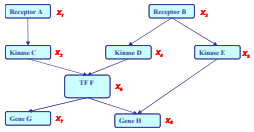
School of Computer Science
Carnegie Mellon

Hidden Markov Model and Conditional Random Fields

Probabilistic Graphical Models (10-708)

Lecture 12, Oct 29, 2007

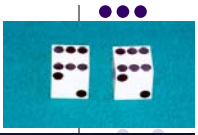


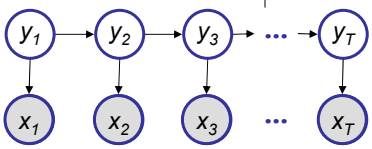
Eric Xing

Reading: J-Chap. 12, and addition papers

- Feedbacks
  - Today
  - Office hour
- Recitation
- Project milestone
  - This Wednesday

Hidden Markov Model revisit





- Transition probabilities between any two states

$$p(y_t^j = 1 \mid y_{t-1}^i = 1) = a_{i,j},$$

or $$p(y_t \mid y_{t-1}^i = 1) \sim \text{Multinomial}(a_{i,1}, a_{i,2}, \ldots, a_{i,M}), \forall i \in \mathrm{I}.$$

- Start probabilities

$$p(y_1) \sim \text{Multinomial}(\pi_1, \pi_2, \ldots, \pi_M).$$

- Emission probabilities associated with each state

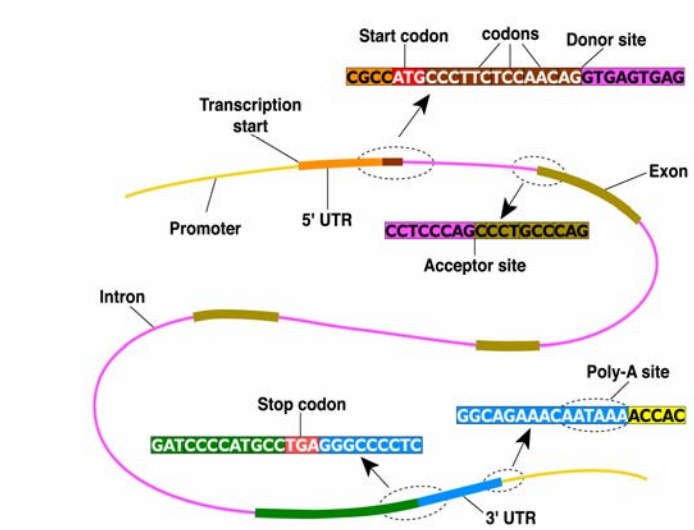
$$p(x_t \mid y_t^i = 1) \sim \text{Multinomial}(b_{i,1}, b_{i,2}, \ldots, b_{i,K}), \forall i \in \mathrm{I}.$$

or in general: $$p(x_t \mid y_t^i = 1) \sim \mathrm{f}(\cdot \mid \theta_i), \forall i \in \mathrm{I}.$$

Applications of HMMs

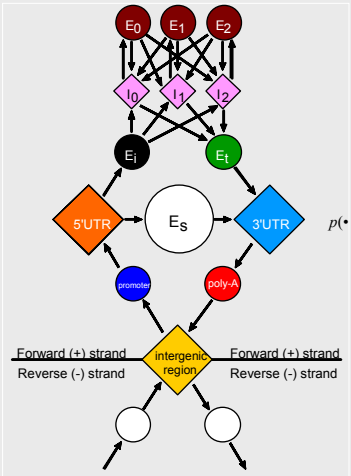
- **Some early applications of HMMs**
  - finance, but we never saw them
  - speech recognition
  - modelling ion channels
- In the mid-late 1980s HMMs entered genetics and molecular biology, and they are now firmly entrenched.
- **Some current applications of HMMs to biology**
  - mapping chromosomes
  - aligning biological sequences
  - predicting sequence structure
  - inferring evolutionary relationships
  - finding genes in DNA sequence

Typical structure of a gene

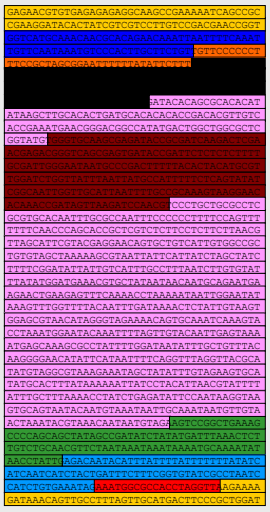


GENSCAN (Burge & Karlin)

