COMS W4701: Artificial Intelligence

Lecture 18: Learning Hidden Markov Models

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Today

- Smoothing: Forward-backward algorithm
- Supervised learning: Maximum likelihood
- Unsupervised learning: Baum-Welch algorithm

Inference

- Inference tasks compute belief states or hidden states given evidence

- **Filtering (state estimation)**: Find $P(X_t \mid e_{1:t})$
  - Estimate the belief state, given a sequence of past observations

- **Smoothing**: Find $P(X_k \mid e_{1:N})$, for $1 \leq k < N$
  - Use both past and future evidence to *smooth* a belief state

- **Learning**: Learn the parameters $P(X_0)$, $P(X_t|X_{t+1})$, $P(E_t|X_t)$ from data

Smoothing

- Suppose we have evidence $e_{1:N}$ and we want to go "back" in time to compute "more informed" belief states $P(X_k|e_{1:N})$, $1 \leq k < N$

- We can derive $P(X_k|e_{1:N}) = P(X_k, e_{1:N})$ using the product rule:

$$P(X_k, e_{1:k}, e_{k+1:N}) = P(X_k, e_{1:k})P(e_{k+1:N}|X_k, \cancel{e_{1:k}}) = \boldsymbol{\alpha}_k * \boldsymbol{\beta}_k$$

Conditional independence

- We have $\boldsymbol{\alpha}_k$ from the forward algorithm
- $\boldsymbol{\beta}_k$ is the joint probability of "future" evidence, conditioned on state at k
- We take the elementwise product of $\boldsymbol{\alpha}_k$ and $\boldsymbol{\beta}_k$ arrays

Backward Algorithm

- As with the forward algorithm, we *iteratively* compute $\boldsymbol{\beta}_k$ but going *backward*
- Let $\boldsymbol{\beta}_{k+1} = P(e_{k+2:N} \mid X_{k+1})$, $\boldsymbol{\beta}'_{k+1} = P(e_{k+1:N} \mid X_{k+1})$, and $\boldsymbol{\beta}_k = P(e_{k+1:N} \mid X_k)$
- Let $\boldsymbol{\beta}_N = (1, \dots, 1)$ (algorithm base case)

- Given X_{k+1}, E_{k+1} is conditionally independent of $E_{k+2}, \dots, E_t$

$$P(e_{k+1:N} \mid X_{k+1}) = P(e_{k+1} | X_{k+1}) P(e_{k+2:N} \mid X_{k+1})$$

$$\boxed{\boldsymbol{\beta}'_{k+1} = \boldsymbol{\beta}_{k+1} * O_{k+1}}$$

- Elapse time *backward*:

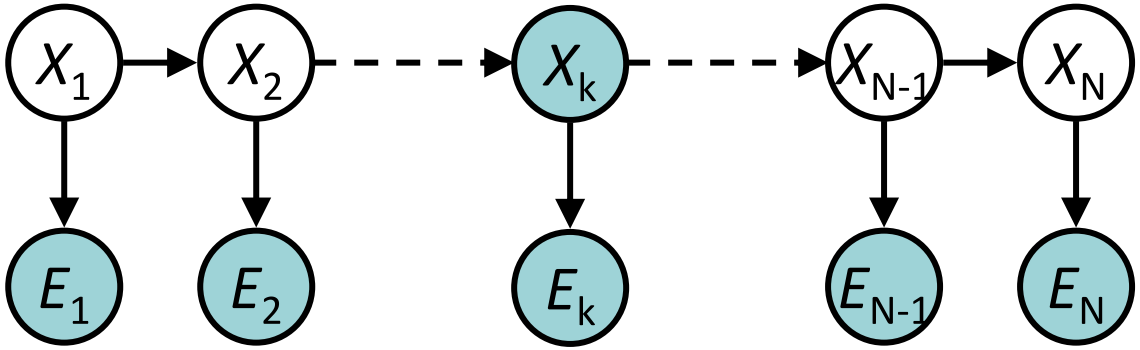
Conditional independence

$$P(e_{k+1:N} \mid X_k) = \sum_{x_{k+1}} P(e_{k+1:N} | x_{k+1}, \cancel{X_k}) P(x_{k+1} | X_k)$$

$$\boxed{\boldsymbol{\beta}_k = \boldsymbol{\beta}'_{k+1} T^{\top}}$$

Forward-Backward Algorithm

- The **forward-backward algorithm** computes $P(X_k|e_{1:N})$ for all k
  - Use forward algorithm to compute and store $\boldsymbol{\alpha}_k$ for all k
  - Use backward algorithm to compute $\boldsymbol{\beta}_k$ and $P(X_k|e_{1:N})$ for all k
  - $P(X_k|e_{1:N}) \propto \boldsymbol{\alpha}_k * \boldsymbol{\beta}_k$: take elementwise product and normalize



