# Machine Learning

**10-701/15-781, Spring 2010**

## Hidden Markov Model (II)

**Eric Xing**

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**Reading: Chap. 13 CB**




# Three Main Questions on HMMs

1. Evaluation

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

2. Decoding

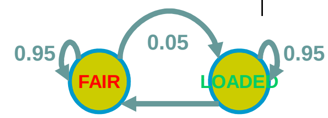
   GIVEN an HMM ***M***, and a sequence ***x***,
   FIND the sequence $\mathbf{y}$ of states that maximizes, e.g., P(***y*** | ***x*** , ***M***), or the most probable subsequence of states
   ALGO. Viterbi, Forward-backward

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 $P(x \mid \theta)$
   ALGO. Baum-Welch (EM)

# 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

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

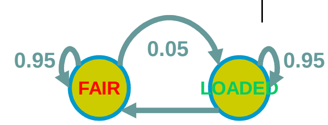
$$\beta_t^k = \sum_i a_{k,i} P(x_{t+1} \mid y_{t+1}^i = 1)\beta_{t+1}^i$$

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





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

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

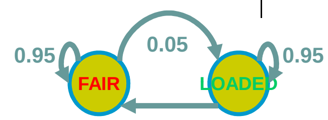
| Alpha (actual) | | Beta (actual) | |
|---|---|---|---|
| 0.0833 | 0.0500 | 0.0000 | 0.0000 |
| 0.0136 | 0.0052 | 0.0000 | 0.0000 |
| 0.0022 | 0.0006 | 0.0000 | 0.0000 |
| 0.0004 | 0.0001 | 0.0000 | 0.0000 |
| 0.0001 | 0.0000 | 0.0001 | 0.0001 |
| 0.0000 | 0.0000 | 0.0007 | 0.0006 |
| 0.0000 | 0.0000 | 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 |

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

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

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

$x$ = 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 (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 |

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

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

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




# What is the probability of a hidden state prediction?

- A single state:

$$P(y_t|\mathbf{X})$$

- What about a hidden state sequence ?

$$P(y_1, \ldots, y_T|\mathbf{X})$$

# 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 |

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# 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:

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

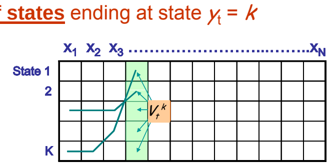
  - Let

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

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

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## The Viterbi Algorithm – derivation

- Define the viterbi probability:

$$V_{t+1}^k = \max_{\{y_1,\dots y_t\}} P(x_1,\dots,x_t, y_1,\dots,y_t, x_{t+1}, y_{t+1}^k = 1)$$

$$= \max_{\{y_1,\dots y_t\}} P(x_{t+1}, y_{t+1}^k = 1 \mid x_1,\dots,x_t, y_1,\dots,y_t) P(x_1,\dots,x_t, y_1,\dots,y_t)$$

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

$$= \max_i P(x_{t+1}, y_{t+1}^k = 1 \mid y_t^i = 1) \max_{\{y_1,\dots y_{t-1}\}} P(x_1,\dots,x_{t-1}, y_1,\dots,y_{t-1}, x_t, y_t^i = 1)$$

