Hidden Markov Models

Filtering, Smoothing & Parameter Estimation

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Bootcamp Talk

7th December 2022

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Recap: Markov Chains

A sequence of random variables $X_1, X_2, \ldots$ taking values in a state space S is a Markov chain if it satisfies the Markov property $\forall t$:

$$\mathbb{P}(X_t = x_t | X_1 = x_1, \ldots, X_{t-1} = x_{t-1}) = \mathbb{P}(X_t = x_t | X_{t-1} = x_{t-1}).$$

That is, the value of X_t depends **only** on the value of X_{t-1}.

Markov Chains

Assume $S = \{1, 2, ..., N\} = [N]$ and that the Markov chain is time homogeneous:

$$\mathbb{P}(X_t = j | X_{t-1} = i) = \mathbb{P}(X_{t'} = j | X_{t'-1} = i) \;\; \forall t, t'.$$

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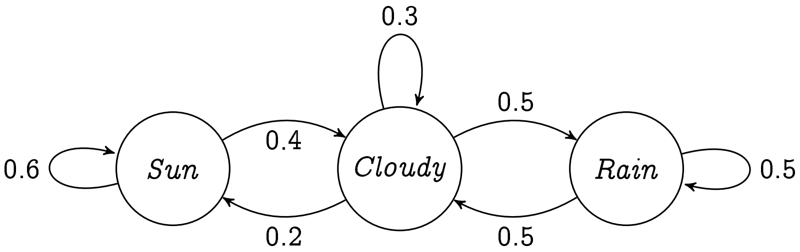
$$a_{ij} = \mathbb{P}(X_t = j | X_{t-1} = i).$$

Markov Chains: Example



$$S = \{Sun, Cloudy, Rain\}, \quad A = \begin{pmatrix} 0.6 & 0.4 & 0 \\ 0.2 & 0.3 & 0.5 \\ 0 & 0.5 & 0.5 \end{pmatrix}$$

Hidden Markov Models

A hidden Markov Model involves an unobservable Markov chain $X_1, X_2, \ldots$ and a sequence of observations $Y_1, Y_2, \ldots$ such that:

$$\mathbb{P}(Y_t = y_t | X_1 = x_1, \ldots, X_t = x_t, Y_1 = y_1, \ldots, Y_{t-1} = y_{t-1}, Y_{t+1} = y_{t+1}, \ldots) \\ = \mathbb{P}(Y_t = y_t | X_t = x_t).$$

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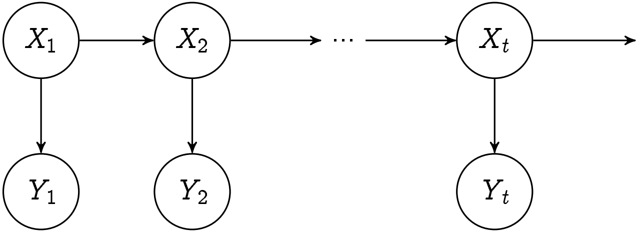
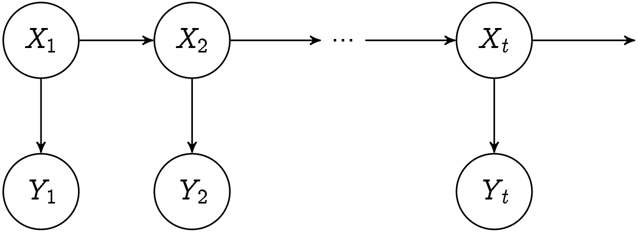


Hidden Markov Models

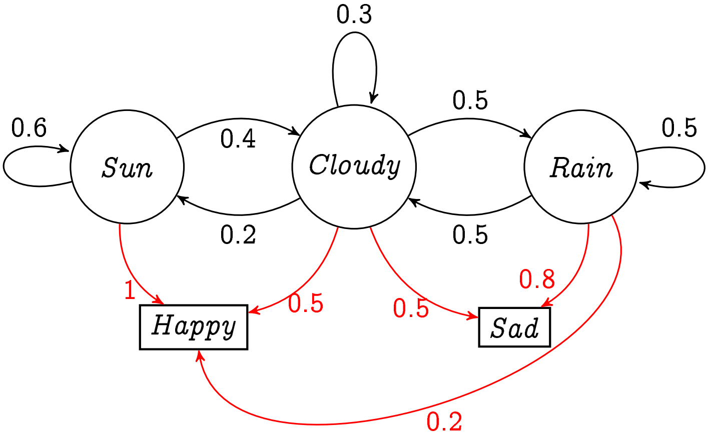


We suppose each Y_t takes values from a set of M possible observations $O = \{o_1, o_2, \ldots, o_M\}$, with emission/observation probabilities:

$$b_j(o_k) = \mathbb{P}(Y_t = o_k | X_t = j)$$

for $k \in [M], j \in [N]$.

