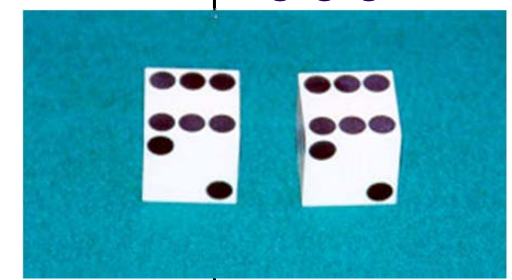
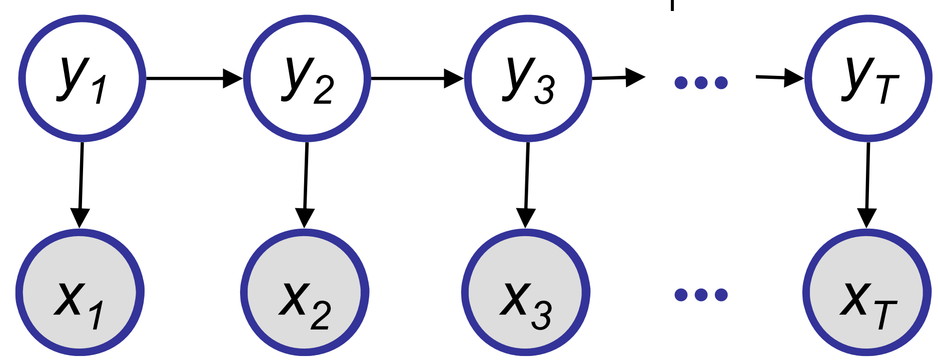
Conditional Random Fields

(slides from Eric Xing)

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

- Start probabilities

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

- Emission probabilities associated with each state

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

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

Inference (review)

- Forward algorithm

$$\alpha_t^k \stackrel{\text{def}}{=} \mu_{t-1\to t}(k) = P(x_1,\dots,x_{t-1},x_t,y_t^k=1)$$

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

- Backward algorithm

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

$$\beta_t^k \stackrel{\text{def}}{=} \mu_{t-1\leftarrow t}(k) = P(x_{t+1},\dots,x_T \mid y_t^k=1)$$

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

$$\xi_t^{i,j} \stackrel{\text{def}}{=} p(y_t^i=1, y_{t+1}^j=1, x_{1:T})$$

$$\propto \mu_{t-1\to t}(y_t^i=1)\mu_{t\leftarrow t+1}(y_{t+1}^j=1)p(x_{t+1} \mid y_{t+1})p(y_{t+1} \mid y_t)$$

$$\xi_t^{i,j} = \alpha_t^i \beta_{t+1}^j a_{i,j}\, p(x_{t+1} \mid y_{t+1}^i=1)$$

The matrix-vector form:

$$B_t(i) \stackrel{\text{def}}{=} p(x_t \mid y_t^i=1)$$

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

$$\alpha_t = \left(A^T\alpha_{t-1}\right).*B_t$$

$$\beta_t = A\left(\beta_{t+1}.*B_{t+1}\right)$$

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

$$\gamma_t = \alpha_t .* \beta_t$$

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:**

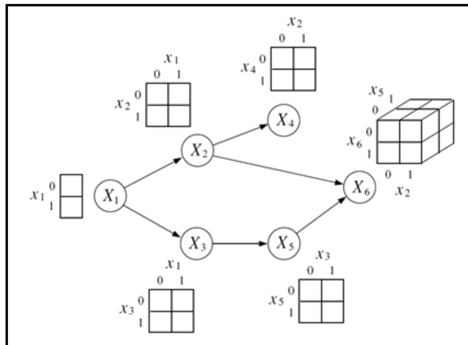
    GIVEN: the porcupine genome; we don't know how frequent are the CpG islands there, neither do we know their composition

    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

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

- 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

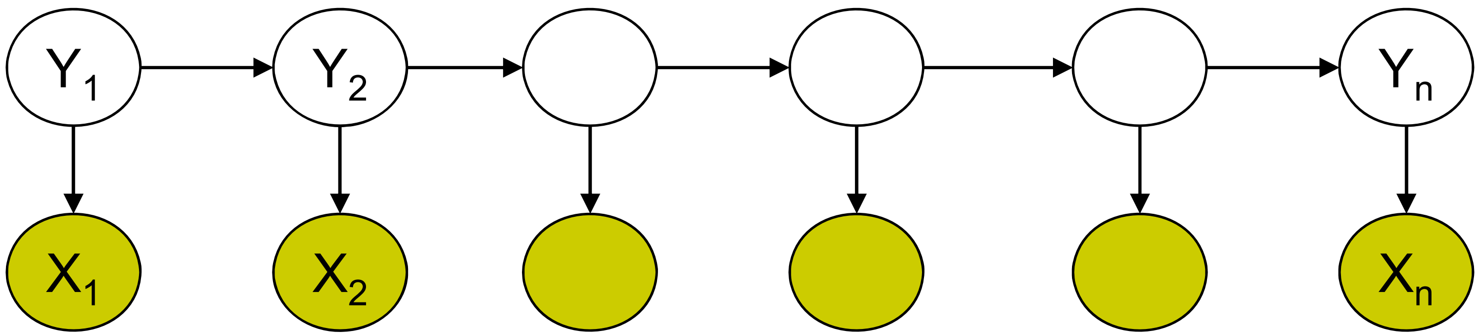
$$\gamma_{n,t}^i = \langle y_{n,t}^i \rangle = p(y_{n,t}^i = 1 \mid \mathbf{x}_n)$$

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

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

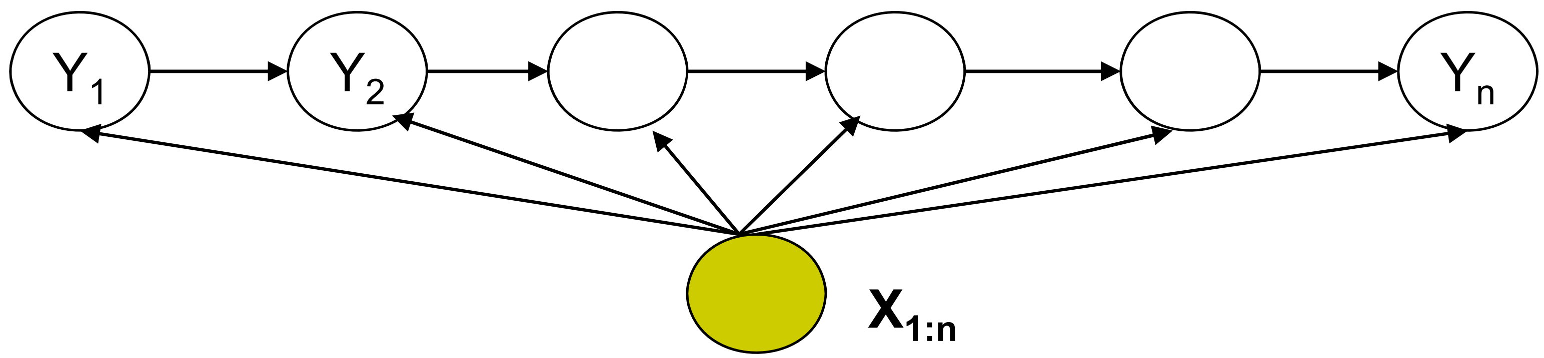
$$\pi_i^{ML} = \frac{\sum_n \gamma_{n,1}^i}{N} \qquad a_{ij}^{ML} = \frac{\sum_n \sum_{t=2}^{T} \xi_{n,t}^{i,j}}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i} \qquad b_{ik}^{ML} = \frac{\sum_n \sum_{t=1}^{T} \gamma_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i}$$

Shortcomings of Hidden Markov Model (1): locality of features



- 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 $P(\mathbf{Y}, \mathbf{X})$, but in a prediction task, we need the conditional probability $P(\mathbf{Y}|\mathbf{X})$

