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# Conditional Random Fields: Probabilistic Models for Segmenting and Labeling Sequence Data

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# Sequence Segmenting and Labeling

- Goal: mark up sequences with content tags
- Application in computational biology
  - DNA and protein sequence alignment
  - Sequence homolog searching in databases
  - Protein secondary structure prediction
  - RNA secondary structure analysis
- Application in computational linguistics & computer science
  - Text and speech processing, including topic segmentation, part-of-speech (POS) tagging
  - Information extraction
  - Syntactic disambiguation

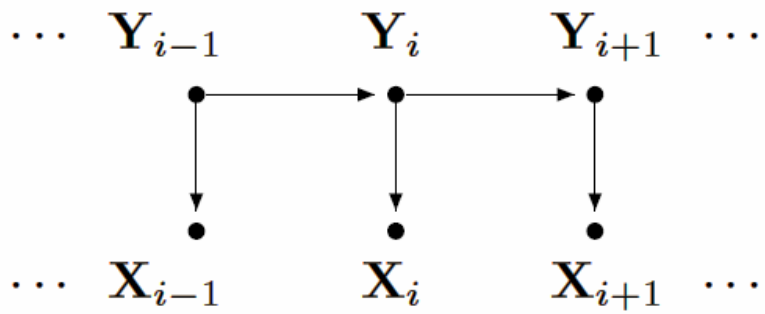
# Example: Protein secondary structure prediction

```
Conf: 977621015677468999723631357600330223342057899861488356412238
Pred: CCCCCCCCCCCCCEEEEEEECCCCCCCCCCCCCHHHHHHHHHHHHHHHHCCCCEEEEHHCC
  AA: EKKSINECDLKGKKVLIRVDFNVPVKNGKITNDYRIRSALPTLKKVLTEGGSCVLMSHLG
              10        20        30        40        50        60

Conf: 855764222454123478985100010478999999874033445740023666631258
Pred: CCCCCCCCCCCCCCCCCCCCCCCCCCCHHHHHHHHHHHHHCCCCCCCCCCCCHHHHHHCCC
  AA: RPKGIPMAQAGKIRSTGGVPGFQQKATLKPVAKRLSELLLRPVTFAPDCLNAADVVSKMS
              70        80        90       100       110       120

Conf: 8746886110023430443100178999998750533552122443345520013224 52
Pred: CCCEEEECCCHHHHHHCCCCCHHHHHHHHHHHHHCCEEEECCCCCCCCCCCCCCCCHHHH
  AA: PGDVVLLENVRFYKEEGSKKAKDREAMAKILASYGDVYISDAFGTAHRDSATMTGIPKIL
             130       140       150       160       170       180
```

# Generative Models

- Hidden Markov models (HMMs) and stochastic grammars
  - Assign a joint probability to paired observation and label sequences
  - The parameters typically trained to maximize the joint likelihood of train examples

Standard tool is the hidden Markov Model (HMM).




$$P(\mathbf{X}, \mathbf{Y}) = \prod_i P(\mathbf{X}_i \mid \mathbf{Y}_i)\, P(\mathbf{Y}_i \mid \mathbf{Y}_{i-1})$$

# Generative Models (cont'd)

- Difficulties and disadvantages
  - Need to enumerate all possible observation sequences
  - Not practical to represent multiple interacting features or long-range dependencies of the observations
  - Very strict independence assumptions on the observations

# Conditional Models

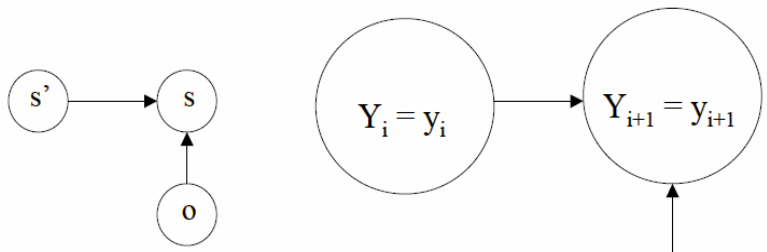
- Conditional probability *P(label sequence* **y** | *observation sequence* **x***)* rather than joint probability *P*(**y, x**)
  - Specify the probability of possible label sequences given an observation sequence