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

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





## The Viterbi Algorithm

- Input: $\mathbf{x} = x_1, \dots, x_T$,

**Initialization:**

$$V_1^k = P(x_1 \mid y_1^k = 1)\pi_k$$

**Iteration:**

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

$$\text{Ptr}(k,t) = \arg\max_i a_{i,k} V_{t-1}^i$$

**Termination:**

$$P(\mathbf{x}, \mathbf{y}^*) = \max_k V_T^k$$

**TraceBack:**

$$y_T^* = \arg\max_k V_T^k$$

$$y_{t-1}^* = \text{Ptr}(y_t^*, t)$$

# Viterbi Vs. MPA (individual)

| $V_t^k$ (log) | | $ptr(k,t)$ | | Seq | Veterbi | MPA | $p(y_t^k=1\mid x)$ | |
|---|---|---|---|---|---|---|---|---|
| --2.4849 | -2.9957 | N/A | | 1 | 1 | 1 | 0.8128 | 0.1872 |
| -4.3280 | -5.3496 | 1 | 2 | 2 | 1 | 1 | 0.8238 | 0.1762 |
| -6.1710 | -7.7035 | 1 | 2 | 1 | 1 | 1 | 0.8176 | 0.1824 |
| -8.0141 | -10.0574 | 1 | 2 | 5 | 1 | 1 | 0.7925 | 0.2075 |
| -9.8571 | -10.8018 | 1 | 2 | 6 | 1 | 1 | 0.7415 | 0.2585 |
| -11.7002 | -13.1557 | 1 | 2 | 2 | 1 | 1 | 0.7505 | 0.2495 |
| -13.5432 | -15.5096 | 1 | 2 | 1 | 1 | 1 | 0.7386 | 0.2614 |
| -15.3863 | -16.2540 | 1 | 2 | 6 | 1 | 1 | 0.7027 | 0.2973 |
| -17.2293 | -18.6079 | 1 | 2 | 2 | 1 | 1 | 0.7251 | 0.2749 |
| -19.0724 | -20.9618 | 1 | 2 | 4 | 1 | 1 | 0.7251 | 0.2749 |



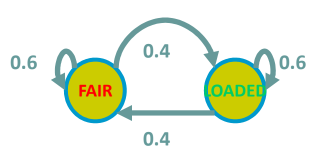


# Another Example

X = 6, 2, 3, 5, 6, 2, 6, 3, 6, 6

| $V_t^k$ (log) | | $ptr(k,t)$ | | Seq | Veterbi | MPA | $p(y_t^k=1\mid x)$ | |
|---|---|---|---|---|---|---|---|---|
| -2.4849 | -1.3863 | N/A | | 6 | 2 | 2 | 0.2733 | 0.7267 |
| -4.0943 | -4.1997 | 2 | 2 | 2 | 1 | 1 | 0.6040 | 0.3960 |
| -6.3969 | -7.0131 | 1 | 2 | 3 | 1 | 1 | 0.6538 | 0.3462 |
| -8.6995 | -9.6158 | 1 | 1 | 5 | 1 | 1 | 0.6062 | 0.3938 |
| -11.0021 | -10.3090 | 1 | 1 | 6 | 2 | 2 | 0.2861 | 0.7139 |
| -13.0170 | -13.1224 | 2 | 2 | 2 | 2 | 1 | 0.5342 | 0.4658 |
| -15.3196 | -14.3263 | 1 | 2 | 6 | 2 | 2 | 0.2734 | 0.7266 |
| -17.0344 | -17.1397 | 2 | 2 | 3 | 2 | 1 | 0.5226 | 0.4774 |
| -19.3370 | -18.3437 | 1 | 2 | 6 | 2 | 2 | 0.2252 | 0.7748 |
| -21.0518 | -19.5477 | 2 | 2 | 6 | 2 | 2 | 0.2159 | 0.7841 |

max




Same transition probabilities

# 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





# Three Main Questions on HMMs

1. Evaluation

   GIVEN an HMM $\boldsymbol{M}$, and a sequence $\boldsymbol{x}$,
   FIND Prob ($\boldsymbol{x} \mid \boldsymbol{M}$)
   ALGO. Forward

2. Decoding

   GIVEN an HMM $\boldsymbol{M}$, and a sequence $\boldsymbol{x}$,
   FIND the sequence $\mathbf{y}$ of states that maximizes, e.g., P($\boldsymbol{y} \mid \boldsymbol{x}$, $\boldsymbol{M}$), or the most probable subsequence of states
   ALGO. Viterbi, Forward-backward