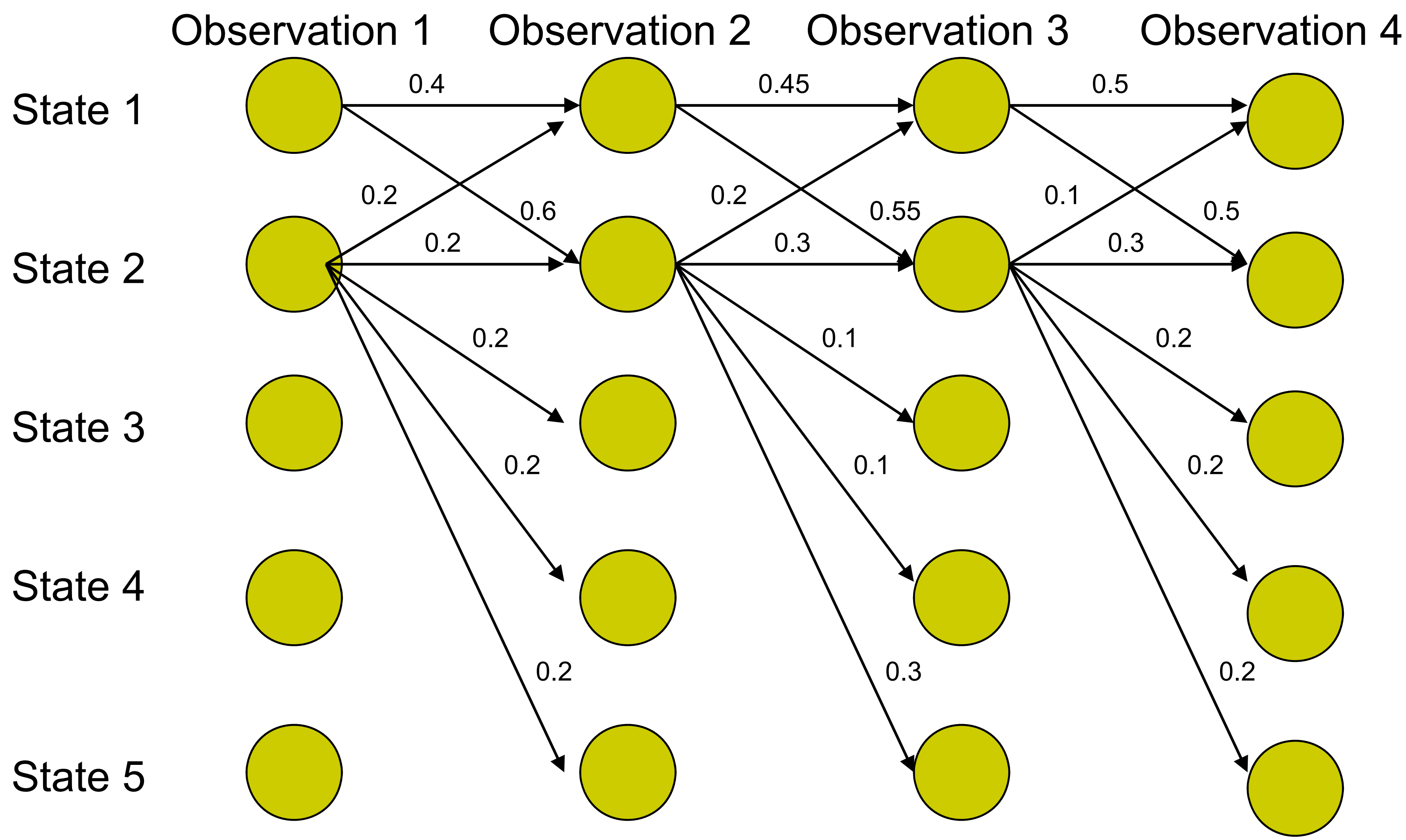
Solution:
Maximum Entropy Markov Model (MEMM)



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

- 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**)

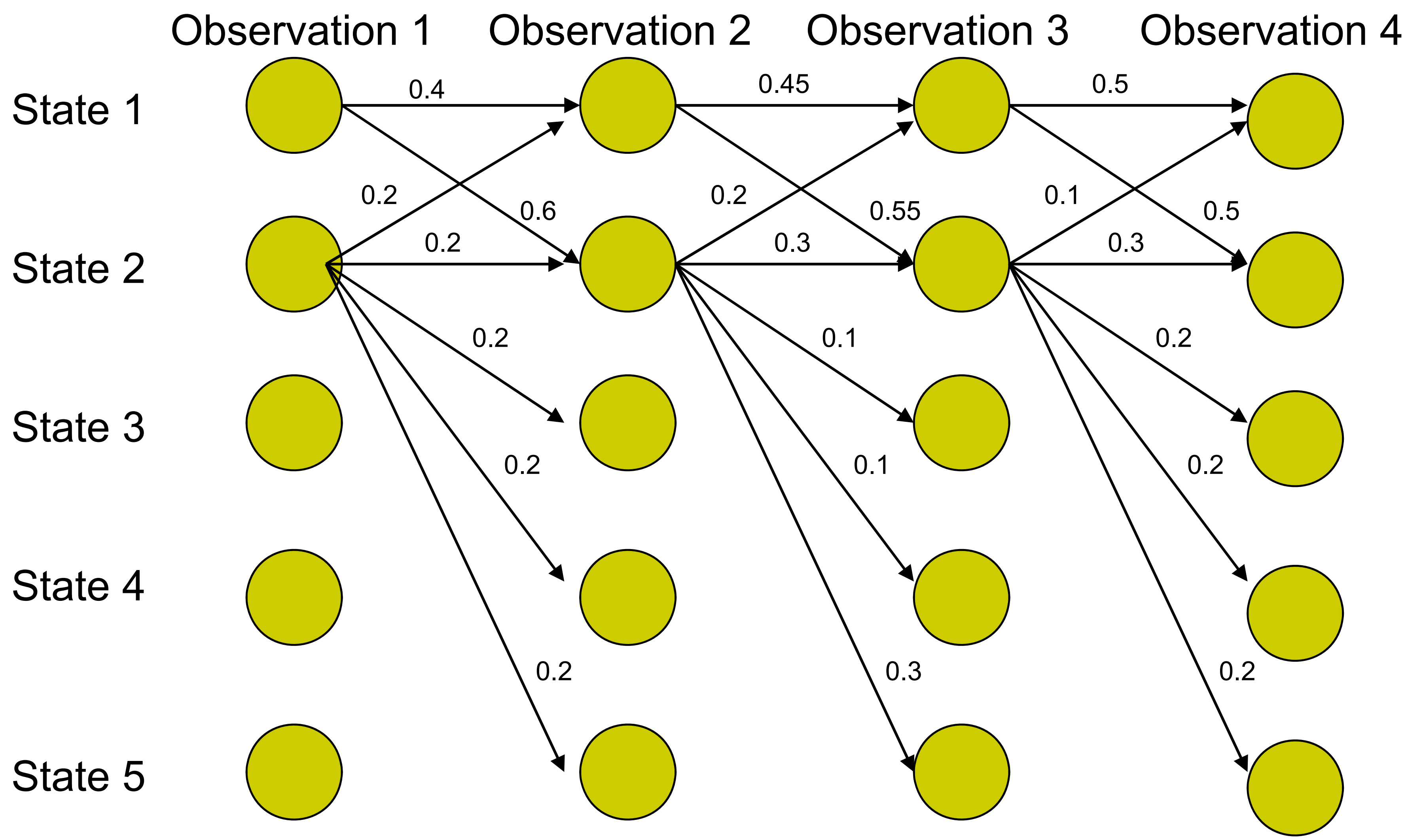
Then, shortcomings of MEMM (and HMM) (2): the Label bias problem