- Allow arbitrary, non-independent features on the observation sequence X

- The probability of a transition between labels may depend on past and future observations
  - Relax strong independence assumptions in generative models

# Discriminative Models
# Maximum Entropy Markov Models (MEMMs)

- Exponential model
- Given training set X with label sequence Y:
  - Train a model θ that maximizes P(Y|X, θ)
  - For a new data sequence **x**, the predicted label **y** maximizes P(**y**|**x**, θ)
  - Notice the per-state normalization




A = a, where A is a random variable, and a is an outcome

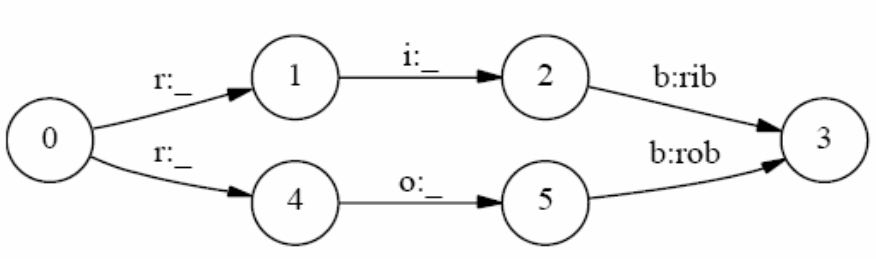
$$P(y' \mid y, x) = \frac{1}{Z(y, x)} \exp\left(\sum_k \underbrace{\lambda_k}_{\text{weight}} \underbrace{f_k(x, y, y')}_{\text{feature}}\right)$$

# MEMMs (cont'd)

- MEMMs have all the advantages of Conditional Models
- Per-state normalization: all the mass that arrives at a state must be distributed among the possible successor states ("conservation of score mass")
- Subject to Label Bias Problem
  - Bias toward states with fewer outgoing transitions

# Label Bias Problem

- Consider this MEMM:




- **P(1 and 2 | ro) = P(2 | 1 and ro)P(1 | ro) = P(2 | 1 and o)P(1 | r)**
  **P(1 and 2 | ri) = P(2 | 1 and ri)P(1 | ri) = P(2 | 1 and i)P(1 | r)**

- Since **P(2 | 1 and x) = 1 for all x, P(1 and 2 | ro) = P(1 and 2 | ri)**

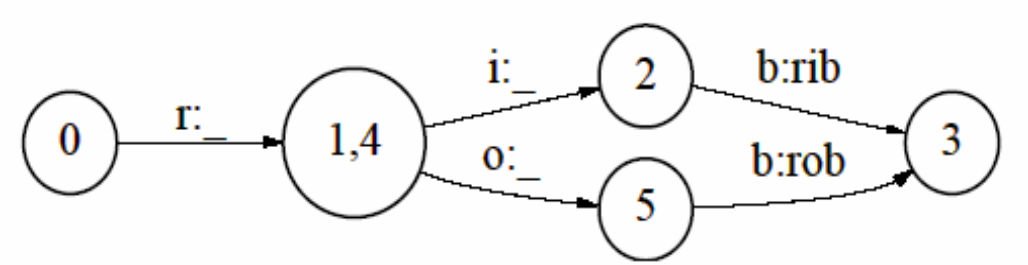
In the training data, label value 2 is the only label value observed after label value 1
Therefore **P(2 | 1) = 1, so P(2 | 1 and x) = 1 for all x**

