

#### Machine Learning & Data Mining CS/CNS/EE 155

#### Lecture 17: Survey of Advanced Topics

#### What We Covered

## **Basic Supervised Learning**

- Training Data:  $S = \{(x_i, y_i)\}_{i=1}^N$   $x \in \mathbb{R}^D$  $y \in \{-1, +1\}$
- Model Class:  $f(x | w, b) = w^T x b$  Linear Models

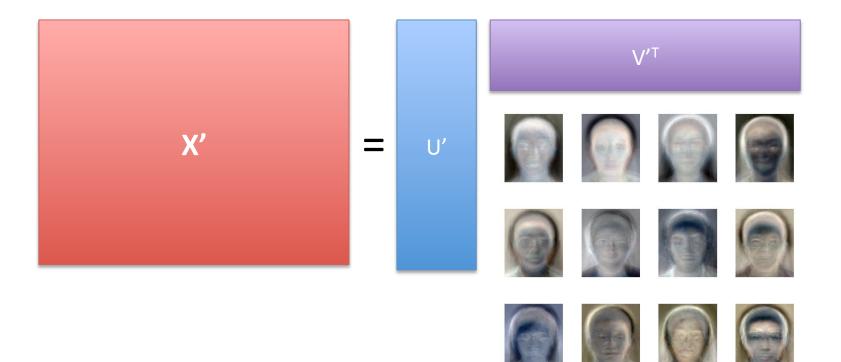
• Loss Function:  $L(a,b) = (a-b)^2$  Squared Loss

• Learning Objective:

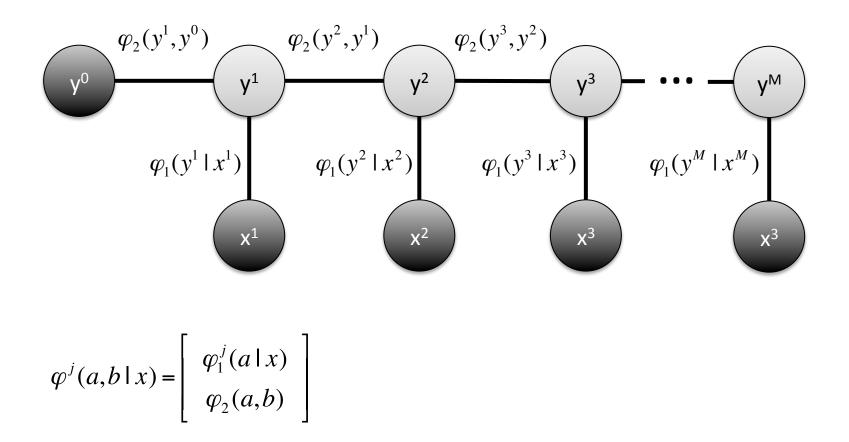
$$\operatorname{argmin}_{w,b} \sum_{i=1}^{N} L(y_i, f(x_i \mid w, b))$$

**Optimization Problem** 

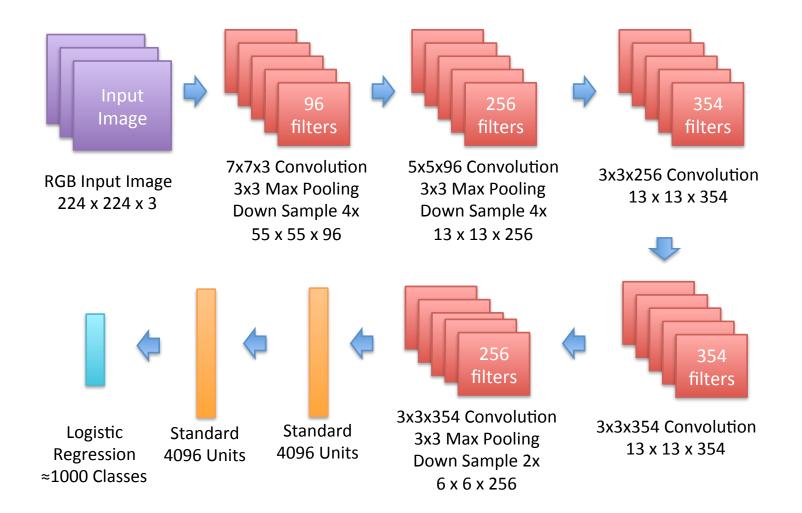
## **Basic Unsupervised Learning**



#### **Sequence Prediction**



#### Intro to Deep Learning



# Simple Optimization Algorithms

• Stochastic Gradient Descent

• EM algorithm (for HMMs)

# **Other Basic Concepts**

Cross Validation

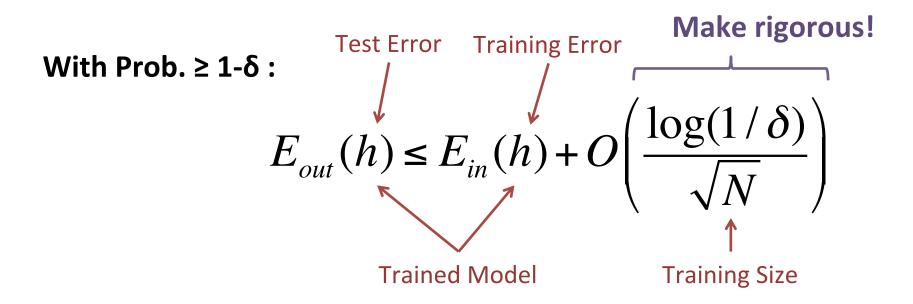
• Overfitting

• Bias-Variance Tradeoff

Learning Theory

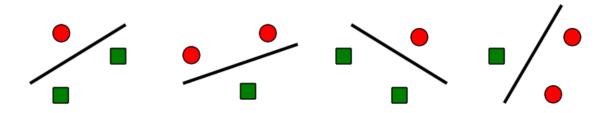
# **Generalization Bounds**

- Formal characterization of overfitting
- Example result:



# Shattering

 Definition: A set of points is shattered by H if for all possible binary labelings of points, there exists some h that classifies perfectly.

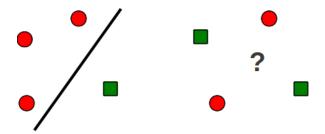


In 2D, any 3 points can always be shattered by linear models!

Slide Material Borrowed From Piyush Rai: https://www.cs.utah.edu/~piyush/teaching/27-9-print.pdf

# Shattering

 Definition: A set of points is shattered by H if for all possible binary labelings of points, there exists some h that classifies perfectly.



