# 16.410/413 <br> Principles of Autonomy and Decision Making 

Lecture 21: Intro to Hidden Markov Models the Baum-Welch algorithm

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## Assignments

## Readings

- Lecture notes
- [AIMA] Ch. 15.1-3, 20.3.
- Paper on Stellar: L. Rabiner, "A tutorial on Hidden Markov Models..."


## Outline

## (1) Decoding and Viterbi's algorithm

## 2 Learning and the Baum-Welch algorithm

## Decoding

- Filtering and smoothing produce distributions of states at each time step.
- Maximum likelihood estimation chooses the state with the highest probability at the "best" estimate at each time step.
- However, these are pointwise best estimate: the sequence of maximum likelihood estimates is not necessarily a good (or feasible) trajectory for the HMM!
- How do we find the most likely state history, or state trajectory? (As opposed to the sequence of point-wise most likely states?)


## Example: filtering/smoothing vs. decoding

- Three states:

$$
\mathcal{X}=\left\{x_{1}, x_{2}, x_{3}\right\} .
$$

- Three possible observations:

$$
\mathcal{Z}=\{2,3\}
$$

- Initial distribution: $\pi=(1,0,0)$.
- Transition probabilities:


$$
T=\left[\begin{array}{ccc}
0 & 0.5 & 0.5 \\
0 & 0.9 & 0.1 \\
0 & 0 & 1
\end{array}\right]
$$

- Observation probabilities:

Observation sequence:

$$
M=\left[\begin{array}{ll}
0.5 & 0.5 \\
0.9 & 0.1 \\
0.1 & 0.9
\end{array}\right] \quad Z=(2,3,3,2,2,2,3,2,3)
$$

## Example: filtering/smoothing vs. decoding

- Using filtering:

| $t$ | $x_{1}$ | $x_{2}$ | $x_{3}$ |
| ---: | ---: | ---: | ---: |
| 1 | $\mathbf{1 . 0 0 0 0}$ | 0 | 0 |
| 2 | 0 | 0.1000 | $\mathbf{0 . 9 0 0 0}$ |
| 3 | 0 | 0.0109 | $\mathbf{0 . 9 8 9 1}$ |
| 4 | 0 | 0.0817 | $\mathbf{0 . 9 1 8 3}$ |
| 5 | 0 | 0.4165 | $\mathbf{0 . 5 8 3 5}$ |
| 6 | 0 | $\mathbf{0 . 8 4 3 7}$ | 0.1563 |
| 7 | 0 | 0.2595 | $\mathbf{0 . 7 4 0 5}$ |
| 8 | 0 | $\mathbf{0 . 7 3 2 8}$ | 0.2672 |
| 9 | 0 | 0.1771 | $\mathbf{0 . 8 2 2 9}$ |

- The sequence of point-wise most likely states is:

$$
(1,3,3,3,3,2,3,2,3)
$$

- The above sequence is not feasible for the HMM model!

Example: filtering vs. smoothing vs. decoding $\quad 3 / 4$

- Using smoothing:

| $t$ | $x_{1}$ | $x_{2}$ | $x_{3}$ |
| ---: | ---: | ---: | ---: |
| 1 | $\mathbf{1 . 0 0 0 0}$ | 0 | 0 |
| 2 | 0 | $\mathbf{0 . 6 2 9 7}$ | 0.3703 |
| 3 | 0 | $\mathbf{0 . 6 2 5 5}$ | 0.3745 |
| 4 | 0 | $\mathbf{0 . 6 2 5 1}$ | 0.3749 |
| 5 | 0 | $\mathbf{0 . 6 2 1 8}$ | 0.3782 |
| 6 | 0 | $\mathbf{0 . 5 9 4 8}$ | 0.4052 |
| 7 | 0 | 0.3761 | $\mathbf{0 . 6 2 3 9}$ |
| 8 | 0 | 0.3543 | $\mathbf{0 . 6 4 5 7}$ |
| 9 | 0 | 0.1771 | $\mathbf{0 . 8 2 2 9}$ |

- The sequence of point-wise most likely states is:

$$
(1,2,2,2,2,2,3,3,3)
$$

## Viterbi's algorithm

- As before, let us use the Markov property of the HMM.
- Define

$$
\delta_{k}(s)=\max _{X_{1:(k-1)}} \operatorname{Pr}\left[X_{1: k}=\left(X_{1:(k-1)}, s\right), Z_{1: k} \mid \lambda\right]
$$

(i.e., $\delta_{k}(s)$ is the joint probability of the most likely path that ends at state $s$ at time $k$, generating observations $Z_{1: k}$.)

