Advanced Introduction to Machine Learning

10715, Fall 2014

Structured Models:

Hidden Markov Models versus Conditional Random Fields

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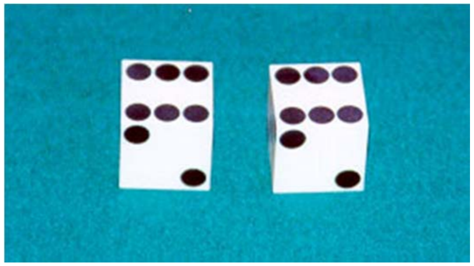
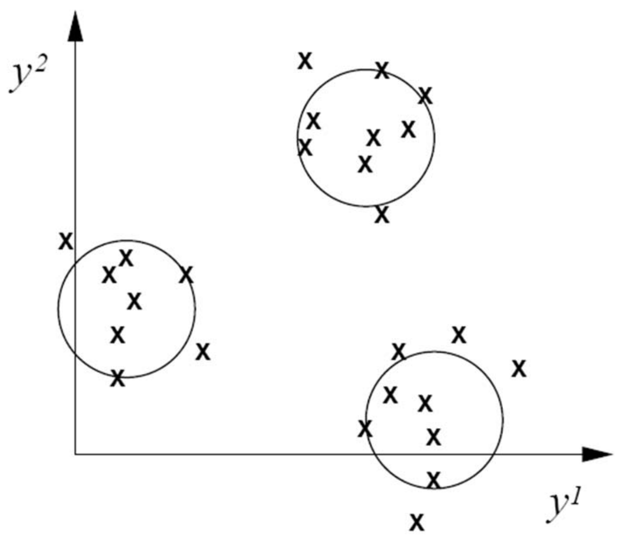
Lecture 11, October 13, 2014

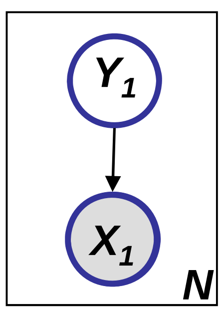


Reading:

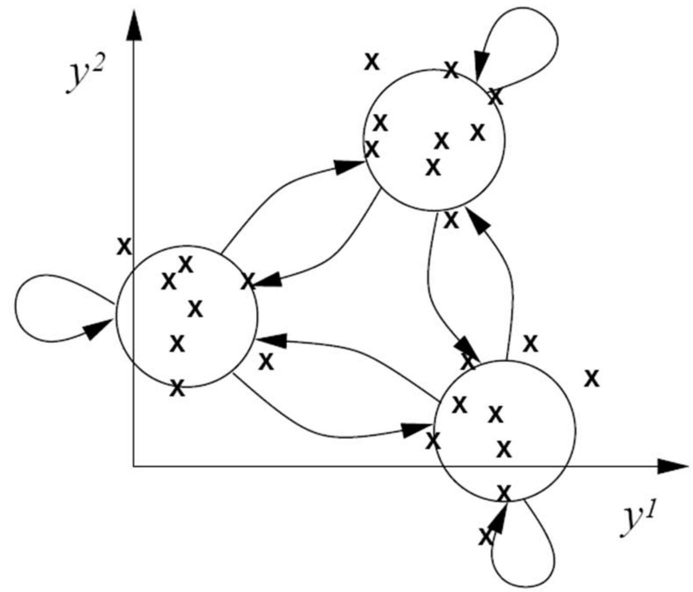
From static to dynamic mixture models

Static mixture





Dynamic mixture



The underlying source:

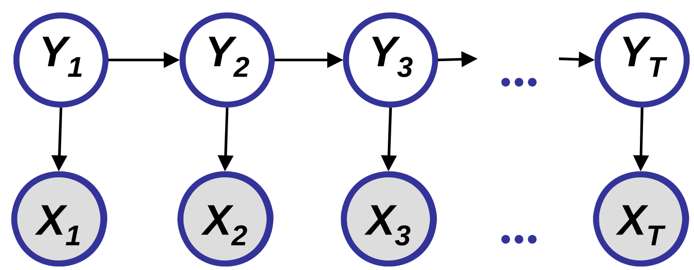
Speech signal,

dice,

The sequence:

Phonemes,

sequence of rolls,



Hidden Markov Model

- Observation space
  - **Alphabetic set:** $\mathbb{C} = \{c_1, c_2, \cdots, c_K\}$
  - **Euclidean space:** $\mathbb{R}^d$
- Index set of hidden states

$$\mathbb{I} = \{1, 2, \cdots, M\}$$

- Transition probabilities between any two states

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

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

- Start probabilities

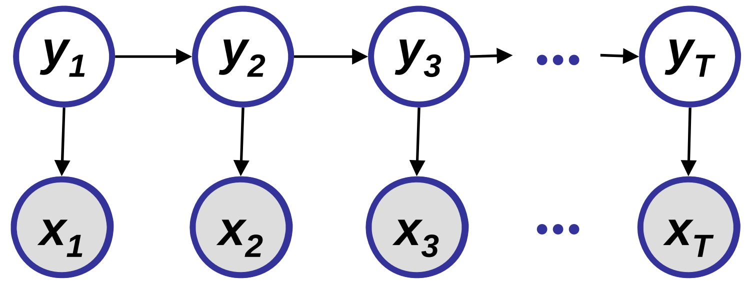
$$p(y_1) \sim \text{Multinomial}(\pi_1, \pi_2, \ldots, \pi_M).$$

- Emission probabilities associated with each state

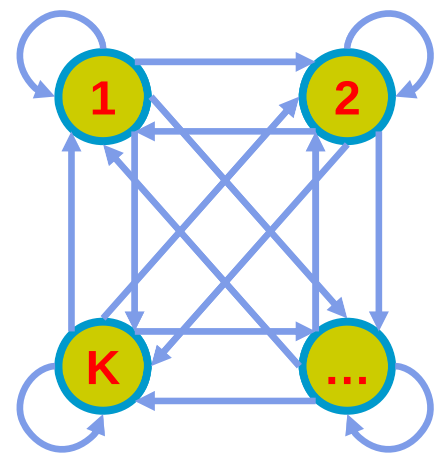
$$p(x_t \mid y_t^i = 1) \sim \text{Multinomial}(b_{i,1}, b_{i,2}, \ldots, b_{i,K}), \forall i \in \mathbb{I}.$$

or in general:

$$p(x_t \mid y_t^i = 1) \sim \text{f}(\cdot \mid \theta_i), \forall i \in \mathbb{I}.$$



Graphical model

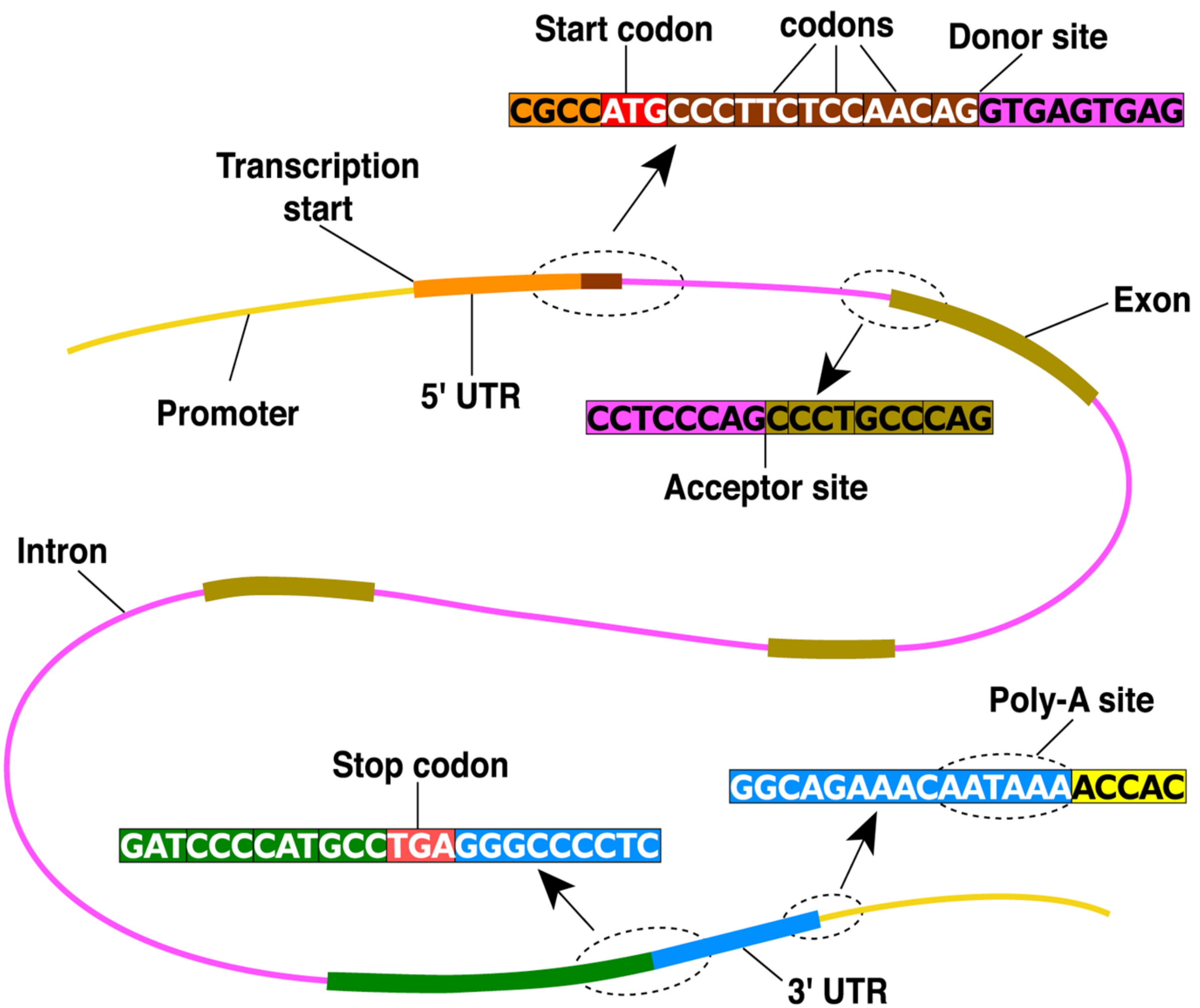


State automata

Applications of HMMs

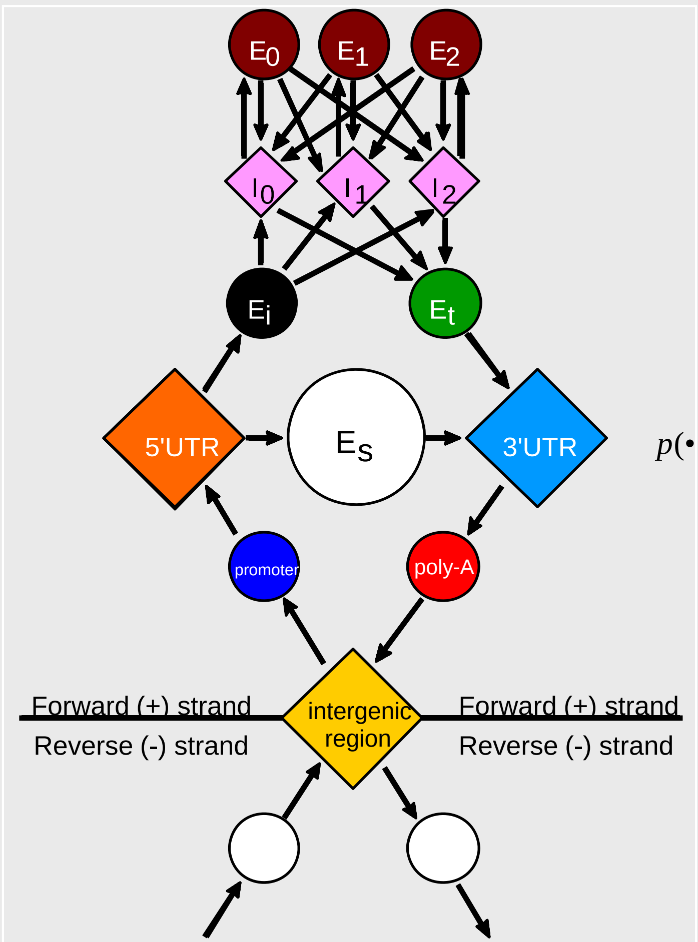
- **Some early applications of HMMs**
  - finance, but we never saw them
  - speech recognition
  - modelling ion channels
- In the mid-late 1980s HMMs entered genetics and molecular biology, and they are now firmly entrenched.
- **Some current applications of HMMs to biology**
  - mapping chromosomes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