In 2D, linear models cannot shatter 4 points!

Slide Material Borrowed From Piyush Rai: https://www.cs.utah.edu/~piyush/teaching/27-9-print.pdf

## VC Dimension

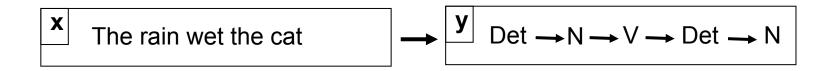
- VC(H) = most # points that can be shattered
   If H is linear models in 2D feature space:
  - VC(H) = 3

With Prob. 
$$\geq 1-\delta$$
:  
 $E_{out}(h) \leq E_{in}(h) + O\left(\frac{\log\left(\frac{2N}{VC(H)} + 1\right) + \log\left(\frac{1}{\delta}\right)}{\sqrt{N}}\right)$ 

#### **Structured Prediction**

### **Examples of Complex Output Spaces**

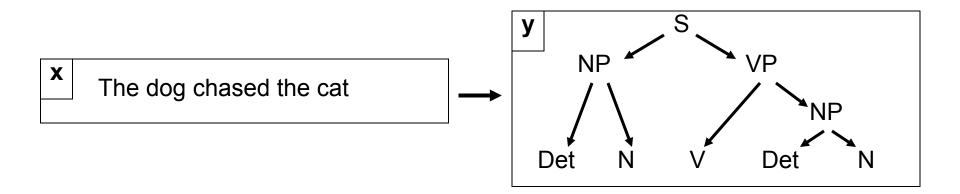
- Part-of-Speech Tagging
  - Given a sequence of words *x*, predict sequence of tags *y*.
  - Dependencies from tag-tag transitions in Markov model.



→ Similarly for other sequence labeling problems, e.g., RNA Intron/ Exon Tagging.

#### **Examples of Complex Output Spaces**

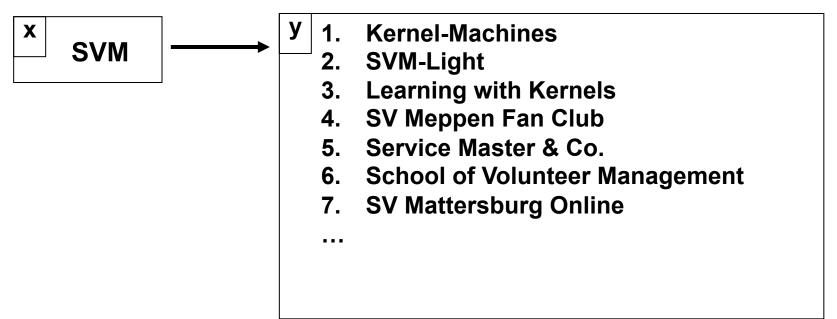
- Natural Language Parsing
  - Given a sequence of words *x*, predict the parse tree *y*.
  - Dependencies from structural constraints, since y has to be a tree.



#### **Examples of Complex Output Spaces**

#### Information Retrieval

- Given a query x, predict a ranking y.
- Dependencies between results (e.g. avoid redundant hits)
- Loss function over rankings (e.g. Average Precision)



# General Formula (Linear Models)

Assume scoring function F

$$h(\mathbf{x}; w) = \underset{\mathbf{y} \in Y(\mathbf{x})}{\operatorname{argmax}} F(\mathbf{x}, \mathbf{y}; w)$$

• Assume F is linear:

$$F(\mathbf{x},\mathbf{y};w) = w^T \Psi(\mathbf{x},\mathbf{y})$$

#### Example 1

 $h(\mathbf{x}; w) = \underset{\mathbf{y} \in Y(\mathbf{x})}{\operatorname{argmax}} F(\mathbf{x}, \mathbf{y}; w) \qquad F(\mathbf{x}, \mathbf{y}; w) = w^T \Psi(\mathbf{x}, \mathbf{y})$ 

**Binary Classification:** 

$$\Psi(\mathbf{x}, y) = y\mathbf{x}$$

 $Y(\mathbf{x}) = \{-1, +1\}$ 

 $F(\mathbf{x}, y; w) = y(w^T \mathbf{x})$ 

$$h(\mathbf{x}; w) = \underset{y \in \{-1,+1\}}{\operatorname{argmax}} y(w^T \mathbf{x})$$

#### Examples

 $h(\mathbf{x}; w) = \underset{\mathbf{y} \in Y(\mathbf{x})}{\operatorname{argmax}} F(\mathbf{x}, \mathbf{y}; w) \qquad F(\mathbf{x}, \mathbf{y}; w) = w^T \Psi(\mathbf{x}, \mathbf{y})$ 

**1**<sup>st</sup> Order Sequences:

 $Y(\mathbf{x})$  = all possible output sequences

$$\Psi(\mathbf{x},\mathbf{y}) = \sum_{j} \phi(y^{j}, y^{j-1} | \mathbf{x})$$

$$F(\mathbf{x}, \mathbf{y}; w) = w^T \sum_{j} \phi(y^j, y^{j-1} | \mathbf{x})$$

Solve using Viterbi!

#### Examples

 $h(\mathbf{x}; w) = \underset{\mathbf{y} \in Y(\mathbf{x})}{\operatorname{argmax}} F(\mathbf{x}, \mathbf{y}; w) \qquad F(\mathbf{x}, \mathbf{y}; w) = w^T \Psi(\mathbf{x}, \mathbf{y})$ 

#### **Integer Linear Program:**

 $Y(\mathbf{x})$  = Feasible settings of **y** Each y<sup>j</sup>  $\in$  {0,1}

$$\Psi(\mathbf{x},\mathbf{y}) = \sum_{j} y^{j} \phi^{j}(\mathbf{x})$$

$$F(\mathbf{x}, \mathbf{y}; w) = \mathbf{y}^T \mathbf{c} \qquad \mathbf{c} = \begin{bmatrix} w^T \phi^1(\mathbf{x}) \\ w^T \phi^2(\mathbf{x}) \\ \vdots \end{bmatrix}$$

 $h(\mathbf{x}; w) = \underset{\mathbf{y} \in Y(\mathbf{x})}{\operatorname{argmax}} \mathbf{y}^{T} \mathbf{c}$ 

#### **Structured Prediction Learning Problem**

Efficient Inference/Prediction

$$h(\mathbf{x}; w) = \underset{\mathbf{y}}{\operatorname{argmax}} w^{T} \Psi(\mathbf{y}, \mathbf{x})$$

- Viterbi in sequence labeling
- CKY Parser for parse trees
- Sorting for ranking

#### Efficient Learning/Training

- Learn parameters w from training data  $\{x_i, y_i\}_{i=1..N}$
- Structural SVM: Hinge Loss Minimization
- Conditional Random Fields: Log Loss Minimization
- Structured Perceptron, etc...

