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/max-sum message passing

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Program

1. Markov models

2. Inference by message passing

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Program

1. Markov models

- Markov chains
- Transition distribution
- Hidden Markov models
- Emission distribution
- Mixture of Gaussians as special case
- Linear Dynamical System (LDS)

2. Inference by message passing

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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)

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Markov chains

ightharpoonup Chain rule with ordering x_1, \ldots, x_d

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

- 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: $\pi_i = \{x_{i-1}, \dots, x_{i-1}\}$

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

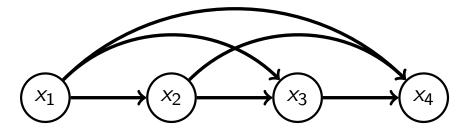
▶ 1st order Markov chain: $\pi_i = \{x_{i-1}\}$

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

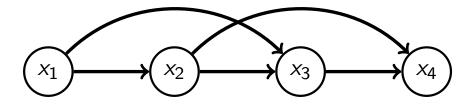
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Markov chain — DAGs

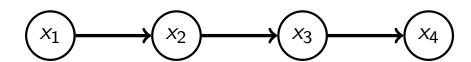
Chain rule



Second-order Markov chain



First-order Markov chain

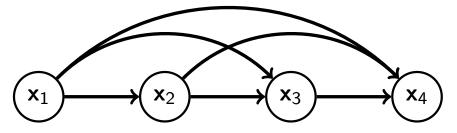


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Vector-valued Markov chains

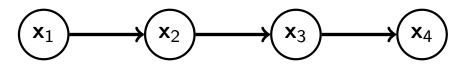
- While not explicitly discussed, the graphical models extend to vector-valued variables.
- ightharpoonup Chain rule with ordering $\mathbf{x}_1, \dots, \mathbf{x}_d$

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



► 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*
- \triangleright For example, 1st order Markov chain of length T:

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

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

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Transition distribution

(Consider 1st order Markov chain.)

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

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

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 function f_i

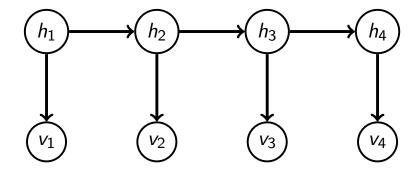
► Homogeneous Markov chain: $p(x_i|x_{i-1})$ does not depend on i, e.g.

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

▶ 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
- \triangleright The h_i s model/explain all dependencies between the v_i s

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Emission distribution

- $ightharpoonup p(v_i|h_i)$ 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 (HMM).

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Gaussian emission model with discrete-valued latents

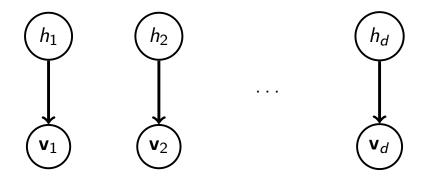
▶ Special case: $h_i \perp \!\!\! \perp h_{i-1}$, and $\mathbf{v}_i \in \mathbb{R}^m, h_i \in \{1, \ldots, K\}$

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

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

for all h_i and \mathbf{v}_i .

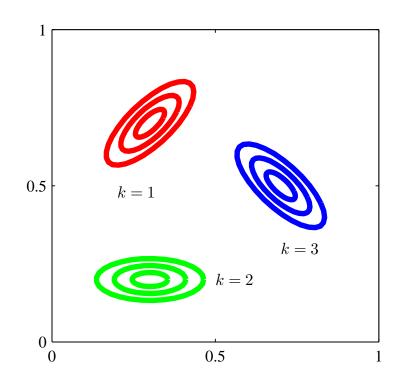
DAG

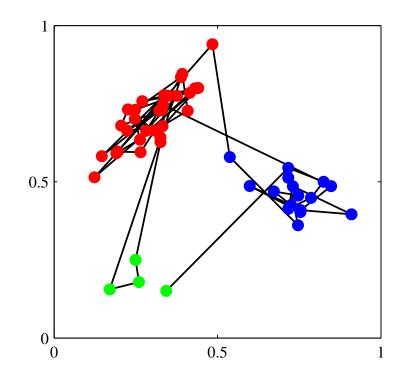


- Corresponds to d iid draws from a Gaussian mixture model with K mixture components
 - $lackbox{\sf Mean } \mathbb{E}[\mathbf{v}|h=k]=oldsymbol{\mu}_k$
 - ightharpoonup Covariance matrix $\mathbb{V}[\mathbf{v}|h=k]=\mathbf{\Sigma}_k$