Forward algorithm

Backward algorithm

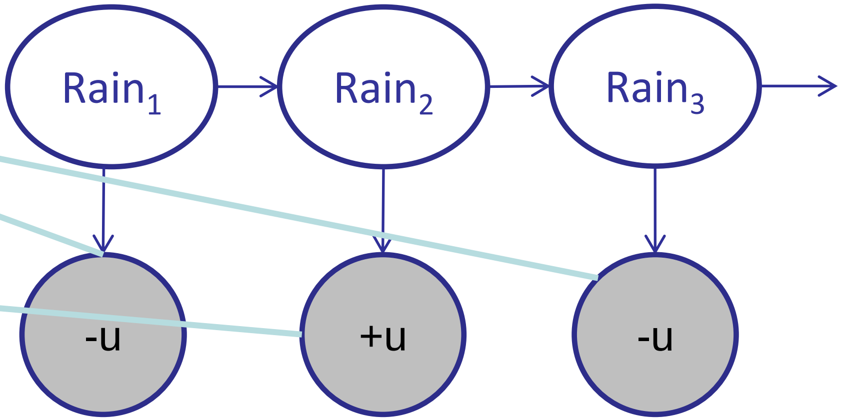
$\boldsymbol{\alpha}_k = P(X_k, e_{1:k})$ $\times$ $\boldsymbol{\beta}_k = P(e_{k+1:N}|X_k)$

Example: Weather HMM

$$T = \begin{array}{cc} \begin{pmatrix} 0.7 & 0.3 \\ 0.3 & 0.7 \end{pmatrix} & \begin{array}{c} +r \\ -r \end{array} \\ \begin{array}{cc} +r & -r \end{array} & \end{array}$$

$$O_1 = O_3 = \begin{pmatrix} 0.1 \\ 0.8 \end{pmatrix}$$

$$O_2 = \begin{pmatrix} 0.9 \\ 0.2 \end{pmatrix}$$



$$\boxed{\begin{aligned} \boldsymbol{\beta}'_{k+1} &= \boldsymbol{\beta}_{k+1} * O_{k+1} \\ \boldsymbol{\beta}_k &= \boldsymbol{\beta}'_{k+1} T^\top \end{aligned}}$$

Initialize $\beta_3 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$\beta'_3 = \beta_3 * O_3 = \begin{pmatrix} 0.1 \\ 0.8 \end{pmatrix} \qquad \beta_2 = {\beta'_3}^\top T^\top = P(e_3 | X_2) = \begin{pmatrix} 0.31 \\ 0.59 \end{pmatrix}$$

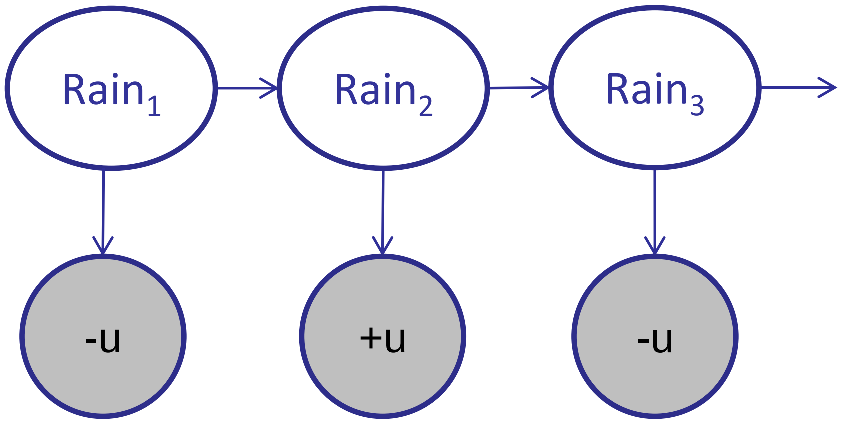
$$\beta'_2 = \beta_2 * O_2 = \begin{pmatrix} .279 \\ .118 \end{pmatrix} \qquad \beta_1 = {\beta'_2}^\top T^\top = P(e_{2:3} | X_1) = \begin{pmatrix} .2307 \\ .1663 \end{pmatrix}$$