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

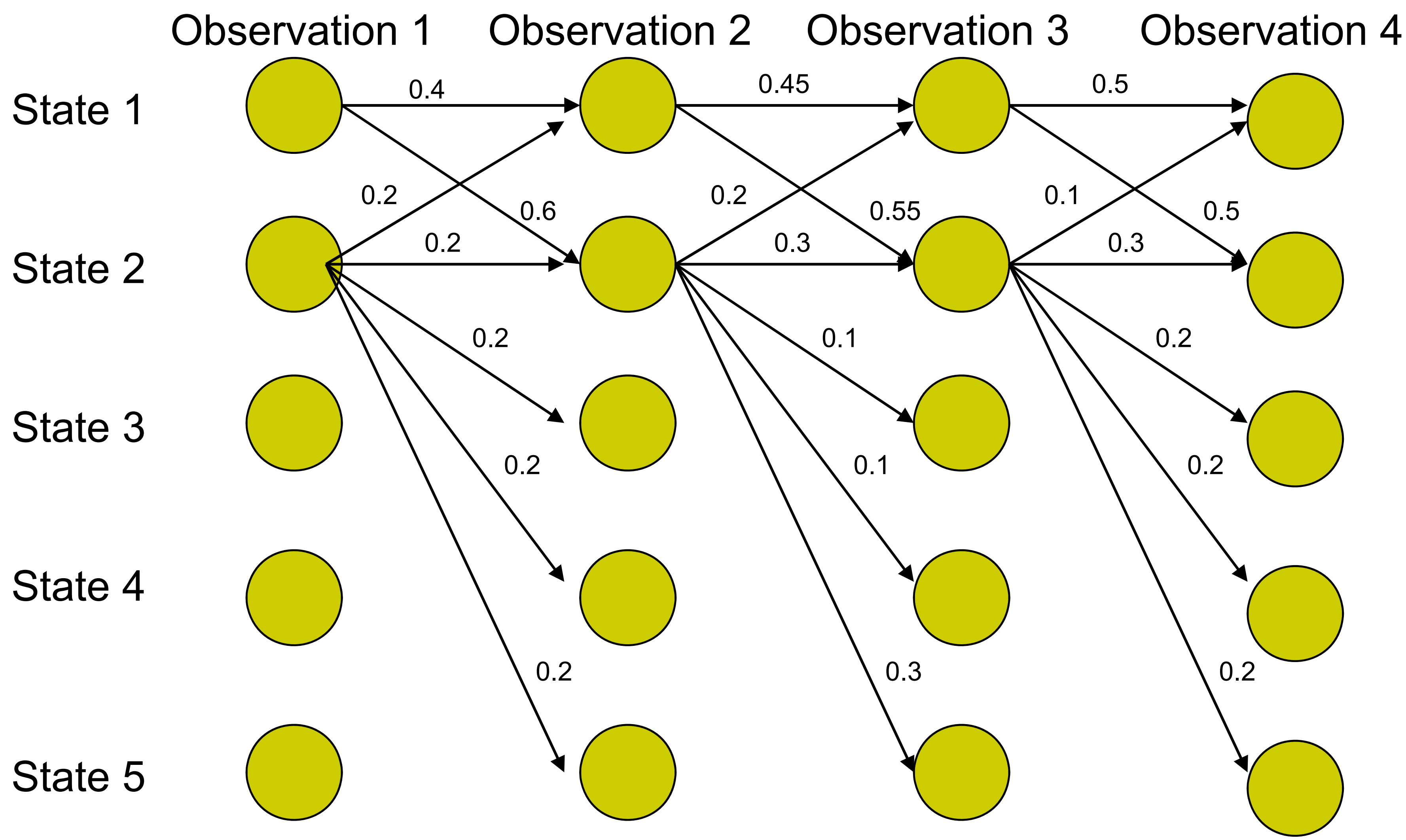
MEMM: the Label bias problem



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

- 0.4 x 0.45 x 0.5 = 0.09

MEMM: the Label bias problem

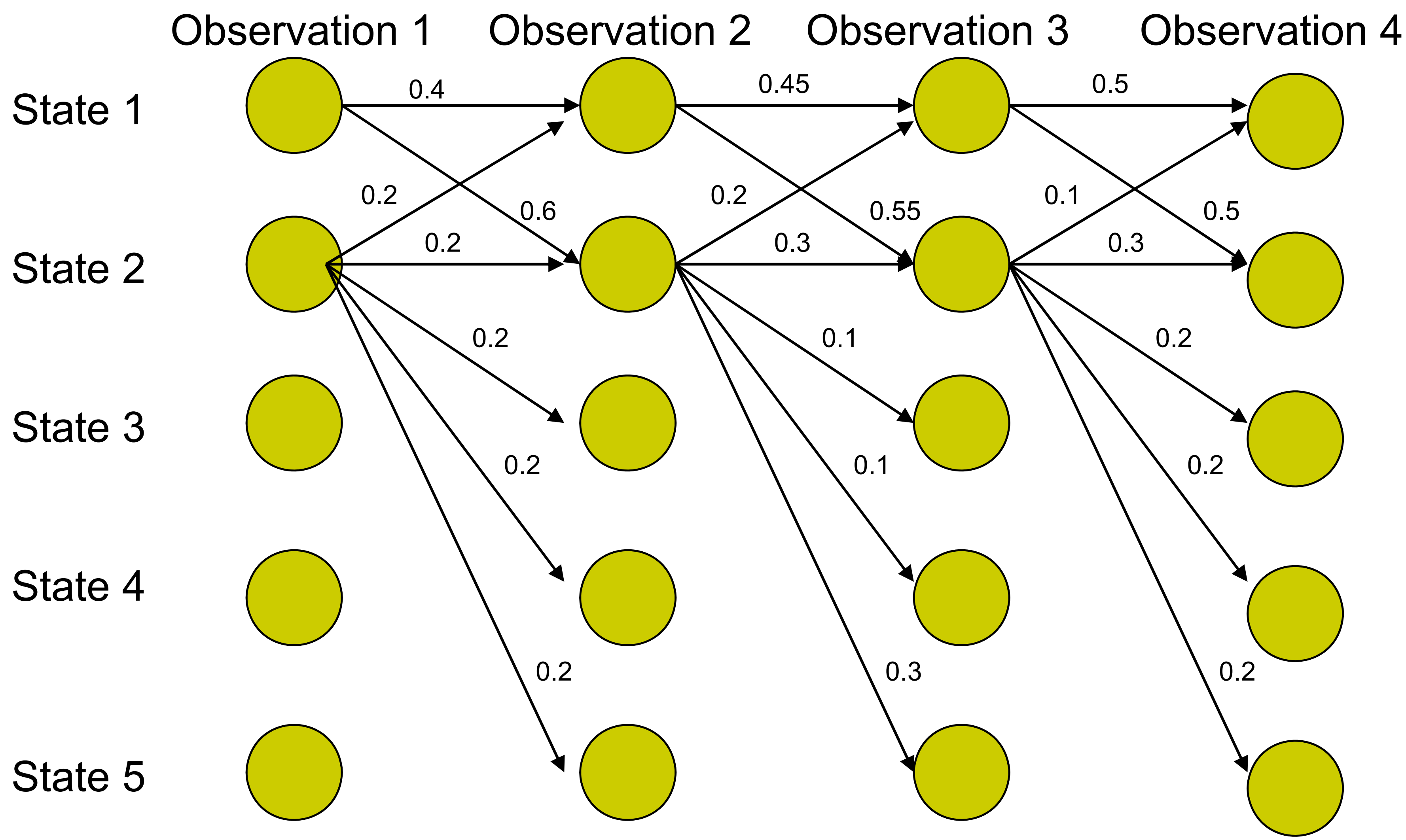


Probability of path 2->2->2->2 :