- Clearly,

$$
\delta_{k+1}(s)=\max _{q}\left(\delta_{k}(q) T_{q, s}\right) M_{s, z_{k+1}}
$$

- This can be iterated to find the probability of the most likely path that ends at each possible state $s$ at the final time. Among these, the highest probability path is the desired solution.
- We need to keep track of the path...


## Viterbi's algorithm 2/3

- Initialization, for all $s \in \mathcal{X}$ :
- $\delta_{1}(s)=\pi_{s} M_{s, z_{1}}$
- $\operatorname{Pre}_{1}(s)=$ null.
- Repeat, for $k=1, \ldots, t-1$, and for all $s \in \mathcal{X}$ :
- $\delta_{k+1}(s)=\max _{q}\left(\delta_{k}(q) T_{q, s}\right) M_{s, z_{k+1}}$
- $\operatorname{Pre}_{k+1}(s)=\arg \max _{q}\left(\delta_{k}(q) T_{q, s}\right)$
- Select most likely terminal state: $s_{t}^{*}=\arg \max _{s} \delta_{t}(s)$
- Backtrack to find most likely path. For $k=t-1, \ldots, 1$
- $q_{k}^{*}=\operatorname{Pre}_{k+1}\left(q_{k+1}^{*}\right)$
- The joint probability of the most likely path + observations is found as $p^{*}=\delta_{t}\left(s_{t}^{*}\right)$.


## Whack-the-mole example

- Viterbi's algorithm
- $\delta_{1}=(0.6,0,0)$
- $\delta_{2}=(0.012,0.048,0.18)$

$$
\text { - } \delta_{3}=(0.0038,0.0216,0.0432)
$$

$$
\begin{array}{r}
\operatorname{Pre}_{1}=(\text { null }, \text { null, null }) \\
\operatorname{Pre}_{2}=(1,1,1) . \\
\operatorname{Pre}_{3}=(2,3,3) .
\end{array}
$$

- Joint probability of the most likely path + observations: 0.0432
- End state of the most likely path: 3
- Most likely path: $3 \leftarrow 3 \leftarrow 1$.

Example: filtering vs. smoothing vs. decoding $\quad 4 / 4$

- Using Viterbi's algorithm:

| $t$ | $x_{1}$ | $x_{2}$ | $x_{3}$ |
| ---: | ---: | ---: | ---: |
| 1 | $0.5 / 0$ | 0 | 0 |
| 2 | $0 / 1$ | $0.025 / 1$ | $0.225 / 1$ |
| 3 | $0 / 1$ | $0.00225 / 2$ | $0.2025 / 3$ |
| 4 | $0 / 1$ | $0.0018225 / 2$ | $0.02025 / 3$ |
| 5 | $0 / 1$ | $0.0014762 / 2$ | $0.002025 / 3$ |
| 6 | $0 / 1$ | $0.0011957 / 2$ | $0.0002025 / 3$ |
| 7 | $0 / 1$ | $0.00010762 / 2$ | $0.00018225 / 3$ |
| 8 | $0 / 1$ | $8.717 \mathrm{e}-05 / 2$ | $1.8225 \mathrm{e}-05 / 3$ |
| 9 | $0 / 1$ | $7.8453 \mathrm{e}-06 / 2$ | $1.6403 \mathrm{e}-05 / 3$ |

- The most likely sequence is:

$$
(1,3,3,3,3,3,3,3,3)
$$

- Note: Based on the first 8 observations, the most likely sequence would have been
$(1,2,2,2,2,2,2,2)$ !
E. Frazzoli (MIT)


## Viterbi's algorithm 3/3

- Viterbi's algorithm is similar to the forward algorithm, with the difference that the summation over the states at time step $k$ becomes a maximization.
- The time complexity is, as for the forward algorithm, linear in $t$ (and quadratic in $\operatorname{card}(\mathcal{X}))$.
- The space complexity is also linear in $t$ (unlike the forward algorithm), since we need to keep track of the "pointers" Pre ${ }_{k}$.
- Viterbi's algorithm is used in most communication devices (e.g., cell phones, wireless network cards, etc.) to decode messages in noisy channels; it also has widespread applications in speech recognition.


