Markov and Hidden Markov Models

COMP9418 — Advanced Topics in Statistical Machine Learning

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Acknowledgments

- [Barber, BRML, 2012] Bayesian Reasoning and Machine Learning, David Barber, 2012
  `www.cs.ucl.ac.uk/staff/D.Barber/brml`

Aims (1)

This lecture will allow you to understand and apply some common probabilistic models for sequential data. In particular, following it you should be able to:

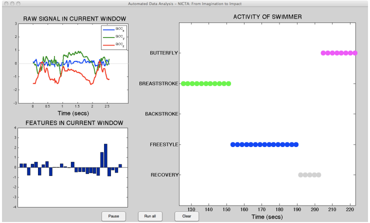
- Apply fully-observable Markov models to the analysis of sequential data.
- Carry out parameter estimation in first-order Markov chains and understand the complexity of this task for higher-order models.
- Carry out clustering of sequential data via mixtures of Markov chains.
- Understand how state space models capture long-term dependencies via the introduction of latent variables.

Aims (2)

- Distinguish the main inference problems, namely smoothing, filtering and prediction, that we can address with Hidden Markov Models (HMMs).
- Solve the above inferential problems along with the most-likely-hidden-path problem via efficient recursions in HMMs.
- Train HMMs for whole-sequence classification and time-dependent classification using a generative or a discriminative approach.

Dealing with Sequential Data (1)

Activity Recognition using Wearable Sensors



Observations may be correlated in time.

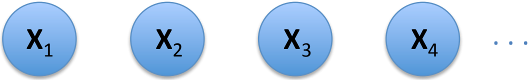
Dealing with Sequential Data (2)

- So far we have assumed iid data
  - Likelihood factorizes across observations
- This is unrealistic for many situations where data is inherently **sequential**
- Temporal data: financial forecasting, currency exchange rate, speech, sensor data, tracking
- Non-temporal data: sequence of characters in an english sentence, sequence of nucleotides in DNA
- We will assume stationary distributions, i.e. independence of time
  - But only the data evolves in time

How to Model Dependencies in Sequential Data?

- Recent observations are more informative than historical ones
- Can have fully observed models where variables are linked through statistical dependencies
- Alternative, we can introduce latent variables (cf Gaussian mixtures)

- We can simply ignore the sequential nature of the data.



Simplest Approach First?

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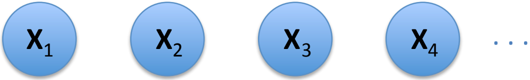

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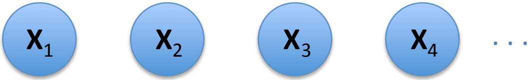

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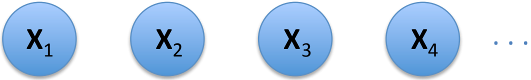

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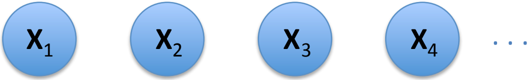

- Example: Binary variable: rain/not rain a day
- Predicting rain/not rain tomorrow would simply account for frequencies
- Clearly historical observations (at least short term) are important!
- But if you live in Scotland you do not need any model!

Outline

1. Markov Chains

2. Mixtures of Markov Chains

3. Hidden Markov Models

General Formulation for Fully Observable Models

Notation: We will denote $\mathbf{y}_{1:T} \stackrel{\text{def}}{=} \mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_T$

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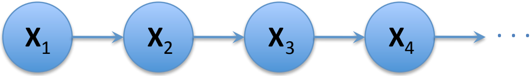
Our initial approach will be to drop some of the long-term dependencies in: $p(\mathbf{x}_t|\mathbf{x}_{1:t-1}) = p(\mathbf{x}_t|\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{t-1})$

First Order Markov Chain

- A Markov chain is defined on either discrete or continuous variables.
- In a first order Markov chain each observation only depends on its immediate past:



$$p(\mathbf{x}_{1:t}) = p(\mathbf{x}_1) \prod_{t=1}^{T} p(\mathbf{x}_t | \mathbf{x}_{t-1}).$$

- If the chain is **stationary** $p(\mathbf{x}_t = \mathbf{s} | \mathbf{x}_{t-1} = \mathbf{s}') = f(\mathbf{s}, \mathbf{s}')$
    - Sometimes this is also called homogeneous

Transition Diagram

Consider a discrete state Markov chain with 3 states and define the **transition probabilities**: $A_{ij} = p(x_t = i | x_{t-1} = j)$:

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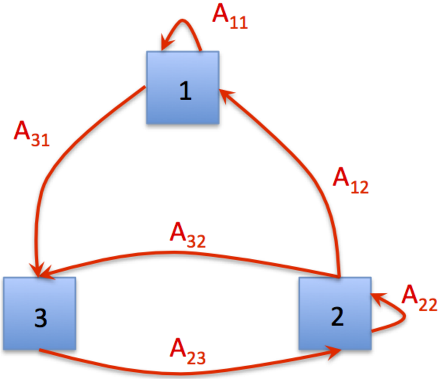

