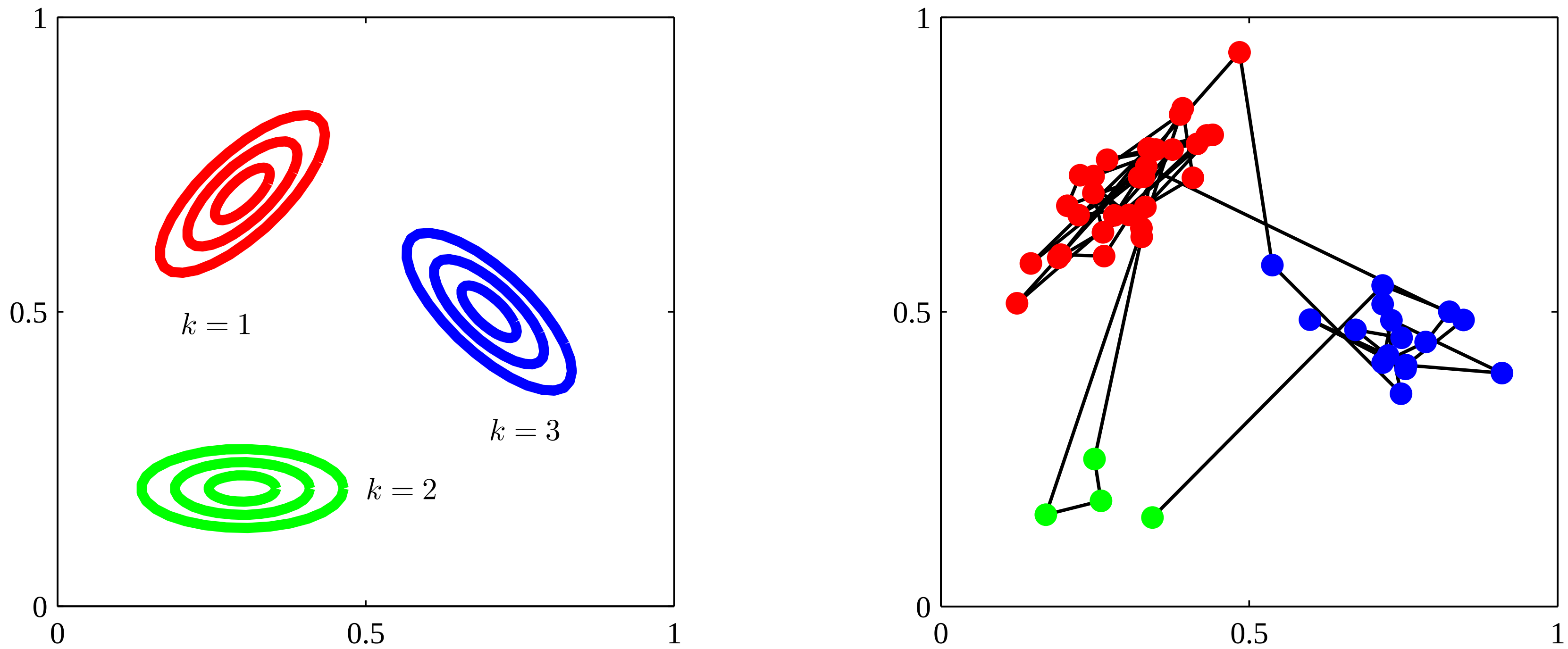
- DAG



- 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)

Program

1. Markov models
    - Markov chains
    - Transition distribution
    - Hidden Markov models
    - Emission distribution
    - Mixture of Gaussians as special case

2. Inference by message passing

Program

1. Markov models

2. Inference by message passing
   - Inference: filtering, prediction, smoothing, Viterbi
   - Filtering: Sum-product message passing yields the alpha-recursion from the HMM literature
   - Smoothing: Sum-product message passing yields the alpha-beta recursion from the HMM literature
   - Sum-product message passing for prediction, inference of most likely hidden path, and for inference of joint distributions