Example: Weather HMM

$$\alpha_1 = \begin{pmatrix} 0.05 \\ 0.4 \end{pmatrix} \quad \alpha_2 = \begin{pmatrix} .1395 \\ .059 \end{pmatrix} \quad \alpha_3 = \begin{pmatrix} .0115 \\ .0665 \end{pmatrix}$$

normalize

$$P(X_1|e_1) = \begin{pmatrix} 0.11 \\ 0.89 \end{pmatrix} \quad P(X_2|e_{1:2}) = \begin{pmatrix} .703 \\ .297 \end{pmatrix} \quad P(X_3|e_{1:3}) = \begin{pmatrix} .148 \\ .852 \end{pmatrix}$$



$$\beta_1 = \begin{pmatrix} .2307 \\ .1663 \end{pmatrix} \quad \beta_2 = \begin{pmatrix} 0.31 \\ 0.59 \end{pmatrix} \quad \beta_3 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

multiply

$$\alpha_1 * \beta_1 = \begin{pmatrix} .012 \\ .067 \end{pmatrix} \quad \alpha_2 * \beta_2 = \begin{pmatrix} .043 \\ .035 \end{pmatrix} \quad \alpha_3 * \beta_3 = \begin{pmatrix} .0115 \\ .0664 \end{pmatrix}$$

normalize

$$P(X_1|e_{1:3}) = \begin{pmatrix} .148 \\ .852 \end{pmatrix} \quad P(X_2|e_{1:3}) = \begin{pmatrix} .554 \\ .446 \end{pmatrix} \quad P(X_3|e_{1:3}) = \begin{pmatrix} .148 \\ .852 \end{pmatrix}$$

Supervised Learning

- We now want to *learn* the *parameters* θ (probabilities) of a HMM from data
- Suppose we have a sequence of states and observations: $\mathbf{d} = \left((x_1, e_1), \dots, (x_N, e_N)\right)$

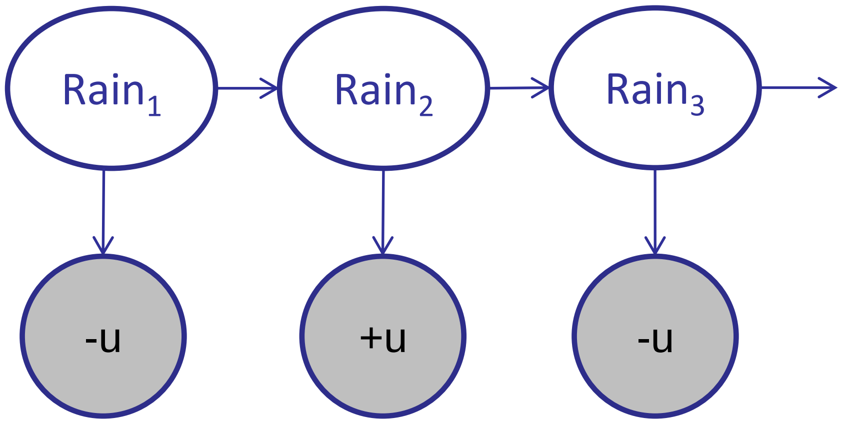
- **Maximum-likelihood learning**: Find parameters that maximize likelihood of data
- Likelihood is joint probability of observed data using transition/observation models:

$$\max_{\theta} \Pr(\mathbf{d}|\theta) = \max_{P(X_0),P(X_{i+1}|X_i),P(E_i|X_i)} \left\{ P(x_0) \prod_{i=1}^{N} P(x_{i+1}|x_i)\, P(e_i\,|x_i) \right\}$$

- Intuitive solution: We can simply count the *proportions* of transitions $x_i \to x_{i+1}$ and *proportions* of observations (x_i, e_i) in our data

Example: Weather HMM

- Given (state, observation) sequences:
- (+r,+u), (+r,-u), (-r,-u), (+r,+u)
- (-r,-u), (-r,+u), (+r,+u)
- (+r,-u), (+r,+u), (-r,-u), (-r,+u), (+r,+u)