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)

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Linear Dynamical System (LDS)

- Continuous-valued hidden and visible state
- Transition model is linear

$$\mathbf{h}_{t+1} = A\mathbf{h}_t + \mathbf{n}_{t+1}^h, \qquad \mathbf{n}_{t+1}^h \sim N(0, \Sigma^h)$$

- ightharpoonup Stable dynamics if all eigenvalues of A have magnitude < 1
- Emission model is linear

$$\mathbf{v}_t = C\mathbf{h}_t + \mathbf{n}_t^v, \qquad \mathbf{n}_t^v \sim N(0, \Sigma^v)$$

- ▶ 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 LDS, this was solved by Kalman (1960), hence it is termed Kalman filtering
- Uses: navigational and guidance systems

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Program

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- Hidden Markov models
- Emission distribution
- Mixture of Gaussians as special case
- Linear Dynamical System (LDS)

2. Inference by message passing

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Program

1. Markov models

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

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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)	$\operatorname{argmax}_{h_{1:t}} p(h_{1:t} v_{1:t})$
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/max-product algorithm).

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The classical inference problems

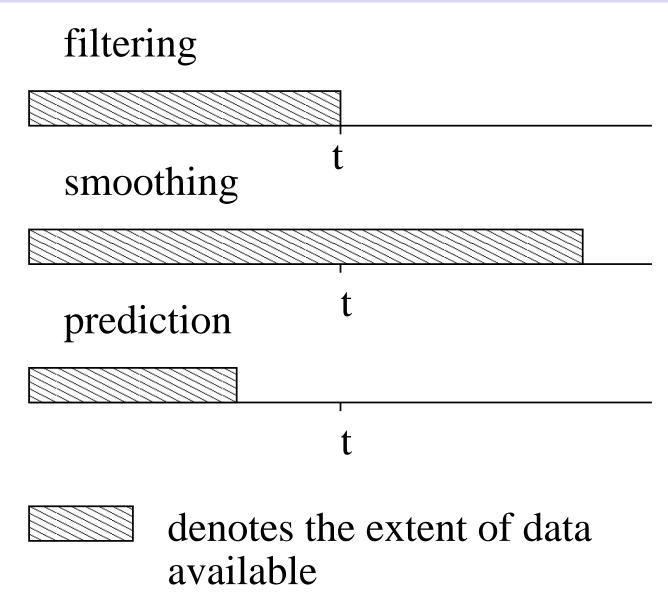
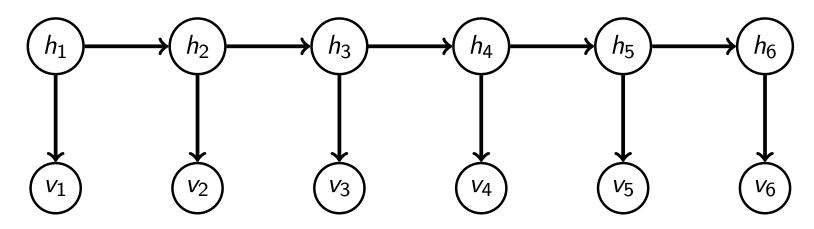


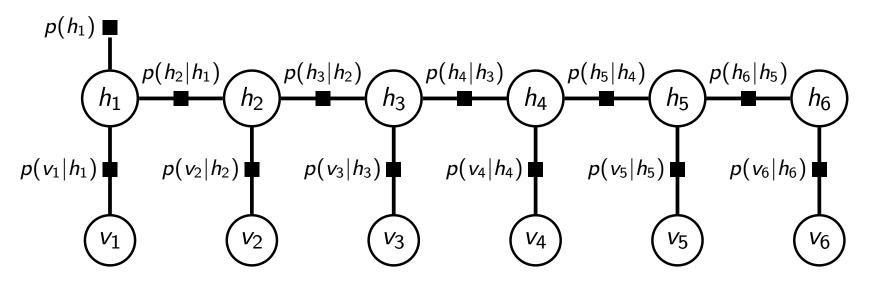
Figure based on Fig. 1.0-1 of Gelb et al (1974)

Factor graph for hidden Markov model

DAG:



Factor graph:



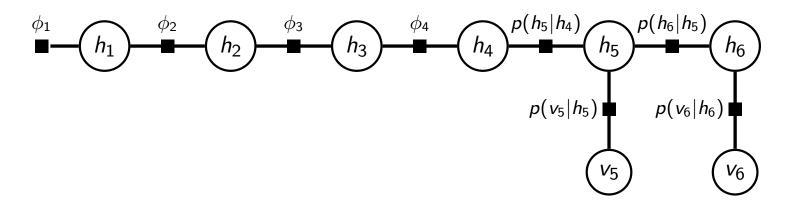
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Filtering $p(h_t|v_{1:t})$: factor graph

- 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

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

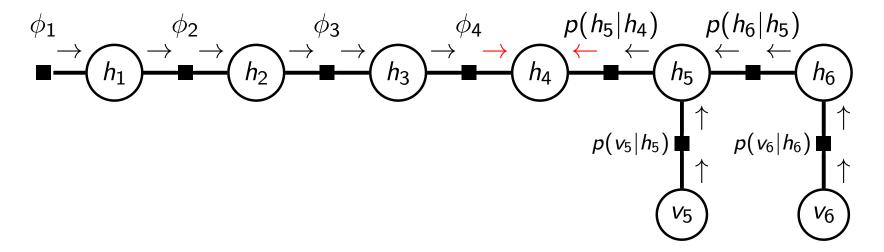
► Factor graph



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

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



There is a simplification:

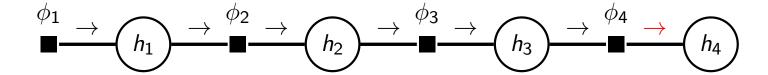
- ▶ The message from $p(h_5|h_4)$ to h_4 equals 1!
- ▶ Follows from message passing starting at leaves v_5 and v_6 since the factors p(.|.) are conditionals and sum to one, e.g.

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

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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.



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

- lnitialisation: $\mu_{\phi_1 \to h_1}(h_1) = \phi_1(h_1)$
- \triangleright 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 :

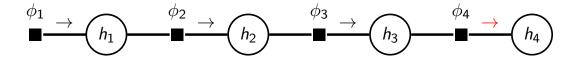
$$\mu_{\phi_2 \to h_2}(h_2) = \sum_{h_1} \phi_2(h_1, h_2) \mu_{\phi_1 \to h_1}(h_1)$$

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

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

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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: $\alpha(h_1) = \phi_1(h_1) = \rho(v_1|h_1)\rho(h_1)$
 - ▶ Update rule for s = 2, ... t:

$$\alpha(h_s) = \sum_{h_{s-1}} \phi_s(h_{s-1}, h_s) \alpha(h_{s-1})$$

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

- ► Algorithm known as "alpha-recursion".
- Desired probability:

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

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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

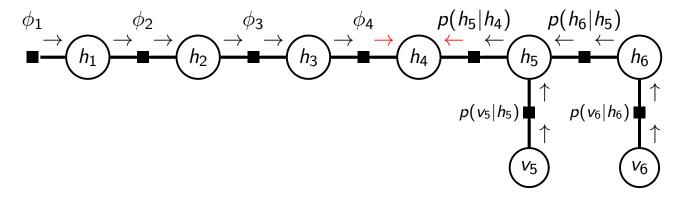
$$p(h_{1:t}|v_{1:t}) \propto p(v_1|h_1)p(h_1)\prod_{i=2}^t p(v_i|h_i)p(h_i|h_{i-1})$$

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

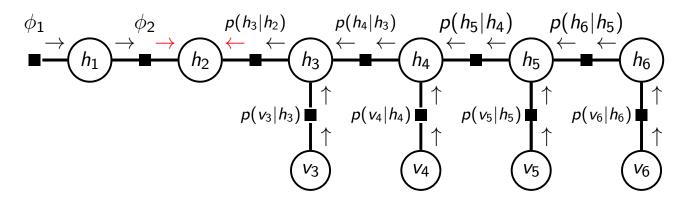
$$Z_t = \sum_{h_t} \alpha(h_t) = p(v_{1:t})$$

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▶ 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 $p(h_t|v_{1:t})$.
- \blacktriangleright Messages to the right of h_s are all equal to one.

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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 $s=1,\ldots,t$.

