732A96 Advanced Machine Learning Graphical Models and Hidden Markov Models

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Lecture 5: Dynamic Bayesian Networks and Hidden Markov Models

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Literature

Main source

 Bishop, C. M. Pattern Recognition and Machine Learning. Springer, 2006. Chapter 13.1-13.2.

Additional source

 Ghahramani, Z. An Introduction to Hidden Markov Models and Bayesian Networks. International Journal of Pattern Recognition and Artificial Intelligence 15, 9-42, 2001.

Dynamic Bayesian Networks: Definition

- ▶ To model **sequential data**, e.g. time series data.
- **Simplification**: Time is discretized in equal width intervals, i.e. t = 0, 1, ...
- Consider a finite set of discrete random variables $X^t = \{X_1^t, \dots, X_n^t\}$ representing the state at time t of a system described by $V = \{X_1, \dots, X_n\}$.
- A dynamic Bayesian network (DBN) is a BN over $X^{0:T} = \{X^0, \dots, X^T\}$. Thus, it defines $p(X^{0:T})$.

▶ **Assumption**: The system is Markovian, i.e. $X^{t+1} \perp_p X^{0:t-1} | X^t$.

$$\begin{array}{c|ccccc} X_1^0 \longrightarrow X_1^1 & X_1^2 & X_1^3 \longrightarrow X_1^4 \\ \downarrow & \uparrow & \downarrow & \downarrow \\ X_2^0 \longrightarrow X_2^1 & X_2^2 \longrightarrow X_2^3 & X_2^4 \\ \downarrow & \uparrow & \uparrow & \downarrow \\ X_3^0 \longrightarrow X_3^1 & X_3^2 \longrightarrow X_3^3 & X_3^4 \end{array}$$

▶ **Assumption**: The system is stationary, i.e. $p(X^{t+1}|X^t) = p(X'|X)$.

$$\begin{array}{c} X_1^0 \longrightarrow X_1^1 \longrightarrow X_1^2 \longrightarrow X_3^3 \longrightarrow X_4^4 \\ \downarrow \qquad \qquad \uparrow \qquad \qquad \uparrow \qquad \uparrow \qquad \uparrow \\ X_2^0 \qquad X_2^1 \qquad X_2^2 \qquad X_2^3 \qquad X_2^4 \\ \downarrow \qquad \qquad \uparrow \qquad \qquad \uparrow \qquad \uparrow \qquad \uparrow \\ X_3^0 \longrightarrow X_3^1 \longrightarrow X_3^2 \longrightarrow X_3^3 \longrightarrow X_3^4 \end{array}$$

Dynamic Bayesian Networks

- ▶ Then, a DBN over $X^{0:T}$ can be defined as
 - ▶ a BN over X^0 , and
 - a BN over $X^t \cup X^{t+1}$ where the nodes in X^t are parentless.

Initial model	Transition model
X_1^0	$X_1^t \rightarrow X_1^{t+1}$
1	↑
X_{2}^{0}	$X_2^t X_2^{t+1}$
1	1
X_3^0	$X_3^t \rightarrow X_3^{t+1}$

The DBN defines

$$p(X^{0:T}) = p(X^0) \prod_{t=0}^{T} p(X^{t+1}|X^t) = \left[\prod_{i=1}^{n} p(X_i^0|pa_G(X_i^0))\right] \left[\prod_{t=0}^{T} \prod_{i=1}^{n} p(X_i^{t+1}|pa_G(X_i^{t+1}))\right]$$

DBN unrolled for T = 4.

$$\begin{array}{c} X_1^0 \longrightarrow X_1^1 \longrightarrow X_1^2 \longrightarrow X_1^3 \longrightarrow X_1^4 \\ \downarrow \qquad \uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow \\ X_2^0 \qquad X_2^1 \qquad X_2^2 \qquad X_2^3 \qquad X_2^4 \\ \downarrow \qquad \uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow \\ X_3^0 \longrightarrow X_3^1 \longrightarrow X_3^2 \longrightarrow X_3^3 \longrightarrow X_3^4 \end{array}$$

Hidden Markov Models: Definition

- ▶ To overcome the **Markovian limitation** of DBNs, while keeping sparsity.
- A hidden Markov model (HMM) over $\{Z^{0:T}, X^{0:T}\}$ where $X^{0:T}$ are observed and $Z^{0:T}$ are unobserved consists of
 - ightharpoonup a DBN over $Z^{0:T}$, and
 - ▶ a BN over $Z^t \cup X^t$ where the nodes in Z^t are parentless.