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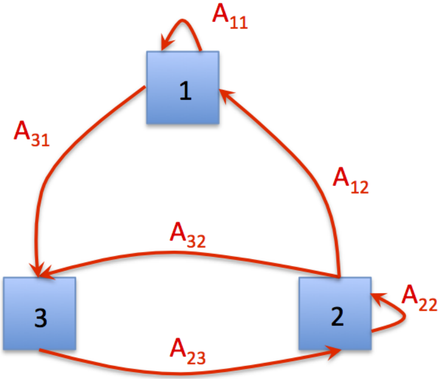

Missing link from i to j simply indicates that $A_{ji} = 0$.

Inference on a Markov Chain

Marginal Distribution

Given a discrete-state first-order Markov chain with K states, we are interested in the marginal:

$$p(x_t = i) = \sum_{j=1}^{K} \underbrace{p(x_t = i | x_{t-1} = j)}_{A_{ij}} p(x_{t-1} = j)$$

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Interpretation: The frequency that we visit a state at (time) step t given that we started from $p(x_1)$ and drew samples from the transition model.

Equilibrium Distribution of a Markov Chain

$$A = \begin{pmatrix} 0.9000 & 0.3000 \\ 0.1000 & 0.7000 \end{pmatrix} \quad A^5 = \begin{pmatrix} 0.7694 & 0.6917 \\ 0.2306 & 0.3083 \end{pmatrix}$$

$$A^{10} = \begin{pmatrix} 0.7515 & 0.7455 \\ 0.2485 & 0.2545 \end{pmatrix} \quad A^{20} = \begin{pmatrix} 0.7500 & 0.7500 \\ 0.2500 & 0.2500 \end{pmatrix}$$

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Do all Markov chains have an equilibrium distribution?

Let us define the matrix $\mathbf{H}$ such that:

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An overly simplistic search engine:

1. For each website list the words associated with it
2. Make an "inverse" list of websites containing word w
3. Rank websites containing w according to equilibrium distribution

Learning the Parameters of a Markov Chain

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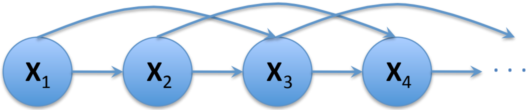
Simply counting occurrences and transitions!

Second Order Markov Chains

We can consider more complex dependencies:



Now the current observation depends on the two previous time steps.

The parameterization for the transitions would be:

$$p(\mathbf{x}_t | \mathbf{x}_{t-2}, \mathbf{x}_{t-1}),$$

which for K-state discrete variables would correspond to $(K-1)(K^2)$ parameters.

How many parameters did we need for the first order Markov chain?

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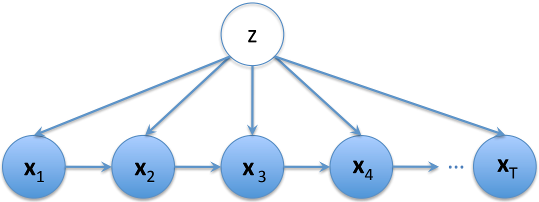
  - Our old trick of introducing latent variables
  - As e.g. in the mixture of Gaussians case

Mixtures of Markov Chains

How do we **cluster** a set of observation sequences $\mathcal{D} = \{x_{1:T}^n\}_{n=1}^N$ where $x_t \in \{1, \ldots, K\}$?



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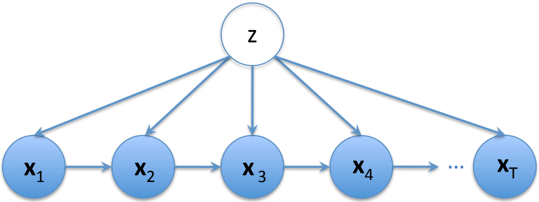

- Mixture model with latent variable $z \in \{1, \ldots, M\}$.
- Markov chain conditioned on the latent variable z:

$$p(x_{1:T}|z) = p(x_1|z) \prod_{t=2}^{T} p(x_t|x_{t-1}, z)$$

The marginal distribution is given by:

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As with the GMM, direct likelihood optimization is hard.

Instead we use EM obtaining the following updates:

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These are similar updates to the single Markov chain's but weighted by the posterior $P(z^i = m|\mathbf{x}^i, \theta^{old})$.

The posterior $P(z^i = m|\mathbf{x}^i, \theta^{old})$ can be computed from the above updates straightforwardly (E step). How?