Transition probabilities: $p(y_t^j = 1 \mid y_{t-1}^i = 1) = a_{i,j}$,



$$p(\bullet \mid y) = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \end{bmatrix}$$



The Forward Algorithm

- We want to calculate $P(\mathbf{x})$, the likelihood of $\mathbf{x}$, given the HMM
  - Sum over all possible ways of generating $\mathbf{x}$:

$$p(\mathbf{x}) = \sum_{\mathbf{y}} p(\mathbf{x},\mathbf{y}) = \sum_{y_1}\sum_{y_2}\cdots\sum_{y_N} \pi_{y_1}\prod_{t=2}^{T} a_{y_{t-1},y_t}\prod_{t=1}^{T} p(x_t \mid y_t)$$

  - To avoid summing over an exponential number of paths $\mathbf{y}$, define

$$\alpha(y_t^k = 1) = \alpha_t^k \overset{\text{def}}{=} P(x_1,\ldots,x_t, y_t^k = 1)$$ (the forward probability)

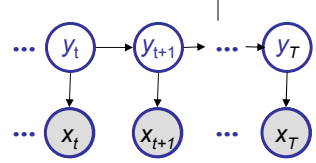
  - The recursion:

$$\alpha_t^k = p(x_t \mid y_t^k = 1)\sum_i \alpha_{t-1}^i a_{i,k}$$

$$P(\mathbf{x}) = \sum_k \alpha_T^k$$

The Backward Algorithm

- We want to compute $P(y_t^k = 1 \mid \mathbf{x})$, the posterior probability distribution on the tth position, given $\mathbf{x}$



  - We start by computing

$$P(y_t^k = 1, \mathbf{x}) = P(x_1,\ldots,x_t, y_t^k = 1, x_{t+1},\ldots,x_T)$$

$P(x)$

$$= P(x_1,\ldots,x_t, y_t^k = 1)P(x_{t+1},\ldots,x_T \mid x_1,\ldots,x_t, y_t^k = 1)$$

$$= P(x_1\ldots x_t, y_t^k = 1)P(x_{t+1}\ldots x_T \mid y_t^k = 1)$$

0 t T

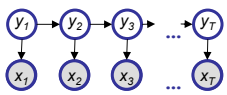
Forward, α_t^k **Backward,** $\beta_t^k = P(x_{t+1},\ldots,x_T \mid y_t^k = 1)$

  - The recursion: $$\beta_t^k = \sum_i a_{k,i}\, p(x_{t+1} \mid y_{t+1}^i = 1)\beta_{t+1}^i$$

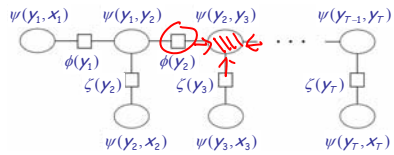
The Junction tree algorithm

$\phi(x_c) = \phi'(x_c) \prod M_{\to x_c}$

- A junction tree for the HMM

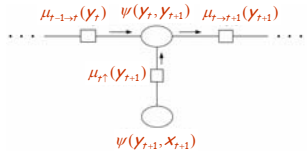


$\Rightarrow$



- Rightward pass

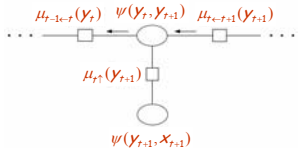
$$\mu_{t\to t+1}(y_{t+1}) = \sum_{y_t} \psi(y_t, y_{t+1}) \mu_{t-1\to t}(y_t) \mu_{t\uparrow}(y_{t+1})$$
$$= \sum_{y_t} p(y_{t+1} \mid y_t) \mu_{t-1\to t}(y_t) p(x_{t+1} \mid y_{t+1})$$
$$= p(x_{t+1} \mid y_{t+1}) \sum_{y_t} a_{y_t, y_{t+1}} \mu_{t-1\to t}(y_t)$$



  - This is exactly the *forward algorithm*!

- Leftward pass …

$$\mu_{t-1\leftarrow t}(y_t) = \sum_{y_{t+1}} \psi(y_t, y_{t+1}) \mu_{t\leftarrow t+1}(y_{t+1}) \mu_{t\uparrow}(y_{t+1})$$
$$= \sum_{y_{t+1}} p(y_{t+1} \mid y_t) \mu_{t\leftarrow t+1}(y_{t+1}) p(x_{t+1} \mid y_{t+1})$$



  - This is exactly the *backward algorithm*!

