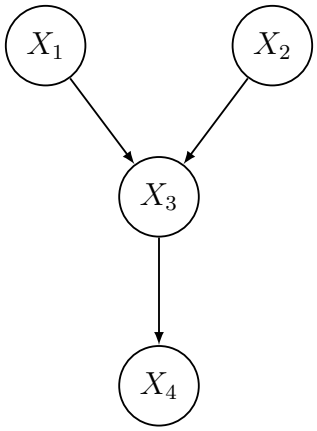
CS 181: Bayesian Networks, HMMs, and Kalman Filters

Week of April 9, 2018
Harvard University

1 Variable Elimination in Bayesian Networks

Recall that a Bayesian network is a graphical model that represents random variables and their dependencies using a directed acyclic graph. They allow us to efficiently model joint distributions over many variables by taking advantage of the local dependencies between variables, and they form the foundation of other models that we'll explore today.

In this section, we discuss an exact inference algorithm called variable elimination. Consider the Bayesian network we saw in lecture:



Assume that all of the random variables are Bernoulli, meaning their domain is $\{0, 1\}$, and thus the domain size $k = 2$. In this network, we can encode the joint distribution as

$$p(x_1, x_2, x_3, x_4) = p(x_3|x_1, x_2)p(x_4|x_3)p(x_1)p(x_2) \tag{1}$$

If we wanted to calculate the marginal distribution of X_4, we could naively marginalize out the other variables, giving us

$$p(x_4) = \sum_{x_1} \sum_{x_2} \sum_{x_3} p(x_3|x_1, x_2)p(x_4|x_3)p(x_1)p(x_2) \tag{2}$$

Calculating this naively requires multiplying 4 values for each of the 8 possible combinations of x_1, x_2, x_3. In general, if there were many variables then

the number of combinations would grow exponentially in the number of variables!

However, note that because we have a compact, Bayesian net representation, we can calculate the marginal distribution more efficiently. By reordering the sums and eliminating one variable at a time, we derive the variable elimination procedure. For example, we can calculate the joint distribution as:

$$
\begin{aligned}
p(x_4) &= \sum_{x_1,x_2,x_3} p(x_3|x_1,x_2)p(x_4|x_3)p(x_1)p(x_2) && (3)\\
&= \sum_{x_2,x_3} p(x_4|x_3)p(x_2) \sum_{x_1} p(x_3|x_1,x_2)p(x_1) && (4)\\
&= \sum_{x_3} p(x_4|x_3) \sum_{x_2} p(x_2)p(x_3|x_2) && (5)\\
&= \sum_{x_3} p(x_4|x_3)p(x_3) && (6)\\
&= p(x_4) && (7)
\end{aligned}
$$

Here, we eliminate x_1, then x_2, then x_3. This is working in 'leaves first' order towards the query, x_4. Alternatively, we could have eliminated variables in a different order, as follows:

$$
\begin{aligned}
p(x_4) &= \sum_{x_1,x_2,x_3} p(x_3|x_1,x_2)p(x_4|x_3)p(x_1)p(x_2) && (8)\\
&= \sum_{x_1,x_2} p(x_1)p(x_2) \sum_{x_3} p(x_3|x_1,x_2)p(x_4|x_3) && (9)\\
&= \sum_{x_1} p(x_1) \sum_{x_2} p(x_2)p(x_4|x_1,x_2) && (10)\\
&= \sum_{x_1} p(x_1)p(x_4|x_1) && (11)\\
&= p(x_4) && (12)
\end{aligned}
$$

Here, we eliminate x_3, then x_2, then x_1.

Variable Elimination. For the following questions, consider the Bayesian network described above, and assume the following CPTs:

x_1	$p(x_1)$
0	0.3
1	0.7

x_2	$p(x_2)$
0	0.6
1	0.4

x_3	x_1	x_2	$p(x_3\|x_1, x_2)$
0	0	0	0.5
0	0	1	0.2
0	1	0	0.9
0	1	1	0.5
1	0	0	0.5
1	0	1	0.8
1	1	0	0.1
1	1	1	0.5

x_4	x_3	$p(x_4\|x_3)$
0	0	0.7
0	1	0.1
1	0	0.3
1	1	0.9

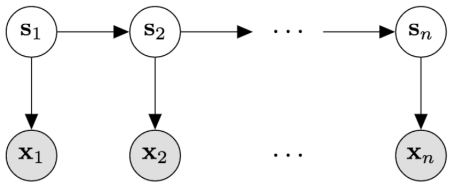
1. First use variable elimination on X_1. Draw the resulting Bayesian network and compute the CPT.
2. First use variable elimination on X_3. Draw the resulting Bayesian network and compute the CPT.