The classical inference problems

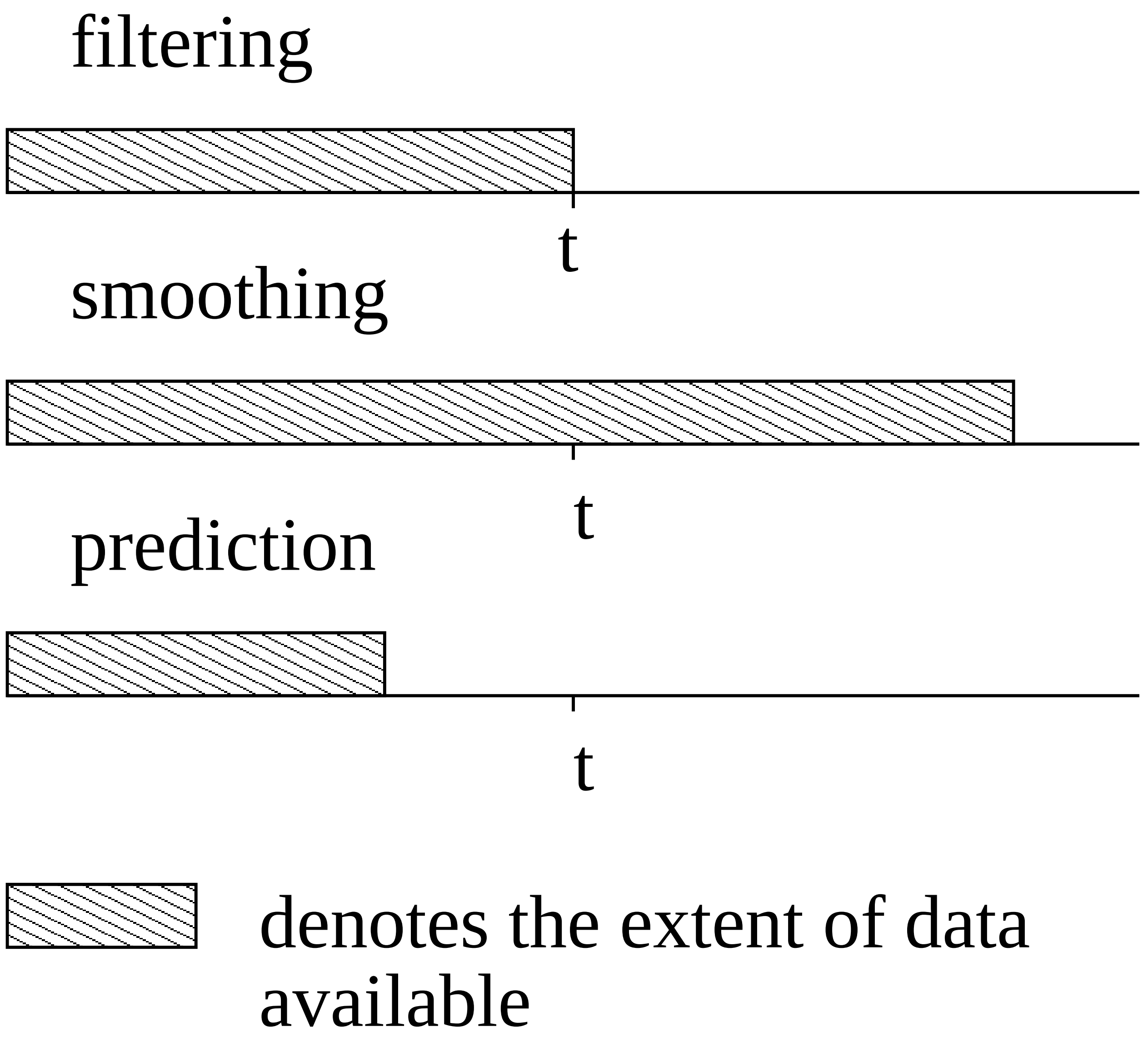
(Considering the index i to refer to time t)

Filtering	(Inferring the present)	$p(h_t \mid v_{1:t})$	
Smoothing	(Inferring the past)	$p(h_t \mid v_{1:u})$	$t < u$
Prediction	(Inferring the future)	$p(h_t \mid v_{1:u})$	$t > u$
Most likely Hidden path	(Viterbi alignment)	$\mathrm{argmax}_{h_{1:t}}\, p(h_{1:t} \mid v_{1:t})$	

For prediction, one is also often interested in $p(v_t \mid v_{1:u})$ for $t > u$.