## Outline

Decoding and Viterbi's algorithm
(2) Learning and the Baum-Welch algorithm

## Problem 3: Learning

## The learning problem

Given a HMM $\lambda$, and an observation history $Z=\left(z_{1}, z_{2}, \ldots, z_{t}\right)$, find a new HMM $\lambda^{\prime}$ that explains the observations at least as well, or possibly better, i.e., such that $\operatorname{Pr}\left[Z \mid \lambda^{\prime}\right] \geq \operatorname{Pr}[Z \mid \lambda]$.

- Ideally, we would like to find the model that maximizes $\operatorname{Pr}[Z \mid \lambda]$; however, this is in general an intractable problem.
- We will be satisfied with an algorithm that converges to local maxima of such probability.
- Notice that in order for learning to be effective, we need lots of data, i.e., many, long observation histories!


## Example: Finding Keyser Söze

Let us consider the following problem.

- The elusive leader of a dangerous criminal organization (e.g., Keyser Söze, from the movie "The Usual Suspects") is known to travel between two cities (say, Los Angeles and New York City)
- The FBI has no clue about his whereabouts at the initial time (e.g., uniform probability being at any one of the cities).
- The FBI has no clue about the probability that he would stay or move to the other city at each time period:

| from $\backslash$ to | LA | NY |
| :---: | :---: | :---: |
| LA | 0.5 | 0.5 |
| NY | 0.5 | 0.5 |

- At each time period the FBI could get sighting reports (or evidence of his presence in a city), including a non-sighting null report. An estimate of the probability of getting such reports is

| where \report | LA | NY | null |
| :---: | :---: | :---: | :---: |
| LA | 0.4 | 0.1 | 0.5 |
| NY | 0.1 | 0.5 | 0.4 |

## Example: Finding Keyser Söze

- Let us assume that the FBI has been tracking sighting reports for, say, 20 periods, with observation sequence $Z$

$$
\begin{aligned}
& Z=(-, L A, L A,-, N Y,-, N Y, N Y, N Y,- \\
& N Y, N Y, N Y, N Y, N Y,-,-, L A, L A, N Y)
\end{aligned}
$$

- We can compute, using the algorithms already discussed:
- the current probability distribution (after the 20 observations):

$$
\gamma_{20}=(0.1667,0.8333)
$$

- the probability distribution at the next period (so that we can catch him):

$$
\gamma_{21}=T^{\prime} \gamma_{20}=(0.5,0.5)
$$

- the probability of getting that particular observation sequence given the model:

$$
\operatorname{Pr}[Z \mid \lambda]=1.9 \cdot 10^{-10}
$$

## Example: Finding Keyser Söze

- Using smoothing:

| $t$ | LA | NY |
| :---: | ---: | ---: |
| 1 | 0.5556 | 0.4444 |
| 2 | 0.8000 | 0.2000 |
| 3 | 0.8000 | 0.2000 |
| $\cdots$ | $\cdots$ | $\ldots$ |
| 18 | 0.8000 | 0.2000 |
| 19 | 0.8000 | 0.2000 |
| 20 | 0.1667 | 0.8333 |

- The sequence of point-wise most likely states is:

$$
\begin{aligned}
&(L A, L A, L A, L A, N Y, L A, N Y, N Y, N Y, L A \\
&N Y, N Y, N Y, N Y, N Y, L A, L A, L A)
\end{aligned}
$$

- The new question is: given all the data, can we improve on our model, in such a way that the observations are more consistent with it?


## Expectation of (state) counts

- Let us define

$$
\gamma_{k}(s)=\operatorname{Pr}\left[X_{k}=s \mid Z, \lambda\right],
$$

i.e., $\gamma_{k}(s)$ is the probability that the system is at state $s$ at the $k$-th time step, given the observation sequence $Z$ and the model $\lambda$.