## **Perceptron Learning Algorithm**

- w<sup>1</sup> = 0, b<sup>1</sup> = 0
- For t = 1 ....
  - Receive example (x,y)
  - $If h(x | w^t) = y$ 
    - $[w^{t+1}, b^{t+1}] = [w^{t}, b^{t}]$

– Else

- w<sup>t+1</sup>= w<sup>t</sup> + yx
- $b^{t+1} = b^t + y$

$$h(x \mid w) = sign(w^T x - b)$$

Training Set:

$$S = \{(x_i, y_i)\}_{i=1}^{N}$$
  
y \le \{+1, -1\}

Go through training set in arbitrary order (e.g., randomly)

#### **Structured Perceptron**

- $W^1 = 0$   $h(x | w) = \underset{y'}{\operatorname{argmax}} w^T \Psi(x, y')$
- For t = 1 ....
  - Receive example (x,y)
  - $If h(x | w^t) = y$ 
    - w<sup>t+1</sup> = w<sup>t</sup>

– Else

•  $w^{t+1} = w^t + \Psi(x,y)$ 

**Training Set:** 

$$S = \{(x_i, y_i)\}_{i=1}^{N}$$

Go through training set in arbitrary order (e.g., randomly)

# **Conventional SVMs**

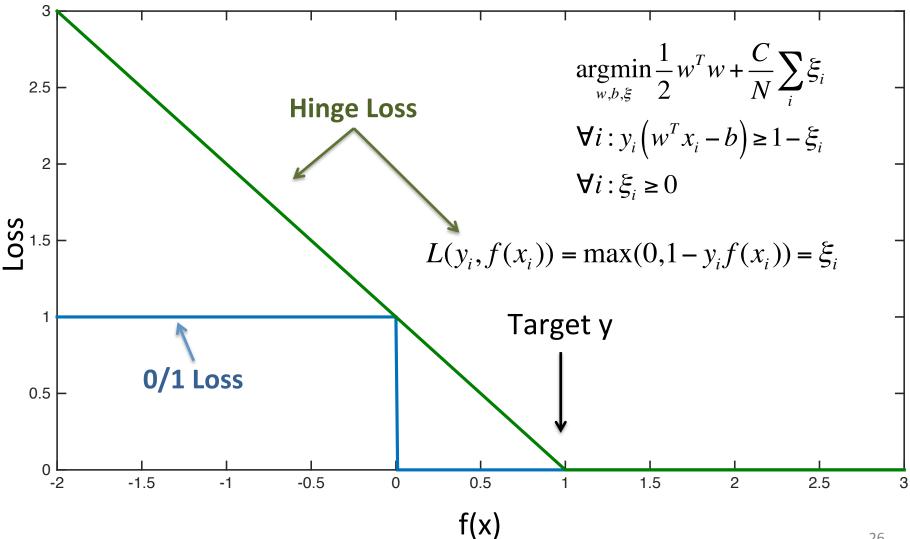
- Input: x (high dimensional point)
- Target: y (either +1 or -1)
- Prediction: sign( $w^T x$ )

• Training: 
$$\underset{w,\xi}{\operatorname{arg\,min}} \frac{1}{2}w^2 + \frac{C}{N}\sum_{i=1}^N \xi_i$$

subject to:  $\forall i: y_i \cdot (w^T x_i) \ge 1 - \xi_i$ 

• The sum of slacks  $\sum_i \xi_i$  upper bounds the 0/1 loss!

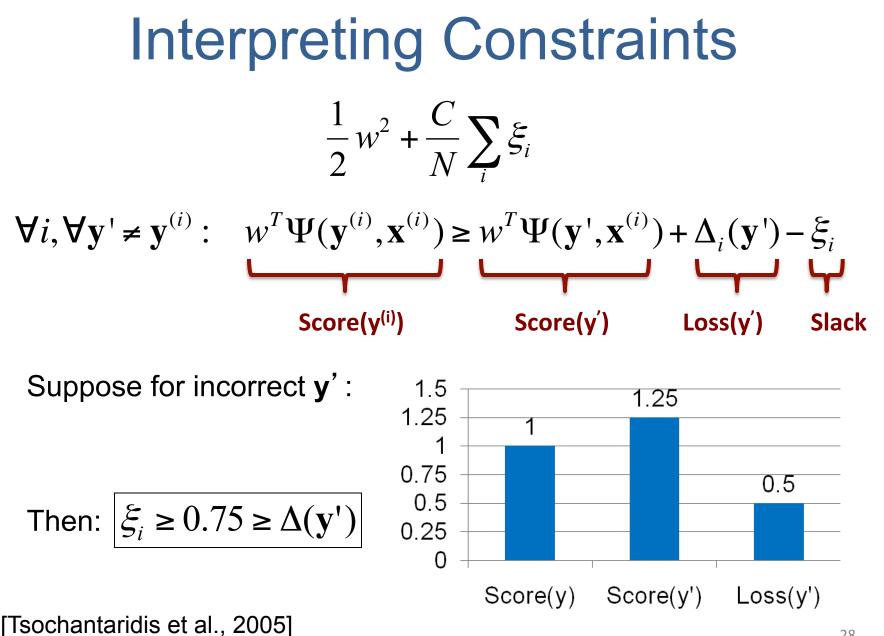
# **Conventional SVMs**



# **Structural SVM**

- Let **x** denote a structured input (sentence)
- Let **y** denote a structured output (POS tags)
- Standard objective function:  $\frac{1}{2}w^2 + \frac{C}{N}\sum_i \xi_i$
- Constraints are defined for each incorrect labeling y' over each x.

[Tsochantaridis et al., 2005]



#### Crowdsourcing

# **Acquiring Labels from Annotators**

Keyword Tagging Attractions in Paris!

- Please inspect the attraction below.
- SELECT ALL keywords that are appropriate for this attraction.
- Selected keywords will turn RED.
- The right pane below displays additional information (e.g., wikipedia page) for your convenience.