- However, we expect **P(1 and 2 | ri)** to be greater than **P(1 and 2 | ro).**

- Per-state normalization does not allow the required expectation

# Solve the Label Bias Problem

- Change the state-transition structure of the model




  - Not always practical to change the set of states

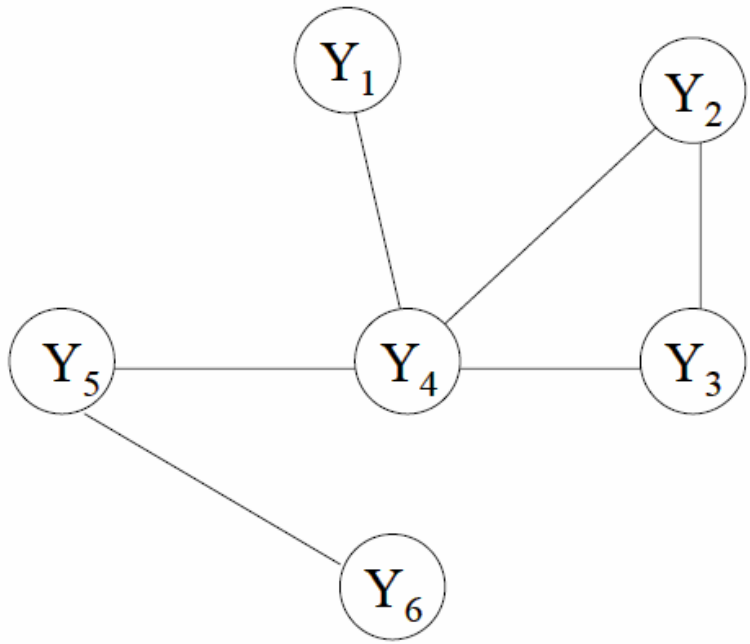
- Start with a fully-connected model and let the training procedure figure out a good structure
  - Prelude the use of prior, which is very valuable (e.g. in information extraction)

# Random Field

Let G = (Y, E) be a graph where each vertex $Y_v$ is a random variable

Suppose $P(Y_v \mid \text{all other } Y) = P(Y_v \mid \text{neighbors}(Y_v))$ then Y is a random field

Example:




- $P(Y_5 \mid \text{all other } Y) = P(Y_5 \mid Y_4, Y_6)$

# Conditional Random Fields (CRFs)

- CRFs have all the advantages of MEMMs without label bias problem
  - MEMM uses per-state exponential model for the conditional probabilities of next states given the current state
  - CRF has a single exponential model for the joint probability of the entire sequence of labels given the observation sequence
- Undirected acyclic graph
- Allow some transitions “vote” more strongly than others depending on the corresponding observations

# Definition of CRFs

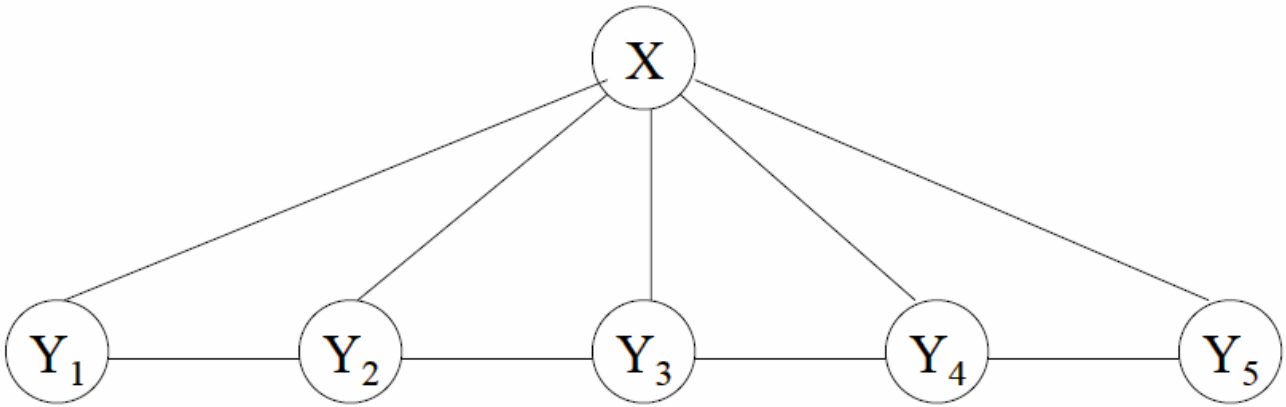
**X** is a random variable over data sequences to be labeled