- Number of initial states: 2 +r, 1 –r
- Transitions: 2 +r to +r, 2 +r to -r, 3 -r to +r, 2 -r to -r
- Observations: 5 +r to +u, 2 +r to –u, 2 –r to +u, 3 –r to -u

$$\widehat{P(U|+r)} = \begin{pmatrix} 5/7 \\ 2/7 \end{pmatrix}$$

$$\widehat{P(X_0)} = \begin{pmatrix} 2/3 \\ 1/3 \end{pmatrix} \qquad \hat{T} = \begin{pmatrix} 2/4 & 2/4 \\ 3/5 & 2/5 \end{pmatrix}$$

$$\widehat{P(U|-r)} = \begin{pmatrix} 2/5 \\ 3/5 \end{pmatrix}$$

Unsupervised Learning

- Problem: State information is generally hidden in HMM problems
- We may only see the observations in a data set

- Suppose we have an *initial guess* about the HMM parameters
- We can compute $\boldsymbol{\gamma}_k = P(X_k | e_{1:N})$ from forward-backward algorithm
- $\boldsymbol{\gamma}_k$ is the *expected* number of occurrences of each state value x at time k

- We can use $\boldsymbol{\gamma}_k$ in place of "true counts" to update HMM parameters!
- New initial distribution: $\widehat{P(X_0)} = \boldsymbol{\gamma}_0 = P(X_0 | e_{1:N})$

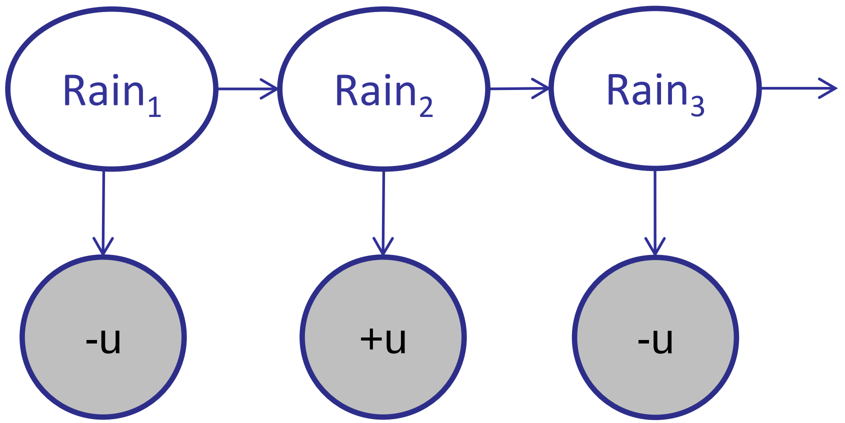
Expected Observations

- Our "data set" now looks like $((\boldsymbol{\gamma}_1, e_1), (\boldsymbol{\gamma}_2, e_2), \ldots, (\boldsymbol{\gamma}_N, e_N))$
- New estimate of $P(e|x)$: number of (x, e) / total number of x

$$\boxed{\widehat{P(e|x)} = \frac{\sum_{e_k=e} \boldsymbol{\gamma}_k(x)}{\sum_{k=1}^{N} \boldsymbol{\gamma}_k(x)}}$$

$$O_1 = O_3 = \begin{pmatrix} 0.1 \\ 0.8 \end{pmatrix} \quad O_2 = \begin{pmatrix} 0.9 \\ 0.2 \end{pmatrix}$$

$$\gamma_0 = \begin{pmatrix} 0.36 \\ .0.64 \end{pmatrix} \quad \gamma_1 = \begin{pmatrix} .148 \\ .852 \end{pmatrix} \quad \gamma_2 = \begin{pmatrix} .554 \\ .446 \end{pmatrix} \quad \gamma_3 = \begin{pmatrix} .148 \\ .852 \end{pmatrix}$$



$$\widehat{P(X_0)} = \gamma_0 = \begin{pmatrix} 0.36 \\ 0.64 \end{pmatrix}$$

$$P(\widehat{+u|X}) = \frac{\gamma_2}{\gamma_1 + \gamma_2 + \gamma_3} = \begin{pmatrix} .652 \\ .207 \end{pmatrix}$$

$$P(\widehat{-u|X}) = \frac{\gamma_1 + \gamma_3}{\gamma_1 + \gamma_2 + \gamma_3} = \begin{pmatrix} .348 \\ .793 \end{pmatrix}$$

Expected Transitions

- In the new “data set” $\big((\boldsymbol{\gamma}_1, e_1), (\boldsymbol{\gamma}_2, e_2), \ldots, (\boldsymbol{\gamma}_N, e_N)\big)$, there are now potential transitions between every pair of states in every timestep