Summary of the F-B algorithm

$$\alpha_t^k \stackrel{\text{def}}{=} \mu_{t-1\to t}(k) = P(x_1, \ldots, x_{t-1}, x_t, y_t^k = 1)$$
$$\alpha_t^k = p(x_t \mid y_t^k = 1) \sum_i \alpha_{t-1}^i a_{i,k}$$
$$\beta_t^k \stackrel{\text{def}}{=} \mu_{t-1\leftarrow t}(k) = P(x_{t+1}, \ldots, x_T \mid y_t^k = 1)$$
$$\beta_t^k = \sum_i a_{k,i} p(x_{t+1} \mid y_{t+1}^i = 1) \beta_{t+1}^i$$

$$\gamma_t^i \stackrel{\text{def}}{=} p(y_t^i = 1 \mid x_{1:T}) \propto \alpha_t^i \beta_t^i = \sum_j \xi_t^{i,j}$$

$$\xi_t^{i,j} \stackrel{\text{def}}{=} p(y_t^i = 1, y_{t+1}^j = 1, x_{1:T})$$
$$\propto \mu_{t-1\to t}(y_t^i = 1) \mu_{t\leftarrow t+1}(y_{t+1}^j = 1) p(x_{t+1} \mid y_{t+1}) p(y_{t+1} \mid y_t)$$
$$\xi_t^{i,j} = \alpha_t^i \beta_{t+1}^j a_{i,j} p(x_{t+1} \mid y_{t+1}^j = 1)$$

The matrix-vector form:

$$B_t(i) \stackrel{\text{def}}{=} p(x_t \mid y_t^i = 1)$$
$$A(i,j) \stackrel{\text{def}}{=} p(y_{t+1}^j = 1 \mid y_t^i = 1)$$

$$\alpha_t = \left(A^T \alpha_{t-1}\right) .* B_t$$
$$\beta_t = A\left(\beta_{t+1} .* B_{t+1}\right)$$
$$\xi_t = \left(\alpha_t \left(\beta_{t+1} .* B_{t+1}\right)^T\right) .* A$$
$$\gamma_t = \alpha_t .* \beta_t$$

$p(\eta) \propto \mu_{\to} \mu_{\leftarrow} \in$

$\to \boxed{\eta} \in$

$\langle v \rangle_t \quad \eta_{t+1}$

$p(\eta_t, \eta_{t+1} \mid x)$

$\beta = ( )$

$A = \square$

Posterior decoding

- We can now calculate

$$P(y_t^k = 1 \mid \mathbf{x}) = \frac{P(y_t^k = 1, \mathbf{x})}{P(\mathbf{x})} = \frac{\alpha_t^k \beta_t^k}{P(\mathbf{x})}$$

- Then, we can ask
  - What is the most likely state at position *t* of sequence **x**:

$$k_t^* = \arg\max_k P(y_t^k = 1 \mid \mathbf{x})$$

  - Note that this is an MPA of a single hidden state, what if we want to a MPA of a whole hidden state sequence?
  - Posterior Decoding: $\left\{ y_t^{k_t^*} = 1 : t = 1 \cdots T \right\}$
  - This is different from MPA of a whole sequence of hidden states
  - This can be understood as *bit error rate* vs. *word error rate*

Example:
MPA of *X* ?
MPA of *(X, Y)* ?

x	y	P(x,y)
0	0	0.35
0	1	0.05
1	0	0.3
1	1	0.3

Viterbi decoding

- GIVEN $\mathbf{x} = x_1, \ldots, x_T$, we want to find $\mathbf{y} = y_1, \ldots, y_T$, such that $P(\mathbf{y}|\mathbf{x})$ is maximized:

$$\mathbf{y}^* = \text{argmax}_{\mathbf{y}}\, P(\mathbf{y}|\mathbf{x}) = \text{argmax}_{\pi}\, P(\mathbf{y},\mathbf{x})$$

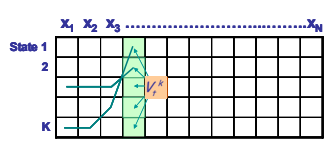
- Let

$$V_t^k = \max_{\{y_1,\ldots,y_{t-1}\}} P(x_1,\ldots,x_{t-1}, y_1,\ldots,y_{t-1}, x_t, y_t^k = 1)$$