#### Place de la Madeleine

Ξ

Ancient Ruin	Palace / Mansion
<ul> <li>Architecture</li> </ul>	Performance
Art	Plaza / Open Area
<ul> <li>Bridge</li> </ul>	Recreational
Cabaret	<ul> <li>Relaxing / Leisure</li> </ul>
Cemetary	Religious
Comedy	<ul> <li>Scenic Nature</li> </ul>
Culture	<ul> <li>Scenic Urban</li> </ul>
Dining	<ul> <li>Scenic Water</li> </ul>
<ul> <li>Fountain</li> </ul>	<ul> <li>Shopping</li> </ul>
Garden / Park	<ul> <li>Sightseeing</li> </ul>
<ul> <li>Historical</li> </ul>	<ul> <li>Spa / Massage</li> </ul>
<ul> <li>Large Building</li> </ul>	Sports
Memorial	Street
<ul> <li>Monument / Statue</li> </ul>	Theater / Opera
Museum Art	Tour
Museum Other	<ul> <li>Transportation</li> </ul>
Nightlife	<ul> <li>Walking / Strolling</li> </ul>
Outdoors	<ul> <li>Zoo / Aquarium</li> </ul>

Search Wikipedia

☆

#### La Madeleine, Paris



The Madeleine church

L'église de la Madeleine (French pronunciation: [legliz de la madelen], Madeleine Church; more formally, L'église Sainte-Marie-Madeleine; less formally, just La Madeleine) is a Roman Catholic church occupying a commanding position in the 8th arrondissement of Paris.

The Madeleine Church was designed in its present form as a temple to the glory of Napoleon's army. To its south lies the Place de la Concorde, to the east is the



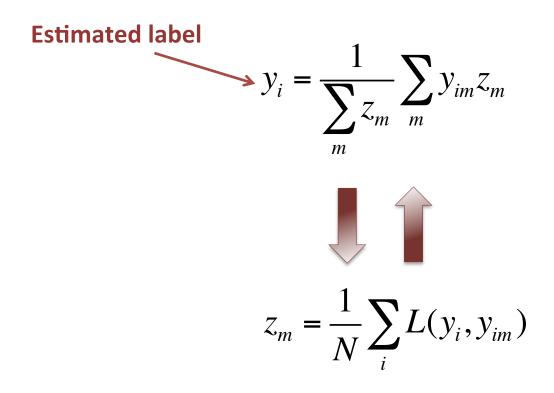
Submit

# How Reliable are Annotators?

- If we knew what the labels were
   Can judge workers on label quality
- If we knew who the good workers were
   Can create labels from their annotations
- Chicken and egg problem!

#### Worker Reliability as Latent Variable

• Let  $z_m$  denote the reliability of worker m



# **Differing Ambiguities Across Tasks**

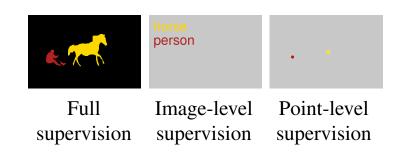
• Often collecting annotations for many tasks

• Some tasks are harder than others

• How many labels to collect for each task?