**Y** is a random variable over corresponding label sequences

**Definition**. *Let* $G = (V, E)$ *be a graph such that* $\mathbf{Y} = (\mathbf{Y}_v)_{v \in V}$, *so that* $\mathbf{Y}$ *is indexed by the vertices of* $G$. *Then* $(\mathbf{X}, \mathbf{Y})$ *is a conditional random field in case, when conditioned on* $\mathbf{X}$, *the random variables* $\mathbf{Y}_v$ *obey the Markov property with respect to the graph:* $p(\mathbf{Y}_v \,|\, \mathbf{X}, \mathbf{Y}_w, w \neq v) = p(\mathbf{Y}_v \,|\, \mathbf{X}, \mathbf{Y}_w, w \sim v)$, *where* $w \sim v$ *means that* $w$ *and* $v$ *are neighbors in* $G$.

# Example of CRFs

Suppose $P(Y_v \mid X$ , all other $Y) = P(Y_v \mid X$, neighbors$(Y_v))$
then X with Y is a **conditional** random field




- $P(Y_3 \mid X$ , all other $Y) = P(Y_3 \mid X, Y_2, Y_4)$
- Think of X as observations and Y as labels

# Graphical comparison among HMMs, MEMMs and CRFs

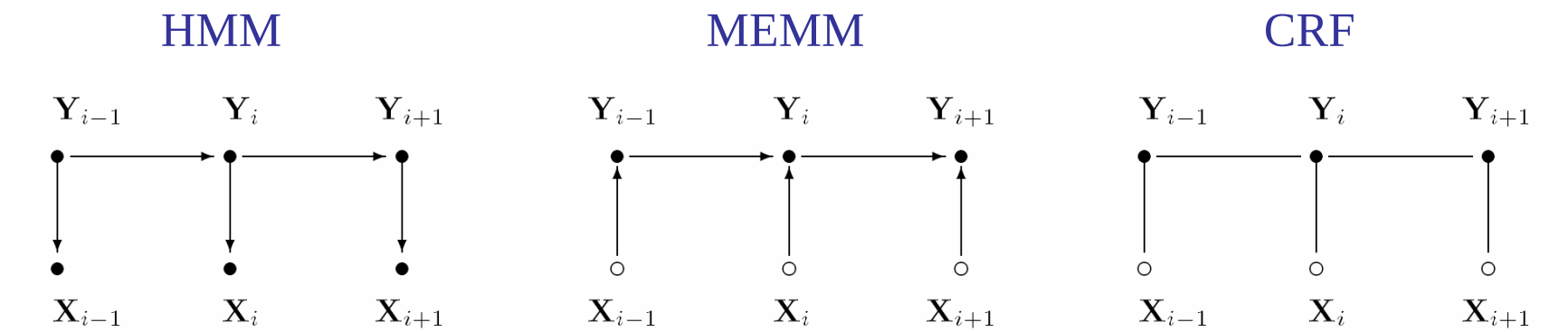



*Figure 2.* Graphical structures of simple HMMs (left), MEMMs (center), and the chain-structured case of CRFs (right) for sequences. An open circle indicates that the variable is not generated by the model.

# Conditional Distribution

If the graph $G = (V, E)$ of Y is a tree, the conditional distribution over the label sequence Y = y, given X = x, by fundamental 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

$\theta = (\lambda_1, \lambda_2, \ldots, \lambda_n; \mu_1, \mu_2, \ldots, \mu_n)$; $\lambda_k$ 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 Distribution (cont'd)

- CRFs use the observation-dependent normalization $Z(\mathrm{x})$ for the conditional distributions:

$$p_\theta(\mathrm{y}\,|\,\mathrm{x}) = \frac{1}{Z(\mathrm{x})} \exp\left( \sum_{e \in E,k} \lambda_k f_k(e, \mathrm{y}|_e, \mathrm{x}) + \sum_{v \in V,k} \mu_k g_k(v, \mathrm{y}|_v, \mathrm{x}) \right)$$