- We can compute the *expected* transitions from a state at step k to a state at step $k+1$

$$P(x_k, x_{k+1} | e_{1:N}) \propto P(x_k, x_{k+1}, e_{1:N})$$

$$= P(x_k, e_{1:k}) P(x_{k+1} | x_k, \cancel{e_{1:k}}) P(e_{k+1} | x_{k+1}, \cancel{x_k}, \cancel{e_{1:k}}) P(e_{k+2:N} | x_{k+1}, \cancel{x_k}, \cancel{e_{1:k+1}})$$

$$= \boldsymbol{\alpha}_k(x_k) P(x_{k+1} | x_k) P(e_{k+1} | x_{k+1}) \boldsymbol{\beta}_{k+1}(x_{k+1})$$

- *Expected* transition matrix: $\boxed{\boldsymbol{\xi}_k = diag(\boldsymbol{\alpha}_k) \cdot T \cdot diag(O_{k+1}) \cdot diag(\boldsymbol{\beta}_{k+1})}$

Expected Transition Matrix

- *Total number* of expected transitions between states is $\sum \boldsymbol{\xi}_k$
- We can normalize each row to obtain new transition probabilities!

$$\boldsymbol{\alpha}_0 = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix} \qquad \boldsymbol{\alpha}_1 = \begin{pmatrix} 0.05 \\ 0.4 \end{pmatrix} \qquad \boldsymbol{\alpha}_2 = \begin{pmatrix} .1395 \\ .059 \end{pmatrix}$$

$$\boxed{P(\widehat{X_{t+1} | X_t} = i) \propto \sum_{k=0}^{N-1} (\boldsymbol{\xi}_k)_i}$$

$$\boldsymbol{\beta}_1 = \begin{pmatrix} .2307 \\ .1663 \end{pmatrix} \qquad \boldsymbol{\beta}_2 = \begin{pmatrix} 0.31 \\ 0.59 \end{pmatrix} \qquad \boldsymbol{\beta}_3 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$T = \begin{pmatrix} 0.7 & 0.3 \\ 0.3 & 0.7 \end{pmatrix} \quad O_1 = O_3 = \begin{pmatrix} 0.1 \\ 0.8 \end{pmatrix} \quad O_2 = \begin{pmatrix} 0.9 \\ 0.2 \end{pmatrix}$$

$$\xi_0 = diag(\boldsymbol{\alpha}_0) \cdot T \cdot diag(O_1) \cdot diag(\boldsymbol{\beta}_1) = \begin{pmatrix} .008 & .020 \\ .003 & .047 \end{pmatrix}$$

$$\xi_1 = diag(\boldsymbol{\alpha}_1) \cdot T \cdot diag(O_2) \cdot diag(\boldsymbol{\beta}_2) = \begin{pmatrix} .010 & .002 \\ .033 & .033 \end{pmatrix}$$

$$\xi_2 = diag(\boldsymbol{\alpha}_2) \cdot T \cdot diag(O_3) \cdot diag(\boldsymbol{\beta}_3) = \begin{pmatrix} .010 & .033 \\ .002 & .033 \end{pmatrix}$$

$$\xi_0 + \xi_1 + \xi_2 = \begin{pmatrix} .028 & .056 \\ .039 & .113 \end{pmatrix}$$

$$\propto$$

$$P(\widehat{X_{k+1} | X_k}) = \begin{pmatrix} .333 & .667 \\ .256 & .744 \end{pmatrix}$$

Baum-Welch Algorithm

- **Baum-Welch** is an *expectation-maximization* algorithm: Learn HMM parameters by alternating between computing expected parameters and maximizing likelihoods

- Initialize HMM parameters $\widehat{P(X_0)}$, $\widehat{P(X_{k+1}|X_k)}$, $\widehat{P(E|X)}$
- Repeat until convergence:
  - **Expectation**: Compute $\boldsymbol{\alpha}_k, \boldsymbol{\beta}_k, \boldsymbol{\gamma}_k, \boldsymbol{\xi}_k\ \forall k$ using current parameters
  - **Maximization**: Compute new parameters $\widehat{P(X_0)}$, $\widehat{P(X_{k+1}|X_k)}$, $\widehat{P(E|X)}$

- The data likelihood $P(e_{1:N})$ will monotonically increase in each iteration
- Will typically reach a *local maximum*, dependent on parameter initialization

Summary

- Smoothing updates belief distributions using past and future observations
- Forward-backward algorithm runs linear in time and space

- Learning HMM parameters: If both hidden states and observations are given, perform supervised learning by counting occurrences

- If states are not given, perform unsupervised learning using Baum-Welch
- Expectation-maximization: Alternate between the two procedures until likelihood converges at local maximum