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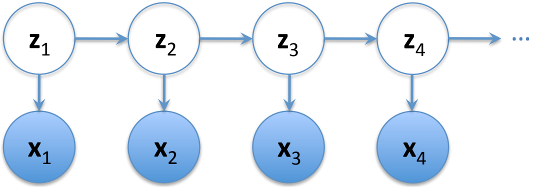

State Space Models

Introducing Complex Dependencies through Latent Variables

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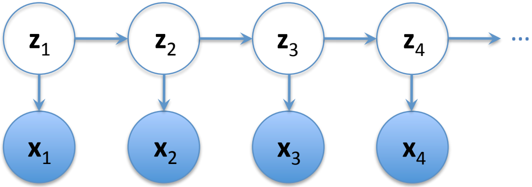
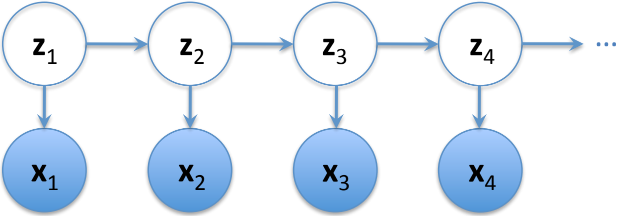


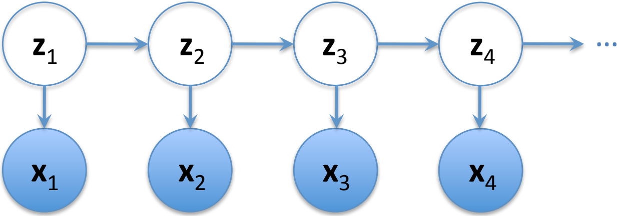
This is known as a state space model.



Joint distribution:

$$p(\mathbf{x}_{1:T}, \mathbf{z}_{1:T}) = p(\mathbf{z}_1)p(\mathbf{x}_1|\mathbf{z}_1)\prod_{t=2}^{T} p(\mathbf{z}_t|\mathbf{z}_{t-1})p(\mathbf{x}_t|\mathbf{z}_t)$$

State Space Models
Properties



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Predictions for $\mathbf{x}_t$ depend on all the previous observations!

State Space Models

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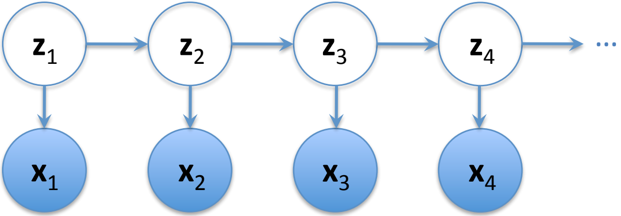

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Predictions for $\mathbf{x}_t$ depend on all the previous observations!

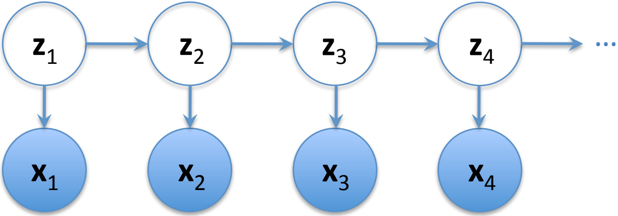
- Can show this using *d-separation*

Hidden Markov models: latent variables are discrete

Linear dynamical systems: latent and visible variables are Gaussian

Hidden Markov Models

Discrete Latent Variables



- Each time slice corresponds to a mixture distribution
- The selection of the mixture component at t depends on the selection of the mixture component at $t-1$
- Widely used in speech recognition, natural language, analysis of biological sequences, etc

Transition Distribution: Assuming $z_t \in \{1, \ldots, K\}$ then:

$$A_{ij} = p(z_t = i | z_{t-1} = j)$$

and an **initial distribution**: $\pi_i = p(z_1 = i)$. So we have a table of $K \times K$ probabilities.

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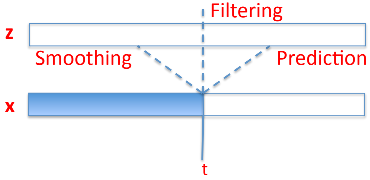
Emission Distribution:

- Discrete states $x_t \in \{1, 2, \ldots S\}$: We have the $S \times K$ emission matrix:

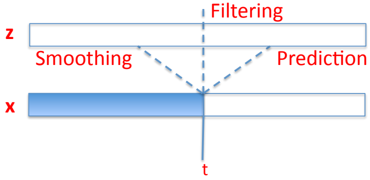
$$B_{ij} = p(x_t = i | z_t = j)$$

- Continuous x_t: z_t selects one of K possible distributions $p(x_t | z_t)$, e.g. a Gaussian: $p(x_t | z_t) = \mathcal{N}(\mathbf{x}_t | \boldsymbol{\mu}_{z_t}, \boldsymbol{\Sigma}_{z_t})$



- Filtering: Inferring the present $p(z_t|x_{1:t})$
- Smoothing: Inferring the past: $p(z_u|x_{1:t})$, $u < t$
- Prediction: Inferring the future: $p(z_s|x_{1:t})$, $s > t$