A Bio Application: gene finding

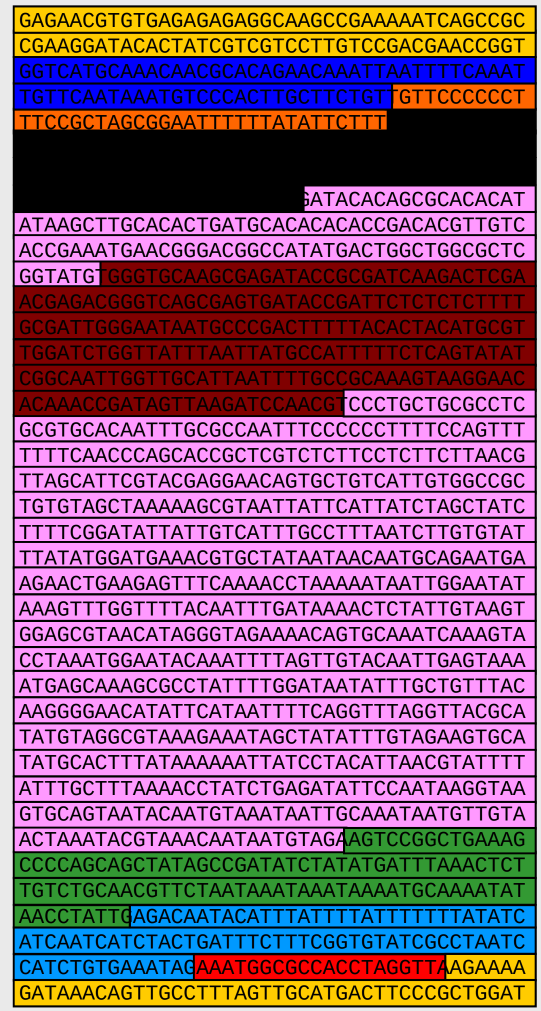


GENSCAN (Burge & Karlin)

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



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



A "Financial" Application: The Dishonest Casino

A casino has two dice:

- Fair die

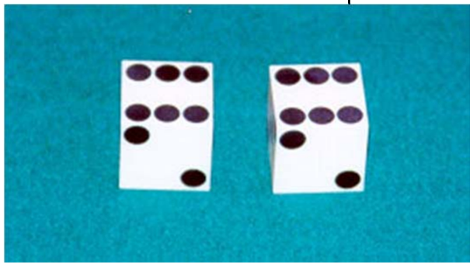
  P(1) = P(2) = P(3) = P(5) = P(6) = 1/6

- Loaded die

  P(1) = P(2) = P(3) = P(5) = 1/10

  P(6) = 1/2

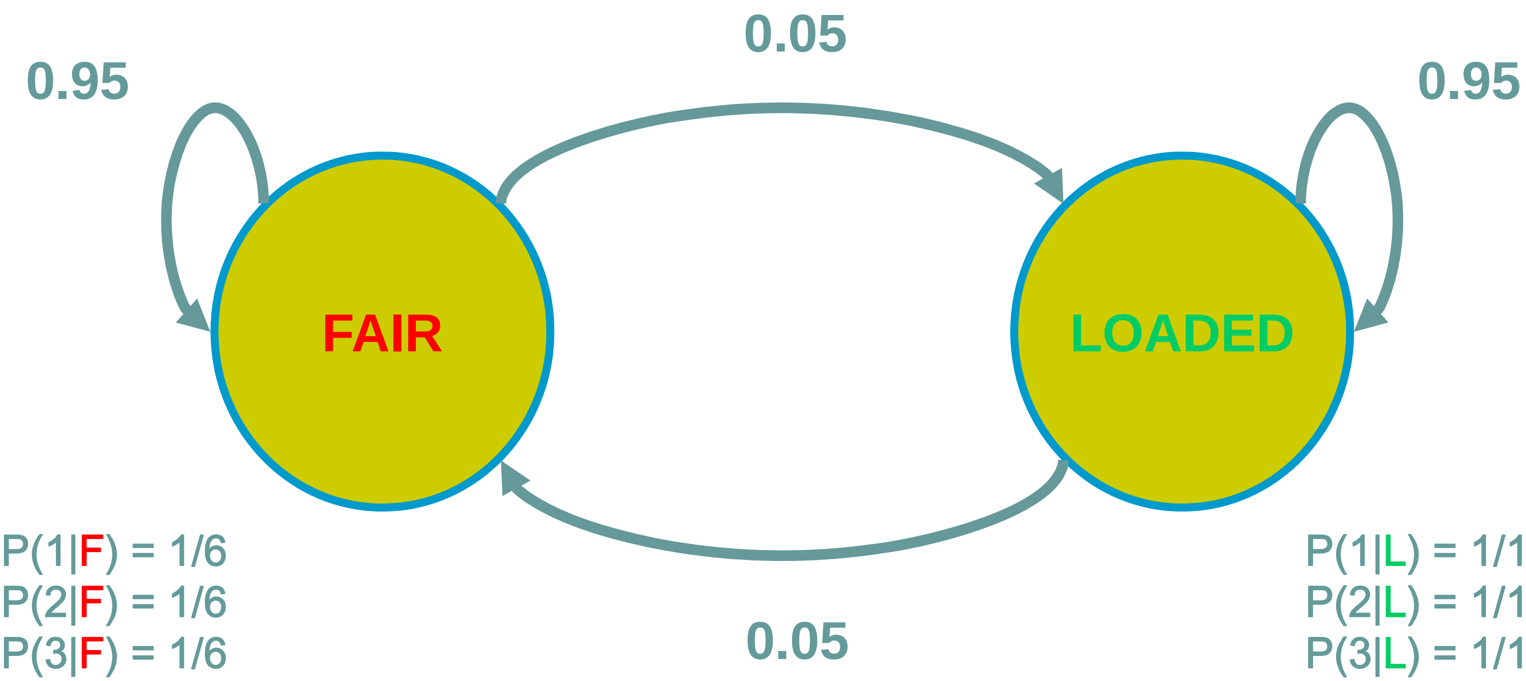
Casino player switches back-&-forth between fair and loaded die once every 20 turns



<u>Game:</u>

1. You bet $1
2. You roll (always with a fair die)
3. Casino player rolls (maybe with fair die, maybe with loaded die)
4. Highest number wins $2

The Dishonest Casino Model



P(1|F) = 1/6
P(2|F) = 1/6
P(3|F) = 1/6
P(4|F) = 1/6
P(5|F) = 1/6
P(6|F) = 1/6

P(1|L) = 1/10
P(2|L) = 1/10
P(3|L) = 1/10
P(4|L) = 1/10
P(5|L) = 1/10
P(6|L) = 1/2

Puzzles Regarding the Dishonest Casino

GIVEN: A sequence of rolls by the casino player

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QUESTION

- How likely is this sequence, given our model of how the casino works?
  - This is the **EVALUATION** problem in HMMs
- What portion of the sequence was generated with the fair die, and what portion with the loaded die?
  - This is the **DECODING** question in HMMs
- How “loaded” is the loaded die? How “fair” is the fair die? How often does the casino player change from fair to loaded, and back?
  - This is the **LEARNING** question in HMMs

Joint Probability

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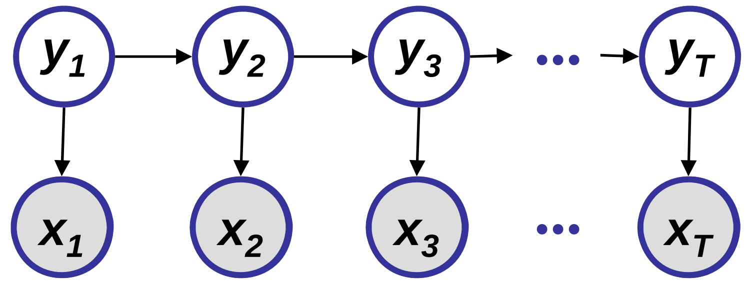
Probability of a Parse

- Given a sequence $\mathbf{x} = x_1 \ldots\ldots x_T$ and a parse $\mathbf{y} = y_1, \ldots\ldots, y_T$,
- To find how likely is the parse: (given our HMM and the sequence)



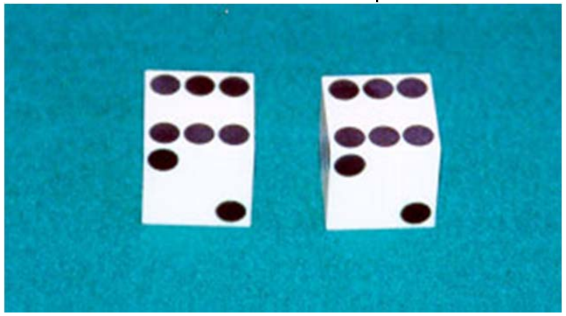
$p(\mathbf{x}, \mathbf{y}) = p(x_1 \ldots\ldots x_T, y_1, \ldots\ldots, y_T)$ (Joint probability)

$= p(y_1)\, p(x_1 \mid y_1)\, p(y_2 \mid y_1)\, p(x_2 \mid y_2) \ldots p(y_T \mid y_{T-1})\, p(x_T \mid y_T)$

$= p(y_1)\, P(y_2 \mid y_1) \ldots p(y_T \mid y_{T-1}) \times p(x_1 \mid y_1)\, p(x_2 \mid y_2) \ldots p(x_T \mid y_T)$

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

Example: the Dishonest Casino



- Let the sequence of rolls be:
  - $\boldsymbol{x}$ = 1, 2, 1, 5, 6, 2, 1, 6, 2, 4
- Then, what is the likelihood of
  - $\boldsymbol{y}$ = Fair, Fair, Fair, Fair, Fair, Fair, Fair, Fair, Fair, Fair?

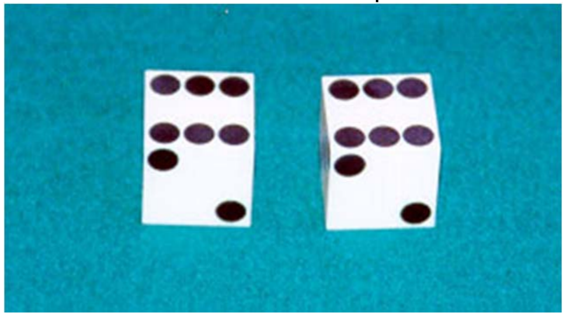
    (say initial probs $a_{0Fair} = ½$, $a_{oLoaded} = ½$)

½ × P(1 | Fair) P(Fair | Fair) P(2 | Fair) P(Fair | Fair) … P(4 | Fair) =

$½ \times (\mathbf{1/6})^{10} \times (\mathbf{0.95})^{9} = .00000000521158647211 = 5.21 \times 10^{-9}$

Example: the Dishonest Casino

- So, the likelihood the die is fair in all this run is just 5.21×10^{-9}



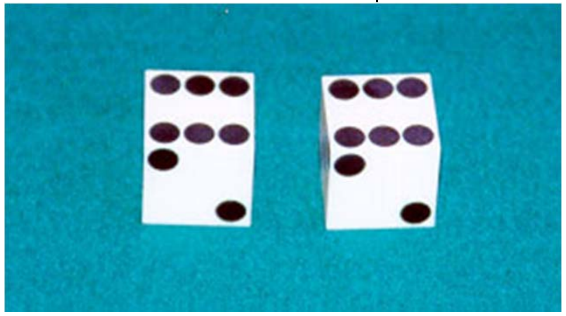
- OK, but what is the likelihood of
  - π = Loaded, Loaded, Loaded, Loaded, Loaded, Loaded, Loaded, Loaded, Loaded, Loaded?