How many sum-product calculations do each of these variable elimination orders require? Which one is preferable?

2 Hidden Markov Models

Last week in lecture, we covered Hidden Markov Models (HMMs). This model is useful for inferring a sequence of unknown states from a corresponding sequence of observed evidence.

2.1 HMM Graphical Model



Consider a sequence of one-hot encoded states $\mathbf{s}_1$,...,$\mathbf{s}_n$ where $\mathbf{s}_t \in \{S_k\}_{k=1}^c$ and a corresponding sequence of observations ($\mathbf{x}_1$,...,$\mathbf{x}_n$) where $\mathbf{x}_t \in \{O_j\}_{j=1}^m$. Each state can be one of c possible states, and each observation can be one of m possible observations. Note that N is the number of data points (each of which is a sequence), where n is the length of a sequence (assume all sequences are the same length). HMMs are characterized by, and help us reason about, the following joint distribution:

$$\begin{aligned} p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_n, \mathbf{x}_1, \ldots, \mathbf{x}_n) = \\ p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_n) p(\mathbf{x}_1, \ldots, \mathbf{x}_n \mid \boldsymbol{s}_1, \ldots, \boldsymbol{s}_n) = \\ p(\boldsymbol{s}_1) \prod_{t=1}^{n-1} p(\boldsymbol{s}_{t+1} \mid \boldsymbol{s}_t) \prod_{t=1}^{n} p(\mathbf{x}_t \mid \boldsymbol{s}_t) \end{aligned}$$

Parameters:

- $\boldsymbol{\theta}$: distribution over initial states, $c \times 1$
- $\mathbf{T}$: $c \times c$ transition matrix such that t_{kj} is the probability of transitioning from S_k to S_j
- $\{\boldsymbol{\pi}\}_{k=1}^c$: state conditional observation probabilities such that $p(\mathbf{x}_t = O_j | \mathbf{s}_t = S_k; \{\boldsymbol{\pi}\}) = \pi_{kj}$. Each $\boldsymbol{\pi}_k$ is $m \times 1$.

Our goals are twofold. First, we need to estimate the parameters from the data. We will do this with a special variant of EM. Then, with our trained HMM, we are able to perform several inference tasks on our data, including smoothing, prediction, and more (see below).

2.2 Properties of HMMs

- future is independent of past given present (Markov Property): $p(\boldsymbol{s}_{t+1} \mid \boldsymbol{s}_1, \ldots \boldsymbol{s}_t, \mathbf{x}_1, \ldots, \mathbf{x}_t) = p(\boldsymbol{s}_{t+1} \mid \boldsymbol{s}_t)$
- observations only depend on present: $p(\mathbf{x}_t \mid \boldsymbol{s}_1, \ldots, \boldsymbol{s}_t, \mathbf{x}_1, \ldots, \mathbf{x}_{t-1}) = p(\mathbf{x}_t \mid \boldsymbol{s}_t)$

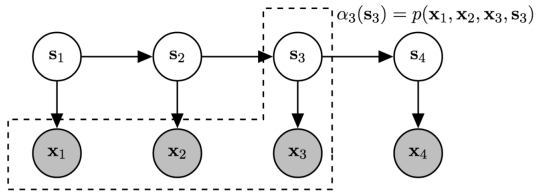
2.3 EM for HMMs: finding parameters with the Baum-Welch Algorithm

Given data points $\{\mathbf{x}^i\}_{i=1}^N$ defined by sequences $(x_1^i, \ldots, x_n^i)$ of length n represented as row vectors, we want to infer the parameters $\{\mathbf{T}, \boldsymbol{\theta}, \{\boldsymbol{\pi}_k\}\}$. Had we been given the true states, we could easily compute joint probability $p(\mathbf{x}^i, \mathbf{s}^i)$ and write the complete-data log likelihood, and maximize with respect to the parameters. Instead, we must proceed by estimating state distributions and parameters iteratively.