3. Learning

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

# 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 $\theta$ of the model to maximize $P(x|\theta)$ --- Maximal likelihood (ML) estimation




# MLE

# 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 $i \to j$ occurs in **y**
    $B_{ik}$ = # times state $i$ in **y** emits $k$ in **x**

  - **We can show that the maximum likelihood parameters $\theta$ are:**

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

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

  - **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 …**




# Supervised ML estimation, ctd.

- **Intuition:**
  - When we know the underlying states, the best estimate of $\theta$ is the average frequency of transitions & emissions that occur in the training data
- **Drawback:**
  - Given little data, there may be **overfitting**:
    - P(x|θ) is maximized, but θ is unreasonable

      **0 probabilities – VERY BAD**
- **Example:**
  - Given 10 casino rolls, we observe

```
x = 2, 1, 5, 6, 1, 2, 3, 6, 2, 3
y = F, F, F, F, F, F, F, F, F, F
```

  - Then: $a_{FF} = 1$; $a_{FL} = 0$

    $b_{F1} = b_{F3} = .2$;

    $b_{F2} = .3$; $b_{F4} = 0$; $b_{F5} = b_{F6} = .1$

## 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 ⇒ strong prior belief
- Small total pseudocounts: just to avoid 0 probabilities --- smoothing





## Unsupervised ML estimation

# 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 $\theta$:
1. Estimate $A_{ij}$ , $B_{ik}$ in the training data
   - How? $A_{ij} = \sum_{n,t} \langle y^i_{n,t-1} y^j_{n,t} \rangle$ $B_{ik} = \sum_{n,t} \langle y^i_{n,t} \rangle x^k_{n,t}$ ,
   - Update $\theta$ according to $A_{ij}$ , $B_{ik}$
   - Now a "supervised learning" problem
2. Repeat 1 & 2, until convergence

**This is called the Baum-Welch Algorithm**

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





# 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

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

- EM
  - The **E** step

$$\gamma^i_{n,t} = \langle y^i_{n,t} \rangle = p(y^i_{n,t} = 1 \mid \mathbf{x}_n)$$

$$\xi^{i,j}_{n,t} = \langle y^i_{n,t-1} y^j_{n,t} \rangle = p(y^i_{n,t-1} = 1, y^j_{n,t} = 1 \mid \mathbf{x}_n)$$

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

$$\pi^{ML}_i = \frac{\sum_n \gamma^i_{n,1}}{N} \qquad a^{ML}_{ij} = \frac{\sum_n \sum_{t=2}^{T} \xi^{i,j}_{n,t}}{\sum_n \sum_{t=1}^{T-1} \gamma^i_{n,t}} \qquad b^{ML}_{ik} = \frac{\sum_n \sum_{t=1}^{T} \gamma^i_{n,t} x^k_{n,t}}{\sum_n \sum_{t=1}^{T-1} \gamma^i_{n,t}}$$

## The Baum-Welch algorithm -- comments

Time Complexity:

# iterations $\times$ $O(K^2N)$

- Guaranteed to increase the log likelihood of the model
- Not guaranteed to find globally best parameters
- Converges to local optimum, depending on initial conditions
- Too many parameters / too large model: Overt-fitting