(slide courtesy of David Barber)

The classical inference problems

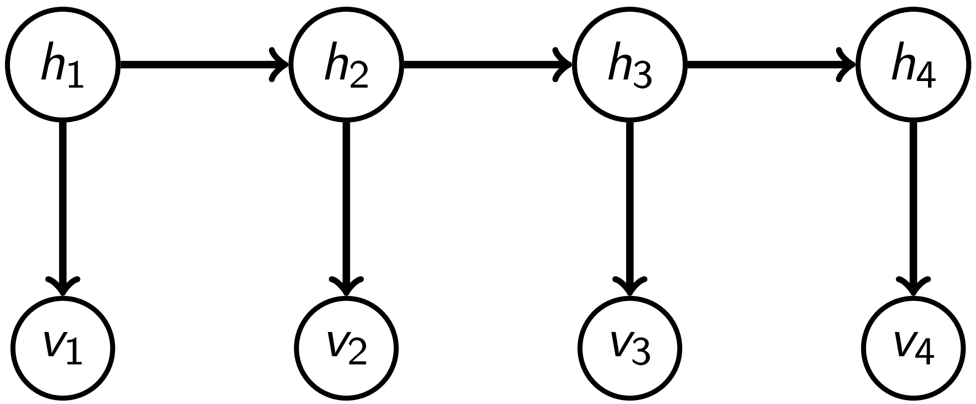


(slide courtesy of Chris Williams)

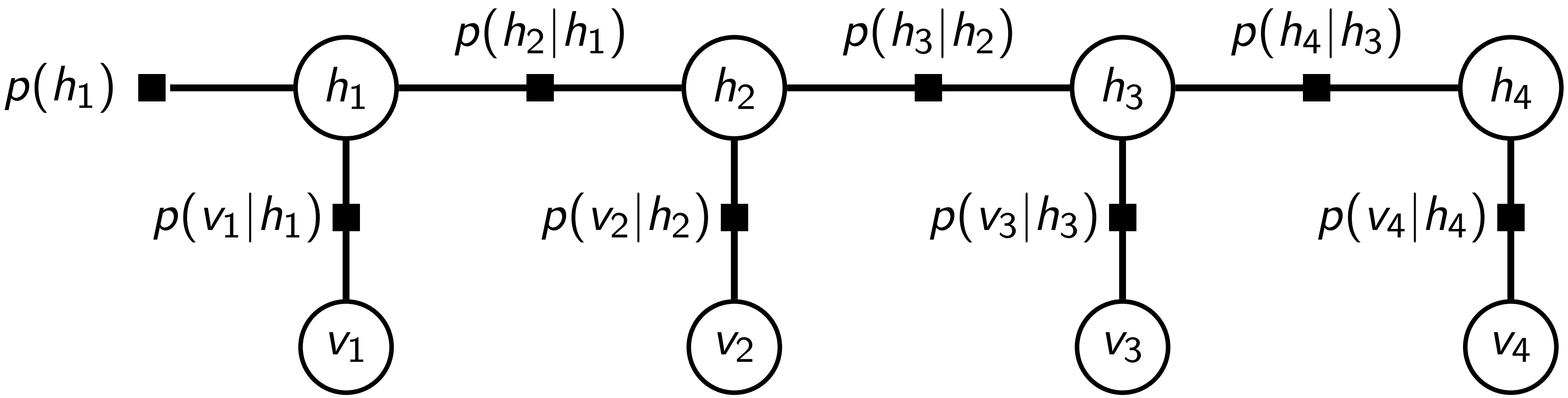
Factor graph for hidden Markov model

(see tutorial 4)

DAG:

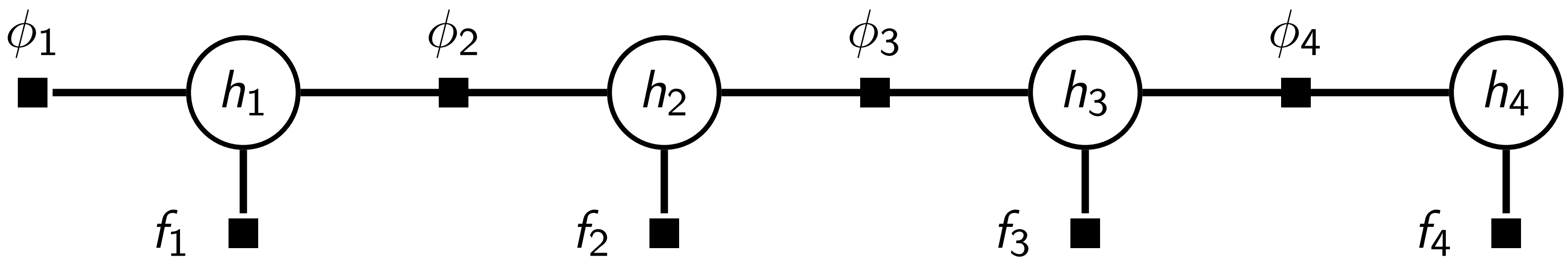


Factor graph:



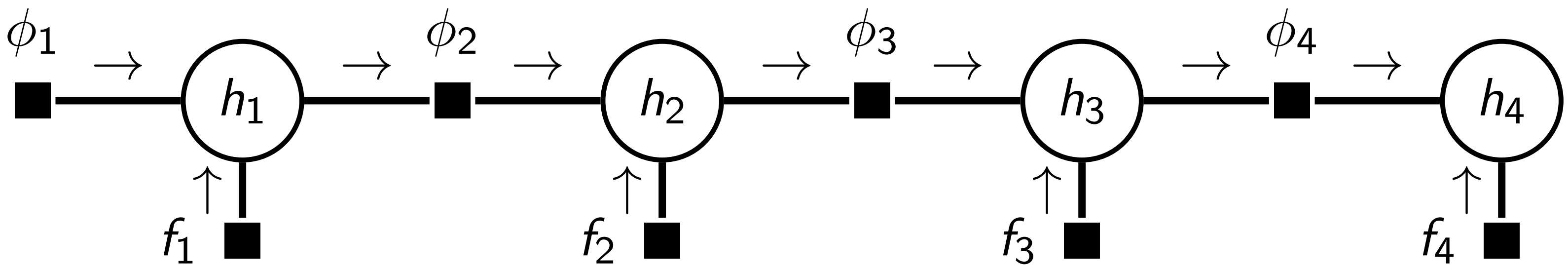
Filtering $p(h_t|v_{1:t})$

- When computing $p(h_t|v_{1:t})$, the $v_{1:t} = (v_1, \ldots, v_t)$ are assumed known and are kept fixed
- Factors $p(v_s|h_s)$ depend on h_s only ($s = 1, \ldots, t$).
- Different options (give the same results):
  - Work with (combined) factors $\phi_s(h_s, h_{s-1}) \propto p(v_s|h_s)p(h_s|h_{s-1})$ and $\phi_1(h_1) = p(v_1|h_1)p(h_1)$.
  - Work with factors $\phi_s(h_s, h_{s-1}) = p(h_s|h_{s-1})$, $f_s(h_s) = p(v_s|h_s)$, and $\phi_1(h_1) = p(h_1)$.
- Factor graph for second option