$\frac{1}{2} \times$ P(1 | Loaded) P(Loaded | Loaded) … P(4 | Loaded) =

$\frac{1}{2} \times (\mathbf{1/10})^8 \times (\mathbf{1/2})^2 (\mathbf{0.95})^9 = .00000000078781176215 = 0.79 \times 10^{-9}$

- Therefore, it is after all 6.59 times more likely that the die is fair all the way, than that it is loaded all the way

Example: the Dishonest Casino



- Let the sequence of rolls be:
  - x = 1, 6, 6, 5, 6, 2, 6, 6, 3, 6
- Now, what is the likelihood π = F, F, …, F?
  - $\frac{1}{2} \times (1/6)^{10} \times (0.95)^{9} = 0.5 \times 10^{-9}$, same as before
- What is the likelihood y = L, L, …, L?

$$\frac{1}{2} \times (1/10)^{4} \times (1/2)^{6} (0.95)^{9} = .00000049238235134735 = 5 \times 10^{-7}$$

- So, it is 100 times more likely the die is loaded

Joint Probability

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Three Main Questions on HMMs

1. Evaluation

GIVEN an HMM ***M***, and a sequence ***x***,
FIND Prob (***x*** | ***M***)
ALGO. Forward

2. Decoding

GIVEN an HMM ***M***, and a sequence ***x*** ,
FIND the sequence **y** of states that maximizes, e.g., P(***y*** | ***x*** , ***M***),
or the most probable subsequence of states
ALGO. Viterbi, Forward-backward

3. Learning

GIVEN an HMM ***M***, with unspecified transition/emission probs.,
and a sequence ***x***,
FIND parameters $\theta = (\pi_i, a_{ij}, \eta_{ik})$ that maximize P(***x*** | θ)
ALGO. Baum-Welch (EM)

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

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

(the forward probability)

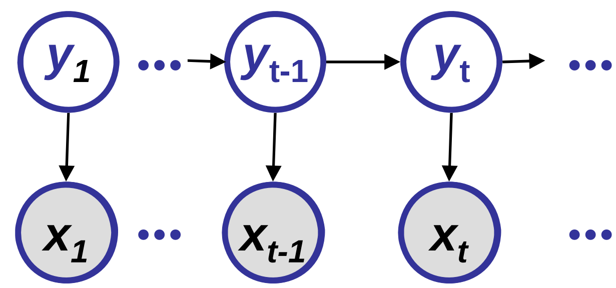
  - The recursion:

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

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

The Forward Algorithm – derivation

- Compute the forward probability:



$$\alpha_t^k = P(x_1,\ldots,x_{t-1},x_t,y_t^k=1)$$

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

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

$$= P(x_t \mid y_t^k=1) \sum_i P(x_1,\ldots,x_{t-1},y_{t-1}^i=1) P(y_t^k=1 \mid y_{t-1}^i=1)$$

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

Chain rule: $P(A,B,C) = P(A)P(B \mid A)P(C \mid A,B)$

The Forward Algorithm

- We can compute α_t^k for all k, t, using dynamic programming!

Initialization:

$$\alpha_1^k = P(x_1, y_1^k = 1)$$
$$= P(x_1 \mid y_1^k = 1) P(y_1^k = 1)$$
$$= P(x_1 \mid y_1^k = 1) \pi_k$$

$$\alpha_1^k = P(x_1 \mid y_1^k = 1) \pi_k$$

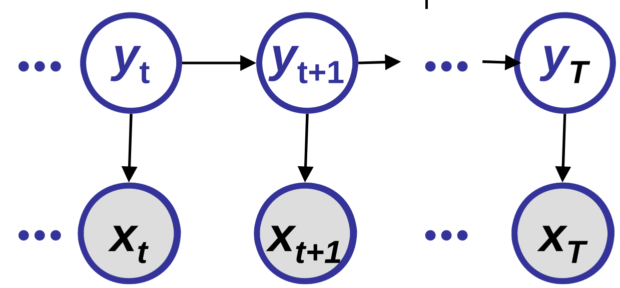
Iteration:

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

Termination:

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

The Backward Algorithm



- We want to compute $P(y_t^k = 1 \mid \mathbf{x})$,

  the posterior probability distribution on the t th position, given $\mathbf{x}$

  - We start by computing

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

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

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

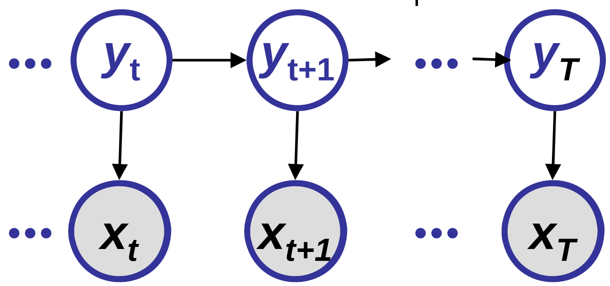
Forward, α_t^k Backward, $\beta_t^k = P(x_{t+1}, \ldots, x_T \mid y_t^k = 1)$

  - 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 Backward Algorithm – derivation

- Define the backward probability:



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

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

$$= \sum_i P(y_{t+1}^i = 1 \mid y_t^k = 1)\, p(x_{t+1} \mid y_{t+1}^i = 1, y_t^k = 1)\, P(x_{t+2},\ldots,x_T \mid x_{t+1}, y_{t+1}^i = 1, y_t^k = 1)$$

$$= \sum_i P(y_{t+1}^i = 1 \mid y_t^k = 1)\, p(x_{t+1} \mid y_{t+1}^i = 1)\, P(x_{t+2},\ldots,x_T \mid y_{t+1}^i = 1)$$

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

Chain rule: $P(A,B,C \mid \alpha) = P(A \mid \alpha) P(B \mid A,\alpha) P(C \mid A,B,\alpha)$

The Backward Algorithm

- We can compute β_t^k for all k, t, using dynamic programming!

Initialization:

$$\beta_T^k = 1, \ \forall k$$

Iteration:

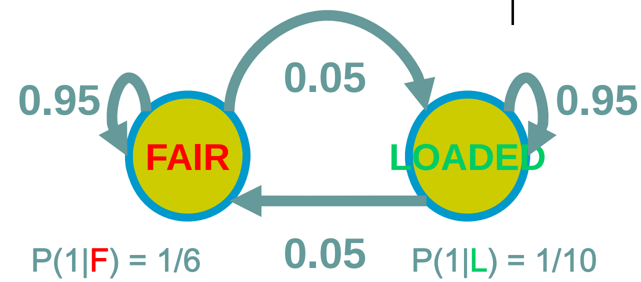
$$\beta_t^k = \sum_i a_{k,i} P(x_{t+1} \mid y_{t+1}^i = 1) \beta_{t+1}^i$$

Termination:

$$P(\mathbf{x}) = \sum_k \alpha_1^k \beta_1^k$$

Example:

x = 1, 2, 1, 5, 6, 2, 1, 6, 2, 4



P(1|F) = 1/6
P(2|F) = 1/6
P(3|F) = 1/6
P(4|F) = 1/6
P(5|F) = 1/6
P(6|F) = 1/6

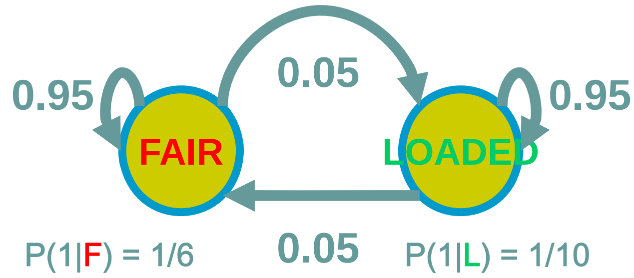
P(1|L) = 1/10
P(2|L) = 1/10
P(3|L) = 1/10
P(4|L) = 1/10
P(5|L) = 1/10
P(6|L) = 1/2

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

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

x = 1, 2, 1, 5, 6, 2, 1, 6, 2, 4

Alpha (actual)		Beta (actual)	
0.0833	0.0500	0.0000	0.0000
0.0136	0.0052	0.0000	0.0000
0.0022	0.0006	0.0000	0.0000
0.0004	0.0001	0.0000	0.0000
0.0001	0.0000	0.0001	0.0001
0.0000	0.0000	0.0007	0.0006
0.0000	0.0000	0.0045	0.0055
0.0000	0.0000	0.0264	0.0112
0.0000	0.0000	0.1633	0.1033
0.0000	0.0000	1.0000	1.0000



P(1|F) = 1/6
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P(5|F) = 1/6
P(6|F) = 1/6

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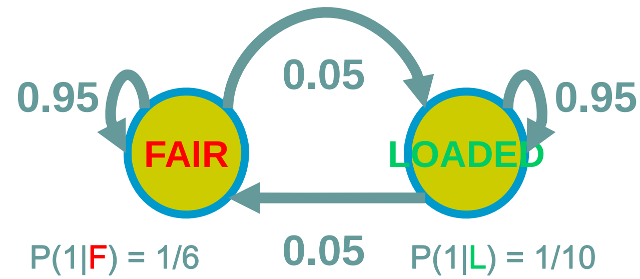
P(2|L) = 1/10
P(3|L) = 1/10
P(4|L) = 1/10
P(5|L) = 1/10
P(6|L) = 1/2

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

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

x = 1, 2, 1, 5, 6, 2, 1, 6, 2, 4



P(1|F) = 1/6	P(1|L) = 1/10
P(2|F) = 1/6	P(2|L) = 1/10
P(3|F) = 1/6	P(3|L) = 1/10
P(4|F) = 1/6	P(4|L) = 1/10
P(5|F) = 1/6	P(5|L) = 1/10
P(6|F) = 1/6	P(6|L) = 1/2

Alpha (logs)		Beta (logs)	
-2.4849	-2.9957	-16.2439	-17.2014
-4.2969	-5.2655	-14.4185	-14.9922
-6.1201	-7.4896	-12.6028	-12.7337
-7.9499	-9.6553	-10.8042	-10.4389
-9.7834	-10.1454	-9.0373	-9.7289
-11.5905	-12.4264	-7.2181	-7.4833
-13.4110	-14.6657	-5.4135	-5.1977
-15.2391	-15.2407	-3.6352	-4.4938
-17.0310	-17.5432	-1.8120	-2.2698
-18.8430	-19.8129	0	0

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

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

What is the probability of a hidden state prediction?

$$P(y_5^1 \mid X) = \frac{(a)}{P(X)}$$
$$P(y_5^2 \mid X) = \frac{(b)}{P(X)}$$
$$\Big] + = 1.$$

$$P(y_5^1 \mid X) = \frac{a}{a+b} = \frac{\exp(-18.8207)}{\exp(-18.8207) + \exp(-19.8743)} = \underline{0.7415}$$

$$P(y_8^1 \mid X) = \exp(-18.8743)/C$$
$$P(y_8^2 \mid X) = \exp(-19.6545)/C$$
$$P(y_8^1 \mid X) = 0.6857.$$

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 $\mathbf{x}$:

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

  - 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:

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

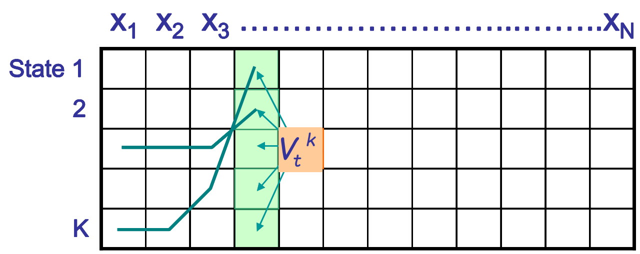
  - Let

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

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

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: two scenarios

- **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

Supervised ML estimation

- Given $x = x_1 \ldots x_N$ for which the true state path $y = y_1 \ldots y_N$ is known,
  - **Define:**

    A_{ij} = # times state transition $i \rightarrow j$ occurs in **y**

    B_{ik} = # times state i in **y** emits k in **x**

  - **We can show that the maximum likelihood parameters θ are:**

$$a_{ij}^{ML} = \frac{\#(i \rightarrow j)}{\#(i \rightarrow \bullet)} = \frac{\sum_n \sum_{t=2}^T y_{n,t-1}^i y_{n,t}^j}{\sum_n \sum_{t=2}^T y_{n,t-1}^i} = \frac{A_{ij}}{\sum_{j'} A_{ij'}}$$

$$b_{ik}^{ML} = \frac{\#(i \rightarrow k)}{\#(i \rightarrow \bullet)} = \frac{\sum_n \sum_{t=1}^T y_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^T y_{n,t}^i} = \frac{B_{ik}}{\sum_{k'} B_{ik'}}$$

(Homework!)