2.3.1 Forward-Backward

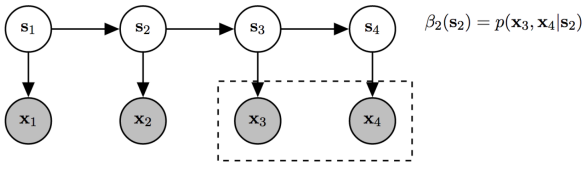
The HMM model is characterized by the joint distribution $p(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_n, \mathbf{x}_1, \ldots, \mathbf{x}_n)$, which means that many of our training and inference tasks are an issue of marginalizing to obtain conditionals. Thus, naive algorithms can be expensive (lots of nested summations over states). EM for HMMs using the efficient Forward-Backward inference algorithm is called the Baum-Welch algorithm. Following the algorithm, we define the recurrence relations $\alpha_t(\boldsymbol{s}_t)$ and $\beta_t(\boldsymbol{s}_t)$ in the E step:

- $\alpha_t(\mathbf{s}_t)$ represents the joint probability of observations $1, \ldots, t$ and state t. α_t can be defined in terms of α_{t-1}. Move **forwards** through the sequence to calculate the α's
- $\beta_t(\mathbf{s}_t)$ represents the joint probability of observations $t+1, \ldots, n$ conditioned on state t. β_t can be defined in terms of β_{t+1}. Move **backwards** through the sequence to calculate the β's.



$$\forall \mathbf{s}_3 : \quad \alpha_3(\mathbf{s}_3) = p(\mathbf{x}_3 \mid \mathbf{s}_3) \sum_{\mathbf{s}_2} p(\mathbf{s}_3 \mid \mathbf{s}_2) \alpha_2(\mathbf{s}_2)$$

(a) alpha



$$\forall \mathbf{s}_2 : \quad \beta_2(\mathbf{s}_2) = \sum_{s_3} p(\mathbf{s}_3 \mid \mathbf{s}_2) p(\mathbf{x}_3 \mid \mathbf{s}_3) \beta_3(\mathbf{s}_3)$$

(b) beta

The probabilities used in the α and β definitions come from the parameters that we fix in the E step.

$$\forall \mathbf{s}_t: \quad \alpha_t(\mathbf{s}_t) = \begin{cases} p(\mathbf{x}_t \,|\, \mathbf{s}_t) \sum_{\mathbf{s}_{t-1}} p(\mathbf{s}_t \,|\, \mathbf{s}_{t-1}) \alpha_{t-1}(\mathbf{s}_{t-1}) & \text{if } 1 < t \leq n \\ p(\mathbf{x}_1 \,|\, \mathbf{s}_1) p(\mathbf{s}_1) & \text{o.w.} \end{cases}$$

$$\forall \mathbf{s}_t: \quad \beta_t(\mathbf{s}_t) = \begin{cases} \sum_{\mathbf{s}_{t+1}} p(\mathbf{s}_{t+1} \,|\, \mathbf{s}_t) p(\mathbf{x}_{t+1} \,|\, \mathbf{s}_{t+1}) \beta_{t+1}(\mathbf{s}_{t+1}) & \text{if } 1 \leq t < n \\ 1 & \text{o.w.} \end{cases}$$

2.3.2 Inference Patterns with $\boldsymbol{\alpha}, \boldsymbol{\beta}$

The following patterns are useful for inference with a trained HMM, but also in the E step during training (basically, any time we are considering the parameters fixed):

- $\alpha_t(\mathbf{s}_t)\beta_t(\mathbf{s}_t) = p(\mathbf{x}_1, \ldots, \mathbf{x}_n, \mathbf{s}_t) \propto p(\mathbf{s}_t | \mathbf{x}_1, \ldots, \mathbf{x}_n)$
- joint of observations: $p(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \sum_{\mathbf{s}_t} \alpha_t(\mathbf{s}_t)\beta_t(\mathbf{s}_t)$ (for any t)
- smoothing: $p(\mathbf{s}_t \,|\, \mathbf{x}_1, \ldots, \mathbf{x}_n) \propto p(\mathbf{x}_1, \ldots, \mathbf{x}_n, \mathbf{s}_t) = \alpha_t(\mathbf{s}_t)\beta_t(\mathbf{s}_t)$
- prediction: $p(\mathbf{x}_{n+1} \,|\, \mathbf{x}_1, \ldots, \mathbf{x}_n) \propto \sum_{\mathbf{s}_n, \mathbf{s}_{n+1}} \alpha_n(\mathbf{s}_n) p(\mathbf{s}_{n+1} \,|\, \mathbf{s}_n) p(\mathbf{x}_{n+1} \,|\, \mathbf{s}_{n+1})$
- transition: $p(\mathbf{s}_t, \mathbf{s}_{t+1} \,|\, \mathbf{x}_1, \ldots, \mathbf{x}_n) \propto \alpha_t(\mathbf{s}_t) p(\mathbf{s}_{t+1} \,|\, \mathbf{s}_t) p(\mathbf{x}_{t+1} \,|\, \mathbf{s}_{t+1}) \beta_{t+1}(\mathbf{s}_{t+1})$