- 0.2 X 0.3 X 0.3 = 0.018

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

MEMM: the Label bias problem

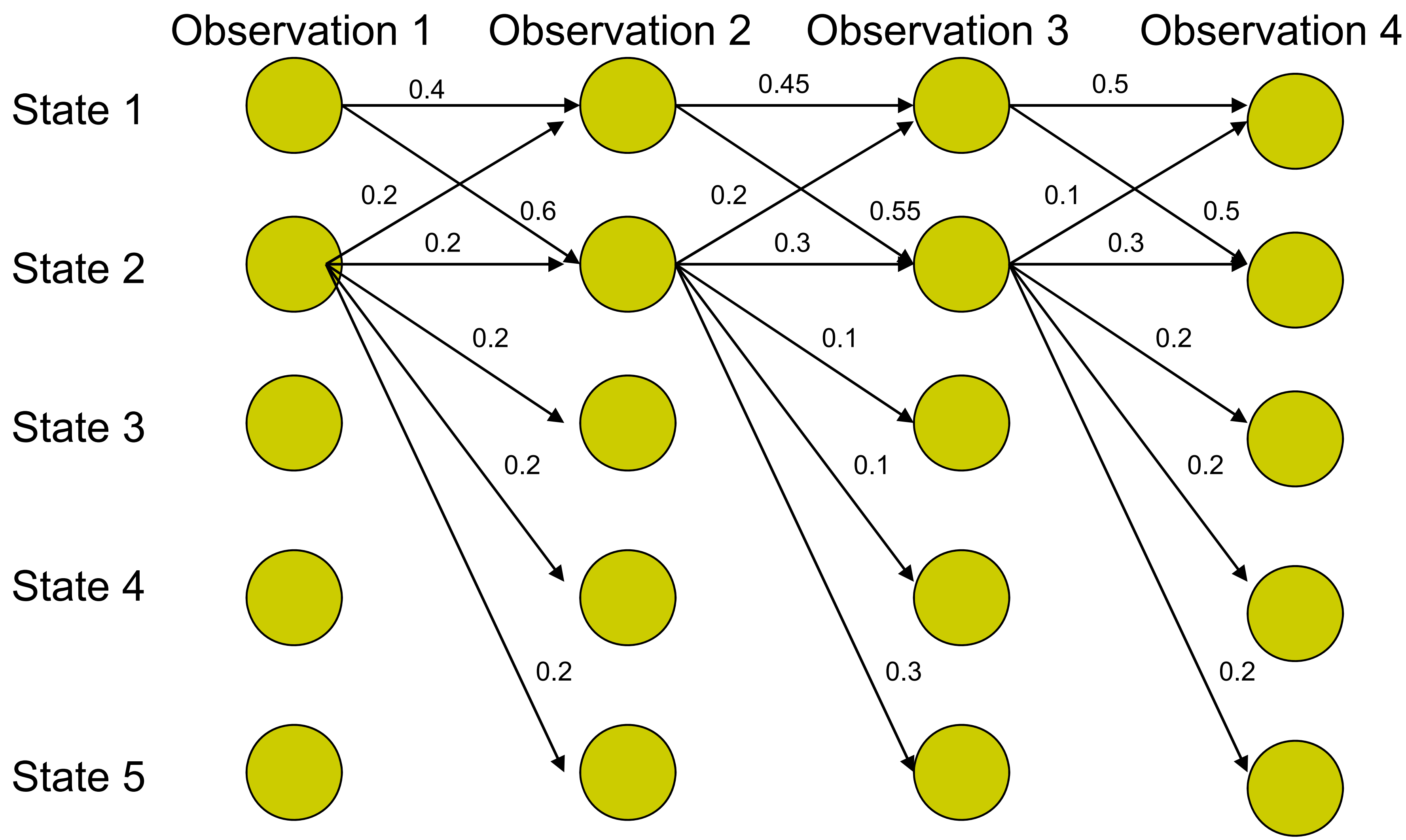


Probability of path 1->2->1->2:

- 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

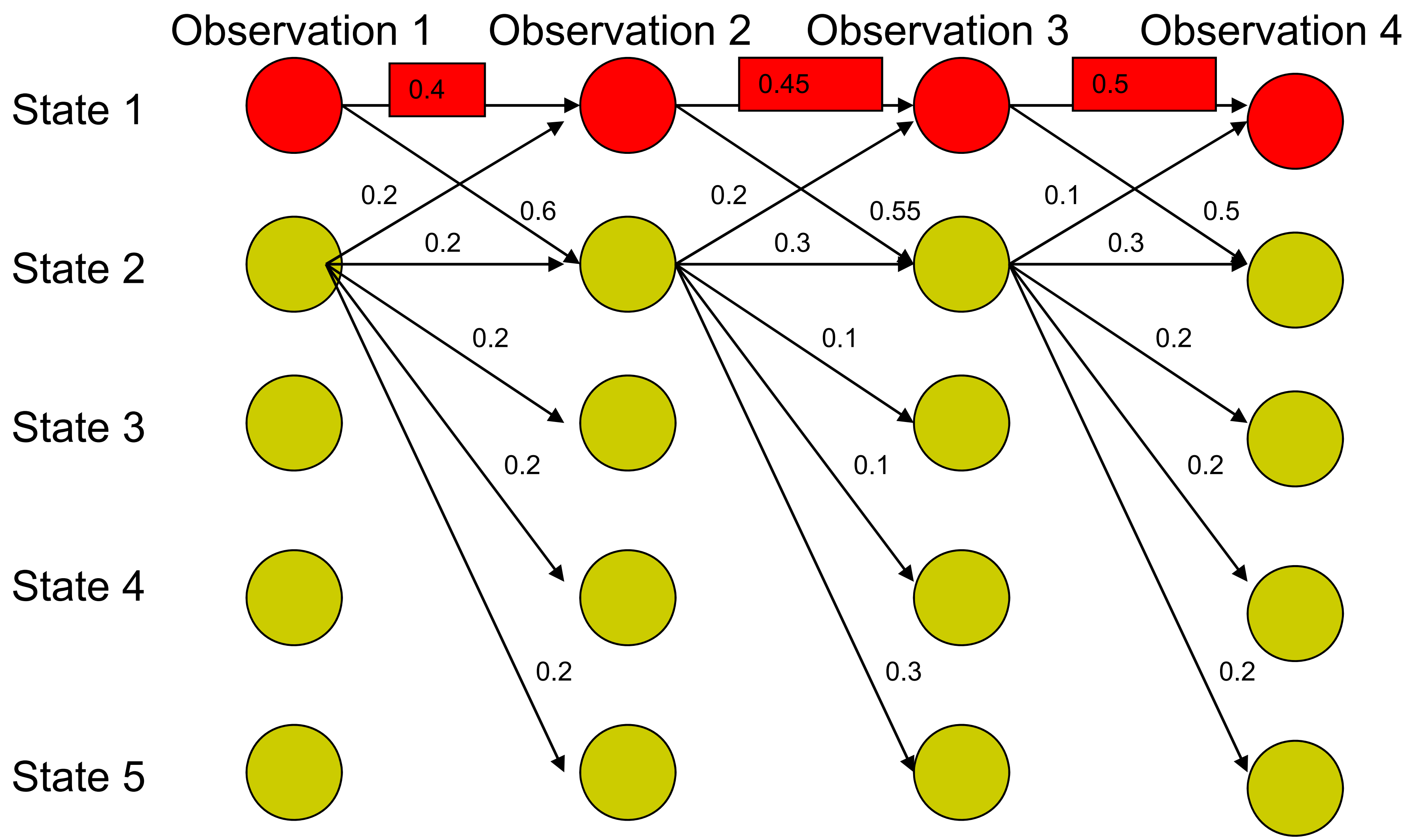


Probability of path 1->1->2->2:

- 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

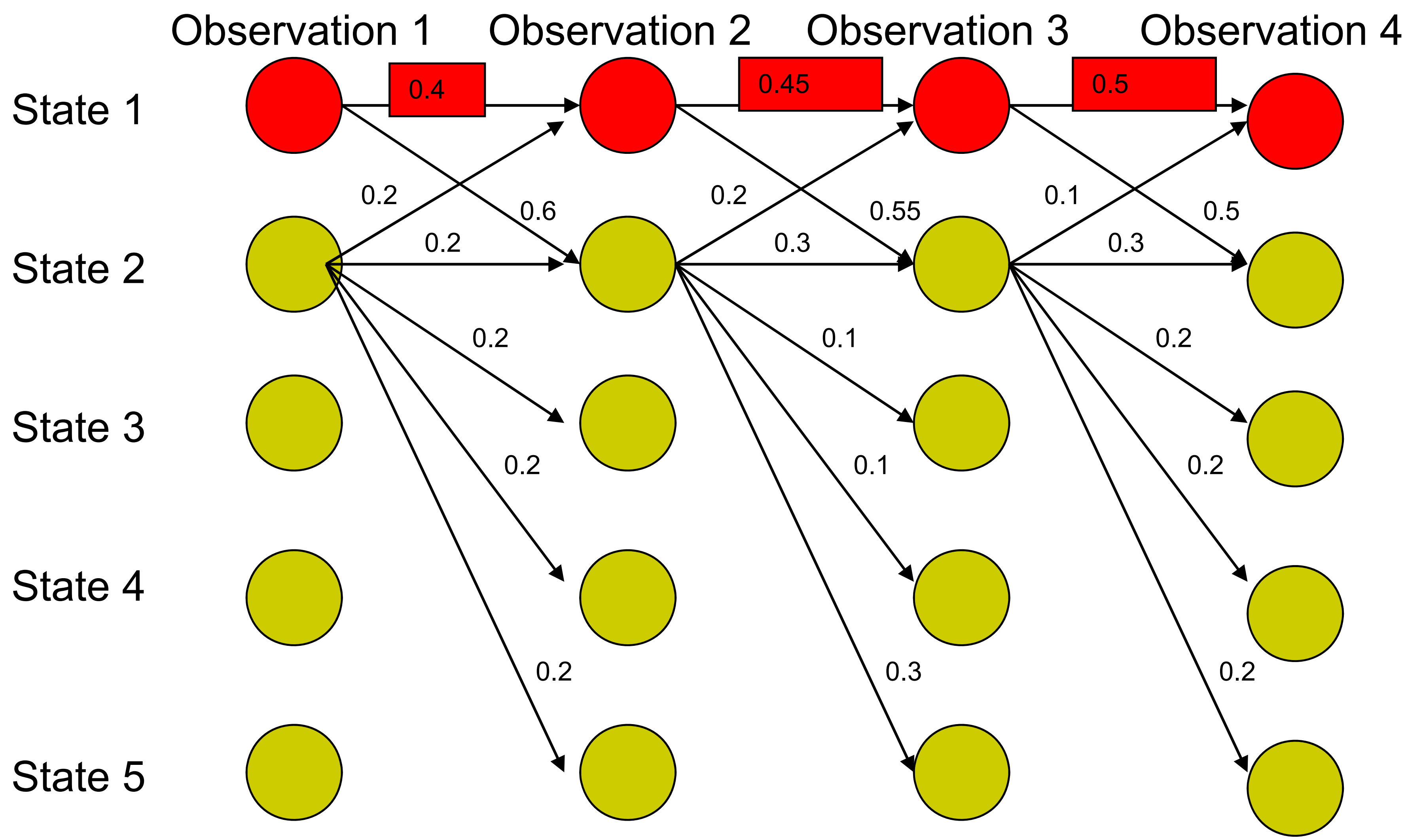
MEMM: the Label bias problem



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?**

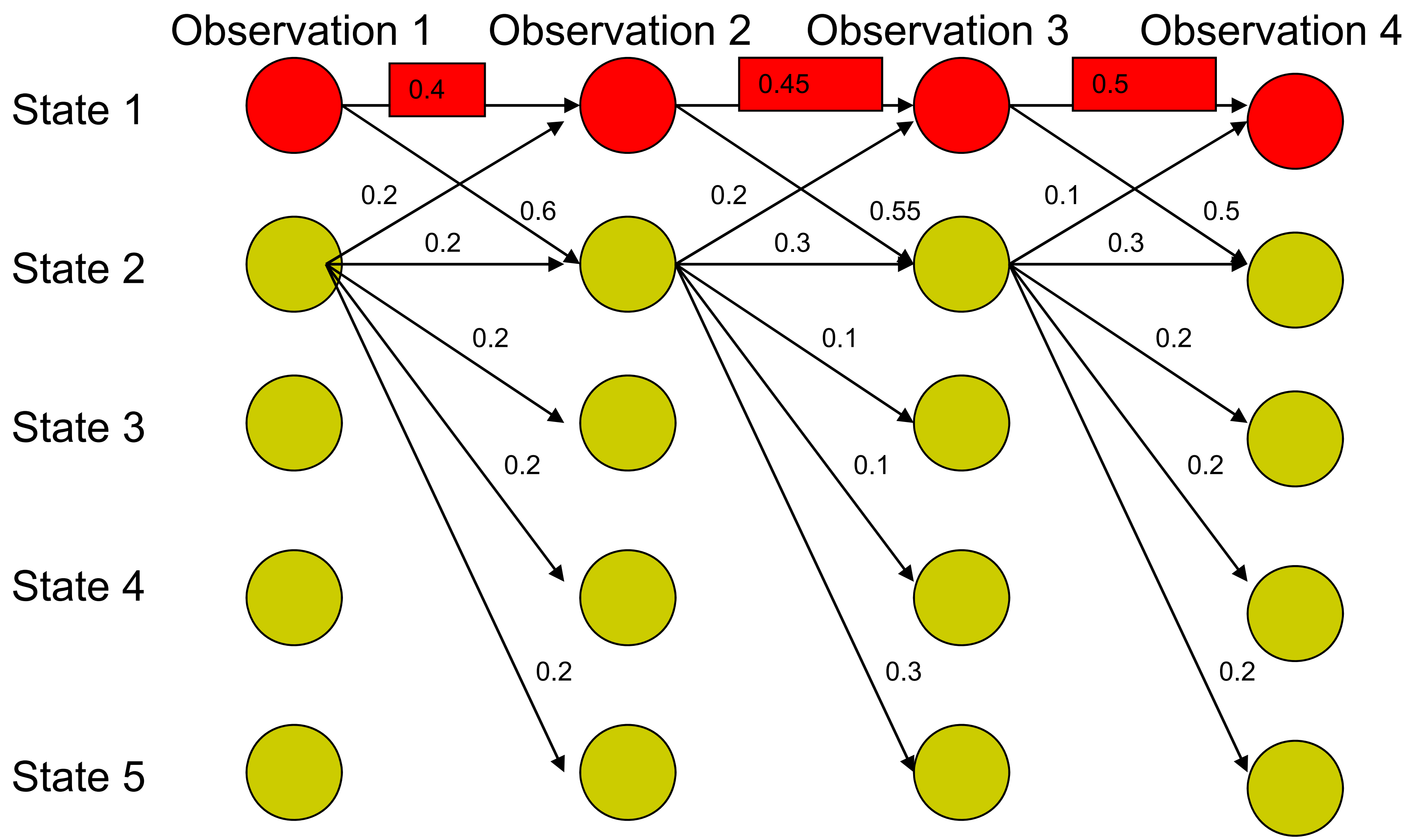
MEMM: the Label bias problem



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

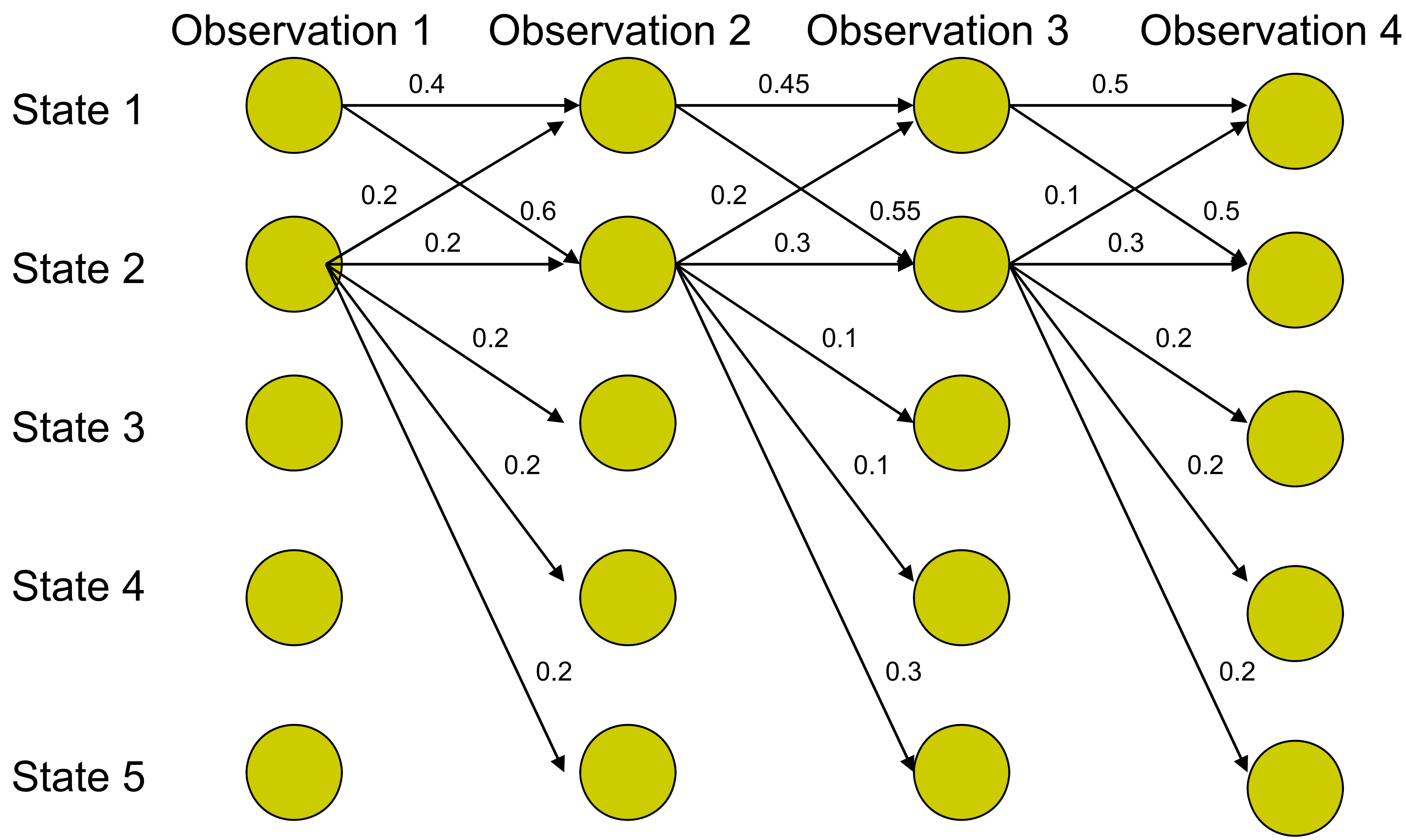
MEMM: the Label bias problem



Label bias problem in MEMM:

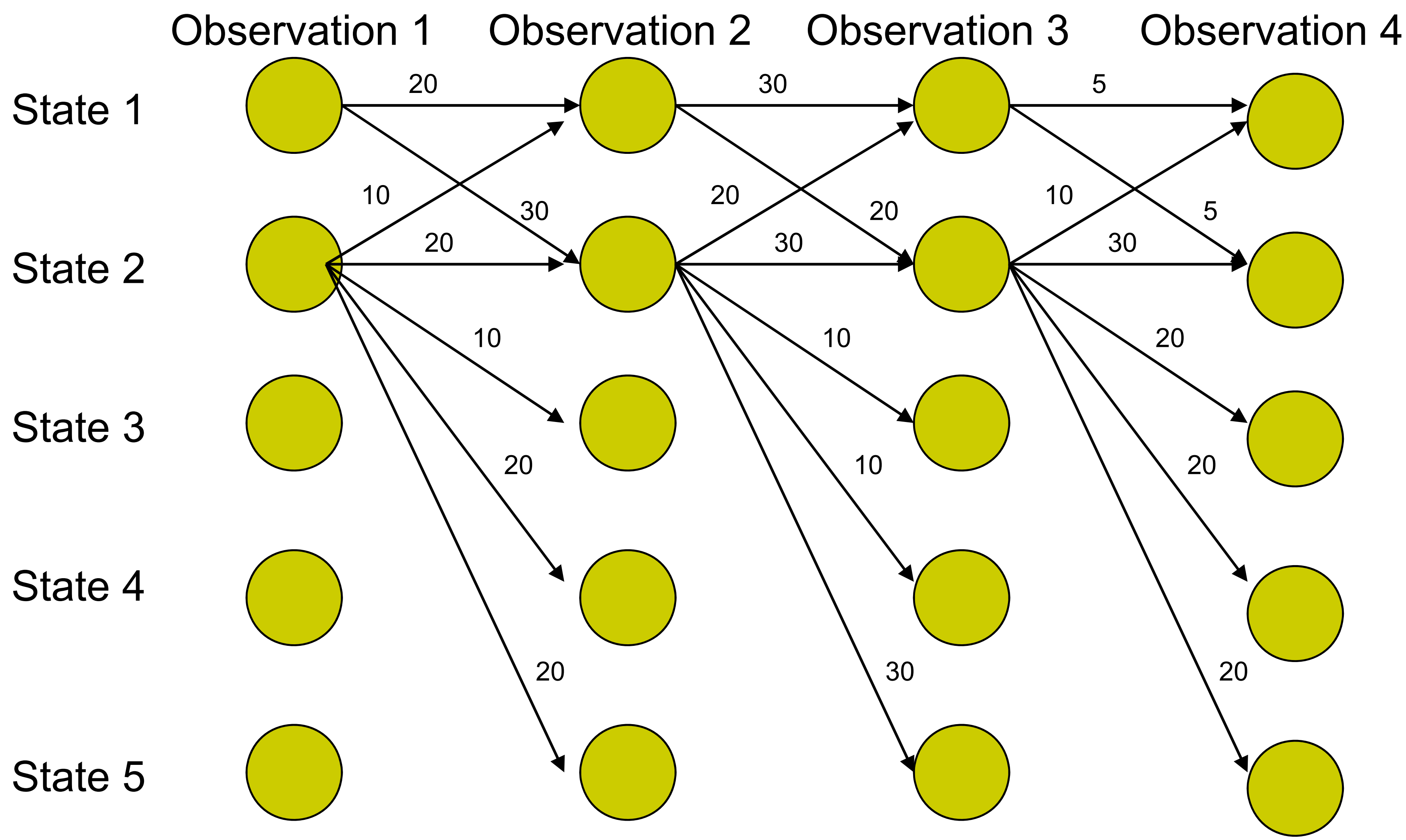
- Preference of states with lower number of transitions over others

Solution:
Do not normalize probabilities locally



From local probabilities .

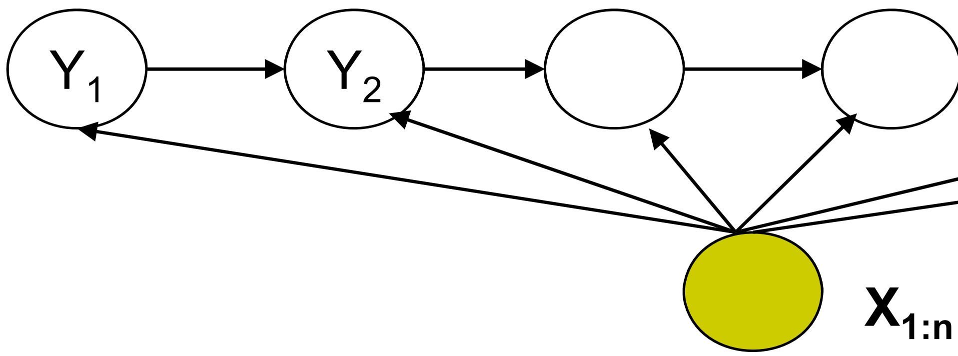
Solution:
Do not normalize probabilities locally



From local probabilities to local potentials

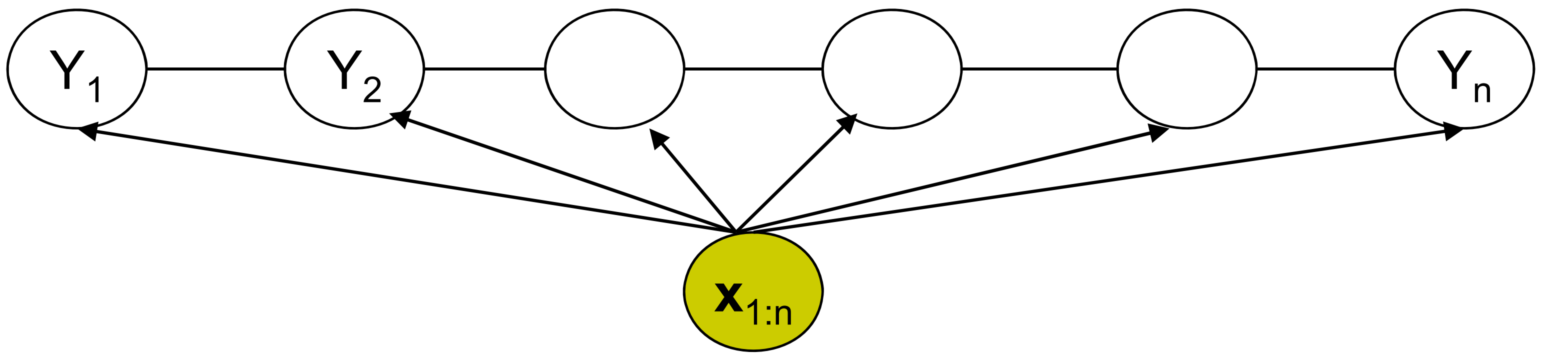
- States with lower transitions do not have an unfair advantage!

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

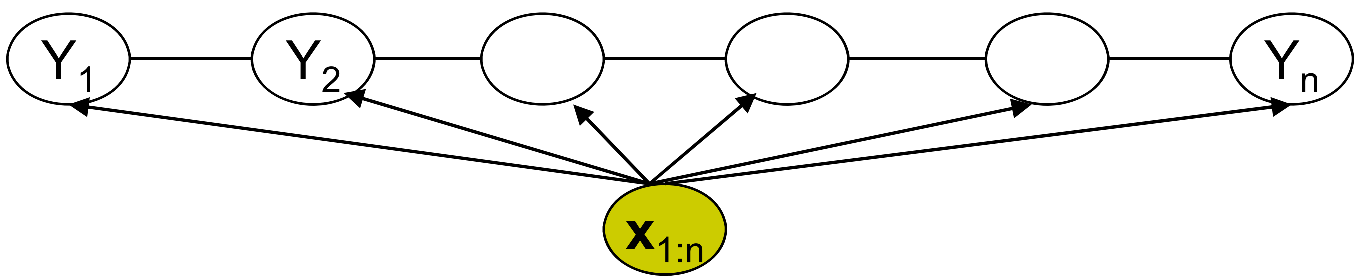


$$P(\mathbf{y}_{1:n}|\mathbf{x}_{1:n}) = \frac{1}{Z(\mathbf{x}_{1:n})}\prod_{i=1}^{n}\phi(y_i, y_{i-1}, \mathbf{x}_{1:n}) = \frac{1}{Z(\mathbf{x}_{1:n}, \mathbf{w})}\prod_{i=1}^{n}\exp(\mathbf{w}^T\mathbf{f}(y_i, y_{i-1}, \mathbf{x}_{1:n}))$$