  - **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 Gaussian, and apply learning rules for Gaussian …**

(Homework!)

Pseudocounts

- Solution for small training sets:
  - Add pseudocounts

    A_{ij} = # times state transition $i \rightarrow j$ occurs in $\mathbf{y}$ + R_{ij}

    B_{ik} = # times state i in $\mathbf{y}$ emits k in $\mathbf{x}$ + S_{ik}

  - R_{ij}, S_{ij} are pseudocounts representing our prior belief
  - Total pseudocounts: $R_i = \Sigma_j R_{ij}$, $S_i = \Sigma_k S_{ik}$,
    - --- "strength" of prior belief,
    - --- total number of imaginary instances in the prior

- Larger total pseudocounts $\Rightarrow$ strong prior belief

- Small total pseudocounts: just to avoid 0 probabilities --- smoothing

Unsupervised ML estimation

- Given $x = x_1 \ldots x_N$ for which the true state path $y = y_1 \ldots y_N$ is unknown,

  - **EXPECTATION MAXIMIZATION**

0. Starting with our best guess of a model M, parameters θ:
1. Estimate A_{ij} , B_{ik} in the training data
   - How? $A_{ij} = \sum_{n,t} \langle y_{n,t-1}^i y_{n,t}^j \rangle$ $B_{ik} = \sum_{n,t} \langle y_{n,t}^i \rangle x_{n,t}^k$, How? (homework)
2. Update θ according to A_{ij} , B_{ik}
   - Now a "supervised learning" problem
3. Repeat 1 & 2, until convergence

This is called the Baum-Welch Algorithm

We can get to a provably more (or equally) likely parameter set θ each iteration

The Baum Welch algorithm

- The complete log likelihood

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

- The expected complete log likelihood

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

- EM
  - The **E** step

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

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

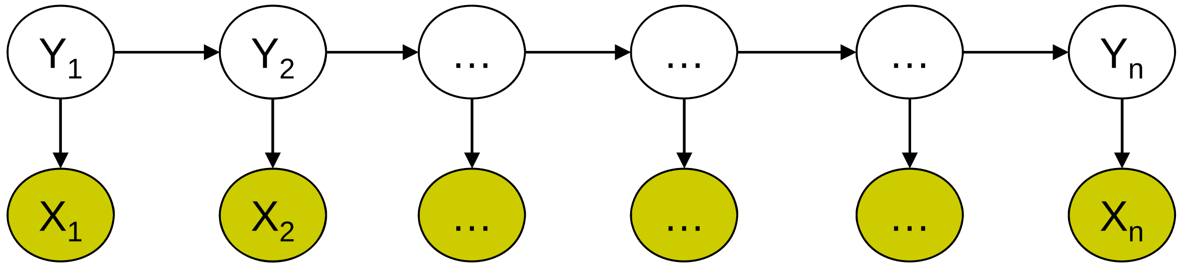
  - The **M** step ("symbolically" identical to MLE)

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

Summary

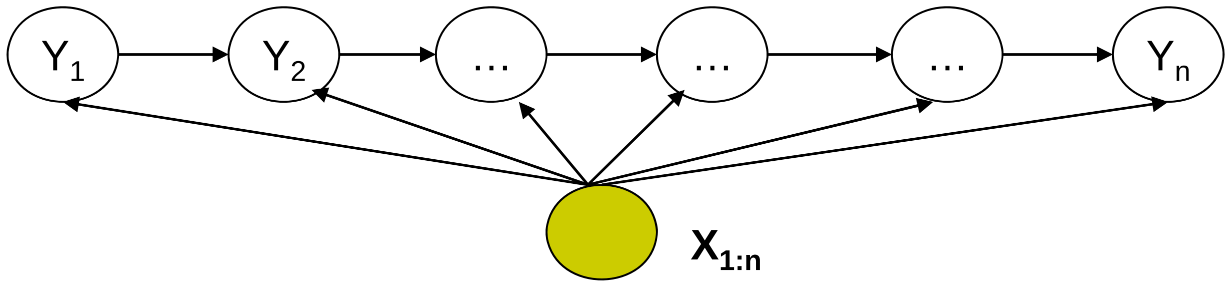
- Modeling hidden transitional trajectories (in discrete state space, such as cluster label, DNA copy number, dice-choice, etc.) underlying observed sequence data (discrete, such as dice outcomes; or continuous, such as CGH signals)
- Useful for parsing, segmenting sequential data
- Important HMM computations:
  - The joint likelihood of a parse and data can be written as a product to local terms (i.e., initial prob, transition prob, emission prob.)
  - Computing marginal likelihood of the observed sequence: forward algorithm
  - Predicting a single hidden state: forward-backward
  - Predicting an entire sequence of hidden states: viterbi
  - Learning HMM parameters: an EM algorithm known as Baum-Welch

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
  - 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**)

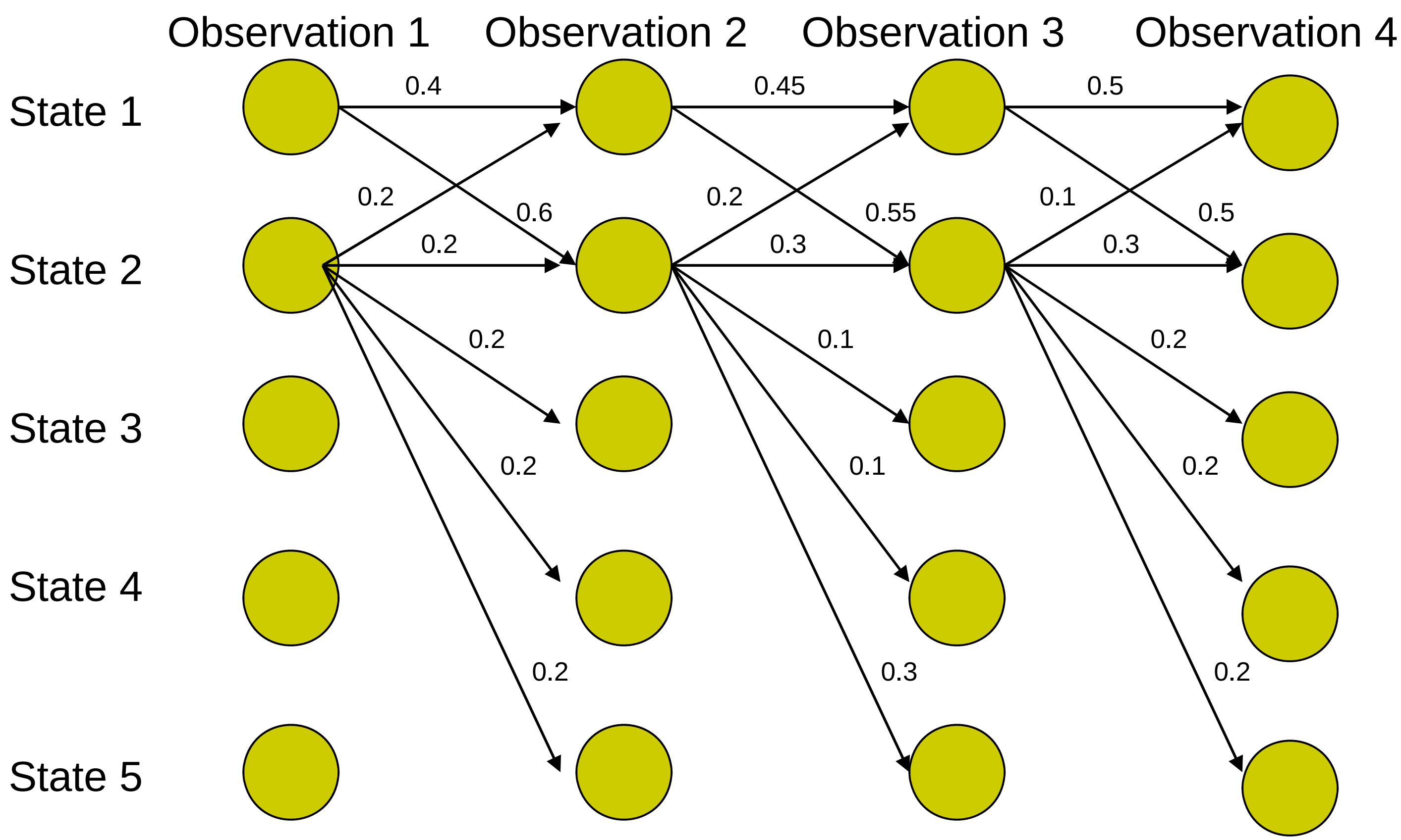
Solution:
Maximum Entropy Markov Model (MEMM)



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

- 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**)