## Summary: the HMM algorithms

**Questions:**

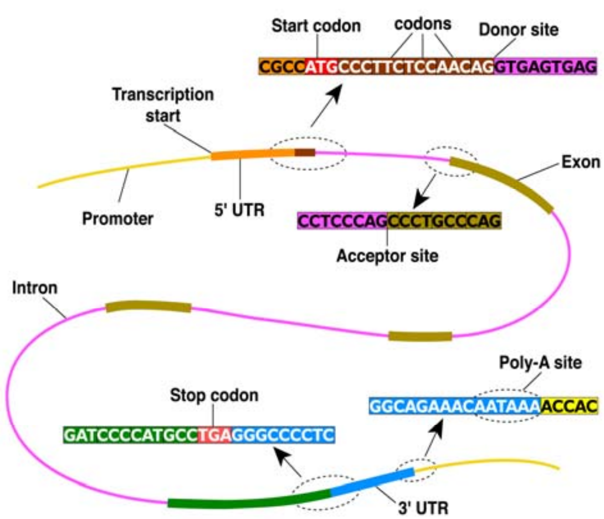
- **Evaluation**: What is the probability of the observed sequence? Forward
- **Decoding**: What is the probability that the state of the 3rd roll is loaded, given the observed sequence? Forward-Backward
- **Decoding**: What is the most likely die sequence? Viterbi
- **Learning**: Under what parameterization are the observed sequences most probable? Baum-Welch (EM)

## Applications of HMMs

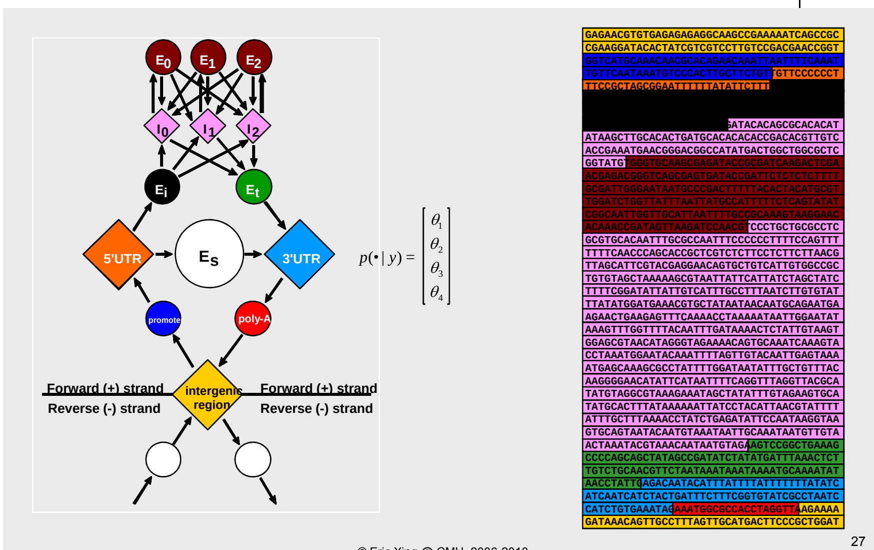
- **Some early applications of HMMs**
  - finance, but we never saw them
  - speech recognition
  - modelling ion channels
- In the mid-late 1980s HMMs entered genetics and molecular biology, and they are now firmly entrenched.
- **Some current applications of HMMs to biology**
  - mapping chromosomes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




## Typical structure of a gene



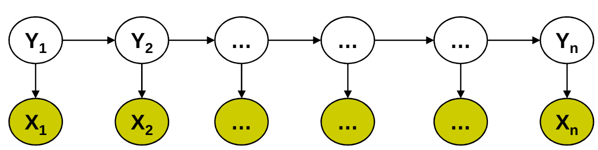
# GENSCAN (Burge & Karlin)








# Shortcomings of Hidden Markov Model

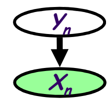



- HMM models capture dependences between each state and only its corresponding observation
  - NLP example: In a sentence segmentation task, each segmental state may depend not just on a single word (and the adjacent segmental stages), but also on the (non-local) features of the whole line such as line 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**)

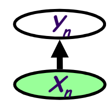
## Recall Generative vs. Discriminative Classifiers

- Goal: Wish to learn f: X → Y, e.g., P(Y|X)

- Generative classifiers (e.g., Naïve Bayes):
  - Assume some functional form for P(X|Y), P(Y)
    This is a **'*generative*'** model of the data!
  - Estimate parameters of P(X|Y), P(Y) directly from training data
  - Use Bayes rule to calculate P(Y|X= x)