Initial model	Transition model	Emission model
$U_1^0 \\ \downarrow \\ U_2^0 \\ \downarrow \\ U_3^0$	$U_1^t \rightarrow U_1^{t+1}$ $\downarrow U_2^t \qquad U_2^{t+1}$ $\downarrow U_3^t \rightarrow U_3^{t+1}$	U ₁ ^t U ₂ ^t U ₃ ^t U ₃ ^t O ₁ ^t

A HMM is a DBN that defines

$$p(Z^{0:T}, X^{0:T}) = p(Z^0) \prod_{t=1}^{T} p(Z^{t+1}|Z^t) \prod_{t=0}^{T} p(X^t|Z^t)$$

▶ HMM unrolled for T = 4.

Hidden Markov Models: Learning

The structure is typically fixed to

- Consider a sample with a single observation over $X^{0:T}$.
- Parameter learning: EM algorithm.
- ightharpoonup Cardinality of Z^t ? BIC score to select among a set of plausible values.

Hidden Markov Models: Learning

- Recall that maximizing the log likelihood function over $x^{0:T}$ is inefficient (no closed form solution) and ineffective (multimodal).
- Consider instead maximizing its expectation

$$E_{Z^{0:T}}[\log p(Z^{0:T}, x^{0:T})] = \sum_{z^{0:T}} p(z^{0:T}|x^{0:T}) \log p(z^{0:T}, x^{0:T})$$

$$= \sum_{z^{0:T}} p(z^{0:T}|x^{0:T}) [\log \theta_{z^{0}} + \sum_{t=1}^{T} \log \theta_{z^{t+1}|z^{t}} + \sum_{t=1}^{T} \log \theta_{x^{t}|z^{t}}]$$

$$= \sum_{z^0} p(z^0|x^{0:T}) \log \theta_{z^0} + \sum_{t=1}^{T} \sum_{z^t} \sum_{z^{t+1}} p(z^t, z^{t+1}|x^{0:T}) \log \theta_{z^{t+1}|z^t} + \sum_{t=1}^{T} \sum_{z_t} p(z^t|x^{0:T}) \log \theta_{x^t|z^t}$$

Then

$$\begin{array}{l} & \theta \mathop{\mathcal{M}L}_{z^0} = \frac{\rho(z^0|x^{0:T})}{\sum_{z^0}\rho(z^0|x^{0:T})} \\ & \bullet \ \theta \mathop{\mathcal{M}L}_{z^{t+1}|z^t} = \frac{\sum_{t=1}^T \rho(z^t,z^{t+1}|x^{0:T})}{\sum_{t=1}^T \sum_{z^{t+1}} \rho(z^t,z^{t+1}|x^{0:T})} \\ & \bullet \ \theta \mathop{\mathcal{M}L}_{x^t|z^t} = \frac{\sum_{t=1}^T \rho(z^t|x^{0:T}) \mathbf{1}_{\{x^t \in x^{0:T}\}}}{\sum_{t=1}^T \rho(z^t|x^{0:T})} \end{array}$$

Note that computing $p(Z^0|x^{0:T})$, $p(Z^t, Z^{t+1}|x^{0:T})$ and $p(Z^t|x^{0:T})$ requires inference: Forward-backward algorithm.

Hidden Markov Models: Forward-Backward Algorithm

$$\begin{split} \rho(Z^{t}|x^{0:T}) &= \frac{\rho(x^{0:T}|Z^{t})\rho(Z^{t})}{\rho(x^{0:T})} \\ &= \frac{\rho(x^{0:t}|Z^{t})\rho(Z^{t})\rho(x^{t+1:T}|Z^{t})}{\rho(x^{0:T})} \text{ by } X^{0:t} \bot_{\rho} X^{t+1:T}|Z^{t} \\ &= \frac{\rho(x^{0:t},Z^{t})\rho(x^{t+1:T}|Z^{t})}{\rho(x^{0:T})} = \frac{\alpha(Z^{t})\beta(Z^{t})}{\sum_{Z^{t}}\alpha(z^{t})\beta(z^{t})} \\ \rho(Z^{t},Z^{t+1}|x^{0:T}) &= \frac{\rho(x^{0:T}|Z^{t},Z^{t+1})\rho(Z^{t},Z^{t+1})}{\rho(x^{0:T})} \\ &= \frac{\rho(x^{0:t}|Z^{t})\rho(x^{t+1}|Z^{t+1})\rho(x^{t+2:T}|Z^{t+1})\rho(Z^{t+1}|Z^{t})\rho(Z^{t})}{\rho(x^{0:T})} \\ \text{by } X^{0:t} \bot_{\rho} X^{t+1:T}|Z^{t} \cup Z^{t+1} \\ &\quad X^{0:t} \bot_{\rho} Z^{t+1}|Z^{t} \\ &\quad X^{t+1:T} \bot_{\rho} Z^{t}|Z^{t+1} \\ &\quad X^{t+1} \bot_{\rho} X^{t+2:T}|Z^{t+1} \\ &= \frac{\alpha(Z^{t})\beta(Z^{t+1})\rho(x^{t+1}|Z^{t+1})\rho(Z^{t+1}|Z^{t})}{\sum_{Z^{t}} \sum_{Z^{t+1}} \alpha(Z^{t})\beta(Z^{t+1})\rho(x^{t+1}|Z^{t+1})\rho(Z^{t+1}|Z^{t})} \end{split}$$