- Likelihood: $p(x_{1:T})$
- Most likely hidden path (Viterbi alignment): $\text{argmax}_{z_{1:T}}\, p(z_{1:T}|x_{1:T})$



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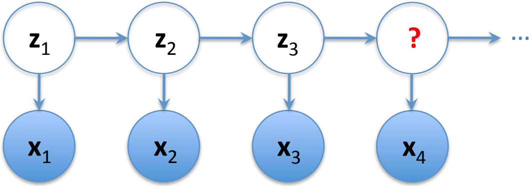
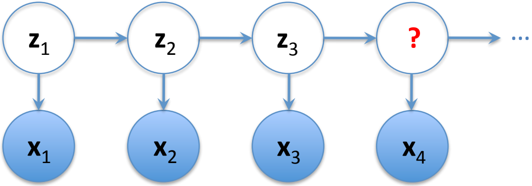
We can use any standard inference method in *graphical models* to solve this problems, e.g. using the Junction Tree Algorithm.

- Instead, we will derive recursions directly.



We can find $p(z_t|x_{1:t})$ by considering $p(z_t, x_{1:t})$ and normalizing accordingly.



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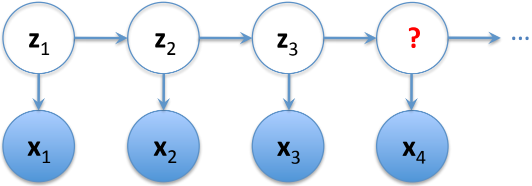
$$p(z_t, x_{1:t}) = \sum_{z_{t-1}} p(z_t, z_{t-1}, x_{1:t-1}, x_t) \quad \text{Def. marginal prob.}$$



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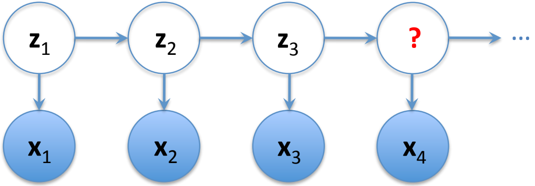
Hidden Markov Models

Filtering (1)



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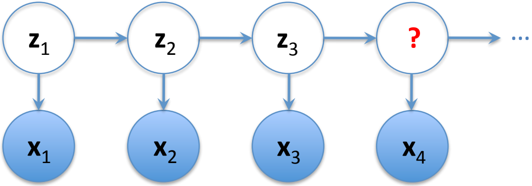
$$\alpha(z_t) = p(x_t|z_t) \sum_{z_{t-1}} p(z_t|z_{t-1}) \alpha(z_{t-1}), \quad t > 1$$



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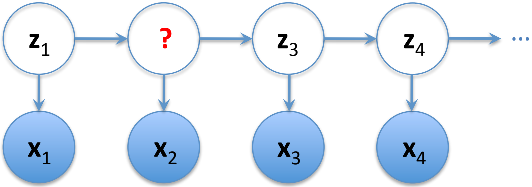
and $\alpha(z_1) = p(z_1)p(x_1|z_1)$

$$\alpha(z_t) = \underbrace{p(x_t|z_t)}_{\text{New evidence}} \underbrace{\sum_{z_{t-1}} \underbrace{p(z_t|z_{t-1})}_{\text{Dynamics}} \alpha(z_{t-1})}_{\text{New prior}}$$

- Filtered distribution propagated forward through the dynamics to reveal a new "prior" at time t
- This distribution is modulated by the observation x_t to incorporate the new evidence

Hidden Markov Models

Smoothing: $p(z_t|x_{1:T})$



Hidden Markov Models

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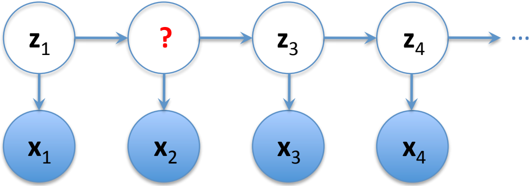

$$p(z_t, x_{1:T}) = p(z_t, x_{1:t}, x_{t+1:T})$$

Hidden Markov Models

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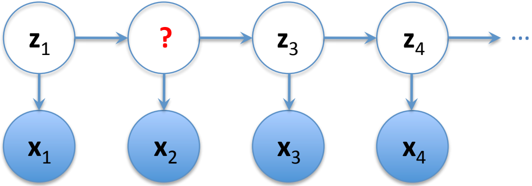

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Hidden Markov Models

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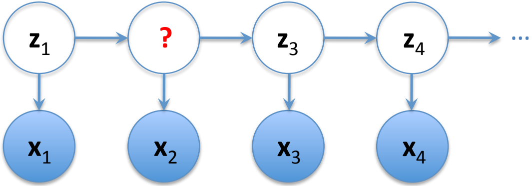

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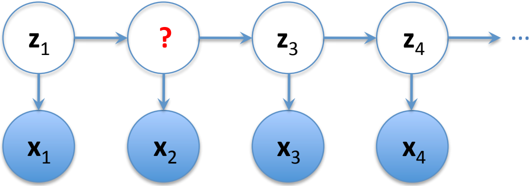

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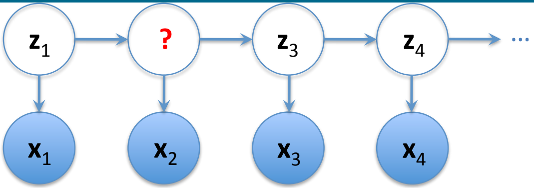
Recursive form for $\alpha(z_t)$ as in filtering. what is $\beta(z_t)$?