= Probability of most likely **sequence of states** ending at state $y_t = k$

- The recursion:

$$V_t^k = p(x_t \mid y_t^k = 1) \max_i a_{i,k} V_{t-1}^i$$



- Underflows are a significant problem

$$p(x_1,\ldots,x_t, y_1,\ldots,y_t) = \pi_{y_1} a_{y_1,y_2} \cdots a_{y_{t-1},y_t} b_{y_1,x_1} \cdots b_{y_t,x_t}$$

  - These numbers become extremely small – underflow
  - Solution: Take the logs of all values: $V_t^k = \log p(x_t \mid y_t^k = 1) + \max_i \left(\log(a_{i,k}) + V_{t-1}^i \right)$

The Viterbi Algorithm – derivation

- Define the viterbi probability:

$$
\begin{aligned}
V_{t+1}^k &= \max_{\{y_1,\ldots,y_t\}} P(x_1,\ldots,x_t,y_1,\ldots,y_t,x_{t+1},y_{t+1}^k=1) \\
&= \max_{\{y_1,\ldots,y_t\}} P(x_{t+1},y_{t+1}^k=1 \mid x_1,\ldots,x_t,y_1,\ldots,y_t)P(x_1,\ldots,x_t,y_1,\ldots,y_t) \\
&= \max_{\{y_1,\ldots,y_t\}} P(x_{t+1},y_{t+1}^k=1 \mid y_t)P(x_1,\ldots,x_{t-1},y_1,\ldots,y_{t-1},x_t,y_t) \\
&= \max_i P(x_{t+1},y_{t+1}^k=1 \mid y_t^i=1)\max_{\{y_1,\ldots,y_{t-1}\}} P(x_1,\ldots,x_{t-1},y_1,\ldots,y_{t-1},x_t,y_t^i=1) \\
&= \max_i P(x_{t+1}, \mid y_{t+1}^k=1)a_{i,k}V_t^i \\
&= P(x_{t+1}, \mid y_{t+1}^k=1)\max_i a_{i,k}V_t^i
\end{aligned}
$$

Computational Complexity and implementation details

- What is the running time, and space required, for Forward, and Backward?

$$\alpha_t^k = p(x_t \mid y_t^k=1)\sum_i \alpha_{t-1}^i a_{i,k}$$

$$\beta_t^k = \sum_i a_{k,i}\, p(x_{t+1} \mid y_{t+1}^i=1)\beta_{t+1}^i$$

$$V_t^k = p(x_t \mid y_t^k=1)\max_i a_{i,k}V_{t-1}^i$$

Time: $O(K^2N)$; Space: $O(KN)$.

- Useful implementation technique to avoid underflows
  - Viterbi: sum of logs
  - Forward/Backward: rescaling at each position by multiplying by a constant

Learning HMM

- **Supervised learning**: estimation when the "right answer" is known
  - **Examples:**

    GIVEN: a genomic region $x = x_1 \ldots x_{1,000,000}$ where we have good (experimental) annotations of the CpG islands

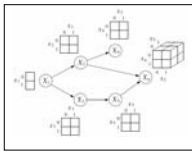
    GIVEN: the casino player allows us to observe him one evening, as he changes dice and produces 10,000 rolls
- **Unsupervised learning**: estimation when the "right answer" is unknown
  - **Examples:**

    GIVEN: the porcupine genome; we don't know how frequent are the CpG islands there, neither do we know their composition

    GIVEN: 10,000 rolls of the casino player, but we don't see when he changes dice
- **QUESTION:** Update the parameters θ of the model to maximize $P(x|\theta)$ --- Maximal likelihood (ML) estimation

Learning HMM: two scenarios

- Supervised learning: if only we knew the true state path then ML parameter estimation would be trivial
  - E.g., recall that for complete observed tabular BN:



$$\theta_{ijk}^{ML} = \frac{n_{ijk}}{\sum_{i',j',k} n_{ij'k}}$$

$$a_{ij}^{ML} = \frac{\#(i \to j)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=2}^{T} y_{n,t-1}^{i} y_{n,t}^{j}}{\sum_n \sum_{t=2}^{T} y_{n,t-1}^{i}}$$

$$b_{ik}^{ML} = \frac{\#(i \to k)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=1}^{T} y_{n,t}^{i} x_{n,t}^{k}}{\sum_n \sum_{t=1}^{T} y_{n,t}^{i}}$$