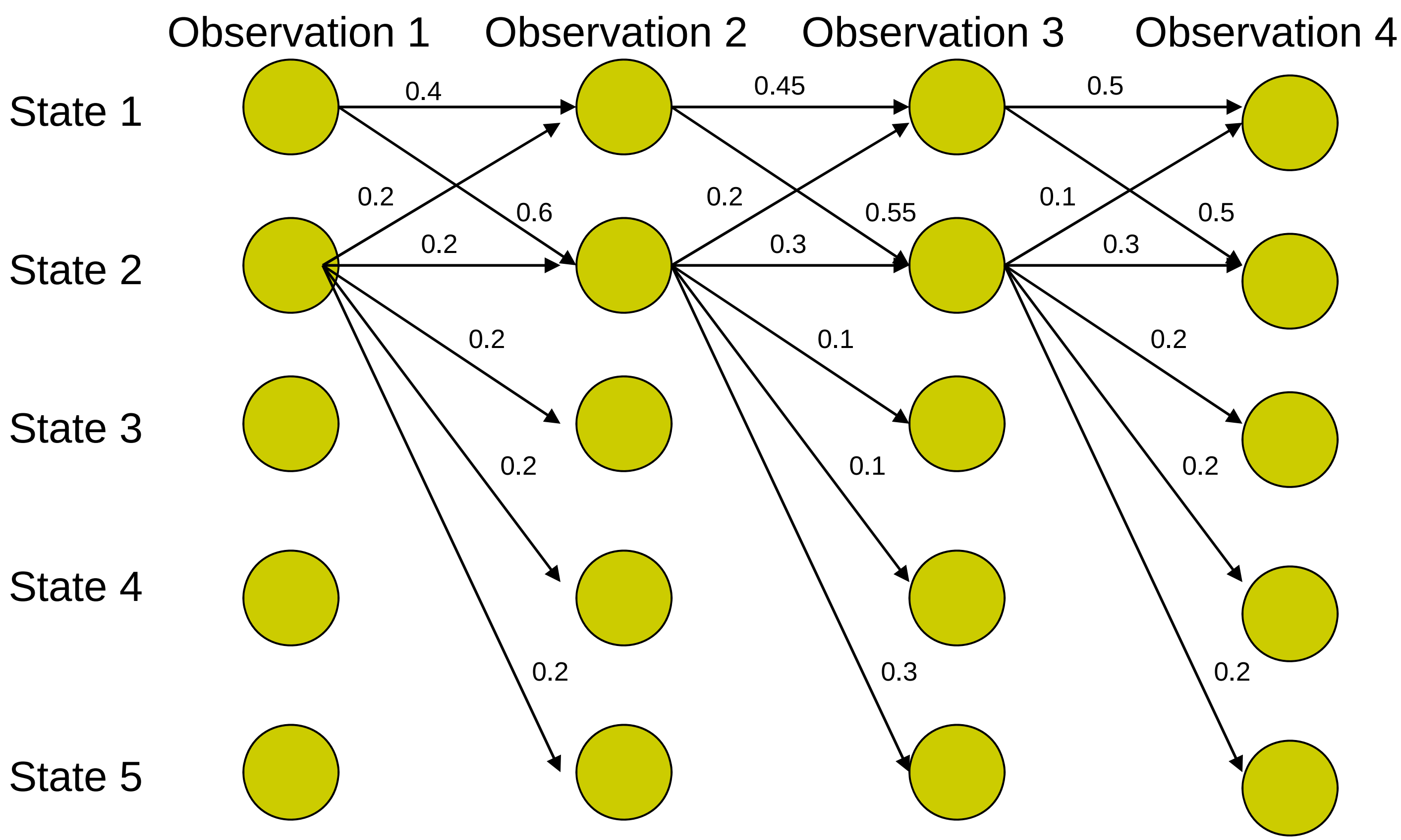
MEMM: the Label bias problem



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

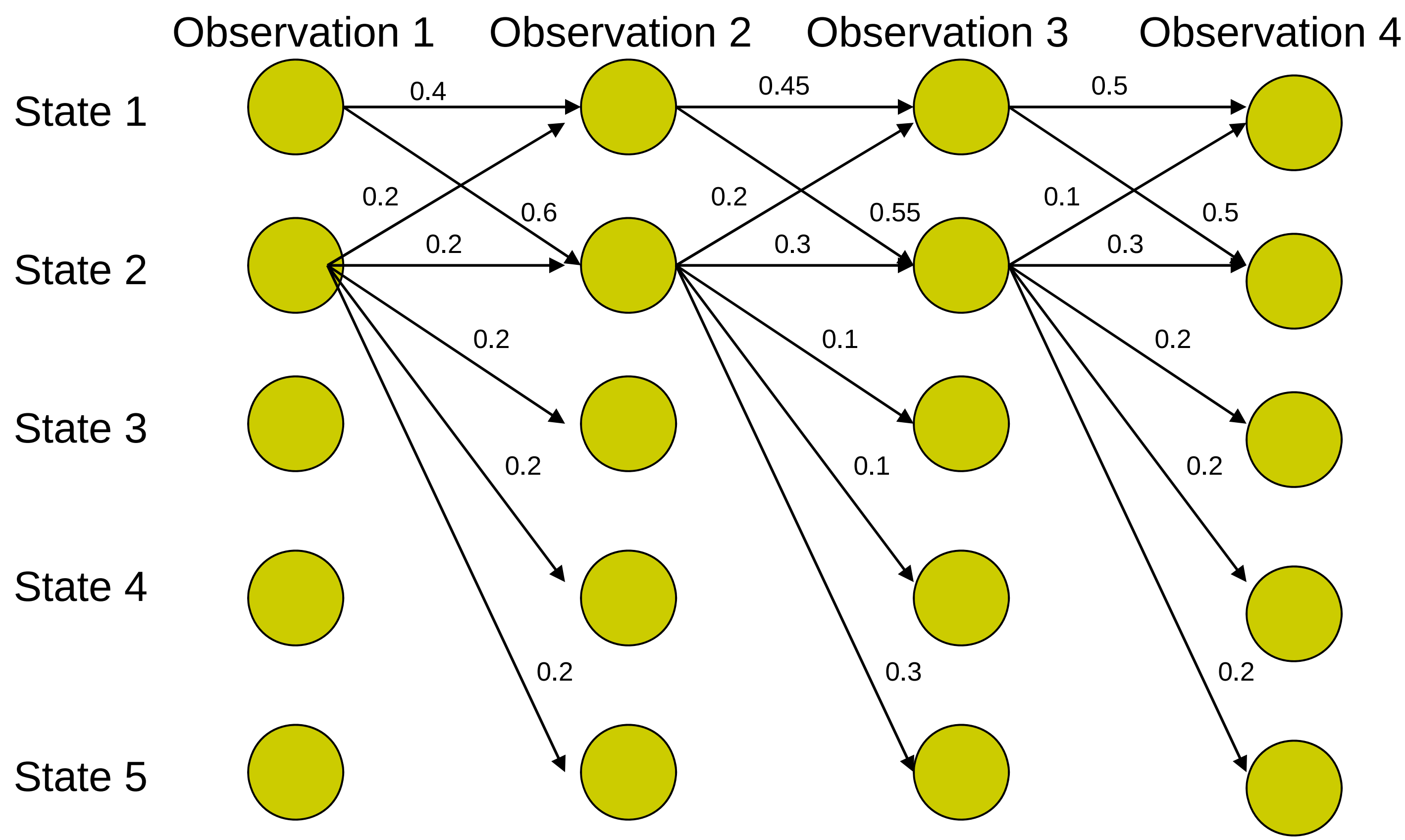
MEMM: the Label bias problem



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

- 0.4 x 0.45 x 0.5 = 0.09

MEMM: the Label bias problem

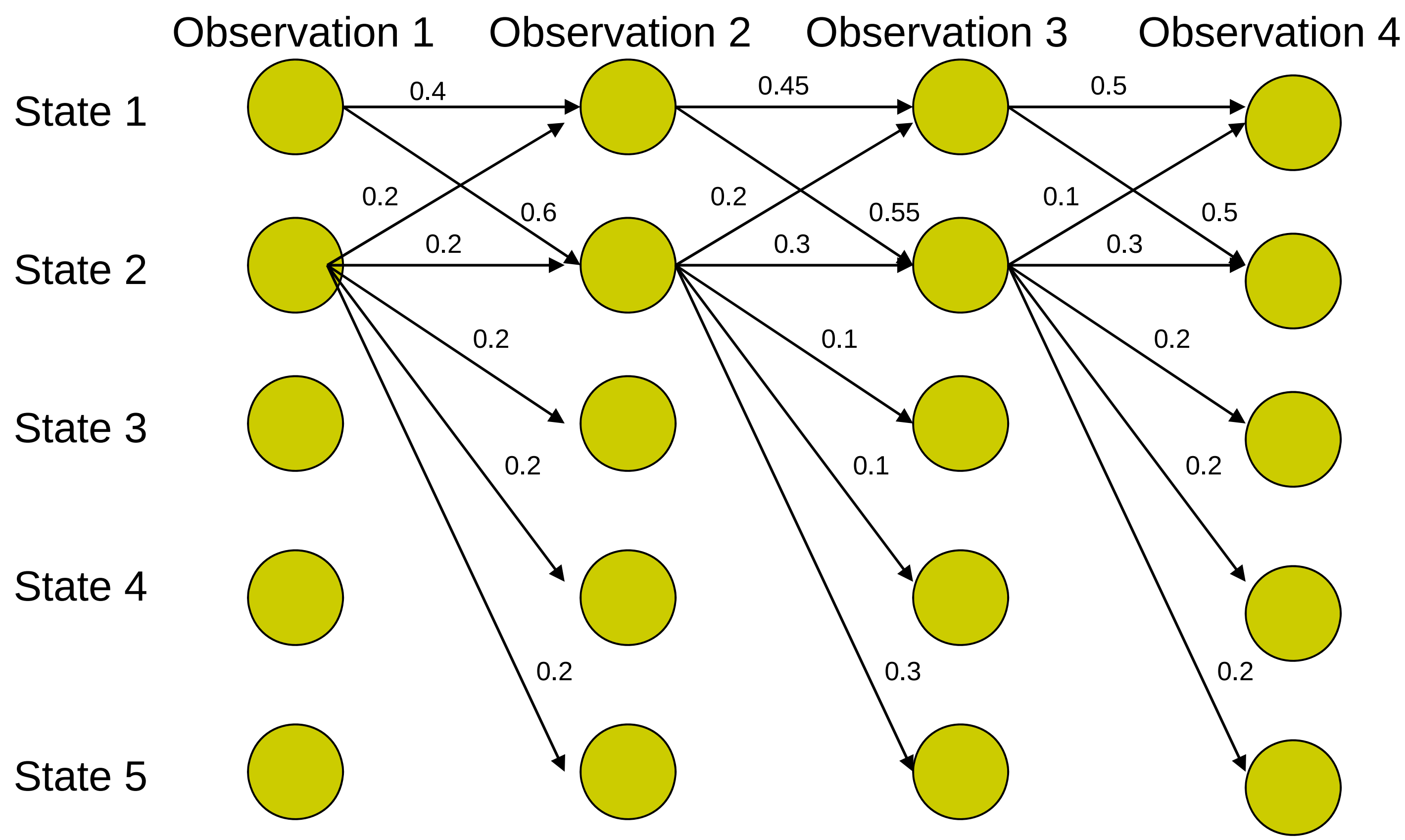


Probability of path 2->2->2->2 :

- 0.2 X 0.3 X 0.3 = 0.018

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

MEMM: the Label bias problem

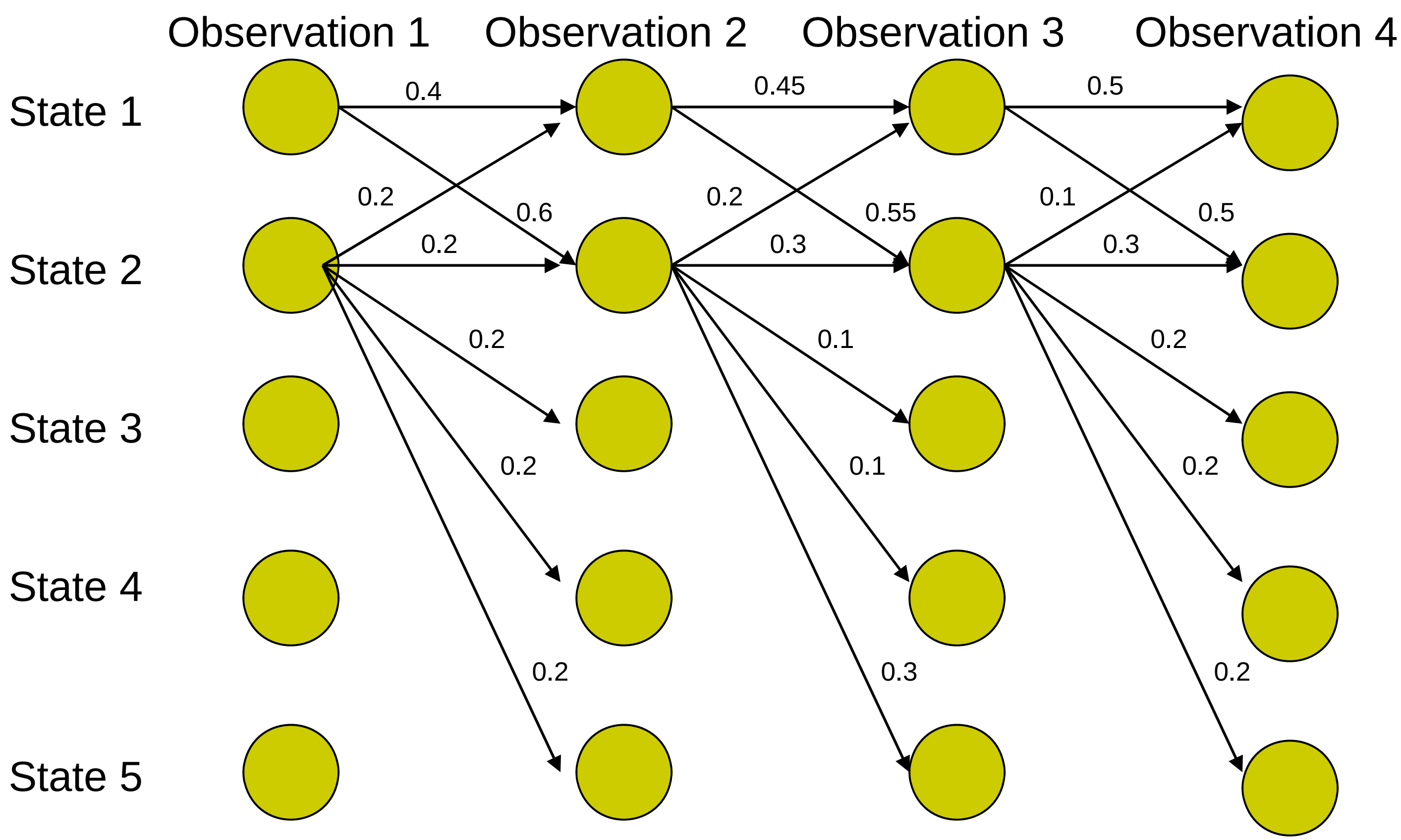


Probability of path 1->2->1->2:

- 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

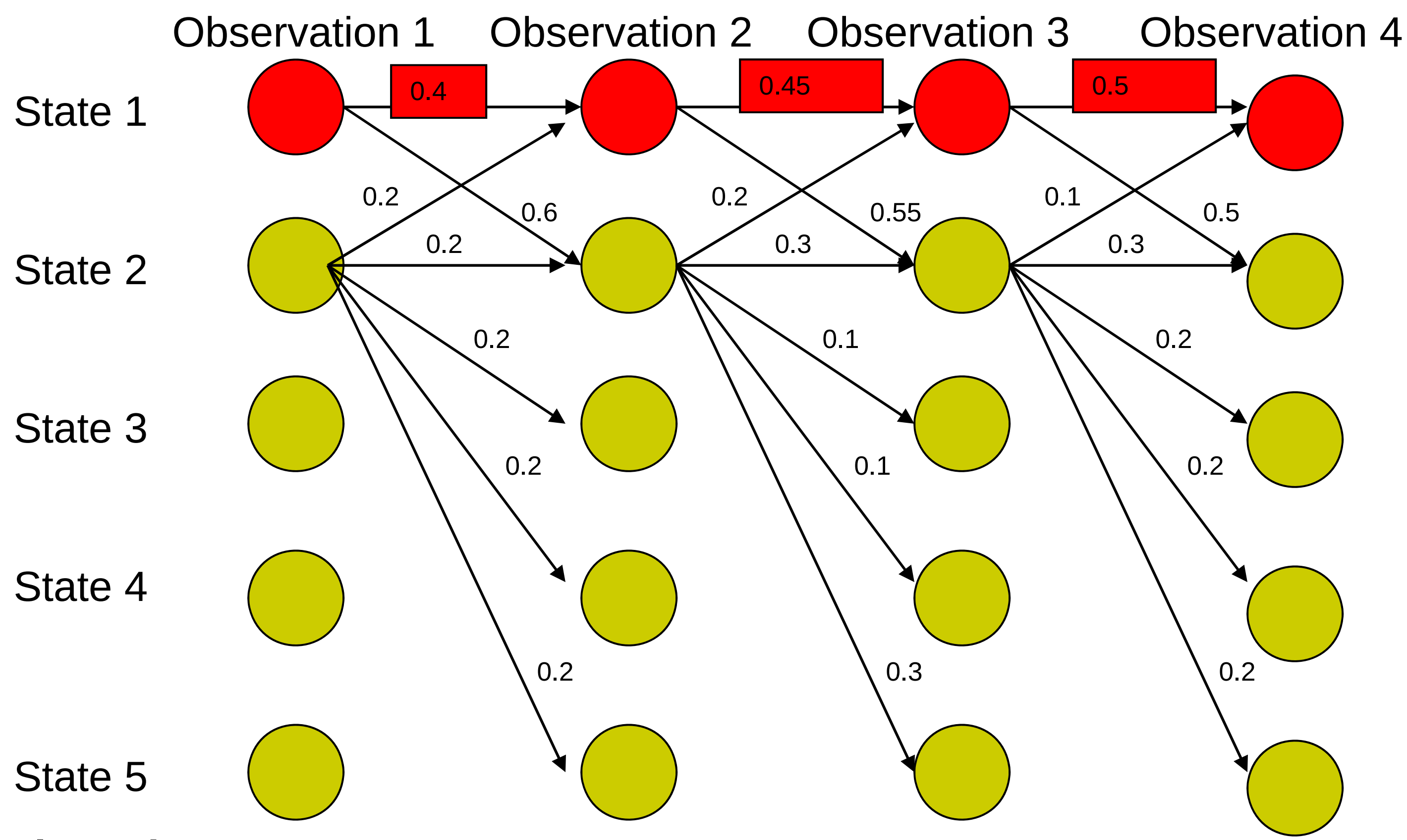


Probability of path 1->1->2->2:

- 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

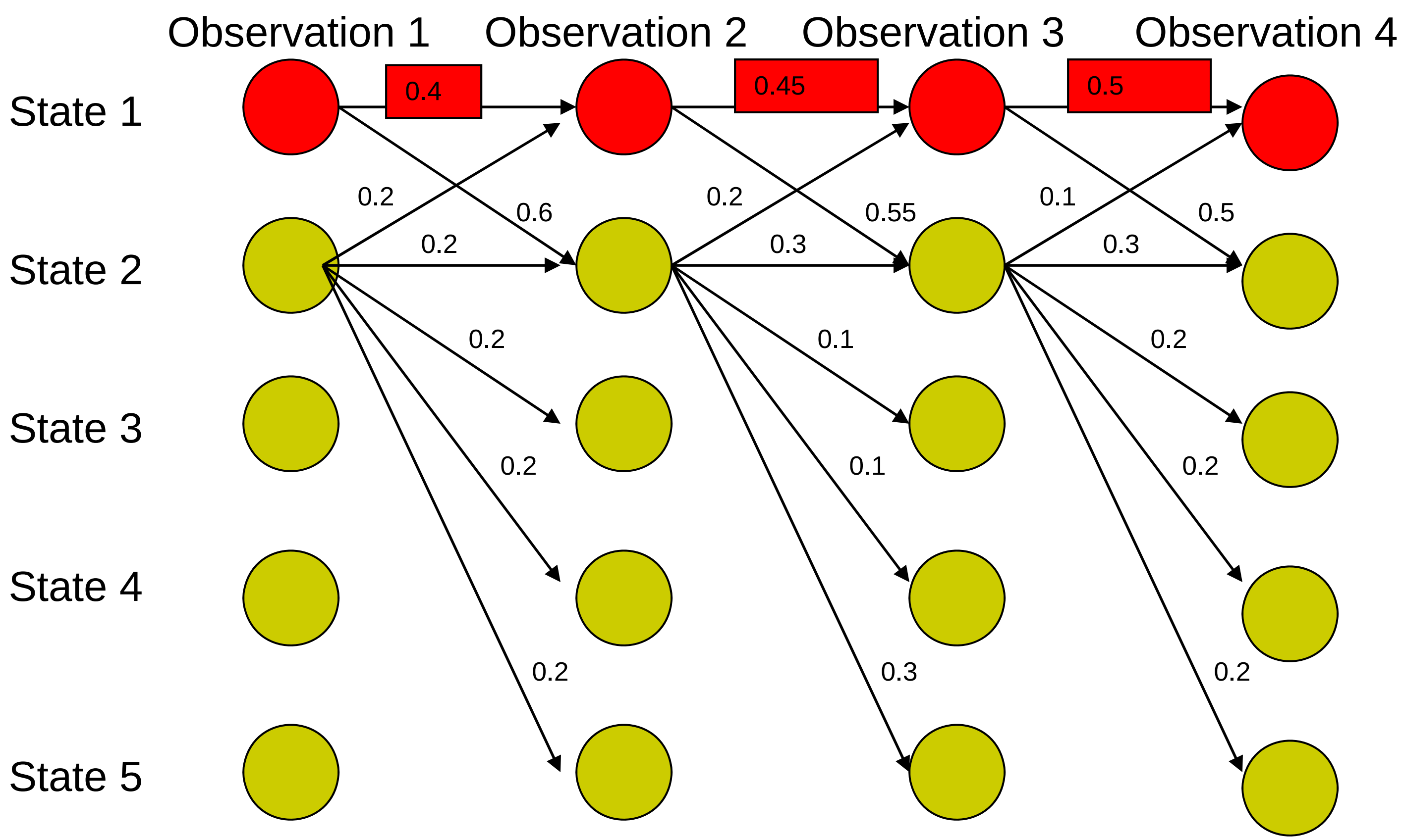
MEMM: the Label bias problem



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?**

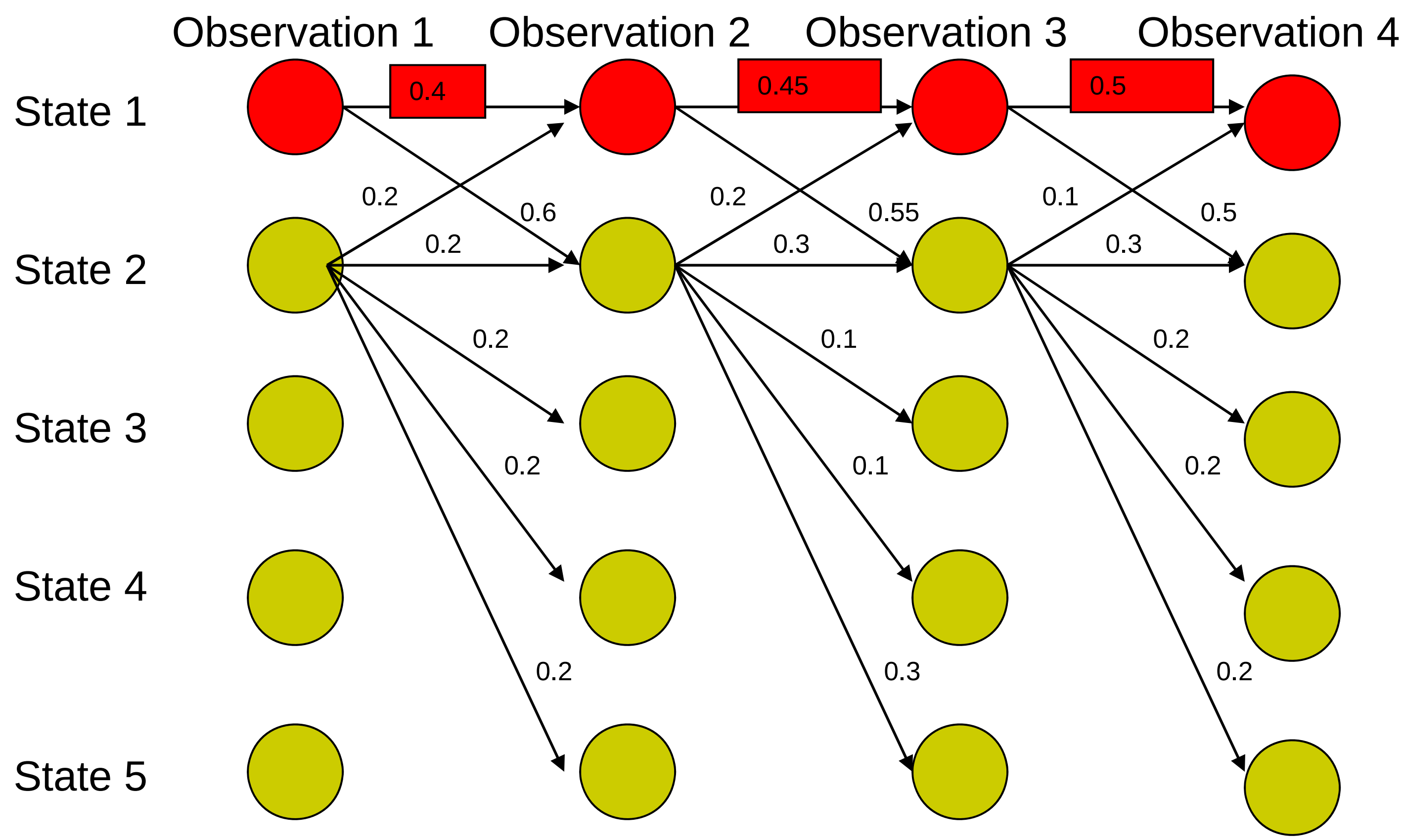
MEMM: the Label bias problem



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

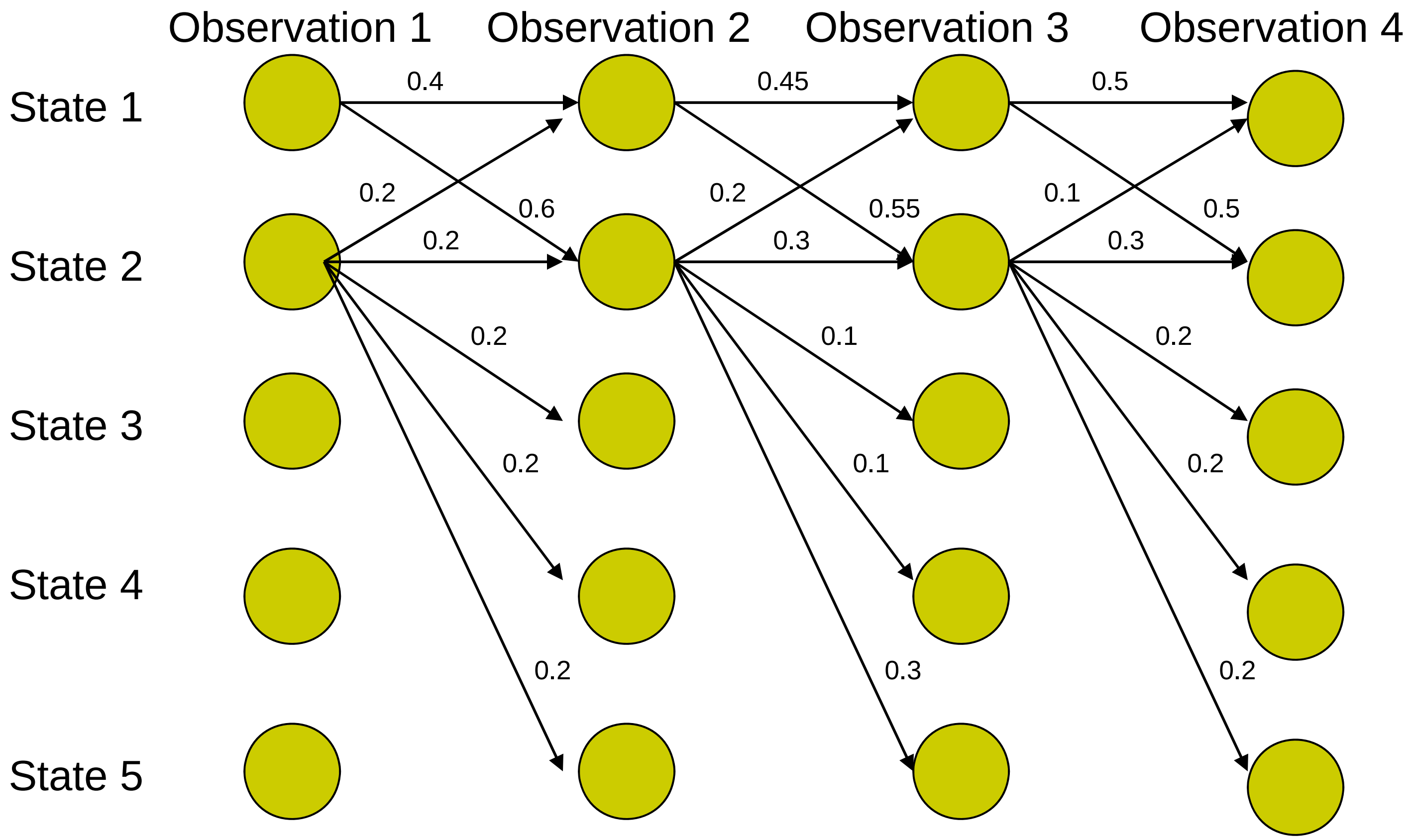
MEMM: the Label bias problem



Label bias problem in MEMM:

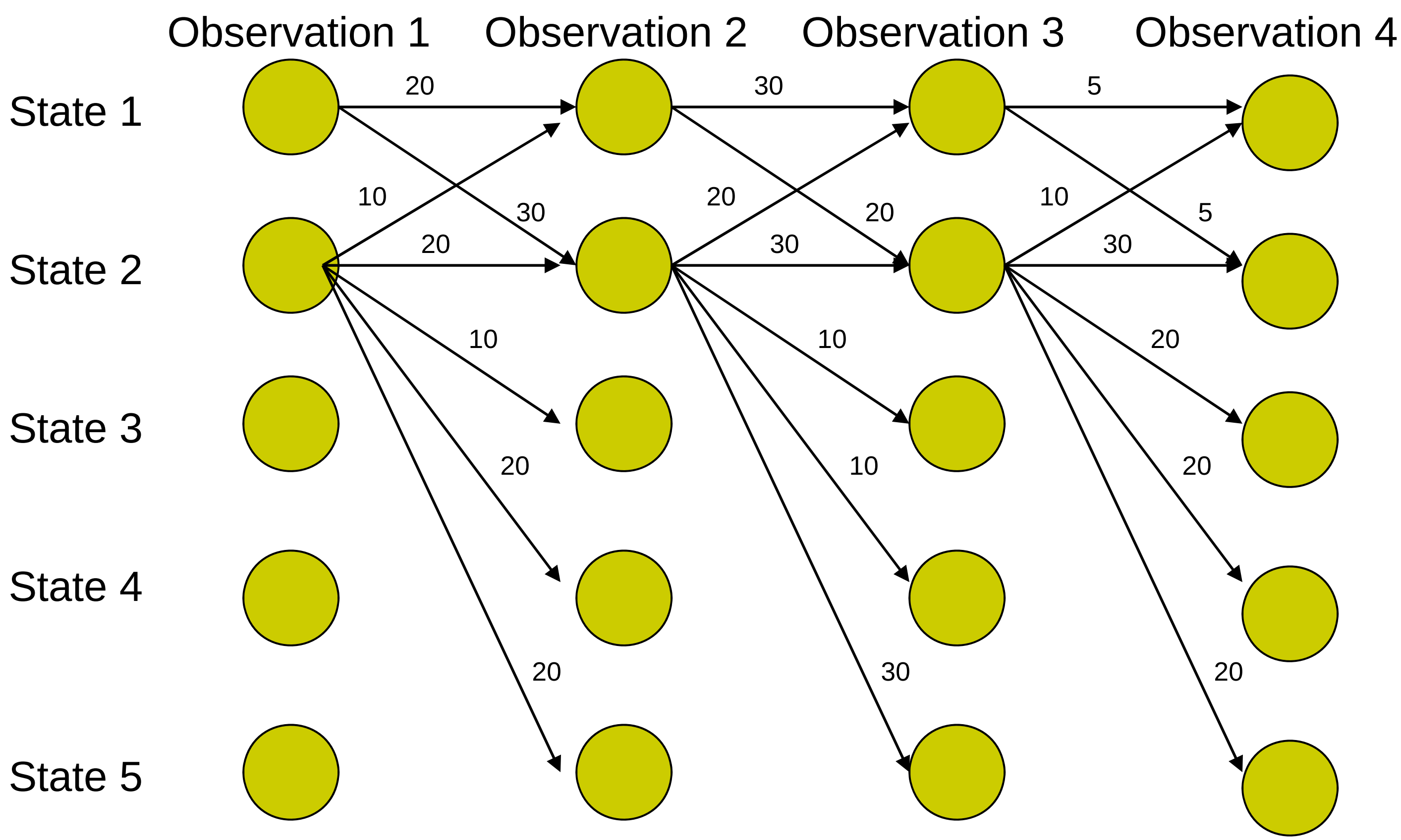
- Preference of states with lower number of transitions over others

Solution:
Do not normalize probabilities locally



From local probabilities ….

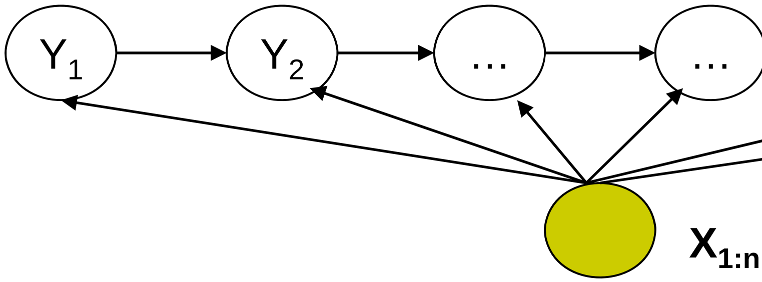
Solution:
Do not normalize probabilities locally



From local probabilities to local potentials

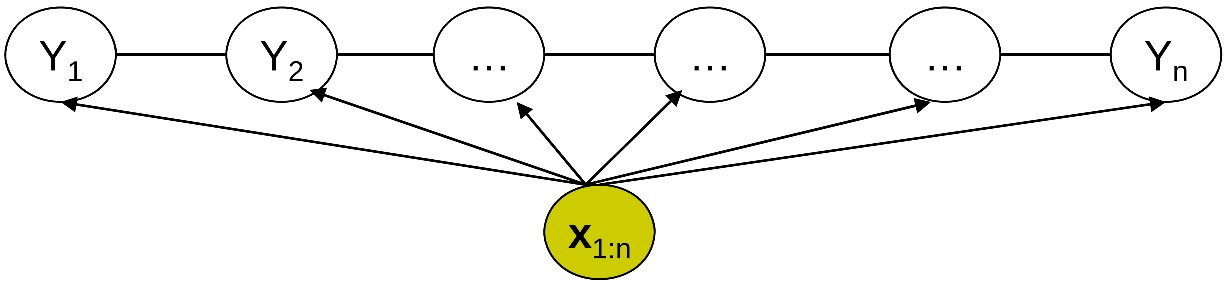
- States with lower transitions do not have an unfair advantage!

From MEMM ....