Hidden Markov Models: Forward-Backward Algorithm

$$\alpha(\mathbf{Z}^{t}) = p(x^{t}|Z^{t})p(Z^{t})p(x^{0:t-1}|Z^{t}) \text{ by } X^{0:t-1} \perp_{p} X^{t}|Z^{t}$$

$$= p(x^{t}|Z^{t})p(x^{0:t-1}, Z^{t}) = p(x^{t}|Z^{t}) \sum_{z^{t-1}} p(x^{0:t-1}, Z^{t}|z^{t-1})p(z^{t-1})$$

$$= p(x^{t}|Z^{t}) \sum_{z^{t-1}} p(x^{0:t-1}|z^{t-1})p(Z^{t}|z^{t-1})p(z^{t-1}) \text{ by } X^{0:t-1} \perp_{p} Z^{t}|Z^{t-1}$$

$$= p(x^{t}|Z^{t}) \sum_{z^{t-1}} p(x^{0:t-1}, z^{t-1})p(Z^{t}|z^{t-1}) = p(x^{t}|Z^{t}) \sum_{z^{t-1}} \alpha(z^{t-1})p(Z^{t}|z^{t-1})$$

$$\alpha(Z^{0}) = p(x^{0}|Z^{0})p(Z^{0})$$

$$\beta(\mathbf{Z}^{t}) = \sum_{z^{t+1}} p(x^{t+1:T}, z^{t+1}|Z^{t}) = \sum_{z^{t+1}} p(x^{t+1:T}|z^{t+1}, Z^{t})p(z^{t+1}|Z^{t})$$

$$= \sum_{z^{t+1}} p(x^{t+1:T}|z^{t+1})p(z^{t+1}|Z^{t}) \text{ by } X^{t+1:T} \perp_{p} Z^{t}|Z^{t+1}$$

$$= \sum_{z^{t+1}} p(x^{t+2:T}|z^{t+1})p(x^{t+1}|z^{t+1})p(z^{t+1}|Z^{t}) \text{ by } X^{t+2:T} \perp_{p} X^{t+1}|Z^{t+1}$$

$$= \sum_{z^{t+1}} \beta(z^{t+1})p(x^{t+1}|z^{t+1})p(z^{t+1}|Z^{t})$$

$$\beta(Z^{T}) = 1 \text{ by } p(Z^{T}|x^{0:T}) = \frac{\alpha(Z^{T})\beta(Z^{T})}{p(x^{0:T})} = p(Z^{T}|x^{0:T})\beta(Z^{T})$$

Hidden Markov Models: Forward-Backward Algorithm

FB algorithm

$$\begin{split} &\alpha(Z^0) \coloneqq p(x^0|Z^0) p(Z^0) \\ &\text{For } t = 1, \dots, T \text{ do} \\ &\alpha(Z^t) \coloneqq p(x^t|Z^t) \sum_{z^{t-1}} \alpha(z^{t-1}) p(Z^t|z^{t-1}) \\ &\beta(Z^T) \coloneqq 1 \\ &\text{For } t = T, \dots, 0 \text{ do} \\ &\beta(Z^t) \coloneqq \sum_{z^{t+1}} \beta(z^{t+1}) p(x^{t+1}|z^{t+1}) p(z^{t+1}|Z^t) \\ &\text{Return } \alpha(Z^0), \dots, \alpha(Z^T), \beta(Z^0), \dots, \beta(Z^T) \end{split}$$

- Unlike the LS algorithm, the FB algorithms cosists of two independent steps.
- Filtering: $p(Z^t|x^{0:t}) = \frac{\alpha(Z^t)}{\sum_{z^t} \alpha(z^t)}$.
- ► Smoothing: $p(Z^t|X^{0:T}) = \frac{\alpha(Z^t)\beta(Z^t)}{\sum_{z^t}\alpha(z^t)\beta(z^t)}$.