## **Structured Annotations**



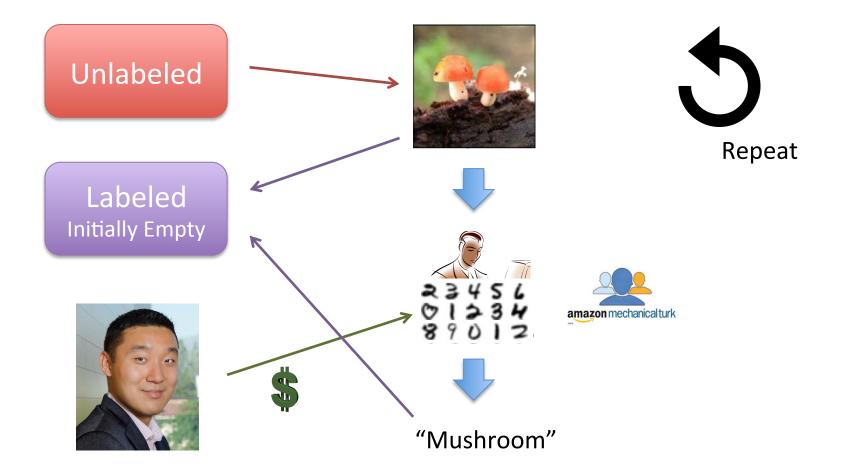




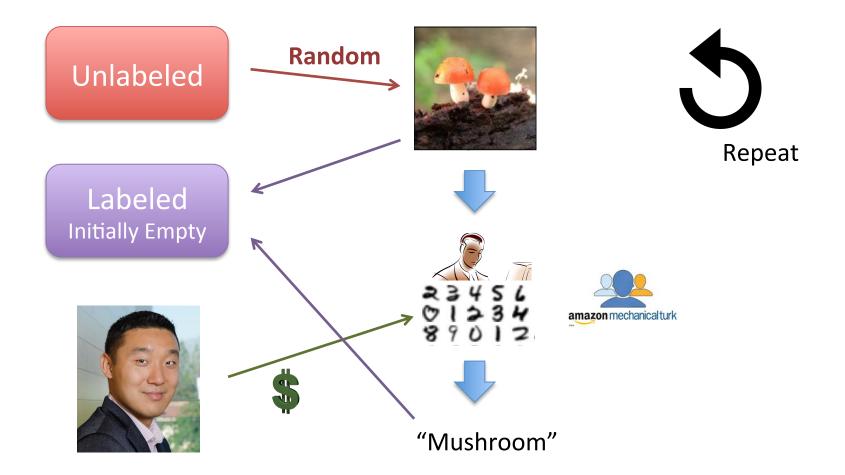
http://arxiv.org/pdf/1506.02106v4.pdf

### **Active Learning**

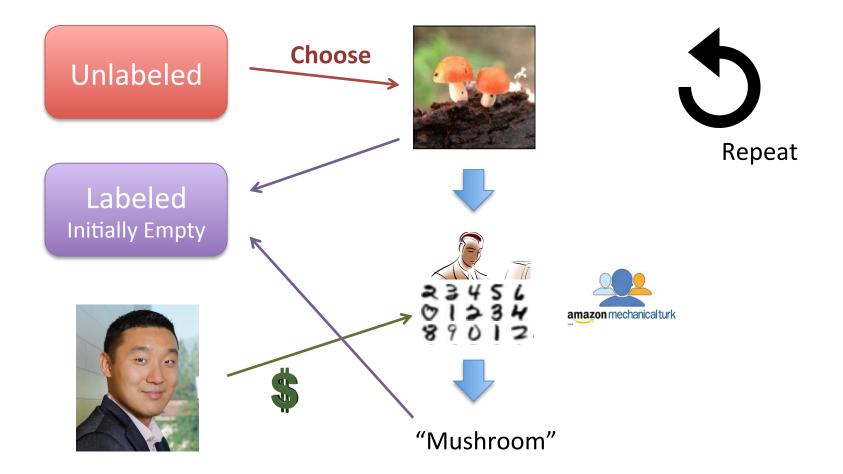
## Crowdsourcing



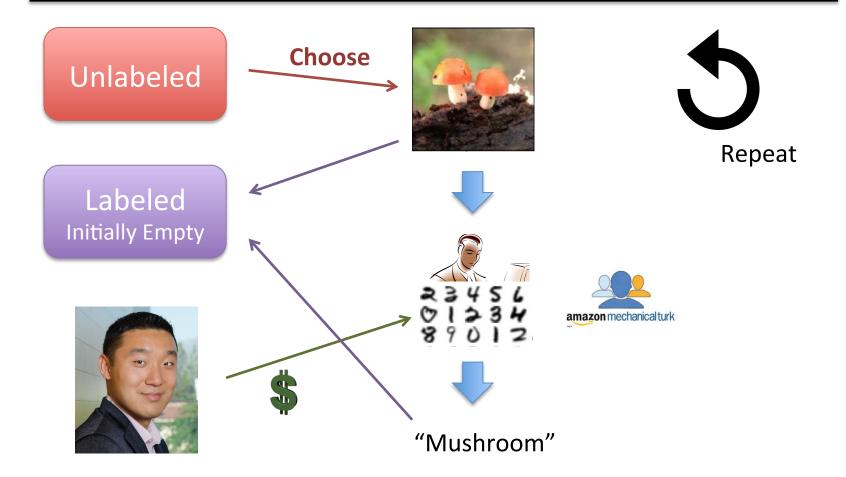
### **Passive Learning**



### **Active Learning**



### **Goal:** Maximize Accuracy with Minimal Cost

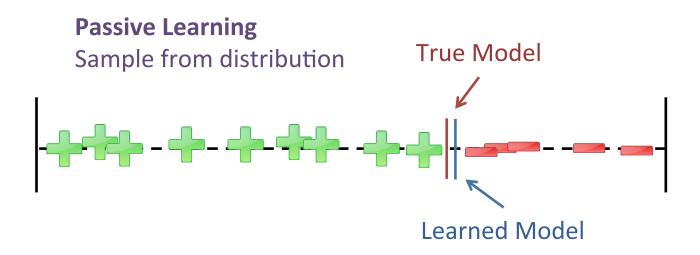


# **Comparison with Passive Learning**

- Conventional Supervised Learning is considered "Passive" Learning
- Unlabeled training set sampled according to test distribution
- So we label it at random
  - Very Expensive!

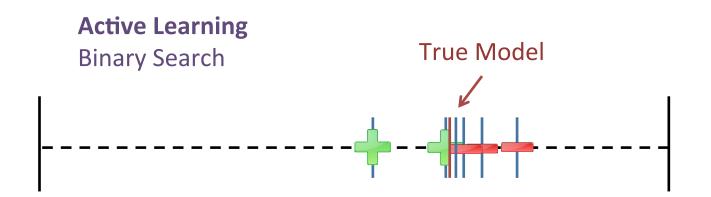
# Simple Example

- 1 feature
- Learn threshold function



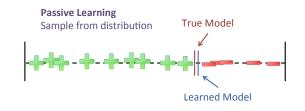
# Simple Example

- 1 feature
- Learn threshold function



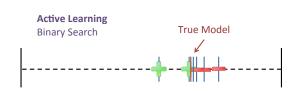
# **Comparison with Passive Learning**

- # samples to be within ε of true model
- Passive Learning:  $O\left(\frac{1}{\epsilon}\right)$



• Active Learning:

$$O\left(\log \frac{1}{2}\right)$$

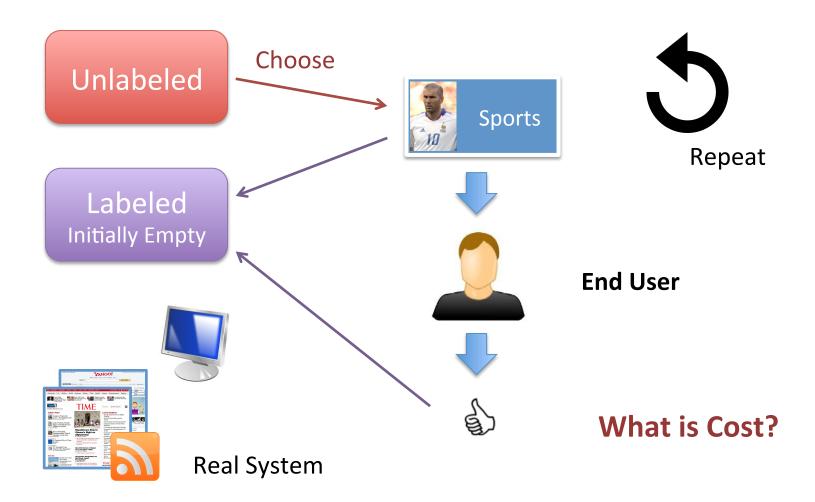


### **Multi-Armed Bandits**

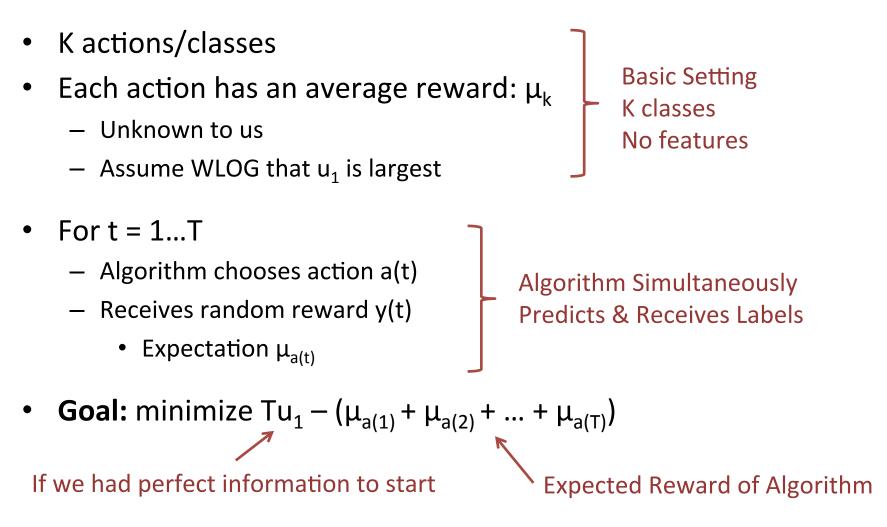
# **Problems with Crowdsourcing**

- Assumes you can label by proxy
  - E.g., have someone else label objects in images
- But sometimes you can't!
  - Personalized recommender systems
    - Need to ask the user whether content is interesting
  - Personalized medicine
    - Need to try treatment on patient
  - Requires actual target domain