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

From MEMM to CRF

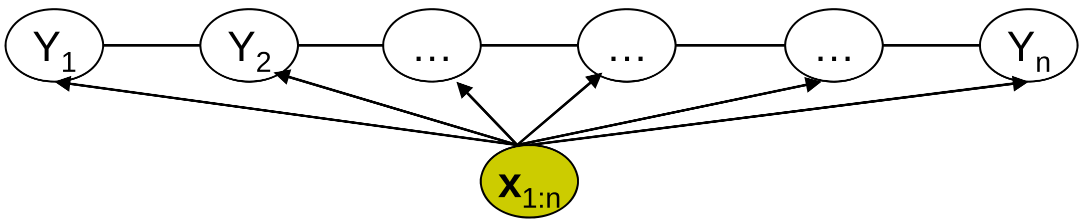


$$P(\mathbf{y}_{1:n}|\mathbf{x}_{1:n}) = \frac{1}{Z(\mathbf{x}_{1:n})}\prod_{i=1}^{n}\phi(y_i, y_{i-1}, \mathbf{x}_{1:n}) = \frac{1}{Z(\mathbf{x}_{1:n}, \mathbf{w})}\prod_{i=1}^{n}\exp(\mathbf{w}^T\mathbf{f}(y_i, y_{i-1}, \mathbf{x}_{1:n}))$$

- CRF is a partially directed model
  - Discriminative model like MEMM
  - Usage of global normalizer Z(**x**) overcomes the label bias problem of MEMM
  - Models the dependence between each state and the entire observation sequence (like MEMM)

Conditional Random Fields

- General parametric form:



$$P(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{x},\lambda,\mu)} \exp\left(\sum_{i=1}^{n}\left(\sum_{k} \lambda_k f_k(y_i, y_{i-1}, \mathbf{x}) + \sum_{l} \mu_l g_l(y_i, \mathbf{x})\right)\right)$$

$$= \frac{1}{Z(\mathbf{x},\lambda,\mu)} \exp\left(\sum_{i=1}^{n}\left(\lambda^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}) + \mu^T \mathbf{g}(y_i, \mathbf{x})\right)\right)$$

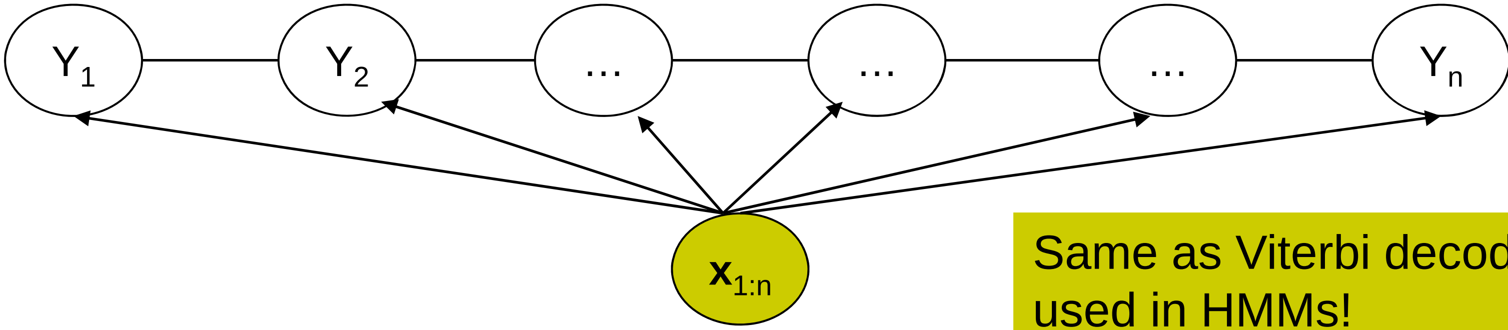
$$\text{where } Z(\mathbf{x},\lambda,\mu) = \sum_{\mathbf{y}} \exp\left(\sum_{i=1}^{n}\left(\lambda^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}) + \mu^T \mathbf{g}(y_i, \mathbf{x})\right)\right)$$

CRFs: Inference

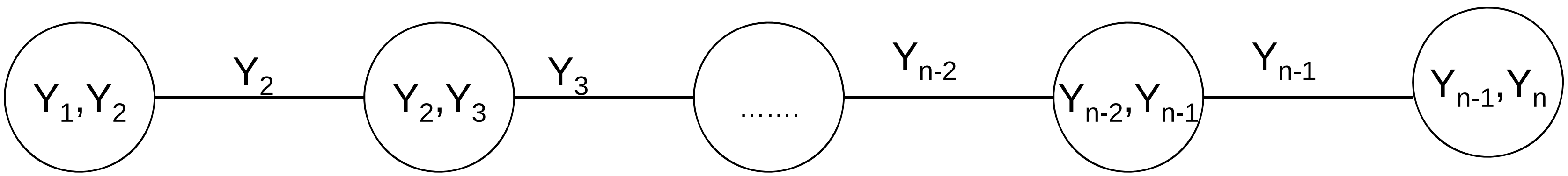
- Given CRF parameters λ and μ, find the **y*** that maximizes P(**y**|**x**)

$$\mathbf{y}^* = \arg\max_{\mathbf{y}} \exp\left(\sum_{i=1}^{n} (\lambda^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}) + \mu^T \mathbf{g}(y_i, \mathbf{x}))\right)$$

  - Can ignore Z(**x**) because it is not a function of **y**
- Run the max-product algorithm on the junction-tree of CRF:



Same as Viterbi decoding used in HMMs!



CRF learning

- Given $\{(\mathbf{x}_d, \mathbf{y}_d)\}_{d=1}^N$, find λ^*, μ^* such that

$$
\begin{aligned}
\lambda*, \mu* &= \arg\max_{\lambda,\mu} L(\lambda, \mu) = \arg\max_{\lambda,\mu} \prod_{d=1}^{N} P(\mathbf{y}_d | \mathbf{x}_d, \lambda, \mu) \\
&= \arg\max_{\lambda,\mu} \prod_{d=1}^{N} \frac{1}{Z(\mathbf{x}_d, \lambda, \mu)} \exp(\sum_{i=1}^{n} (\lambda^T \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_d) + \mu^T \mathbf{g}(y_{d,i}, \mathbf{x}_d))) \\
&= \arg\max_{\lambda,\mu} \sum_{d=1}^{N} (\sum_{i=1}^{n} (\lambda^T \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_d) + \mu^T \mathbf{g}(y_{d,i}, \mathbf{x}_d)) - \log Z(\mathbf{x}_d, \lambda, \mu))
\end{aligned}
$$

- Computing the gradient w.r.t λ:

Gradient of the log-partition function in an exponential family is the expectation of the sufficient statistics.

$$
\nabla_\lambda L(\lambda, \mu) = \sum_{d=1}^{N} (\sum_{i=1}^{n} \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_d) - \sum_{\mathbf{y}} (P(\mathbf{y} | \mathbf{x_d}) \sum_{i=1}^{n} \mathbf{f}(y_{d,i}, y_{d,i-1}, \mathbf{x}_d)))
$$

CRF learning

$$\nabla_\lambda L(\lambda,\mu) = \sum_{d=1}^{N}(\sum_{i=1}^{n}\mathbf{f}(y_{d,i},y_{d,i-1},\mathbf{x}_d) - \sum_{\mathbf{y}}(P(\mathbf{y}|\mathbf{x_d})\sum_{i=1}^{n}\mathbf{f}(y_i,y_{i-1},\mathbf{x}_d)))$$

- Computing the model expectations:
  - Requires exponentially large number of summations: Is it intractable?

$$\sum_{\mathbf{y}}(P(\mathbf{y}|\mathbf{x}_d)\sum_{i=1}^{n}\mathbf{f}(y_i,y_{i-1},\mathbf{x}_d)) = \sum_{i=1}^{n}(\sum_{\mathbf{y}}\mathbf{f}(y_i,y_{i-1},\mathbf{x}_d)P(\mathbf{y}|\mathbf{x}_d))$$

$$= \sum_{i=1}^{n}\sum_{y_i,y_{i-1}}\mathbf{f}(y_i,y_{i-1},\mathbf{x}_d)P(y_i,y_{i-1}|\mathbf{x}_d)$$

Expectation of **f** over the corresponding marginal probability of neighboring nodes!!

- Tractable!
  - Can compute marginals using the sum-product algorithm on the chain

CRF learning

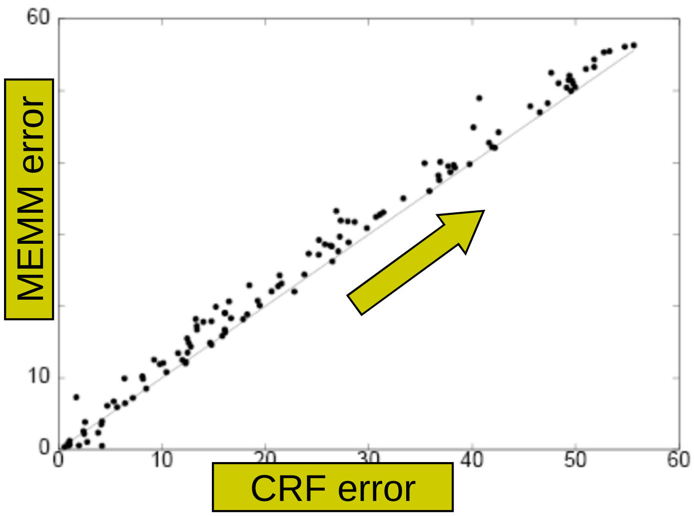
- In practice, we use a Gaussian Regularizer for the parameter vector to improve generalizability

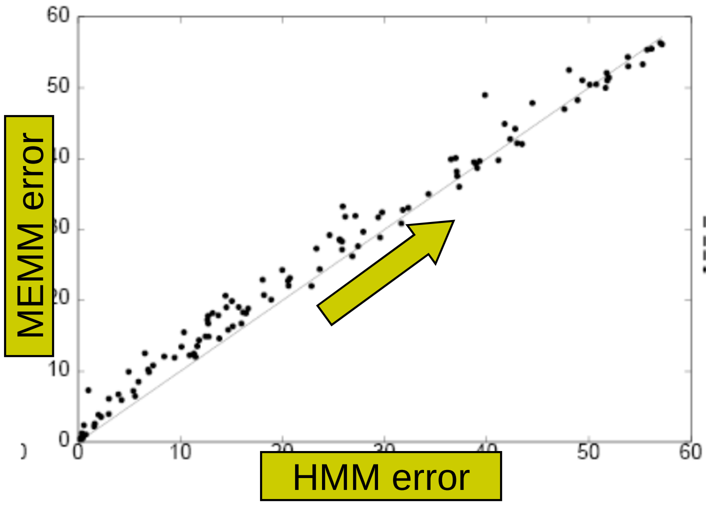
$$\lambda*, \mu* \quad = \quad \arg\max_{\lambda,\mu} \sum_{d=1}^{N} \log P(\mathbf{y}_d | \mathbf{x}_d, \lambda, \mu) - \frac{1}{2\sigma^2}(\lambda^T \lambda + \mu^T \mu)$$

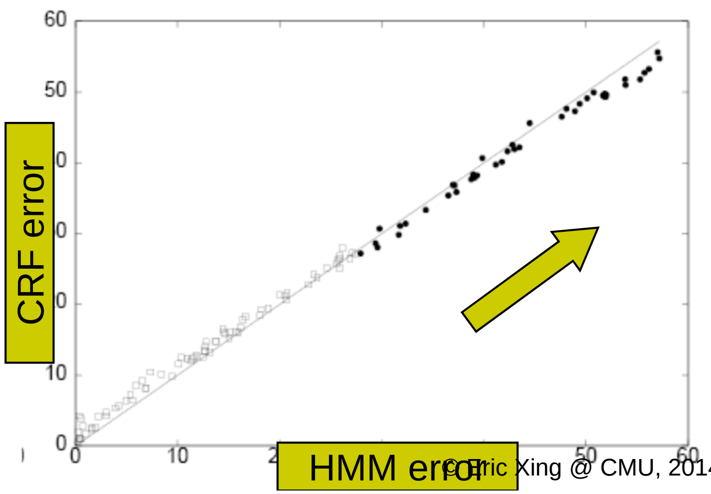
- In practice, gradient ascent has very slow convergence
  - Alternatives:
    - Conjugate Gradient method
    - Limited Memory Quasi-Newton Methods

CRFs: some empirical results

- Comparison of error rates on synthetic data







Data is increasingly higher order in the direction of arrow

CRFs achieve the lowest error rate for higher order data

CRFs: some empirical results

- Parts of Speech tagging

model	*error*	*oov error*
HMM	5.69%	45.99%
MEMM	6.37%	54.61%
CRF	5.55%	48.05%
MEMM$^+$	4.81%	26.99%
CRF$^+$	4.27%	23.76%

$^+$Using spelling features

- Using same set of features: HMM >=< CRF > MEMM
- Using additional overlapping features: CRF$^+$ > MEMM$^+$ >> HMM

Summary

- Conditional Random Fields are partially directed discriminative models
- They overcome the label bias problem of MEMMs by using a global normalizer
- Inference for 1-D chain CRFs is exact
  - Same as Max-product or Viterbi decoding
- Learning also is exact
  - globally optimum parameters can be learned
  - Requires using sum-product or forward-backward algorithm
- CRFs involving arbitrary graph structure are intractable in general
  - E.g.: Grid CRFs
  - Inference and learning require approximation techniques
    - MCMC sampling
    - Variational methods
    - Loopy BP