$Z(\mathrm{x})$ is a normalization over the data sequence x

# Parameter Estimation for CRFs

- The paper provided iterative scaling algorithms
- It turns out to be very inefficient
- Prof. Dietterich's group applied Gradient Descendent Algorithm, which is quite efficient

# Training of CRFs (From Prof. Dietterich)

- First, we take the log of the equation

$$\log p_\theta(y \mid x) = \sum_{e \in E,k} \lambda_k f_k(e, \mathrm{y}|_e, \mathrm{x}) + \sum_{v \in V,k} \mu_k g_k(v, \mathrm{y}|_v, \mathrm{x}) - \log Z(\mathrm{x})$$

- Then, take the derivative of the above equation

$$\frac{\partial \log p_\theta(y \mid x)}{\partial \theta} = \frac{\partial}{\partial \theta}\left( \sum_{e \in E,k} \lambda_k f_k(e, \mathrm{y}|_e, \mathrm{x}) + \sum_{v \in V,k} \mu_k g_k(v, \mathrm{y}|_v, \mathrm{x}) - \log Z(\mathrm{x}) \right)$$

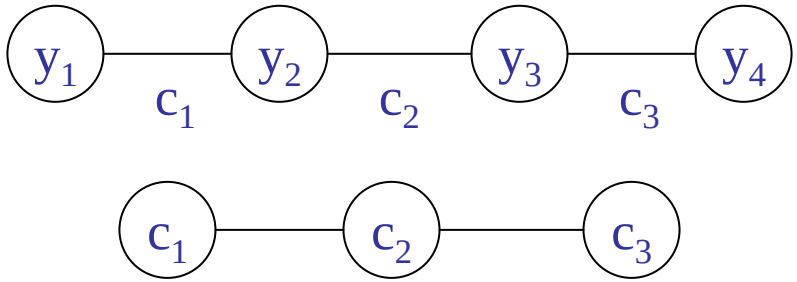
- For training, the first 2 items are easy to get.
- For example, for each $\lambda_k$, $f_k$ is a sequence of Boolean numbers, such as 00101110100111.

$\lambda_k f_k(e, \mathrm{y}|_e, \mathrm{x})$ is just the total number of 1's in the sequence.

- The hardest thing is how to calculate $Z(\mathrm{x})$

# Training of CRFs (From Prof. Dietterich) (cont'd)

- Maximal cliques




$$c_1 : \exp(\varphi(y_1,x) + \varphi(y_2,x) + \psi(y_1,y_2,x)) = c_1(y_1,y_2,x)$$