### **Personalized Labels**



# **Formal Definition**









Average Likes

0	0	0	1	0





			0	
0	0	0	1	0





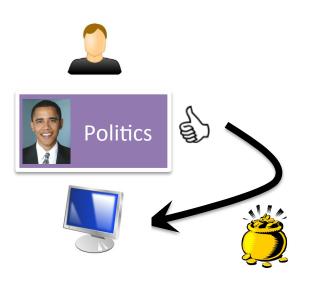


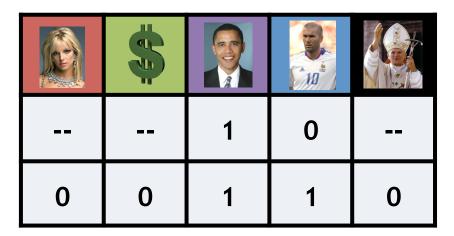


Average Likes

			0	
0	0	1	1	0









#### **Average Likes**

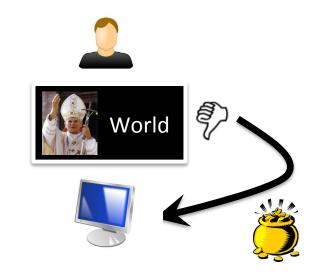




 Image: Second second



**Average Likes** 



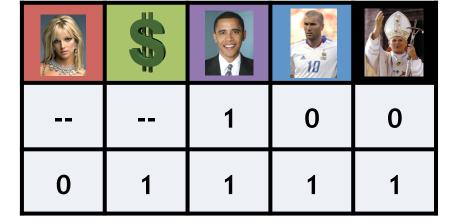


#### **Average Likes**

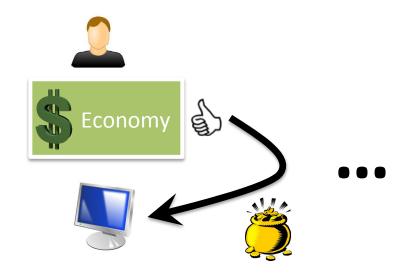


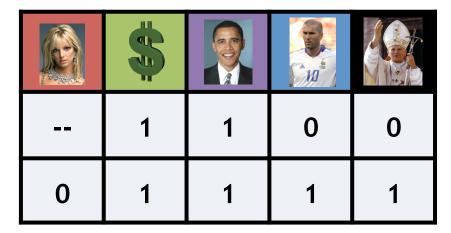


Average Likes









7

**Average Likes** 

### What should Algorithm Recommend?

#### Exploit:



#### **Explore:**





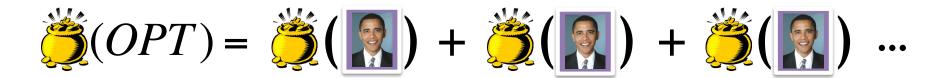


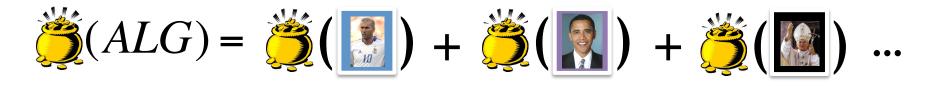
#### How to Optimally Balance Explore/Exploit Tradeoff? Characterized by the Multi-Armed Bandit Problem

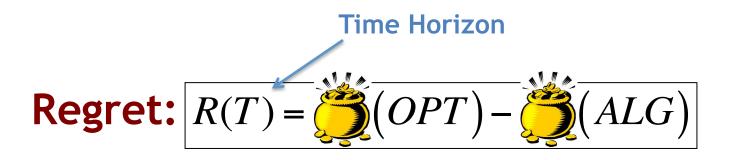
**Average Likes** 

	0.44	0.4	0.33	0.2
0	25	10	15	20





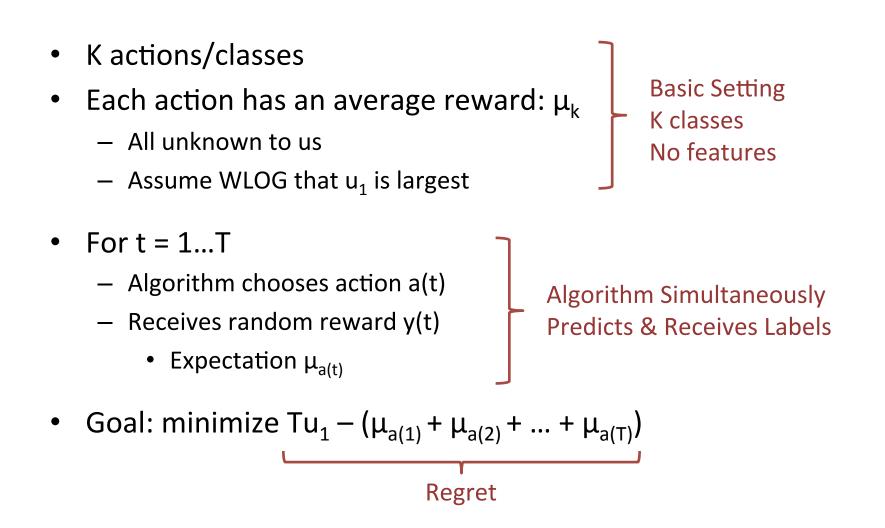




- Opportunity cost of not knowing preferences
- "no-regret" if  $R(T)/T \rightarrow 0$

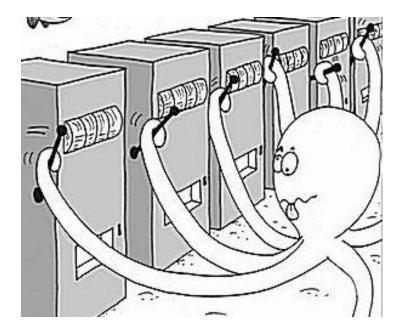
- Efficiency measured by convergence rate