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

Messages for $p(h_4|v_{1:4})$



Marginal posterior:

$$p(h_t|v_{1:t}) \propto \mu_{\phi_t \to h_t}(h_t)\mu_{f_t \to h_t}(h_t)$$

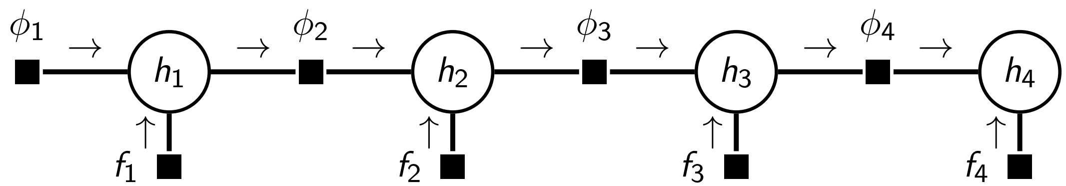
Messages:

- $\mu_{f_i \to h_i}(h_i) = f_i(h_i)$ and $\mu_{\phi_1 \to h_1}(h_1) = \phi_1(h_1)$
- $\mu_{h_1 \to \phi_2}(h_1) = \mu_{\phi_1 \to h_1}(h_1) \cdot \mu_{f_1 \to h_1}(h_1)$
- $\mu_{\phi_2 \to h_2}(h_2) = \sum_{h_1} \phi_2(h_2, h_1)\mu_{h_1 \to \phi_2}(h_1)$

⋮

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

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



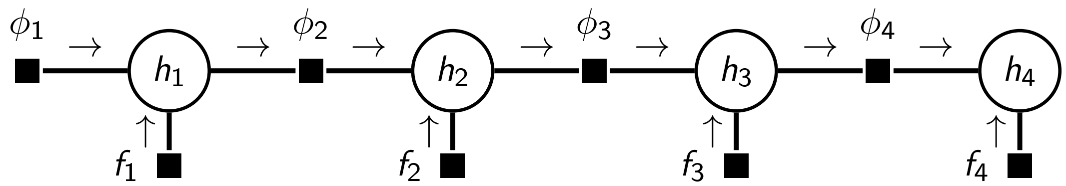
- Recursion:

$$\mu_{h_1\to\phi_2}(h_1) = \phi_1(h_1)\cdot f_1(h_1)$$
$$\mu_{\phi_s\to h_s}(h_s) = \sum_{h_{s-1}} \phi_s(h_s, h_{s-1})\mu_{h_{s-1}\to\phi_s}(h_{s-1})$$
$$\mu_{h_s\to\phi_{s+1}}(h_s) = \mu_{\phi_s\to h_s}(h_s)\cdot \mu_{f_s\to h_s}(h_s)$$

- Inserting the definition of the factors gives:

$$\mu_{h_1\to\phi_2}(h_1) = p(h_1)\cdot p(v_1|h_1)$$
$$\mu_{\phi_s\to h_s}(h_s) = \sum_{h_{s-1}} p(h_s|h_{s-1})\mu_{h_{s-1}\to\phi_s}(h_{s-1})$$
$$\mu_{h_s\to\phi_{s+1}}(h_s) = \mu_{\phi_s\to h_s}(h_s)\cdot p(v_s|h_s)$$

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



- Write recursion in terms of $\mu_{h_s \to \phi_{s+1}}$ only

$$\mu_{h_1 \to \phi_2}(h_1) = p(h_1) \cdot p(v_1|h_1)$$

$$\mu_{h_s \to \phi_{s+1}}(h_s) = p(v_s|h_s) \sum_{h_{s-1}} p(h_s|h_{s-1}) \mu_{h_{s-1} \to \phi_s}(h_{s-1})$$