Hidden Markov Models

Smoothing: β recursion



Hidden Markov Models

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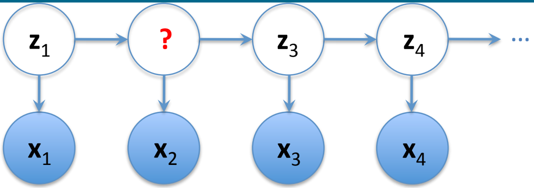

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Hidden Markov Models

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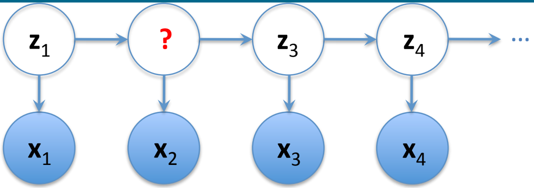

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Hidden Markov Models

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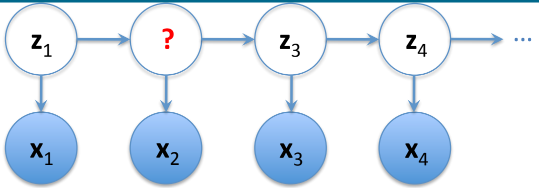

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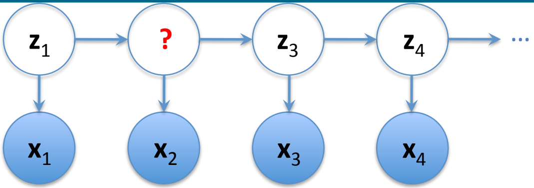
$$\beta(z_{t-1}) = \sum_{z} p(x_t|z_t) p(z_t|z_{t-1}) \beta(z_t) \quad \text{backward recursion!}$$

Hidden Markov Models

Smoothing: β recursion



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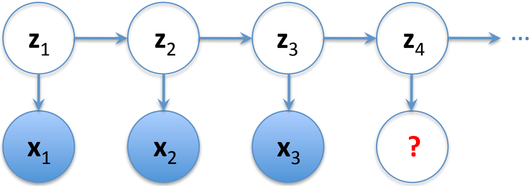
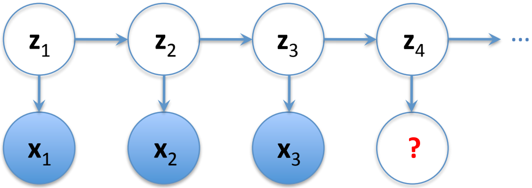
$\beta(z_T) = 1$. **forward-backward algorithm** (or $\alpha - \beta$ recursions)

Recursions can be performed in parallel



$\mathbf{z}_1$
$\mathbf{z}_2$
$\mathbf{z}_3$
$\mathbf{z}_4$
…
$\mathbf{x}_1$
$\mathbf{x}_2$
$\mathbf{x}_3$
?

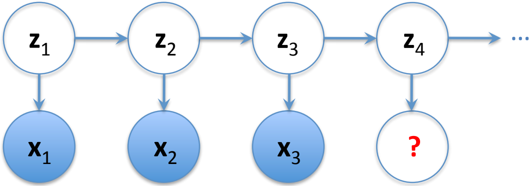


One-step Ahead Prediction:

$$p(x_{t+1}|x_{1:t}) = \sum_{z_t, z_{t+1}} p(x_{t+1}|z_{t+1}) p(z_{t+1}|z_t) \underbrace{p(z_t|x_{1:t})}_{\text{filtering}}$$

Hidden Markov Models

Prediction and Likelihood



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Likelihood Computation:

$$p(x_{1:T}) = \sum_{z_T} p(z_T, x_{1:T}) = \sum_{z_T} \alpha(z_T)$$

It requires only forward computation (filtering).

The most likely hidden path of $p(z_{1:T}|x_{1:T})$ is the same as the most likely state of $p(z_{1:T}, x_{1:T})$.