### Recap: The Multi-Armed Bandit Problem



# The Motivating Problem

• Slot Machine = One-Armed Bandit



#### Each Arm Has Different Payoff

#### • **Goal:** Minimize regret From pulling suboptimal arms

http://en.wikipedia.org/wiki/Multi-armed\_bandit

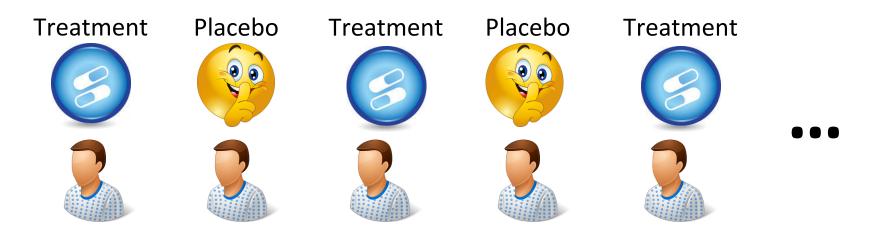
### **Implications of Regret**

**Regret:** 
$$R(T) = \bigotimes(OPT) - \bigotimes(ALG)$$

- If R(T) grows linearly w.r.t. T:
  - Then  $R(T)/T \rightarrow constant > 0$
  - I.e., we converge to predicting something suboptimal
- If R(T) is sub-linear w.r.t. T:
  - Then  $R(T)/T \rightarrow 0$
  - I.e., we converge to predicting the optimal action

# **Experimental Design**

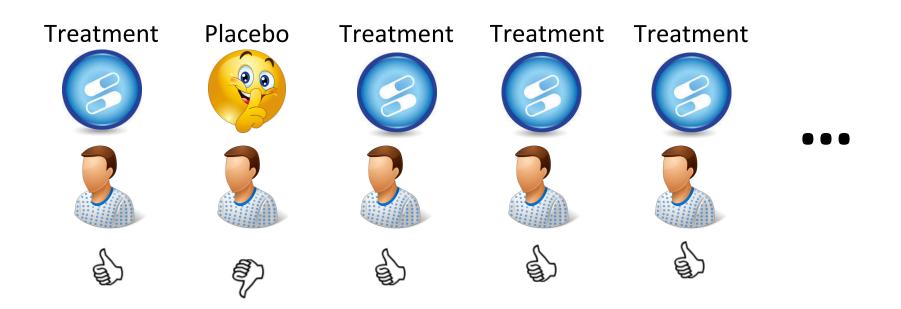
- How to split trials to collect information
- Static Experimental Design
  - Standard practice
  - (pre-planned)



http://en.wikipedia.org/wiki/Design\_of\_experiments

# Sequential Experimental Design

Adapt experiments based on outcomes



### Sequential Experimental Design Matters



Monica Almeida/The New York Times, left

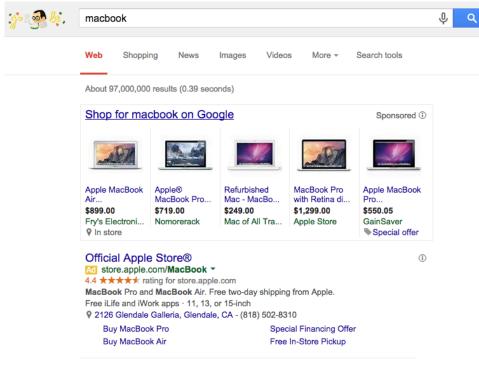
Two Cousins, Two Paths Thomas McLaughlin, left, was given a promising experimental drug to treat his lethal skin cancer in a medical trial; Brandon Ryan had to go without it.

http://www.nytimes.com/2010/09/19/health/research/19trial.html

# Sequential Experimental Design

- MAB models sequential experimental design!
   basic
- Each treatment has hidden expected value
  - Need to run trials to gather information
  - "Exploration"
- In hindsight, should always have used treatment with highest expected value
- Regret = opportunity cost of exploration

### **Online Advertising**



#### Largest Use-Case of Multi-Armed Bandit Problems

#### Apple - MacBook Pro

https://www.apple.com/macbook-pro/ Apple Inc. With the latest-generation Intel processors, all-new graphics, and faster flash storage, MacBook Pro moves further ahead in power and performance.

Buy MacBook Pro with Retin... With top-of-the-line Intel processors, HD graphics, and ... Compare Mac notebooks MacBook Air or iMac. No matter which Mac you choose, you're ...

More results from apple.com »

65

### The UCB1 Algorithm

http://homes.di.unimi.it/~cesabian/Pubblicazioni/ml-02.pdf

# **Confidence Intervals**

- Maintain Confidence Interval for Each Action
  - Often derived using Chernoff-Hoeffding bounds (\*\*)



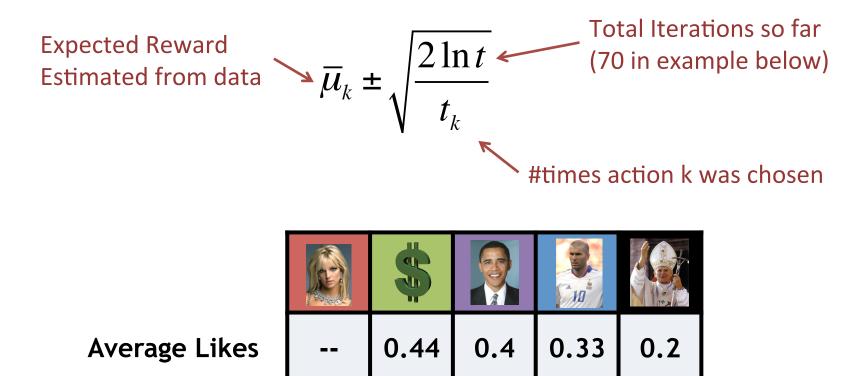




Average Likes		0.44	0.4	0.33	0.2
# Shown	0	25	10	15	20

\*\* http://www.cs.utah.edu/~jeffp/papers/Chern-Hoeff.pdf
http://en.wikipedia.org/wiki/Hoeffding%27s\_inequality