- Called "alpha-recursion": With $\alpha(h_s) = \mu_{h_s \to \phi_{s+1}}(h_s)$

$$\alpha(h_1) = p(h_1) \cdot p(v_1|h_1)$$

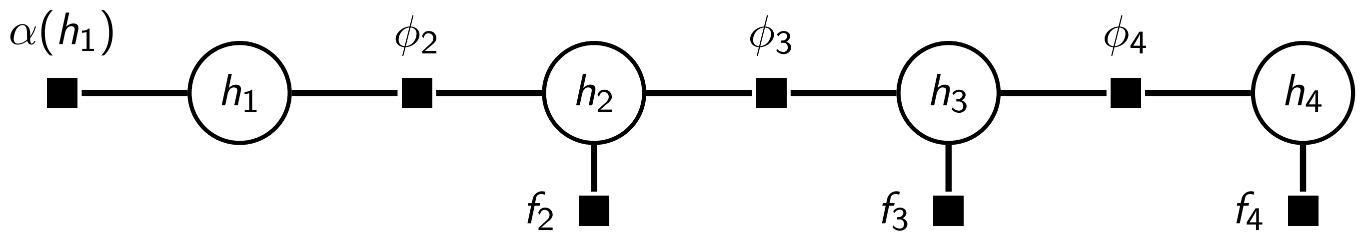
$$\alpha(h_s) = p(v_s|h_s) \sum_{h_{s-1}} p(h_s|h_{s-1}) \alpha(h_{s-1})$$

- Marginal posterior:

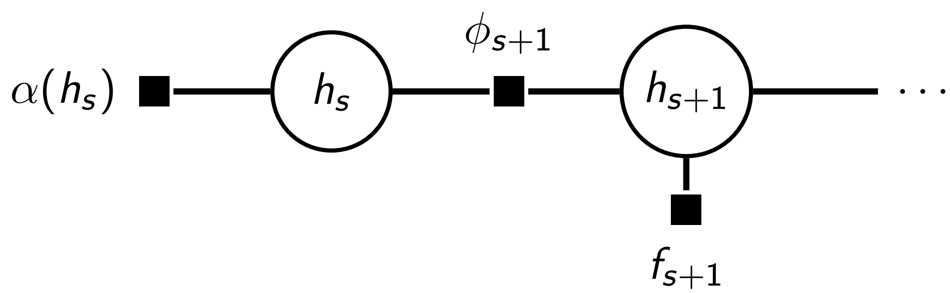
$$p(h_t|v_{1:t}) \propto \alpha(h_t)$$

Filtering $p(h_t|v_{1:t})$ – more on the alpha-recursion

- $\alpha(h_s) = \mu_{h_s \to \phi_{s+1}}(h_s)$ is an effective factor.
- $\alpha(h_1) = p(h_1)p(v_1|h_1) = p(h_1, v_1) \propto p(h_1|v_1)$



- For $\alpha(h_s)$



- We now prove by induction that

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

Filtering $p(h_t|v_{1:t})$ – more on the alpha-recursion

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

- Independencies in the model: $p(h_s|h_{s-1}) = p(h_s|h_{s-1}, v_{1:s-1})$
- With $\alpha(h_{s-1}) = p(h_{s-1}, v_{1:s-1})$ (holds for $s = 2$!)

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

- Independencies in the model: $p(v_s|h_s) = p(v_s|h_s, v_{1:s-1})$

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

which completes the proof.

Filtering $p(h_t|v_{1:t})$ – more on the alpha-recursion

- This kind of approach allows one to obtain the alpha-recursion without message passing (see Barber).
- Interpretation of the alpha-recursion in terms of "prediction and correction"

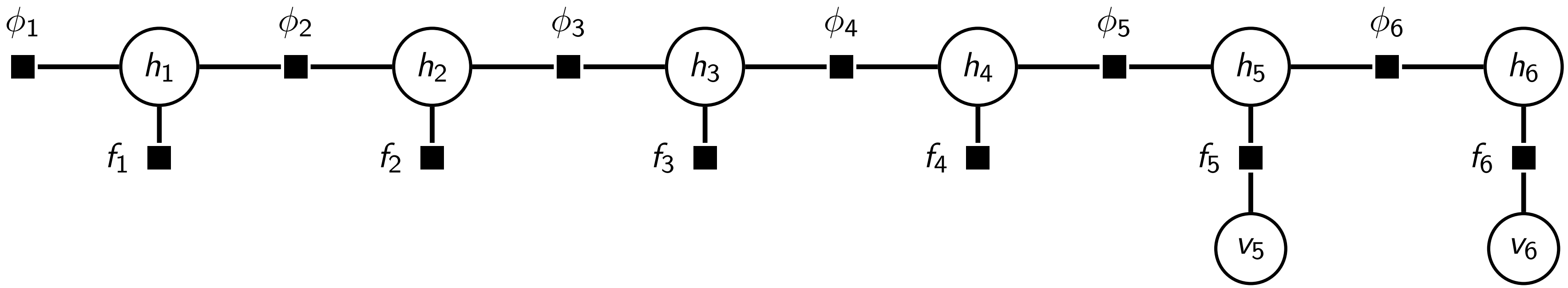
$$
\begin{aligned}
\alpha(h_s) &= p(v_s|h_s) \sum_{h_{s-1}} p(h_s|h_{s-1})\alpha(h_{s-1}) \\
&= p(v_s|h_s) p(h_s, v_{1:s-1}) \\
&\propto \underbrace{p(v_s|h_s)}_{\text{correction}} \underbrace{p(h_s|v_{1:s-1})}_{\text{prediction}} \\
&\propto p(h_s|v_{1:s})
\end{aligned}
$$