2.3.3 E step

For sequence $\mathbf{x}^i$ and a fixed set of parameters $\mathbf{w} = \{\mathbf{T}, \boldsymbol{\theta}, \{\boldsymbol{\pi}_k\}\}$, we estimate the state distribution for $\mathbf{s}_1^i, \ldots, \mathbf{s}_n^i$ given $\mathbf{x}^i$. Let the $c \times 1$ vector $\mathbf{q}_t^i = (q_{t1}^i, \ldots, q_{tc}^i)$ represent $\mathbf{x}^i$'s distribution over states for time t under the current parameters. Let $\mathbf{Q}_{t,t+1}^i$ be the $c \times c$ matrix of transition probabilities under the current parameters.

- α's and β's are defined in terms of fixed parameters.
- $\mathbf{q}$'s defined in terms of α's and β's
- Calculate $q_{tk}^i = p(\mathbf{s}_t^i = S_k | \mathbf{x}^i; \mathbf{w})$ for all t and k (use smoothing eq. just above)
- Calculate $q_{t,t+1,k,\ell}^i = p(\mathbf{s}_t^i = S_k, \mathbf{s}_{t+1}^i = S_\ell | \mathbf{x}^i; \mathbf{w})$ (use transition eq. just above)
- Compute the following $\hat{N}$'s in terms of $\mathbf{q}$'s:

$$\hat{N}_{1k} = \sum_{i=1}^{N} q_{1k}^i \text{ (first period)} \quad \text{and more generally} \quad \hat{N}_k = \sum_{i=1}^{N} \sum_{t=1}^{n} q_{tk}^i \text{ (all periods)}$$

$$\hat{N}_{-nk} = \sum_{i=1}^{N} \sum_{t=1}^{n-1} q_{tk}^i \text{ (without last period)}$$

$$\hat{N}_{k\ell} = \sum_{i=1}^{N} \sum_{t=1}^{n-1} q^i_{t,t+1,k,\ell} \text{ (transitions)}$$

$$\hat{N}_{kj} = \sum_{i=1}^{N} \sum_{t=1}^{n} q^i_{tk} x^i_{tj} \text{ (observations)}$$

2.3.4 M step

Update parameters to maximize the expected complete-data log likelihood $\mathbb{E}_{\mathbf{S}}[\ln p(\mathbf{x}, \mathbf{S}; \mathbf{w})]$. Using the $\hat{N}$'s, we update the parameters in the following way:

$$\hat{\theta}_k = \frac{\hat{N}_{1k}}{N} \quad \hat{\pi}_{kj} = \frac{\hat{N}_{kj}}{\hat{N}_k} \quad \hat{t}_{k\ell} = \frac{\hat{N}_{k\ell}}{\hat{N}_{-nk}}$$

3 Kalman Filters

Now consider the following dynamical system model:

$$z_{t+1} = \Phi z_t + \epsilon_t$$

$$x_t = A z_t + \gamma_t$$

where z are the hidden variables and x are the observed measurements. Φ and A are known constants, while ϵ and γ are random variables drawn from the following normal distributions:

$$\epsilon_t \sim \mathcal{N}(\mu_\epsilon, \sigma_\epsilon^2)$$

$$\gamma_t \sim \mathcal{N}(\mu_\gamma, \sigma_\gamma^2)$$

This is called a (one-dimensional) linear Gaussian state-space model. It is closely related to an HMM – try drawing out the graphical model! – but here the hidden states and the observations are now continuous and normally distributed. Linear Gaussian state-space models have convenient mathematical properties and can be used to describe noisy measurements of a moving object (e.g. missiles, rodents, hands), market fluctuations, and many other processes relevant to computer vision.

The Kalman filter is an algorithm to perform filtering in linear Gaussian state-space models. By filtering, we mean finding the distribution of z_t given observations $x_1, ..., x_t$. The distribution of $z_t \,|\, x_1, ..., x_s$ will be $\mathcal{N}(\mu_{t|s}, \sigma_{t|s}^2)$. If we start with $\mu_{t-1|t-1}$ and $\sigma_{t-1|t-1}^2$, the algorithm tells us to

1. Define the distribution of $z_t \,|\, x_1, ..., x_{t-1}$ by computing $\mu_{t|t-1}$ and $\sigma_{t|t-1}^2$. This is called the prediction step.
2. Define the distribution of $z_t \,|\, x_1, ..., x_t$ by computing $\mu_{t|t}$ and $\sigma_{t|t}^2$. This is called the update step.