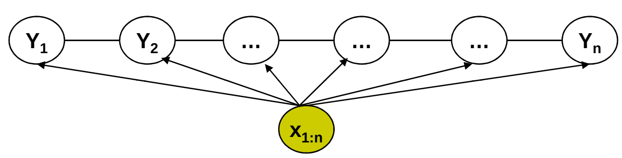

- Discriminative classifiers (e.g., logistic regression)
  - Directly assume some functional form for P(Y|X)
    This is a **'*discriminative*'** model of the data!
  - Estimate parameters of P(Y|X) directly from training data








## Structured Conditional Models




- Conditional probability $P$(label sequence $\mathbf{y}$ | observation sequence $\mathbf{x}$) rather than joint probability $P(\mathbf{y}, \mathbf{x})$
  - Specify the probability of possible label sequences given an observation sequence

- Allow arbitrary, non-independent features on the observation sequence $\mathbf{X}$

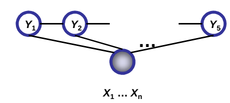
- The probability of a transition between labels may depend on past and future observations

- Relax strong independence assumptions in generative models

# Conditional Distribution

- If the graph $G = (V, E)$ of $\mathbf{Y}$ is a tree, the conditional distribution over the label sequence $\mathbf{Y} = \mathbf{y}$, given $\mathbf{X} = \mathbf{x}$, by the Hammersley Clifford theorem of random fields is:

$$p_\theta(\mathrm{y} \mid \mathrm{x}) \propto \exp\left( \sum_{e \in E,k} \lambda_k f_k(e, \mathrm{y}|_e, \mathrm{x}) + \sum_{v \in V,k} \mu_k g_k(v, \mathrm{y}|_v, \mathrm{x}) \right)$$

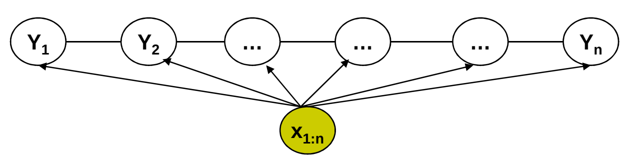


  - x is a data sequence
  - y is a label sequence
  - *v* is a vertex from vertex set V = set of label random variables
  - *e* is an edge from edge set E over V
  - $f_k$ and $g_k$ are given and fixed. $g_k$ is a Boolean vertex feature; $f_k$ is a Boolean edge feature
  - *k* is the number of features
  - $\theta = (\lambda_1, \lambda_2, \cdots, \lambda_n; \mu_1, \mu_2, \cdots, \mu_n); \lambda_k$ and $\mu_k$ are parameters to be estimated
  - $\mathrm{y}|_e$ is the set of components of y defined by edge *e*
  - $\mathrm{y}|_v$ is the set of components of y defined by vertex *v*





# Conditional Random Fields

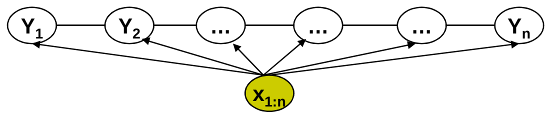



$$P(\mathbf{y}_{1:n}|\mathbf{x}_{1:n}) = \frac{1}{Z(\mathbf{x}_{1:n})}\prod_{i=1}^{n}\phi(y_i, y_{i-1}, \mathbf{x}_{1:n}) = \frac{1}{Z(\mathbf{x}_{1:n}, \mathbf{w})}\prod_{i=1}^{n}\exp(\mathbf{w}^T\mathbf{f}(y_i, y_{i-1}, \mathbf{x}_{1:n}))$$

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

# Conditional Random Fields

- General parametric form:



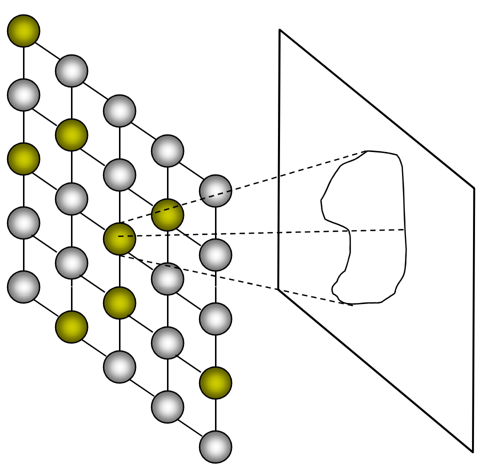

$$P(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{x},\lambda,\mu)} \exp(\sum_{i=1}^{n}(\sum_{k}\lambda_k f_k(y_i,y_{i-1},\mathbf{x}) + \sum_{l}\mu_l g_l(y_i,\mathbf{x})))$$

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

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




# Conditional Random Fields



$$p_\theta(y\,|\,x) = \frac{1}{Z(\theta,x)} \exp\left\{\sum_c \theta_c f_c(x,y_c)\right\}$$

- Allow arbitrary dependencies on input
- Clique dependencies on labels
- Use approximate inference for general graphs

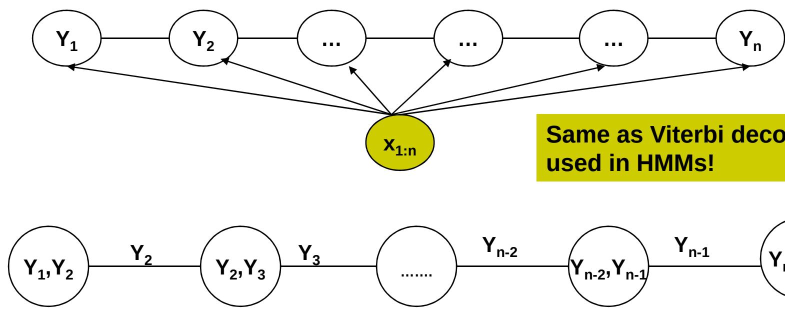
# CRFs: Inference

- Given CRF parameters $\lambda$ and $\mu$, find the $\mathbf{y}^*$ 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!**



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# CRF learning

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

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

- Computing the gradient w.r.t $\lambda$:

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

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



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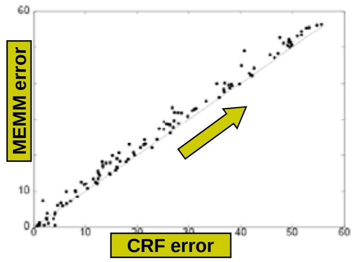
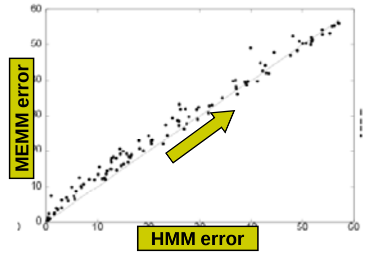
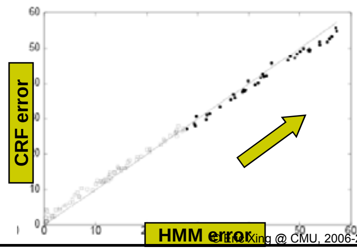
# CRFs: some empirical results

- 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

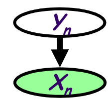
| *model* | *error* | *oov error* |
|---|---|---|
| HMM | 5.69% | 45.99% |
| MEMM | 6.37% | 54.61% |
| CRF | 5.55% | 48.05% |
| MEMM$^+$ | 4.81% | 26.99% |
| CRF$^+$ | 4.27% | 23.76% |

$^+$Using spelling features

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

# Summary

- Conditional Random Fields is a discriminative Structured Input Output model!




- HMM is a generative structured I/O model

- Complementary strength and weakness:

  1.
  2.
  3.
  …