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- 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:

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

Update rule as prediction-correction algorithm:

$$lpha(h_s) \stackrel{(\mathsf{prev \, slide})}{=} p(h_s, v_{1:s})$$

$$\stackrel{(\mathsf{product \, rule})}{=} p(v_s|h_s, v_{1:s-1})p(h_s, v_{1:s-1})$$

$$\stackrel{(\mathsf{Markov \, prop})}{=} p(v_s|h_s)p(h_s, v_{1:s-1})$$

$$\propto \underbrace{p(v_s|h_s)}_{\mathsf{correction \, prediction}} p(h_s|v_{1:s-1})$$

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

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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, ... t:

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

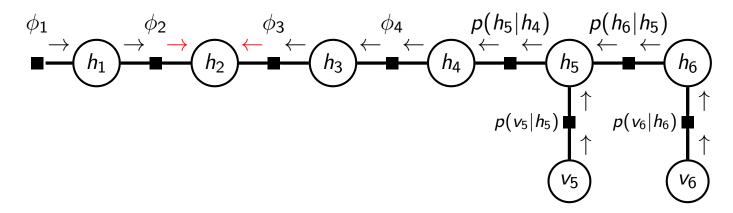
which involves prediction of h_s given $v_{1:s-1}$ and correction using new datum v_s .

ho $\alpha(h_s) = p(h_s, v_{1:s}) \propto p(h_s|v_{1:s})$ and $p(v_{1:s}) = \sum_{h_s} \alpha(h_s)$, for $s = 1, \ldots, t$

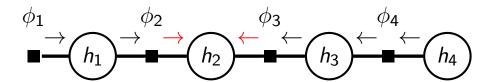
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Smoothing $p(h_t|v_{1:u}), t < u$: reduce to inference on chain

- ▶ 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



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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.
- lnit: $\mu_{h_u \to \phi_u}(h_u) = 1$
- Next message $\mu_{\phi_u \to h_{u-1}}(h_{u-1}) = \sum_{h_u} \phi_u(h_{u-1}, h_u)$
- Variable nodes just copy the incoming message. Write the algorithm in terms of $\beta(h_s) = \mu_{\phi_{s+1} \to h_s}(h_s)$ only:

$$\beta(h_{s-1}) = \sum_{h_s} \phi_s(h_{s-1}, h_s) \beta(h_s)$$

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

Gives "alpha-beta recursion" for smoothing.

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

- ightharpoonup ightharpoonup Forwards via alpha-recursion
 - ► Init: $\alpha(h_1) = p(v_1|h_1)p(h_1)$
 - ▶ Update rule for s = 2, ... t:

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

- ► ← Backwards via beta-recursion
 - lnit: $\beta(h_u) = 1$
 - ▶ Update rule for s = u, ..., 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 ,

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

$$\stackrel{\text{(induction hyp)}}{=} \sum_{h_s} p(v_s|h_s)p(h_s|h_{s-1})p(v_{s+1:u}|h_s)$$

$$\stackrel{\text{(Markov prop)}}{=} \sum_{h_s} p(v_s|h_s)p(h_s|h_{s-1})p(v_{s+1:u}|h_s, v_s)$$

$$\stackrel{\text{(product rule)}}{=} \sum_{h_s} p(v_{s:u}|h_s)p(h_s|h_{s-1})$$

$$\stackrel{\text{(Markov prop)}}{=} \sum_{h_s} p(v_{s:u}|h_s, h_{s-1})p(h_s|h_{s-1})$$

$$\stackrel{\text{(product rule)}}{=} \sum_{h_s} p(v_{s:u}|h_s, h_{s-1})$$

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

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.

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Example: Harmonizing Chorales in the Style of J S Bach

- Moray Allan and Chris Williams (NIPS 2004) "Harmonising Chorales by Probabilistic Inference"
- Visible states are the melody (quarter notes)
- Hidden states are the harmony (which chord)
- Trained using labelled melody/harmony data from Bach chorales
- ► Task: find Viterbi alignment for harmony given melody, or sample from p(harmony|melody.)
- ► Actually it is a bit more complicated. HMMs used for three subtasks: harmonic skeleton, chord skeleton, ornamentation

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Further reading

Exact inference for Hidden Markov models is well-covered in the standard textbooks, e.g.

- ► Bishop (2006) secs. 13.2.2, 13.2.3, 13.2.5
- ► Barber sec. 23.2

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Program recap

1. Markov models

- Markov chains
- Transition distribution
- Hidden Markov models
- Emission distribution
- Mixture of Gaussians as special case
- Linear Dynamical System (LDS)

2. Inference by message passing

- Inference: filtering, prediction, smoothing, Viterbi
- ullet Filtering: Sum-product message passing yields the lpha-recursion
- ullet Smoothing: Sum-product message passing yields the α - β recursion

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Credits

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