Hidden Markov Models: Viterbi Algorithm

▶ To compute the most probable configuration for HMMs.

Viterbi algorithm

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\begin{split} &\omega(Z^0) \coloneqq \log p(Z^0) + \log p(x^0|Z^0) \\ &\text{For } t = 0, \dots, T \text{ do} \\ &\omega(Z^{t+1}) \coloneqq \log p(x^{t+1}|Z^{t+1}) + \max_{z^t} [\log p(z^{t+1}|z^t) + \omega(z^t)] \\ &\psi(Z^{t+1}) \coloneqq \arg \max_{z^t} [\log p(z^{t+1}|z^t) + \omega(z^t)] \\ &\text{For } t = T, \dots, 0 \text{ do} \\ &u_{\max}^{t} \coloneqq \psi(u_{\max}^{t+1}) \\ &\text{Return } u_{\max}^{t:T} \end{split}
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Exercise. Prove that the Viterbi algorithm is correct.

Autoregressive Hidden Markov Models

▶ To overcome the poor modeling of long range correlations in HMMs, by allowing $pa_G(X^t) \neq \emptyset$.

$$Z^{0} \xrightarrow{} Z^{1} \xrightarrow{} Z^{2} \xrightarrow{} Z^{3} \xrightarrow{} Z^{4}$$

$$\downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow$$

$$X^{0} \xrightarrow{} X^{1} \xrightarrow{} X^{2} \xrightarrow{} X^{3} \xrightarrow{} X^{4}$$

- Exercise. Derive the EM algorithm for AR-HMMs with $pa_G(X^t) = \{X^{t-1}\}$. Specifically, derive the recursive expressions for $\alpha(Z^t)$ and $\beta(Z^t)$ to be used in the FB algorithm.
- Hint.

$$\begin{split} \rho(Z^{t}|x^{0:T}) &= \frac{p(x^{0:t-1}, x^{t+1:T}|Z^{t}, x^{t})p(Z^{t}, x^{t})}{p(x^{0:T})} \\ &= \frac{p(x^{0:t-1}|Z^{t}, x^{t})p(Z^{t}, x^{t})p(x^{t+1:T}|Z^{t}, x^{t})}{p(x^{0:T})} \text{ by } X^{0:t-1} \bot_{p} X^{t+1:T}|Z^{t} \cup X^{t} \\ &= \frac{p(x^{0:t}, Z^{t})p(x^{t+1:T}|Z^{t}, x^{t})}{p(x^{0:T})} = \frac{\alpha(Z^{t})\beta(Z^{t})}{\sum_{z^{t}} \alpha(z^{t})\beta(z^{t})} \end{split}$$

Autoregressive Hidden Markov Models

Hint.

$$\begin{split} \rho(Z^{t},Z^{t+1}|x^{0:T}) &= \frac{\rho(x^{0:t-1},x^{t+2:T}|Z^{t},Z^{t+1},x^{t},x^{t+1})\rho(Z^{t},Z^{t+1},x^{t},x^{t+1})}{\rho(x^{0:T})} \\ &= \frac{\rho(x^{0:t-1}|Z^{t},x^{t})\rho(x^{t+2:T}|Z^{t+1},x^{t+1})\rho(x^{t+1}|Z^{t+1},x^{t})\rho(Z^{t+1}|Z^{t})\rho(Z^{t},x^{t})}{\rho(x^{0:T})} \\ & \text{by } X^{0:t-1} \bot_{\rho} X^{t+2:T}|Z^{t} \cup Z^{t+1} \cup X^{t} \cup X^{t+1} \\ & X^{0:t-1} \bot_{\rho} Z^{t+1} \cup X^{t+1}|Z^{t} \cup X^{t} \\ & X^{t+2:T} \bot_{\rho} Z^{t} \cup X^{t}|Z^{t+1} \cup X^{t+1} \\ & X^{t+1} \bot_{\rho} Z^{t}|Z^{t+1} \cup X^{t} \\ & Z^{t+1} \bot_{\rho} X^{t}|Z^{t} \\ &= \frac{\alpha(Z^{t})\beta(Z^{t+1})\rho(x^{t+1}|Z^{t+1},x^{t})\rho(Z^{t+1}|Z^{t})}{\sum_{z^{t}} \sum_{z^{t+1}} \alpha(z^{t})\beta(z^{t+1})\rho(x^{t+1}|z^{t+1},x^{t})\rho(z^{t+1}|z^{t})} \end{split}$$

Exercise. Derive the Viterbi algorithm for AR-HMMs.