- 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:



$$
\begin{aligned}
P(\mathbf{y}|\mathbf{x}) &= \frac{1}{Z(\mathbf{x},\lambda,\mu)} \exp\Big(\sum_{i=1}^{n}\Big(\sum_k \lambda_k f_k(y_i, y_{i-1}, \mathbf{x}) + \sum_l \mu_l g_l(y_i, \mathbf{x})\Big)\Big) \\
&= \frac{1}{Z(\mathbf{x},\lambda,\mu)} \exp\Big(\sum_{i=1}^{n}\big(\lambda^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}) + \mu^T \mathbf{g}(y_i, \mathbf{x})\big)\Big)
\end{aligned}
$$

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

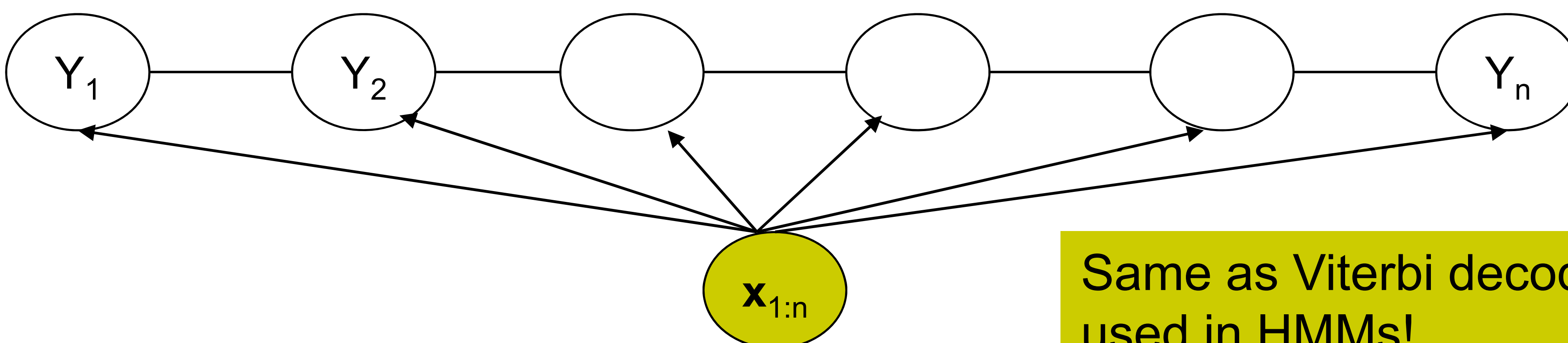
CRFs: Inference

- Given CRF parameters λ and μ, find the $\mathbf{y}^*$ that maximizes $P(\mathbf{y}|\mathbf{x})$

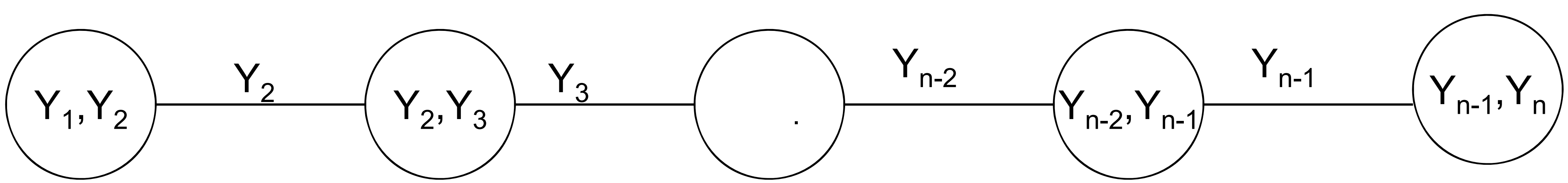
$$\mathbf{y}^* = \arg\max_{\mathbf{y}} \exp\left(\sum_{i=1}^{n} (\lambda^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}) + \mu^T \mathbf{g}(y_i, \mathbf{x}))\right)$$

  - Can ignore $Z(\mathbf{x})$ because it is not a function of $\mathbf{y}$

- 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

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

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

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

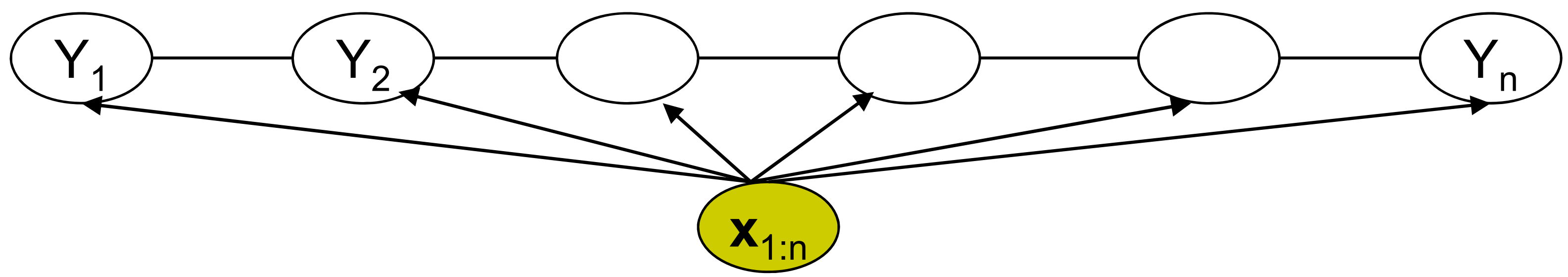
$$= \sum_{i=1}^{n}\sum_{y_i,y_{i-1}}\mathbf{f}(y_i,y_{i-1},\mathbf{x}_d)P(y_i,y_{i-1}|\mathbf{x}_d)$$

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

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

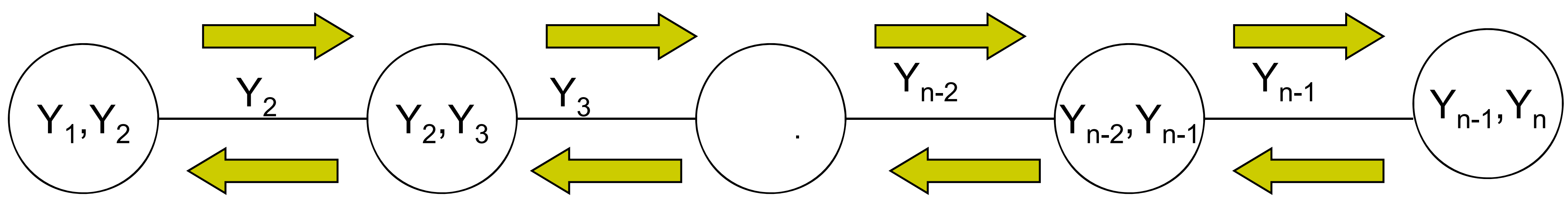
CRF learning

- Computing marginals using junction-tree calibration:



- Junction Tree Initialization:

$$\begin{aligned}\alpha^0(y_i, y_{i-1}) &= \exp(\lambda^T \mathbf{f}(y_i, y_{i-1}, \mathbf{x}_d) \\ &\quad + \mu^T \mathbf{g}(y_i, \mathbf{x}_d))\end{aligned}$$



- After calibration:

Also called forward-backward algorithm

$$\begin{aligned}P(y_i, y_{i-1}|\mathbf{x}_d) &\propto \alpha(y_i, y_{i-1}) \\ \Rightarrow P(y_i, y_{i-1}|\mathbf{x}_d) &= \frac{\alpha(y_i, y_{i-1})}{\sum_{y_i, y_{i-1}} \alpha(y_i, y_{i-1})} = \alpha'(y_i, y_{i-1})\end{aligned}$$

CRF learning

- Computing feature expectations using calibrated potentials:

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

- Now we know how to compute r$_\lambda$L(λ,μ):

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

- Learning can now be done using gradient ascent:

$$\begin{aligned}\lambda^{(t+1)} &= \lambda^{(t)} + \eta \nabla_\lambda L(\lambda^{(t)}, \mu^{(t)}) \\ \mu^{(t+1)} &= \mu^{(t)} + \eta \nabla_\mu L(\lambda^{(t)}, \mu^{(t)})\end{aligned}$$