The Kalman filter alternates between prediction and update steps, assimilating observations one at a time. It requires one forward pass through the data, and is analogous to obtaining the α's in an HMM. You'll be exploring Kalman filters more in depth during this week's homework assignment.

When to Use HMMs (Source: CMU). For each of the following scenarios, is it appropriate to use a Hidden Markov Model? Why or why not? What would the observed data be in each case, and what would the hidden states capture?

1. Stock market price data
2. Recommendations on a database of movie reviews
3. Daily precipitation data in Boston
4. Optical character recognition for identifying words

Parameter Estimation in Supervised HMMs. You are trying to predict the weather using an HMM model. The hidden states of the HMM are the weather of the day, which may be sunny or rainy, and the observable states are the color of the clouds, which can be white or gray. You have data on the weather and clouds from one sequence of four days (note: you have observed the hidden states too!):

Day	Weather	Clouds
1	Sunny	White
2	Rainy	Gray
3	Rainy	Gray
4	Sunny	Gray

1. Draw a graphical model representing the HMM.
2. Write out the values of N, n, c and of the one-hot vectors $\mathbf{s}_1^1, \ldots, \mathbf{s}_4^1, \mathbf{x}_1^1, \ldots, \mathbf{x}_4^1$.
3. Estimate and interpret the values of the parameters $\boldsymbol{\theta}, \mathbf{T}, \{\boldsymbol{\pi}_k\}_{k=1}^c$ using the MLE estimators for the supervised HMM:

$$\hat{\theta}_k = \frac{N_{1k}}{N}, \quad \hat{t}_{kl} = \frac{N_{kl}}{N_{-nk}}, \quad \hat{\pi}_{kj} = \frac{N_{kj}}{N_k}$$

$$N_k = \sum_{i=1}^{N} \sum_{t=1}^{n} s_{tk}^i, \quad N_{1k} = \sum_{i=1}^{N} s_{1,k}^i, \quad N_{-nk} = \sum_{i=1}^{N} \sum_{t=1}^{n-1} s_{tk}^i$$

$$N_{kl} = \sum_{i=1}^{N} \sum_{t=1}^{n-1} s_{t,k}^i s_{t+1,l}^i, \quad N_{kj} = \sum_{i=1}^{N} \sum_{t=1}^{n} s_{tk}^i x_{tj}^i$$

EM for HMMs. You are trying modeling a toy's state using an HMM. At each time step, the toy can be active (state 1) or inactive (state 2), but you can only observe the color of the indicator light, which can be red (observation state 1) or green (observation state 2). You have collected data from one sequence:

Time	Light
1	Green
2	Red
3	Green

You initialize your EM with $\boldsymbol{\theta} = [\frac{1}{2}\ \frac{1}{2}]^\top, \mathbf{T} = \begin{bmatrix} \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} \end{bmatrix}, \boldsymbol{\pi}_1 = [\frac{1}{4}\ \frac{3}{4}]^\top, \boldsymbol{\pi}_2 = [\frac{3}{4}\ \frac{1}{4}]^\top$.

1. Compute $\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3$ for the forward-backward algorithm using the initial parameter values.
2. How is $\mathbf{q}_t^1$ defined? Compute the values of $\mathbf{q}_1^1, \mathbf{q}_2^1$ using the α and β values.
3. How is $\mathbf{Q}_{t,t+1}^1$ defined? Compute the value of $\mathbf{Q}_{1,2}^1$ using the α and β values.

During EM, at one point you obtain the following values after the E step:

$$\mathbf{q}_1^1 = \begin{bmatrix} \frac{2}{3} & \frac{1}{3} \end{bmatrix}^\top, \quad \mathbf{q}_2^1 = \begin{bmatrix} \frac{1}{3} & \frac{2}{3} \end{bmatrix}^\top, \quad \mathbf{q}_3^1 = \begin{bmatrix} \frac{2}{3} & \frac{1}{3} \end{bmatrix}^\top$$

$$\mathbf{Q}_{1,2}^1 = \begin{bmatrix} \frac{1}{6} & \frac{1}{2} \\ \frac{1}{6} & \frac{1}{6} \end{bmatrix}, \quad \mathbf{Q}_{2,3}^1 = \begin{bmatrix} \frac{1}{6} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{6} \end{bmatrix}$$

1. Use the above values to compute $\hat{N}_k, \hat{N}_{kl}, \hat{N}_{kj}$.
2. Complete the M step by updating the parameters $\boldsymbol{\theta}, \mathbf{T}, \boldsymbol{\pi}_1, \boldsymbol{\pi}_2$.