- The correction term updates the predictive distribution of h_s given $v_{1:s-1}$ to include the new data v_s.

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

Consider:

- Hidden Markov model with variables $(h_1, \ldots, h_6, v_1, \ldots, v_6)$
- Observed $v_{1:4} = (v_1, \ldots, v_4)$
- Interest: $p(h_2|v_{1:4})$



Factor graph with factors ϕ_i and $f_1, \ldots, f_4$ defined as before. Factors f_5 and f_6 are: $f_5(h_5, v_5) = p(v_5|h_5)$ and $f_6(h_6, v_6) = p(v_6|h_6)$.

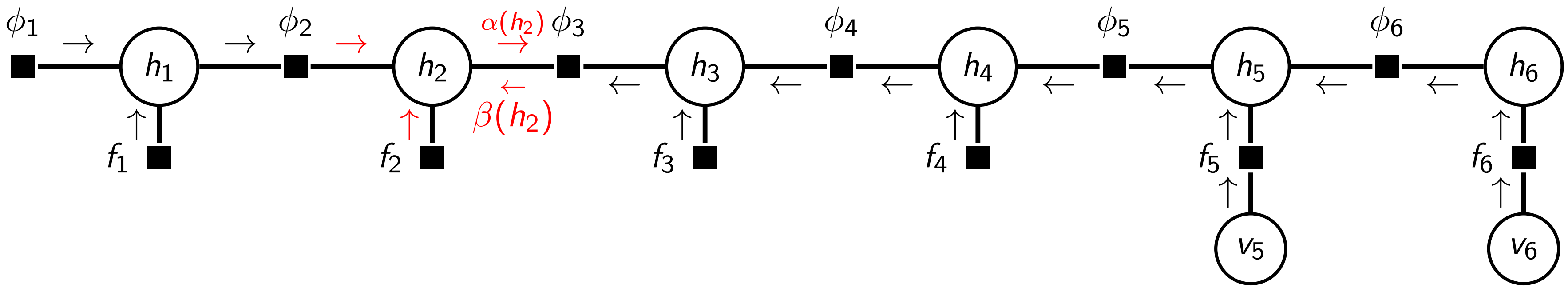
Smoothing $p(h_t|v_{1:u}), t < u$

- $p(h_2|v_{1:4})$ is given by incoming messages

$$p(h_2|v_{1:4}) \propto \underbrace{\mu_{\phi_2\to h_2}(h_2)\mu_{f_2\to h_2}(h_2)}_{\mu_{h_2\to\phi_3}(h_2)=\alpha(h_2)}\mu_{\phi_3\to h_2}(h_2)$$

- Denote $\mu_{\phi_3\to h_2}(h_2)$ by $\beta(h_2)$:

$$p(h_2|v_{1:4}) \propto \alpha(h_2)\beta(h_2)$$



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

- We can compute $\beta(h_2)$ by sum-product message passing.
- Let $\beta(h_s) = \mu_{\phi_{s+1}\to h_s}(h_s)$, then (see tutorial 5)