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Consider maximizing over z_T:

$$
\begin{aligned}
&\max_{z_T} \prod_{t=1}^{T} p(x_t|z_t)p(z_t|z_{t-1}) \\
&= \left(\prod_{t=1}^{T-1} p(x_t|z_t)p(z_t|z_{t-1}) \right) \underbrace{\max_{z_T} p(x_T|z_T)p(z_T|z_{T-1})}_{\mu(z_{T-1})}
\end{aligned}
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$$= \left(\prod_{t=1}^{T-1} p(x_t|z_t)p(z_t|z_{t-1})\right) \underbrace{\max_{z_T} p(x_T|z_T)p(z_T|z_{T-1})}_{\mu(z_{T-1})}$$

Hence we can define:

$$\mu(z_{t-1}) = \max_{z_t} p(x_t|z_t)p(z_t|z_{t-1})\mu(z_t)$$

for $2 \leqslant t \leqslant T$ and with $\mu(z_T) = 1$.

The information propagated backwards regarding maximizing over $z_2, \dots, z_T$ is contained in $\mu(z_1)$. Therefore:

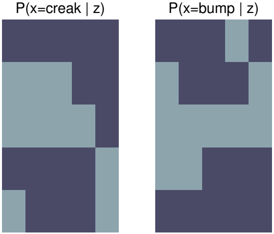
$$z_1^* = \operatorname*{argmax}_{z_1} p(x_1|z_1)p(z_1)\mu(z_1)$$

Then we can compute the others by backtracking:

$$z_t^* = \operatorname*{argmax}_{z_t} p(x_t|z_t)p(z_t|z_{t-1}^*)\mu(z_t)$$

This is a special case of the *max-product* algorithm (in graphical models) and is called **Viterbi Algorithm**.

- You are in bed but have a "mental" partition of the floor as a 5×5 grid
- You know probability of "creak" and "bump" given a position



- Burglar can move only one grid square (left, right, forward, backwards) at time t
- You observe a series of creak/bump information
- Where is the burglar?

Burglar Example (Reproduced from Barber, BRML, 2011): Setting

- Location of the burglar is hidden. Discrete variable $z \in \{1, \ldots, 25\}$
- Absence/presence of creaks and bumps are visible.
- Assume independence and create a new 4-state visible variable using $p(x|z) = p(x^{\text{creak}}|z)p(x^{\text{bump}}|z)$
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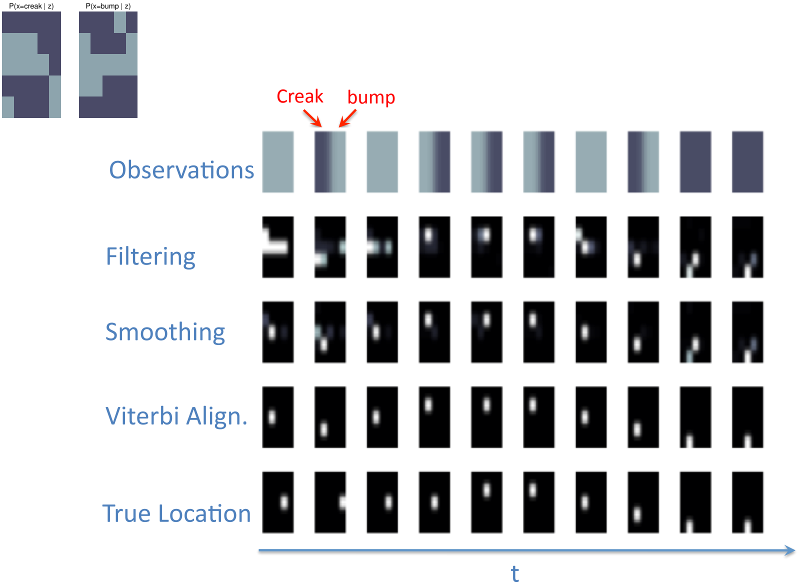
Inference questions:

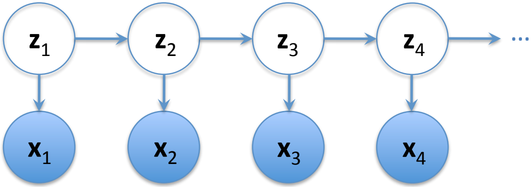
- Where might the burglar be at time t?
- Where could the burglar have been?
  - Important info for the police
- Single best guess for sequence of burglar's positions

HMM Classical Inference Problems

Burglar Example (Reproduced from Barber, BRML, 2011)



Recall our HMM model is given by:



The joint distribution:

$$p(\mathbf{x}_{1:T}, \mathbf{z}_{1:T}) = p(\mathbf{z}_1) p(\mathbf{x}_1|\mathbf{z}_1) \prod_{t=2}^{T} p(\mathbf{z}_t|\mathbf{z}_{t-1}) p(\mathbf{x}_t|\mathbf{z}_t)$$

is parameterized by: $A_{ij} = p(z_t = i|z_{t-1} = j)$, $\pi_i = p(z_1 = i)$ and (assuming discrete observations) $B_{ij} = p(x_t = i|z_t = j)$.

How do we learn these parameters from data?