Hidden Markov Models: Example



With $O = \{Happy, Sad\}$:

- $b_{Sun}(Happy) = 1$
- $b_{Sun}(Sad) = 0$
- $b_{Cloudy}(Happy) = 0.5$
- $b_{Cloudy}(Sad) = 0.5$
- $b_{Rain}(Happy) = 0.2$
- $b_{Rain}(Sad) = 0.8$

Hidden Markov Models

An HHM with hidden state space $S = [N]$ and observation space $O = \{o_1, ..., o_M\}$ can be parameterised fully as $\lambda = (\pi, A, B)$ where:

- $\pi \in \mathbb{R}^N$ is the initial distribution over state space S:

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- $B = \{b_j(o_k) : j \in [N], k \in [M]\}$ gives us the emission/observation probabilities:

$$b_j(o_k) = \mathbb{P}(Y_t = o_k | X_t = j).$$

Hidden Markov Models: Applications

- Speech Recognition (e.g. [Rabiner, 1989]):
  - Hidden states: basic parts of speech (e.g. words, syllables, phonemes etc.).
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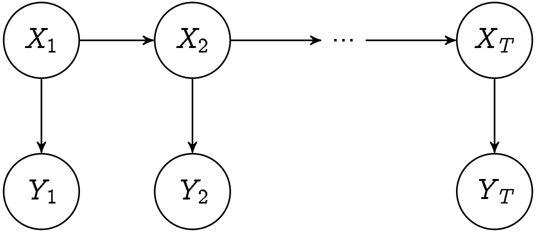
- Bioinformatics (e.g. [Wong et al., 2013]):
  - Hidden states: sequences of nucleotides (A, T, C and G) within a DNA sequence.
  - Observations: intensity of chemical reaction when testing a protein.

HMMs: Important Questions

Given an HHM $\lambda = (\pi, A, B)$ and a sequence of observations $Y = (Y_1, ..., Y_T)$:



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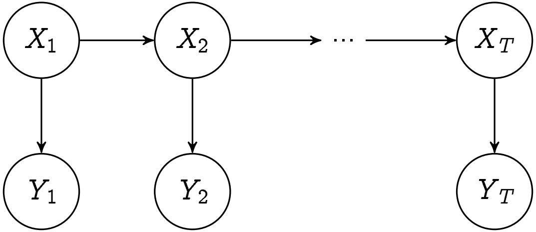

Q1. What is $\mathbb{P}(Y|\lambda)$?

Q2. What value is X_t likely to have taken for any $t \in [T]$?

A Naïve Approach To Q1

The probability of observing $Y = (Y_1, ..., Y_T)$ given an underlying sequence of states $X = (X_1, ..., X_T)$:

$$\mathbb{P}(Y|X, \lambda) = \prod_{t=1}^{T} b_{X_t}(Y_t).$$

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The probability of λ producing $X = (X_1, \ldots, X_T)$:

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Hence, marginalising over all possible X

$$\mathbb{P}(Y|\lambda) = \sum_{X} \mathbb{P}(Y|X,\lambda)\mathbb{P}(X|\lambda) = \sum_{X=(X_1,...,X_T)} \pi_{X_1} b_{X_1}(Y_1) \prod_{t=2}^{T} a_{X_{t-1},X_t} b_{X_t}(Y_t).$$

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- There are N^T possible values for X.
- Hence this calculation has $\mathcal{O}(TN^T)$ complexity.
- We can do much better if we utilise recursion.

Filtering

Predict X_t based on $Y_1, \ldots, Y_t$.

For $i \in [N]$, $t \in [T]$ let our *forward* probabilities be:

$$\alpha_t(i) = \mathbb{P}(Y_1, \ldots, Y_t, X_t = i | \lambda).$$

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Calculate inductively:

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We can now calculate $\mathbb{P}(Y|\lambda)$ as:

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  - (We calculate the probability of an i-to-j transition for every possible (i, j) pair.)
- Calculating $\mathbb{P}(Y|\lambda)$ requires summing T values hence the overall complexity is $\mathcal{O}(TN^2)$.