CRF learning

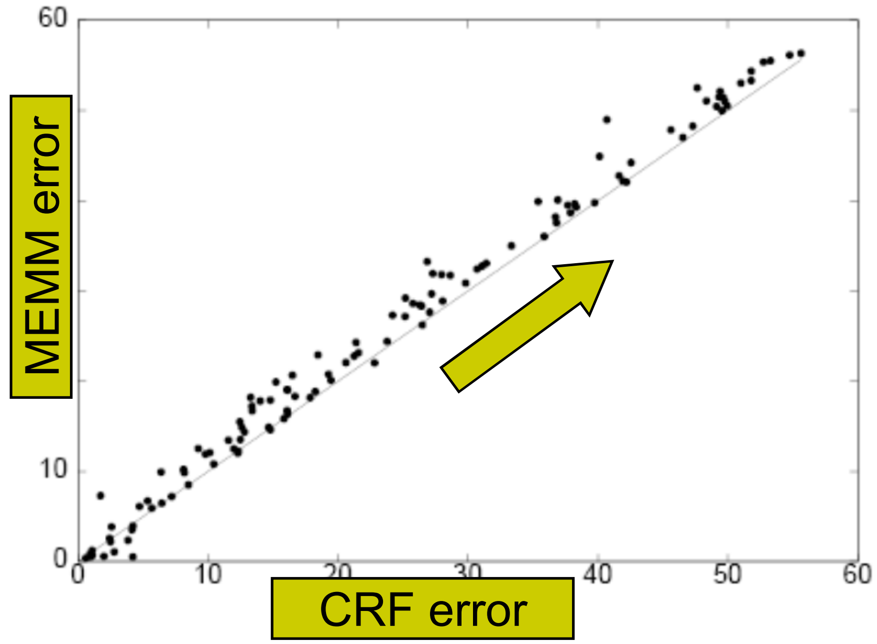
- In practice, we use a Gaussian Regularizer for the parameter vector to improve generalizability

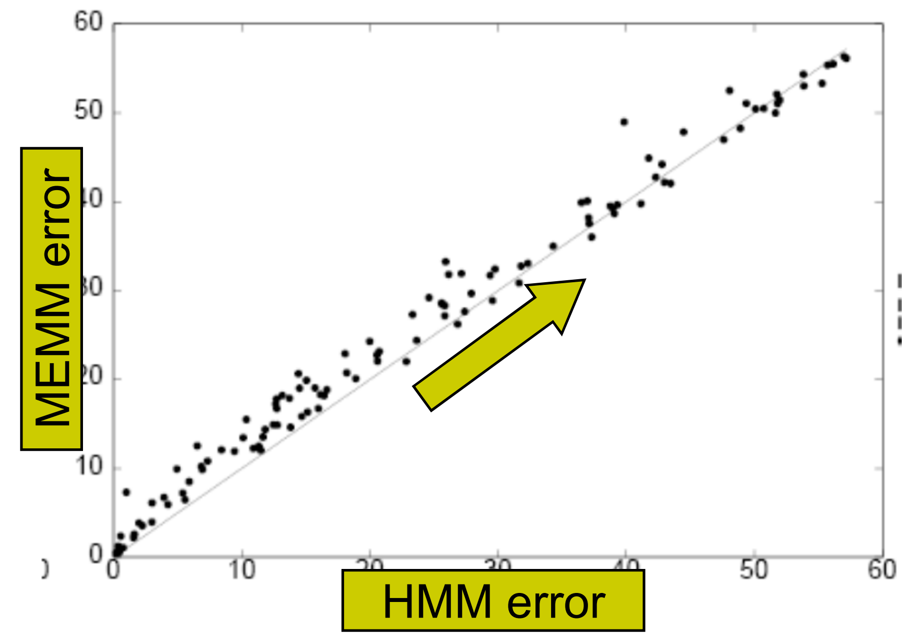
$$\lambda*, \mu* \quad = \quad \arg\max_{\lambda,\mu} \sum_{d=1}^{N} \log P(\mathbf{y}_d | \mathbf{x}_d, \lambda, \mu) - \frac{1}{2\sigma^2}(\lambda^T \lambda + \mu^T \mu)$$

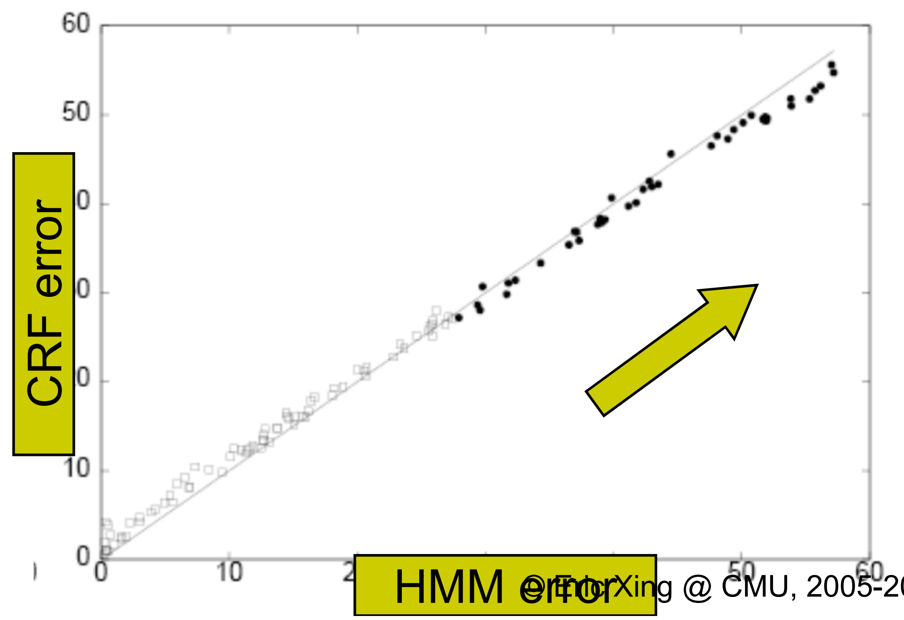
- In practice, gradient ascent has very slow convergence
  - Alternatives:
    - Conjugate Gradient method
    - Limited Memory Quasi-Newton Methods

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

Other CRFs

- So far we have discussed only 1-dimensional chain CRFs
  - Inference and learning: exact
- We could also have CRFs for arbitrary graph structure
  - E.g: Grid CRFs
  - Inference and learning no longer tractable
  - Approximate techniques used
    - MCMC Sampling
    - Variational Inference
    - Loopy Belief Propagation
  - We will discuss these techniques soon

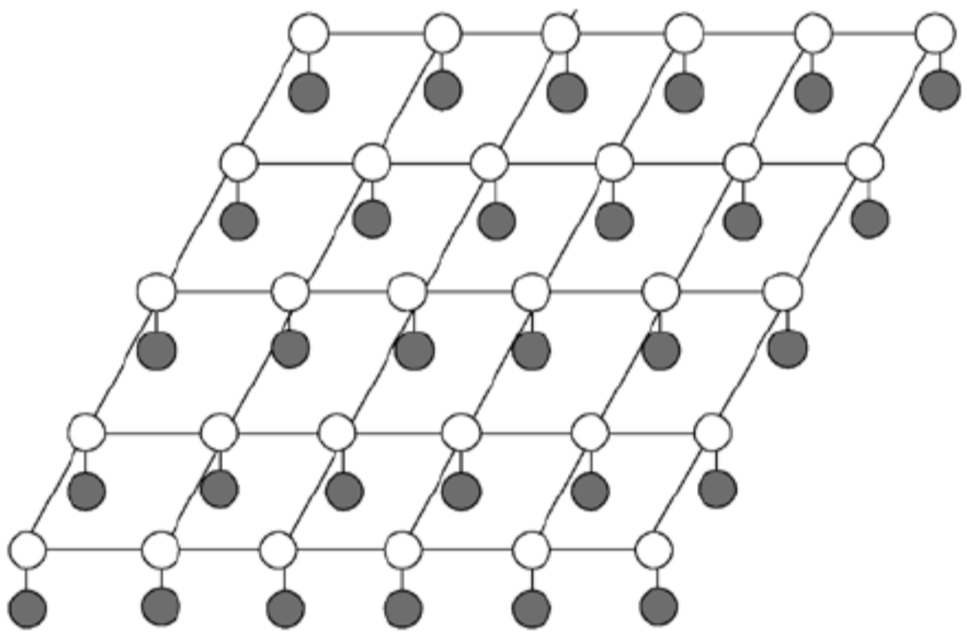


Image Segmentation

- Image segmentation (FG/BG) by modeling of interactions btw RVs
  - Images are noisy.
  - Objects occupy continuous regions in an image.

[Nowozin,Lampert 2012]

Input image

Pixel-wise separate optimal labeling

Locally-consistent joint optimal labeling

$$Y^* = \underset{y \in \{0,1\}^n}{\arg\max} \left[\underbrace{\sum_{i \in S} V_i(y_i, X)}_{\text{Unary Term}} + \underbrace{\sum_{i \in S} \sum_{j \in N_i} V_{i,j}(y_i, y_j)}_{\text{Pairwise Term}} \right].$$

Y: labels
X: data (features)
S: pixels
N_i: neighbors of pixel i