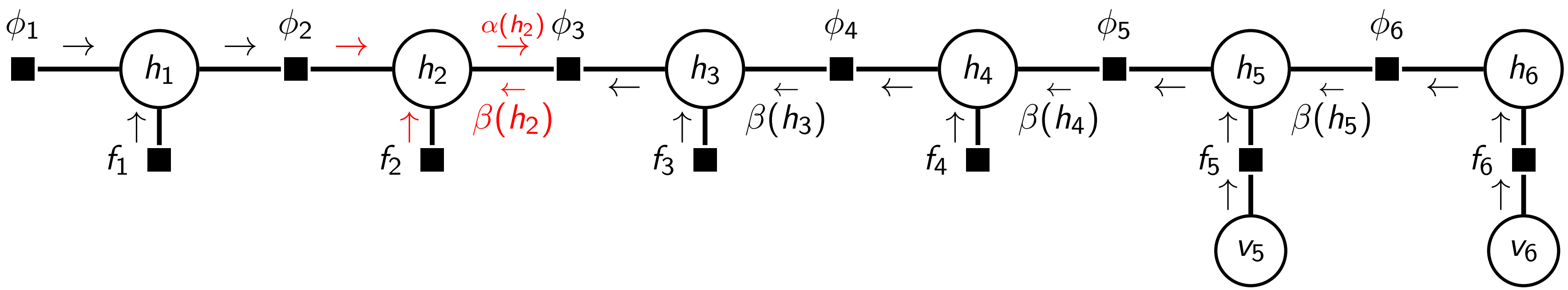
$$\beta(h_4) = \beta(h_5) = 1$$

$$\beta(h_3) = \sum_{h_4} \underbrace{p(h_4|h_3)}_{\phi_4} \underbrace{p(v_4|h_4)}_{f_4} \underbrace{\beta(h_4)}_{1}$$

$$\vdots$$

$$\beta(h_s) = \sum_{h_{s+1}} \underbrace{p(h_{s+1}|h_s)}_{\phi_{s+1}} \underbrace{p(v_{s+1}|h_{s+1})}_{f_{s+1}} \beta(h_{s+1}) \quad (s < u)$$

- From independencies: $\beta(h_s) = p(v_{s+1:u}|h_s)$ (see Barber 23.2.3)



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

- Recursive computation of $\beta(h_s)$ via message passing is known as "beta-recursion" in the HMM literature
- Smoothing via "alpha-beta recursion"

$$p(h_t|v_{1:u}) \propto \alpha(h_t)\beta(h_t)$$

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

$$\alpha(h_1) = p(h_1)p(v_1|h_1) \propto p(h_1|v_1)$$

$$\beta(h_s) = \sum_{h_{s+1}} p(h_{s+1}|h_s)p(v_{s+1}|h_{s+1})\beta(h_{s+1})$$

$$\beta(h_u) = 1$$

- Also known as forward-backward algorithm.
- Due to correspondence to message passing: Knowing all $\alpha(h_s), \beta(h_s) \Longleftrightarrow$ knowing all marginals and all joints of neighbouring latents given the observed data $v_{1:u}$.

Prediction, most likely hidden path, and joint distribution

- Sum-product algorithm can similarly be used for
  - prediction: $p(h_t|v_{1:u})$ and $p(v_t|v_{1:u})$, with $t > u$
  - inference of the most likely hidden path: $\mathrm{argmax}_{h_{1:t}}\, p(h_{1:t}|v_{1:t})$
  - computing pairwise marginals $p(h_t, h_{t+1}|v_{1:u})$, $u \geq t$ or $u < t$.
- Can be written in terms of $\alpha(h_t)$ and $\beta(h_t)$
- See Barber Section 23.2
  (does not use message passing)

Program recap

1. Markov models
   - Markov chains
   - Transition distribution
   - Hidden Markov models
   - Emission distribution
   - Mixture of Gaussians as special case

2. Inference by message passing
   - Inference: filtering, prediction, smoothing, Viterbi
   - Filtering: Sum-product message passing yields the alpha-recursion from the HMM literature
   - Smoothing: Sum-product message passing yields the alpha-beta recursion from the HMM literature
   - Sum-product message passing for prediction, inference of most likely hidden path, and for inference of joint distributions