- We already know how to compute this, e.g., using smoothing:

$$
\gamma_{k}(s)=\frac{\alpha_{k}(s) \beta_{k}(s)}{\operatorname{Pr}[Z \mid \lambda]}=\frac{\alpha_{k}(s) \beta_{k}(s)}{\sum_{s \in \mathcal{X}} \alpha_{t}(s)}
$$

- New concept: how many times is the state trajectory expected to transition from state $s$ ?

$$
\mathrm{E}[\# \text { of transitions from } s]=\sum_{k=1}^{t-1} \gamma_{k}(s)
$$

## Expectation of (transition) counts

- In much the same vein, let us define

$$
\xi_{k}(q, s)=\operatorname{Pr}\left[X_{k}=q, X_{k+1}=s \mid Z, \lambda\right]
$$

(i.e., $\xi_{k}(q, s)$ is the probability of being at state $q$ at time $k$, and at state $s$ at time $k+1$, given the observations and the current HMM model)

- We have that

$$
\xi_{k}(q, s)=\eta_{k} \alpha_{k}(q) T_{q, s} M_{s, z_{k+1}} \beta_{k+1}(s)
$$

where $\eta_{k}$ is a normalization factor, such that $\sum_{q, s} \xi_{k}(q, s)=1$.

- New concept: how many times it the state trajectory expected to transition from state $q$ to state $s$ ?

$$
\mathrm{E}[\# \text { of transitions from } q \text { to } s]=\sum_{k=1}^{t-1} \xi_{k}(q, s)
$$

## Baum-Welch algorithm

- Based on the probability estimates and expectations computed so far, using the original HMM model $\lambda=(T, M, \pi)$, we can construct a new model $\lambda^{\prime}=\left(T^{\prime}, M^{\prime}, \pi^{\prime}\right)$ (notice that the two models share the states and observations):
- The new initial condition distribution is the one obtained by smoothing:

$$
\pi_{s}^{\prime}=\gamma_{1}(s)
$$

- The entries of the new transition matrix can be obtained as follows:

$$
T_{q s}^{\prime}=\frac{E[\# \text { of transitions from state } q \text { to state } s]}{E[\# \text { of transitions from state } q]}=\frac{\sum_{k=1}^{t-1} \xi_{k}(q, s)}{\sum_{k=1}^{t-1} \gamma_{k}(q)}
$$

## Baum-Welch algorithm

- The entries of the new observation matrix can be obtained as follows:

$$
\begin{array}{r}
M_{s m}^{\prime}=\frac{E[\# \text { of times in state } s, \text { when the observation was } m \text { ] }}{E[\# \text { of times in state } s]} \\
=\frac{\sum_{k=1}^{t} \gamma_{k}(s) \cdot \mathbf{1}\left(z_{k}=m\right)}{\sum_{k=1}^{t} \gamma_{k}(s)}
\end{array}
$$

- It can be shown [Baum et al., 1970] that the new model $\lambda^{\prime}$ is such that
- $\operatorname{Pr}\left[Z \mid \lambda^{\prime}\right] \geq \operatorname{Pr}[Z \mid \lambda]$, as desired.
- $\operatorname{Pr}\left[Z \mid \lambda^{\prime}\right]=\operatorname{Pr}[Z \mid \lambda]$ only if $\lambda$ is a critical point of the likelihood function $f(\lambda)=\operatorname{Pr}[Z \mid \lambda]$


## Example: Finding Keyser Söze

Let us apply the method to the example. We get

- Initial condition: $\pi=(1,0)$.
- Transition matrix:

$$
\left[\begin{array}{ll}
0.6909 & 0.3091 \\
0.0934 & 0.9066
\end{array}\right]
$$

- Observation matrix:

$$
\left[\begin{array}{lll}
0.5807 & 0.0010 & 0.4183 \\
0.0000 & 0.7621 & 0.2379
\end{array}\right]
$$



- Note that it is possible that $\operatorname{Pr}\left[Z \mid \lambda^{\prime}\right]>\operatorname{Pr}\left[Z \mid \lambda_{\text {true }}\right]$ ! This is due to overfitting over one particular data set.


## Recursive Bayesian estimation: HMMs and Kalman filters



- The idea of the filtering/smoothing techniques for HMM is in fact broader. In general it applies to any system where the state at a time step only depends on the state at the previous time step (Markov property), and the observation at a time step only depends on the state at that time step.
- HMMs: discrete state (Markov chain), arbitrary transition and observation matrices.
- Kalman filter: continuous state (Markov process), (Linear-)Gaussian transitions, Gaussian observations.

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