Given a set of observation sequences $\mathcal{D} = \{x_{1:T}^n\}_{n=1}^N$ where $x_t \in \{1, \ldots, S\}$ (assume we know the number of hidden states K)

Goal: learn $\theta = \{\mathbf{A}, \boldsymbol{\pi}, \mathbf{B}\}$

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We can try direct log likelihood maximization:

$$\mathcal{L}(\theta) = \sum_{n=1}^{N} \log \sum_{\mathbf{z}} p(\mathbf{x}_{1:T}^n, z_{1:T}^n | \theta)$$

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What can we do?

As in GMMs, we can use the complete data log-likelihood:

$$\mathcal{L}^{\text{comp}}(\theta) = \sum_{n=1}^{N} \log p(\mathbf{x}^n, \mathbf{z}^n | \theta),$$

and iterate:

1. compute its **expectation** over the posterior $\langle \mathcal{L}^{\text{comp}} \rangle_{p(\mathbf{Z}|\mathbf{X},\theta^{\text{old}})}$
2. **Maximize** this expectation wrt θ

In the M-step we need to maximize the objective function:

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \left\langle \sum_{n=1}^{N} \log p(\mathbf{x}^n, \mathbf{z}^n | \boldsymbol{\theta}) \right\rangle_{p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})}$$

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\end{aligned}
$$

wrt $\theta = \{\mathbf{A}, \pi, \mathbf{B}\}$ subject to the usual normalization constraints.

Performing the corresponding derivatives we get the following updates:

$$\pi_i = p(z_1 = i) = \frac{1}{N}\sum_{n=1}^{N} p(z_1^n = i | x_{1:T}^n, \theta^{\text{old}})$$

$$A_{ij} = p(z_t = i | z_{t-1} = j) \propto \sum_{n=1}^{N}\sum_{t=2}^{T} p(z_t^n = i, z_{t-1}^n = j | x_{1:T}^n, \theta^{\text{old}})$$

$$B_{sj} = p(x_t = s | z_t = j) \propto \sum_{n=1}^{N}\sum_{t=1}^{T} \mathbb{I}[x_t^n = s] p(z_t^n = j | x_{1:T}^n, \theta^{\text{old}})$$

Interpretation?

how to deal with different-length sequences?

In the E-step, based on the old parameters, we need to update the distributions:

$$p(z_1 = i | x_{1:T}, \theta^{\text{old}}) \quad \text{and} \quad p(z_t = j | x_{1:T}, \theta^{\text{old}})$$

What classical inference problem are we addressing there?

What about $p(z_t = i, z_{t-1} = j | x_{1:T}, \theta^{\text{old}})$?

- This is a pairwise marginal, which can be shown to be:

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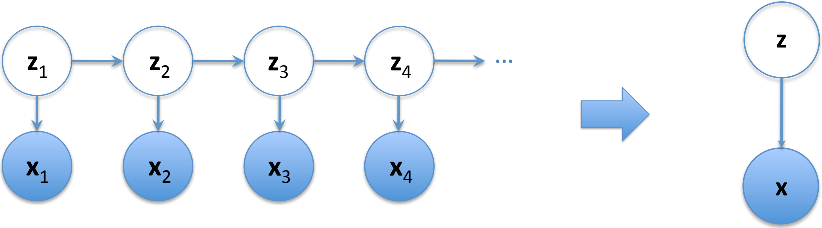
This is an interesting example where learning requires the computation of non-straightforward marginals (inference)

Repeat Until convergence (e.g. using data likelihood):

1. Initialize parameters $\theta^{\text{old}} = \{\mathbf{A}, \boldsymbol{\pi}, \mathbf{B}\}$
2. Run forward-backward recursions to compute corresponding posteriors $p(z_1 = i | x_{1:T}, \theta^{\text{old}})$, $p(z_t = j | x_{1:T}, \theta^{\text{old}})$, $p(z_t = i, z_{t-1} = j | x_{1:T}, \theta^{\text{old}})$
3. Update parameters $\mathbf{A}$, $\boldsymbol{\pi}$, $\mathbf{B}$ using these posteriors accordingly
4. Evaluate likelihood as convergence criterion

- EM is plagued with local optima and a good parameter initialization is needed
- This is specially critical for the emission distribution
- Can initialize $p(x_t|z_t)$ with a simple (non-temporal) mixture model, i.e. $p(x) = \sum_z p(z)p(x|z)$



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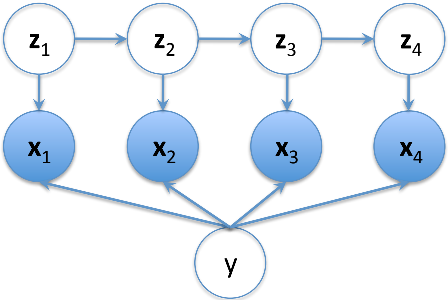
- The **HMM-GMM** model uses a mixture of Gaussians as the emission distribution
  - Popular in tracking and speech recognition