Q2 Using Forward Probabilities: Filtering

Having these forward probabilities allows us to calculate $\mathbb{P}(X_t | Y_1, \ldots, Y_t, \lambda)$:

$$\mathbb{P}(X_t | Y_1, \ldots, Y_t, \lambda) = \frac{\mathbb{P}(X_t, Y_1, \ldots, Y_t | \lambda)}{\mathrm{P}(Y_1, \ldots, Y_t | \lambda)} = \frac{\alpha_t(X_t)}{\sum_{i=1}^{N} \alpha_T(i)}.$$

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We can also get maximum a posteriori (MAP) estimates:

$$X_t^{\text{MAP}} = \operatorname*{argmax}_i \frac{\alpha_t(i)}{\sum_{j=1}^{N} \alpha_T(j)} = \operatorname*{argmax}_i \alpha_t(i)$$

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Smoothing: can we improve this by also using $Y_{t+1}, ..., Y_T$?

Smoothing: Backwards Probabilities

For each $i \in [N]$ and $t \in [T]$ we define

$$\beta_t(i) = \mathbb{P}(Y_{t+1}, \ldots, Y_T | X_t = i, \lambda)$$

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Smoothing: Forward-Backward Algorithm

How can we combine the information given by Y_1, ..., Y_t (via $\alpha_t(i)$) and by Y_{t+1}, ..., Y_T (via $\beta_t(i)$)?

Smoothing: Forward-Backward Algorithm

How can we combine the information given by $Y_1, \ldots, Y_t$ (via $\alpha_t(i)$) and by $Y_{t+1}, \ldots, Y_T$ (via $\beta_t(i)$)?

$$\gamma_t(i) = \mathbb{P}(X_t = i | Y, \lambda) = \frac{\mathbb{P}(X_t = i, Y_1, \ldots, Y_t | \lambda)\mathbb{P}(Y_{t+1}, \ldots, Y_T | X_t = i, \lambda)}{\mathbb{P}(Y|\lambda)}$$

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NOTE: X_1^{MAP}, ..., X_T^{MAP} is not necessarily the most probable sequence of X_1, ..., X_T given Y; it might even include impossible transitions from X_t to X_{t+1}.

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To find the most probable sequence $X = X_1, \ldots, X_T$ that maximises $\mathbb{P}(X \mid Y, \lambda)$, we'd have to use other techniques (e.g. Viterbi algorithm).

Parameter Estimation

What if we don't know $\lambda = (\pi, A, B)$?

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What if we don't know $\lambda = (\pi, A, B)$?

Given an observed sequence $Y = Y_1, ..., Y_T$ we can estimate λ using the forward-backward algorithm's machinery via the Baum-Welch Algorithm.

Parameter Estimation: The Baum-Welch Algorithm

Choose some initial parameter values $\lambda = (\pi, A, B)$.

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Choose some initial parameter values $\lambda = (\pi, A, B)$.

Introduce $\xi_t(i,j)$ where:

$$\xi_t(i,j) = \mathbb{P}(X_t = i, X_{t+1} = j \mid Y, \lambda) = \frac{\overbrace{\alpha_t(i)}^{\substack{\text{being in state} \\ i \text{ at time } t}} \cdot \overbrace{a_{ij}\, b_j(Y_{t+1})}^{\substack{\text{moving from } i \text{ to } j \\ \text{and observing } Y_{t+1}}} \cdot \overbrace{\beta_{t+1}(j)}^{\substack{\text{being in state } j \\ \text{at time } t+1}}}{\mathbb{P}(Y \mid \lambda)}$$

$$= \frac{\alpha_t(i) \cdot a_{ij}\, b_j(Y_{t+1}) \cdot \beta_{t+1}(j)}{\sum_{k=1}^{N} \sum_{l=1}^{N} \alpha_t(k) \cdot a_{kl}\, b_l(Y_{t+1}) \cdot \beta_{t+1}(l)}$$

Parameter Estimation: The Baum-Welch Algorithm

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Note: $\gamma_t(i) = \sum_{j=1}^{N} \xi_t(i, j)$.

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$$\bar{b_j}(o_k) = \frac{\text{expected number of } o_k \text{ observations from state } j}{\text{expected number of time steps in state } j} = \frac{\sum_{t=1}^{T} \mathbb{1}_{\{Y_t = o_k\}} \cdot \gamma_t(j)}{\sum_{t=1}^{T} \gamma_t(j)}$$

Parameter Estimation: The Baum-Welch Algorithm

The Baum-Welch algorithm is a form of expectation maximisation algorithm:

- Once we've found $\bar{\lambda} = (\bar{\pi}, \bar{A}, \bar{B})$ we repeat the procedure with these parameters instead of λ to find another set of (improved) parameters.
- We repeat until the parameters stabilise into a local optimum.

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- Given only a sequence of observations $Y = Y_1, .., Y_T$ we can estimate $\lambda = (\pi, A, B)$ using the Baum-Welch algorithm.

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Thank you

Any questions?