  - What if y is continuous? We can treat $\{(x_{n,t}, y_{n,t}) : t = 1:T, n = 1:N\}$ as $N \times T$ observations of, e.g., a GLIM, and apply learning rules for GLIM …
- Unsupervised learning: when the true state path is unknown, we can fill in the missing values using inference recursions.
  - The Baum Welch algorithm (i.e., EM)
    - Guaranteed to increase the log likelihood of the model after each iteration
    - Converges to local optimum, depending on initial conditions

The Baum Welch algorithm

- The complete log likelihood

$$\ell_c(\boldsymbol{\theta};\mathbf{x},\mathbf{y}) = \log p(\mathbf{x},\mathbf{y}) = \log \prod_n \left(p(y_{n,1}) \prod_{t=2}^{T} p(y_{n,t} \mid y_{n,t-1}) \prod_{t=1}^{T} p(x_{n,t} \mid x_{n,t}) \right)$$

- The expected complete log likelihood

$$\langle \ell_c(\boldsymbol{\theta};\mathbf{x},\mathbf{y}) \rangle = \sum_n \left(\langle y_{n,1}^i \rangle_{p(y_{n,1}|\mathbf{x}_n)} \log \pi_i \right) + \sum_n \sum_{t=2}^{T} \left(\langle y_{n,t-1}^i y_{n,t}^j \rangle_{p(y_{n,t-1},y_{n,t}|\mathbf{x}_n)} \log a_{i,j} \right) + \sum_n \sum_{t=1}^{T} \left(x_{n,t}^k \langle y_{n,t}^i \rangle_{p(y_{n,t}|\mathbf{x}_n)} \log b_{i,k} \right)$$

- EM
  - The E step

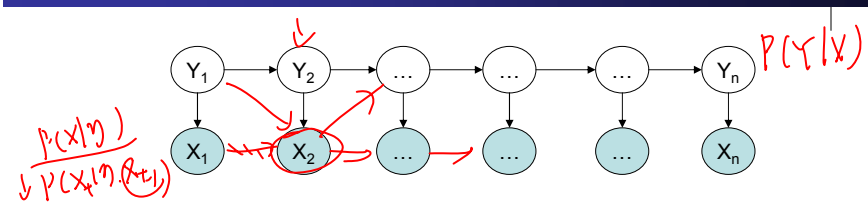
$$\gamma_{n,t}^i = \langle y_{n,t}^i \rangle = p(y_{n,t}^i = 1 \mid \mathbf{x}_n)$$

$$\xi_{n,t}^{i,j} = \langle y_{n,t-1}^i y_{n,t}^j \rangle = p(y_{n,t-1}^i = 1, y_{n,t}^j = 1 \mid \mathbf{x}_n)$$

  - The M step ("symbolically" identical to MLE)

$$\pi_i^{ML} = \frac{\sum_n \gamma_{n,1}^i}{N} \qquad a_{ij}^{ML} = \frac{\sum_n \sum_{t=2}^{T} \xi_{n,t}^{i,j}}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i} \qquad b_{ik}^{ML} = \frac{\sum_n \sum_{t=1}^{T} \gamma_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i}$$

Shortcomings of Hidden Markov Model



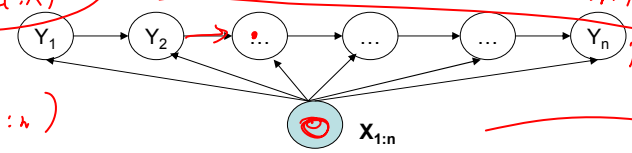
- HMM models capture dependences between each state and only its corresponding observation
  - NLP example: In a sentence segmentation task, each segmental state may depend not just on a single word (and the adjacent segmental stages), but also on the (non-local) features of the whole line such as line length, indentation, amount of white space, etc.
- Mismatch between learning objective function and prediction objective function

  $P(X, Y) \to P(X) \to P(Y|X) = \frac{P(X,Y)}{P(X)}$

  - HMM learns a joint distribution of states and observations P(**Y**, **X**), but in a prediction task, we need the conditional probability P(**Y**|**X**)

Solution:

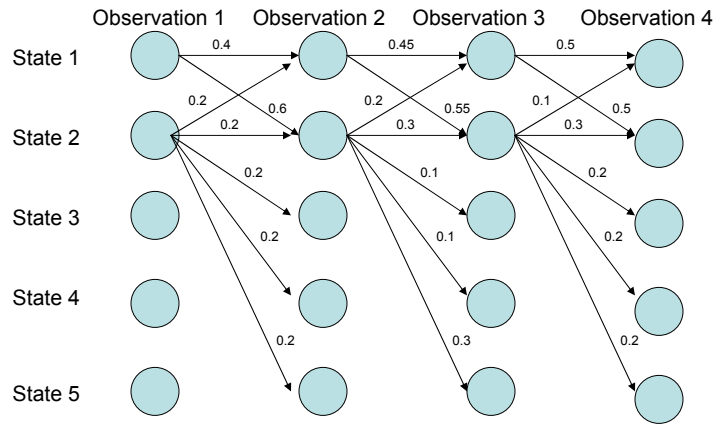
Maximum Entropy Markov Model (MEMM)



$$P(\mathbf{y}_{1:n}|\mathbf{x}_{1:n}) = \prod_{i=1}^{n} P(y_i|y_{i-1},\mathbf{x}_{1:n}) = \prod_{i=1}^{n} \frac{\exp(\mathbf{w}^T\mathbf{f}(y_i, y_{i-1}, \mathbf{x}_{1:n}))}{Z(y_{i-1}, \mathbf{x}_{1:n})}$$

- Models dependence between each state and the full observation sequence explicitly
  - More expressive than HMMs
- Discriminative model
  - Completely ignores modeling P(**X**): saves modeling effort
  - Learning objective function consistent with predictive function: P(**Y**|**X**)

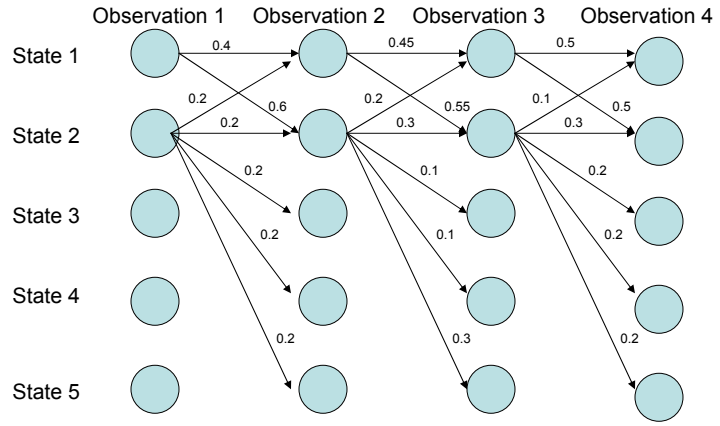
MEMM: the Label bias problem



What the local transition probabilities say:

- State 1 almost always prefers to go to state 2
- State 2 almost always prefer to stay in state 2

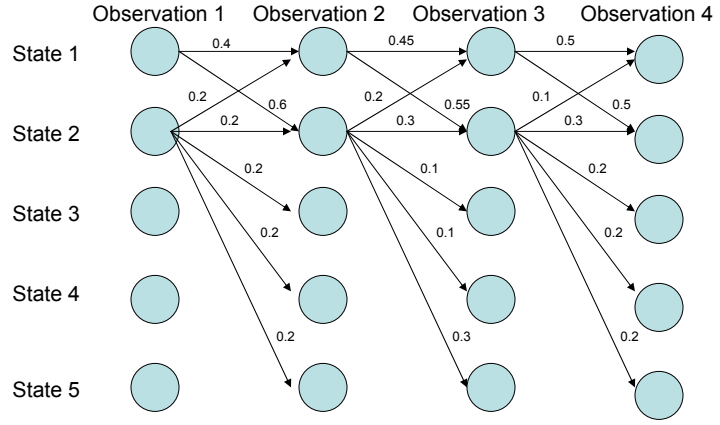
MEMM: the Label bias problem



Probability of path 1-> 1-> 1-> 1:

- 0.4 x 0.45 x 0.5 = 0.09

MEMM: the Label bias problem

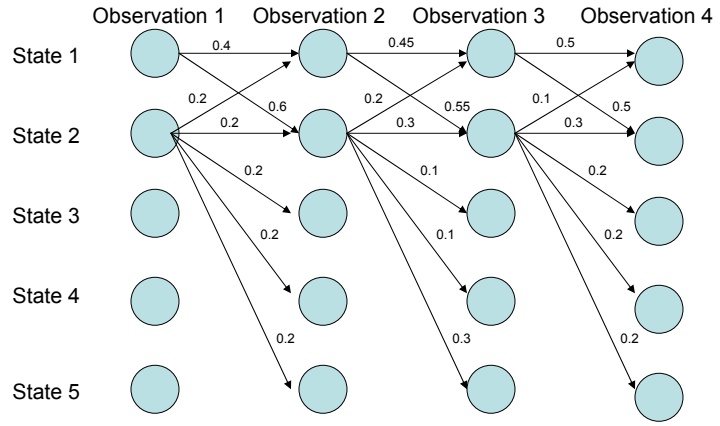


Probability of path 2->2->2->2 :

- 0.2 X 0.3 X 0.3 = 0.018

Other paths:
1-> 1-> 1-> 1: 0.09

MEMM: the Label bias problem

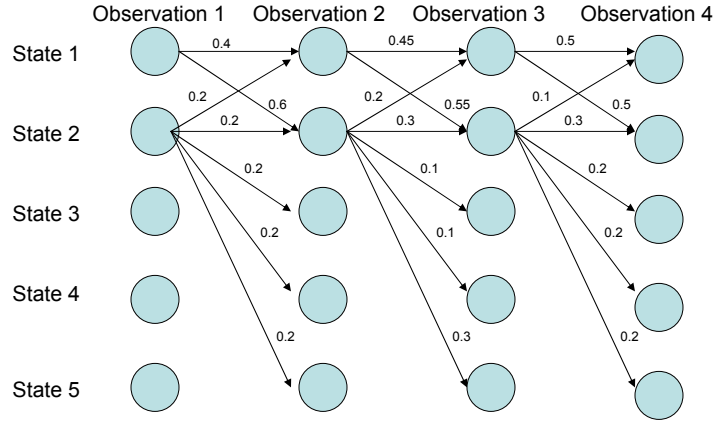


Probability of path 1->2->1->2:

- 0.6 X 0.2 X 0.5 = 0.06

Other paths:
1->1->1->1: 0.09
2->2->2->2: 0.018

MEMM: the Label bias problem

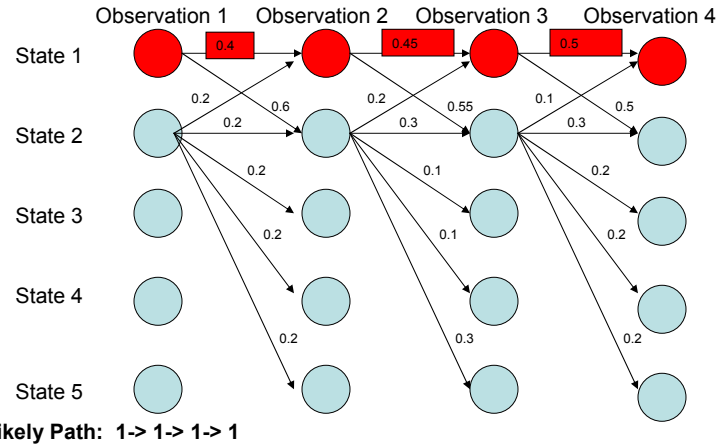


Probability of path 1->1->2->2:

- 0.4 X 0.55 X 0.3 = 0.066

Other paths:
1->1->1->1: 0.09
2->2->2->2: 0.018
1->2->1->2: 0.06

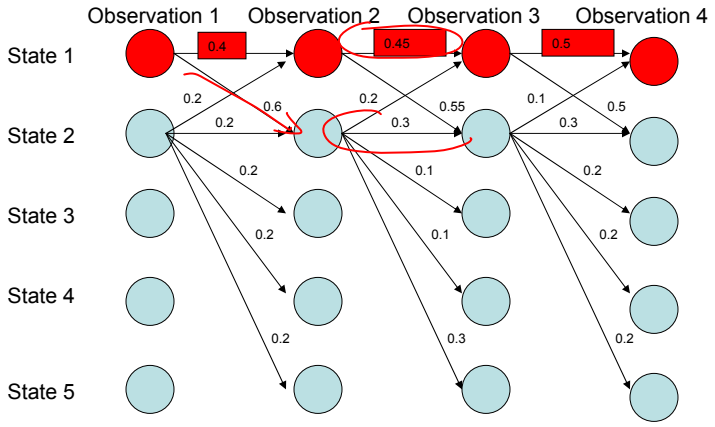
MEMM: the Label bias problem



Most Likely Path: 1-> 1-> 1-> 1

- Although **locally** it seems state 1 wants to go to state 2 and state 2 wants to remain in state 2.
- **why?**