$$c_2 : \exp(\varphi(y_3,x) + \psi(y_2,y_3,x)) = c_2(y_2,y_3,x)$$

$$c_3 : \exp(\varphi(y_4,x) + \psi(y_3,y_4,x)) = c_3(y_3,y_4,x)$$

$$Z(x) = \sum_{y_1,y_2,y_3,y_4} c_1(y_1,y_2,x)c_2(y_2,y_3,x)c_3(y_3,y_4,x)$$

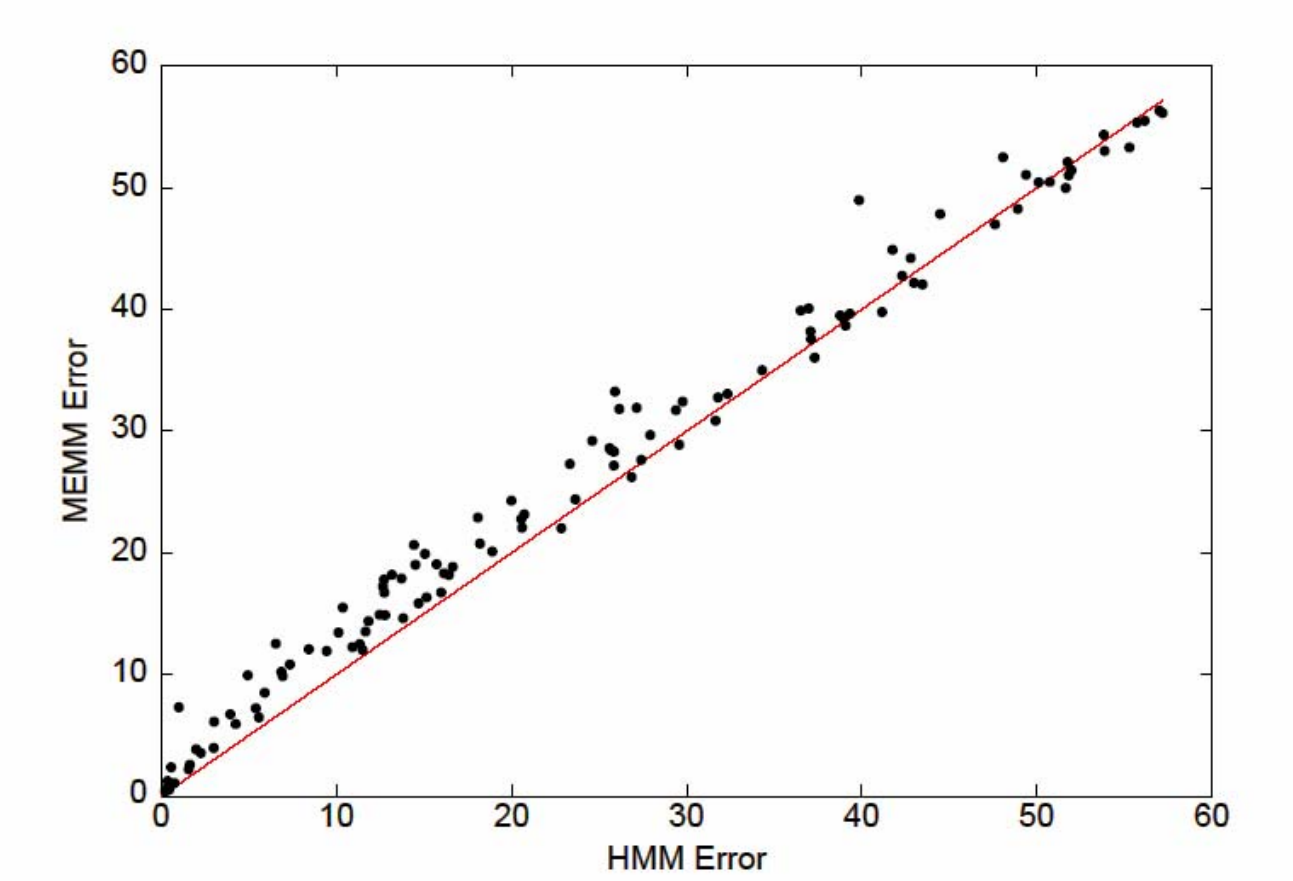
$$= \sum_{y_1}\sum_{y_2} c_1(y_1,y_2,x) \sum_{y_3} c_2(y_2,y_3,x) \sum_{y_4} c_3(y_3,y_4,x)$$

# Modeling the label bias problem

- In a simple HMM, each state generates its designated symbol with probability 29/32 and the other symbols with probability 1/32
- Train MEMM and CRF with the same topologies
- A run consists of 2,000 training examples and 500 test examples, trained to convergence using Iterative Scaling algorithm
- CRF error is 4.6%, and MEMM error is 42%
- MEMM fails to discriminate between the two branches
- CRF solves label bias problem