Sequence Classification with HMMs

We want to classify complete sequences based on labeled data $\mathcal{D} = \{(x^n_{1:T_n}, y^n)\}_{n=1}^N$, e.g. $y \in \{\text{swimming, no swimming}\}$



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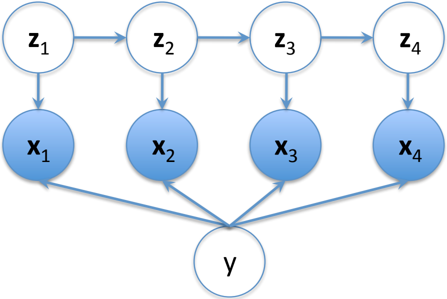

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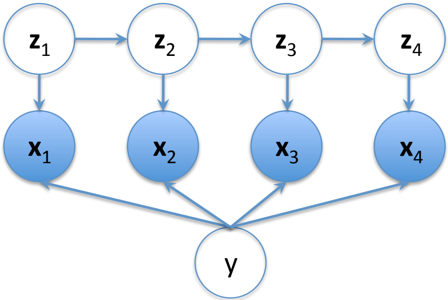

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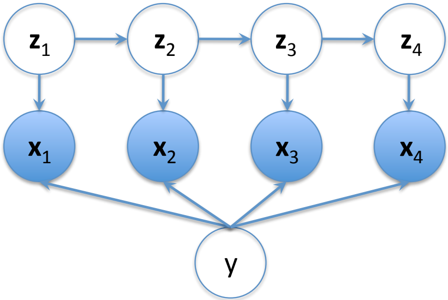

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- However this is inherently **generative**, any problems?
- In many applications, it is customary to train C HMMs in a **discriminative** way

Discriminative Training of HMMs for Sequence Classification

- Define a new single discriminative model using the C HMMs:

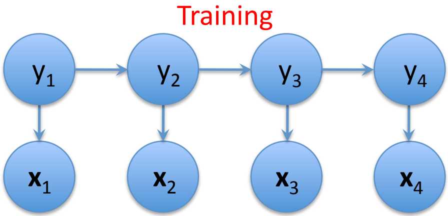
$$p(y|\mathbf{x}_{1:T}) = \frac{p(\mathbf{x}_{1:T}|y)}{\sum_{y'=1}^{C} p(\mathbf{x}_{1:T}|y')p(y')}$$

- Then maximise the likelihood of the classes and corresponding observations $\mathbf{x}_{1:T}$:

$$\mathcal{L} = \sum_{n=1}^{N} \log p(y^{(n)}|\mathbf{x}_{1:T}^{(n)})$$

- EM-style updates no longer possible
- Learning via gradient-based optimization

We can also be given time-dependent labels $\mathcal{D} = \{(\mathbf{x}^n_{1:T_n}, y^n_{1:T_n})\}_{n=1}^N$



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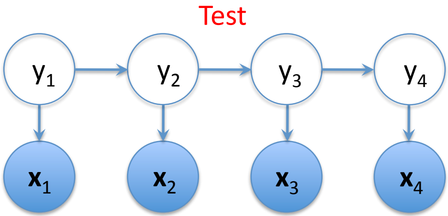

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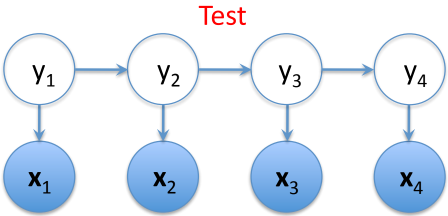

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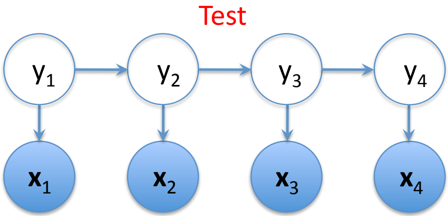

How would you train this model? How would you make predictions?
Alternatively, we can be **discriminative** by realizing that:
$p(x_t|y_t) \propto \tilde{p}(y_t|x_t)\tilde{p}(x_t)$

- Learn transitions and discriminative model $\tilde{p}(y_t|x_t)$ separately and do Viterbi decoding afterwards.

We have seen that standard HMMs are inherently generative.

- We model the joint $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{y})$
- We make predictions $p(\mathbf{y}|\mathbf{x})$ using Bayes' rule

If we lack prior information and only care about discriminating between patterns given a set of features:

- We can model $p(\mathbf{y}|\mathbf{x})$ directly.
- This will avoid making unrealistic assumptions about the density of $\mathbf{x}$

Such an approach is adopted by Conditional Random Fields

Summary and Conclusions

- Modelling dependencies in sequential data is essential
- Difficult trade-off flexibility vs complexity in fully observable models
- Use trick of introducing latent variables
- Hidden Markov Models are an elegant way of modelling long-term dependencies in observations
- Reading: Barber (BRML, 2017) Ch 23 (except sec 23.4)