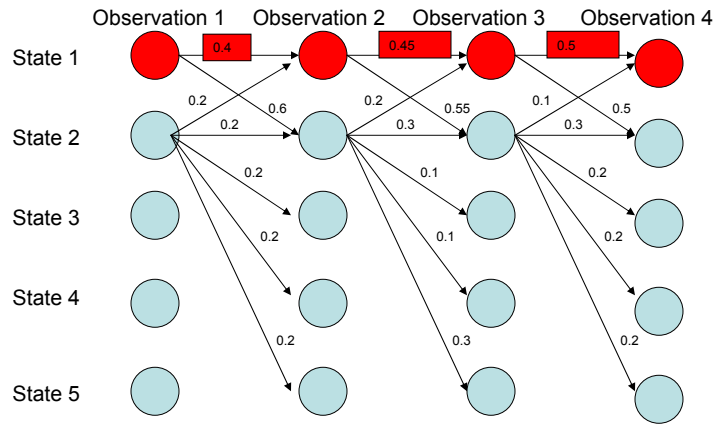
MEMM: the Label bias problem



Most Likely Path: 1-> 1-> 1-> 1

- State 1 has only two transitions but state 2 has 5:
  - Average transition probability from state 2 is lower

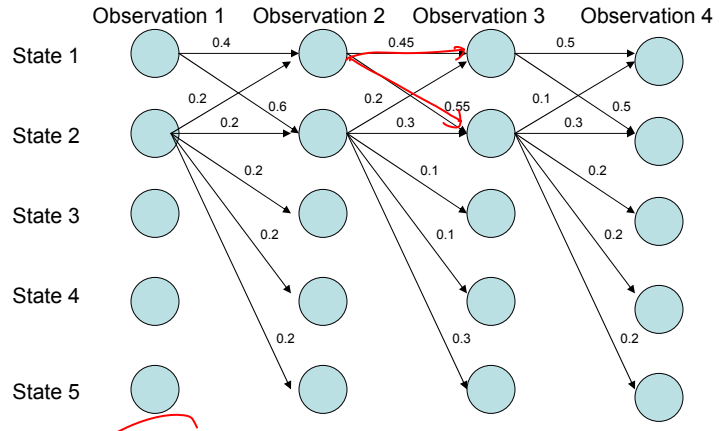
MEMM: the Label bias problem



Label bias problem in MEMM:

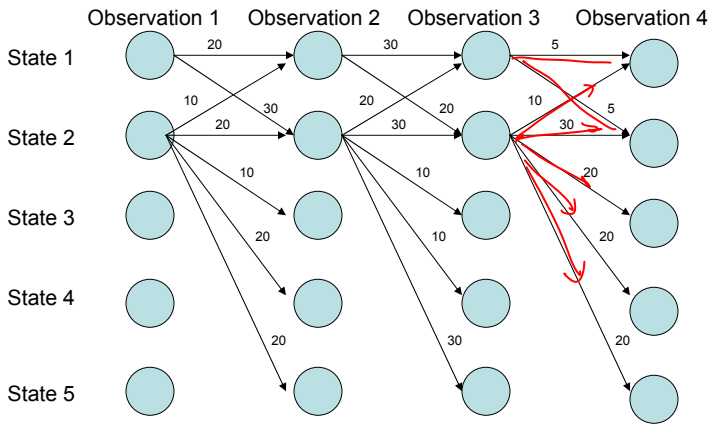
- Preference of states with lower number of transitions over others

Solution: Do not normalize probabilities locally



From local probabilities …

Solution:
Do not normalize probabilities locally



From local probabilities to local potentials

- States with lower transitions do not have an unfair advantage!

- Office hour

  1 – 2 pm Mon

- Mid-term project milestone due today

- Next week

  4:30 – 5:30 this Friday