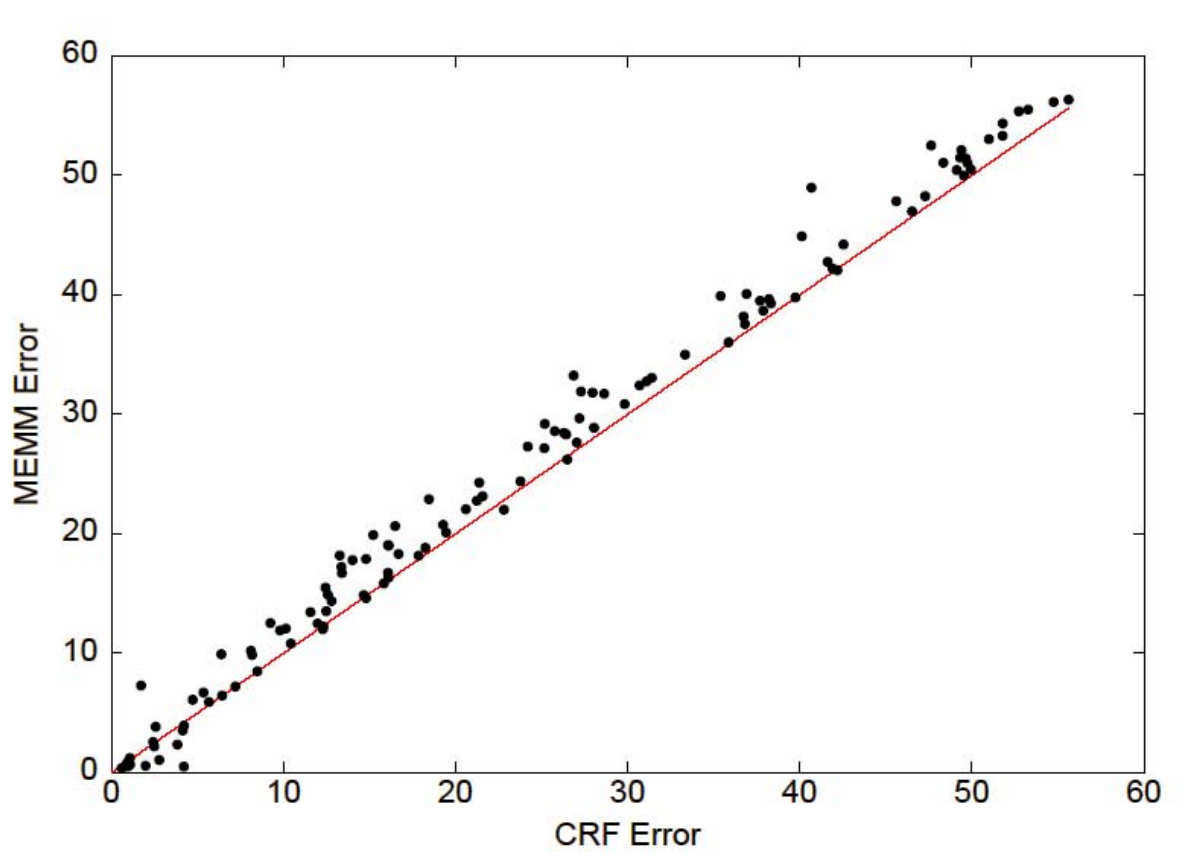
# MEMM vs. HMM

- The HMM outperforms the MEMM



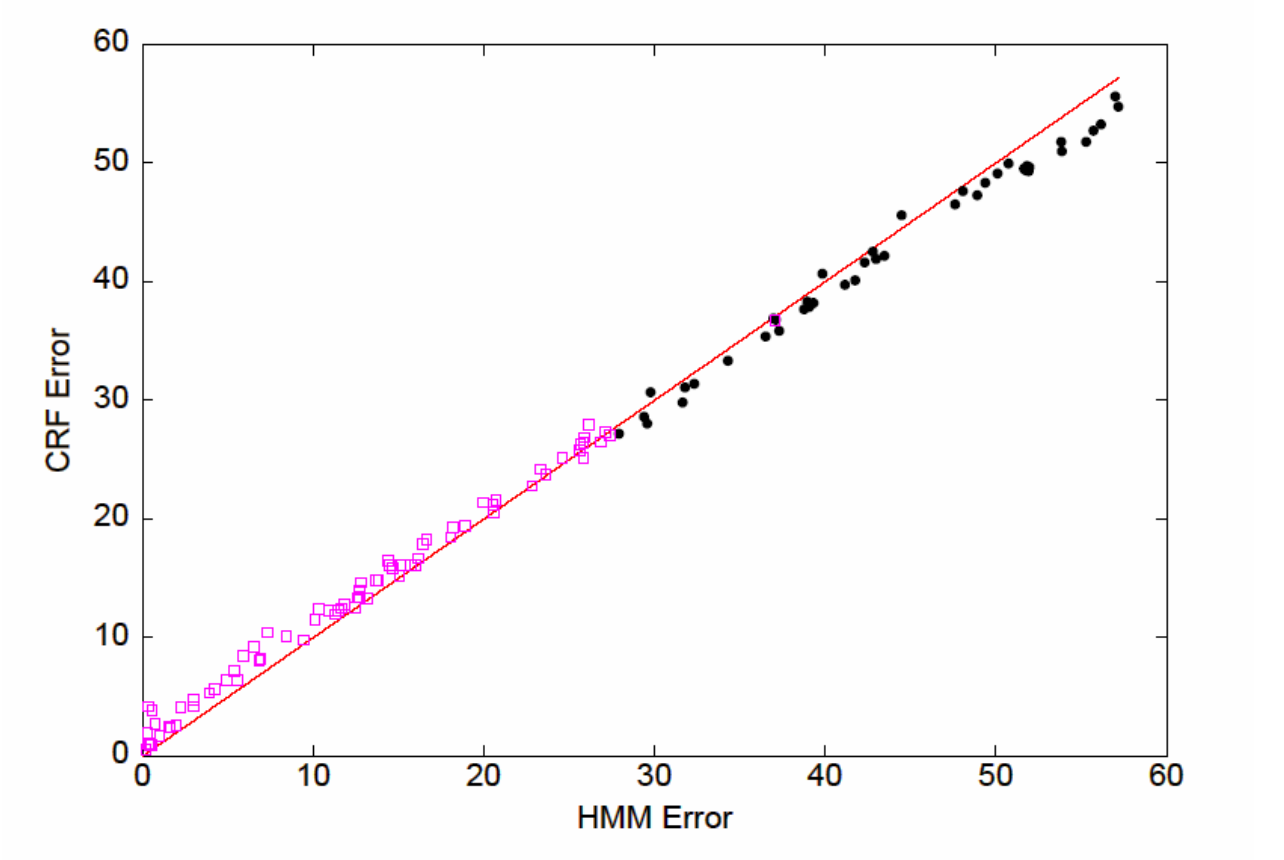
# MEMM vs. CRF

- CRF usually outperforms the MEMM



# CRF vs. HMM

Each open square represents a data set with $\alpha < 1/2$, and a solid circle indicates a data set with $\alpha \geqslant 1/2$; When the data is mostly second order ($\alpha \geqslant 1/2$), the discriminatively trained CRF usually outperforms the HMM



# POS tagging Experiments

UPenn tagging task: 45 tags (syntactic), 1M words training

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| DT | NN | NN | | NN | | VBZ | RB | JJ |
| The | asbestos | fiber | ; | crocidolite | ; | is | unusually | resilient |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| IN | PRP | VBZ | DT | NNS | | IN | RB | JJ | NNS |
| once | it | enters | the | lungs | ; | with | even | brief | exposures |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| TO | PRP | VBG | NNS | WDT | VBP | RP | NNS | JJ | |
| to | it | causing | symptoms | that | show | up | decades | later | ; |

| | | |
|---|---|---|
| NNS | VBD | |
| researchers | said | |

# POS tagging Experiments (cont'd)

- Compared HMMs, MEMMs, and CRFs on Penn treebank POS tagging
- Each word in a given input sentence must be labeled with one of 45 syntactic tags
- Add a small set of orthographic features: whether a spelling begins with a number or upper case letter, whether it contains a hyphen, and if it contains one of the following suffixes: -ing, -ogy, -ed, -s, -ly, -ion, -tion, -ity, -ies
- oov = out-of-vocabulary (not observed in the training set)

| *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

# Summary

- Discriminative models are prone to the label bias problem
- CRFs provide the benefits of discriminative models
- CRFs solve the label bias problem well, and demonstrate good performance

Thanks for your attention!

Special thanks to
Prof. Dietterich & Tadepalli!