# UCB1 Confidence Interval



# Shown

http://homes.di.unimi.it/~cesabian/Pubblicazioni/ml-02.pdf

# The UCB1 Algorithm

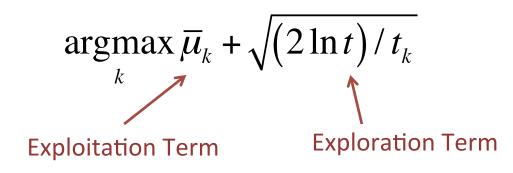
- At each iteration
  - Play arm with highest **Upper Confidence Bound**:

$$\operatorname*{argmax}_{k} \overline{\mu}_{k} + \sqrt{\left(2\ln t\right)/t_{k}}$$

				-ei 11	
Average Likes		0.44	0.4	0.33	0.2
# Shown	0	25	10	15	20

http://homes.di.unimi.it/~cesabian/Pubblicazioni/ml-02.pdf

Balancing Explore/Exploit "Optimism in the Face of Uncertainty"



				ee 11	
Average Likes	-	0.44	0.4	0.33	0.2
# Shown	0	25	10	15	20

http://homes.di.unimi.it/~cesabian/Pubblicazioni/ml-02.pdf

# Analysis (Intuition)

$$a(t+1) = \operatorname*{argmax}_{k} \overline{\mu}_{k} + \sqrt{(2\ln t)/t_{k}}$$

With high probability (\*\*): Upper Confidence Bound of Best Arm  

$$\overline{\mu}_{a(t+1)} + \sqrt{(2\ln t)/t_{a(t+1)}} \ge \overline{\mu}_1 + \sqrt{(2\ln t)/t_1} \ge \mu_1$$
Value of Best Arm

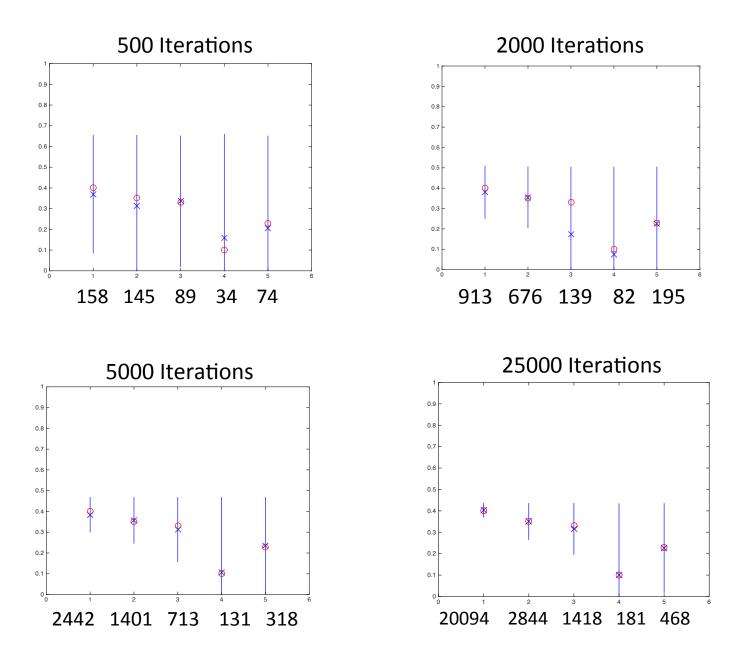
$$\mu_{a(t+1)} \geq \overline{\mu}_{a(t+1)} - \sqrt{\left(2\ln t\right)/t_{a(t+1)}}$$

The true value is greater than the lower confidence bound.

$$\mu_1 - \mu_{a(t+1)} \le 2\sqrt{\left(2\ln t\right)/t_{a(t+1)}}$$

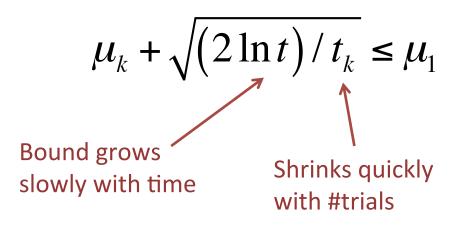
Bound on regret at time t+1

\*\* Proof of Theorem 1 in http://homes.di.unimi.it/~cesabian/Pubblicazioni/ml-02.pdf



### How Often Sub-Optimal Arms Get Played

• An arm never gets selected if:



- The number of times selected:
  - Prove using Hoeffding's Inequality

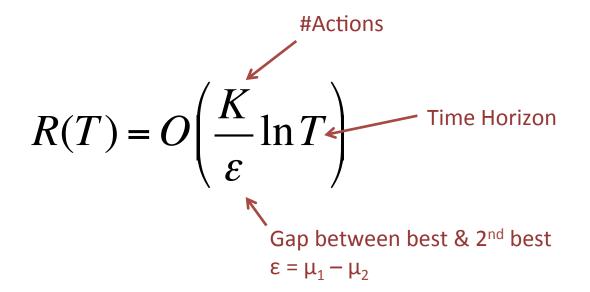
$$I: O\left(\frac{\ln t}{\left(\mu_1 - \mu_k\right)^2}\right)$$

1

# **Regret Guarantee**

• With high probability:

– UCB1 accumulates regret at most:



Theorem 1 in http://homes.di.unimi.it/~cesabian/Pubblicazioni/ml-02.pdf

# Extensions

- Contextual Bandits

   Features of environment
- Dependent-Arms Bandits

   Features of actions/classes
- Dueling Bandits
  - Learn from pairwise feedback

# Recap: MAB & UCB1

Interactive setting

- Receives reward/label while making prediction

• Must balance explore/exploit

- Sub-linear regret is good
  - Average regret converges to 0

## **Reinforcement Learning**

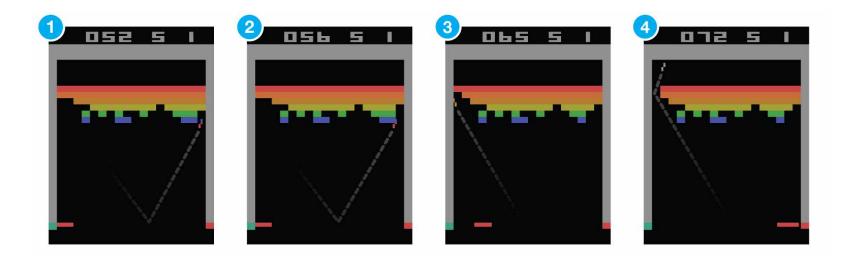
# **Actions Impact State**

- In MAB:
  - Actions do not impact state
  - Constant reward function
- Reinforcement Learning
  - Actions effect state you're in
  - Reward function depends on state

## Video Demo (Deep Reinforcement Learning for Atari)

https://www.youtube.com/watch?v=iqXKQf2BOSE

### What is State?



#### Reward of each action varies depending on state!

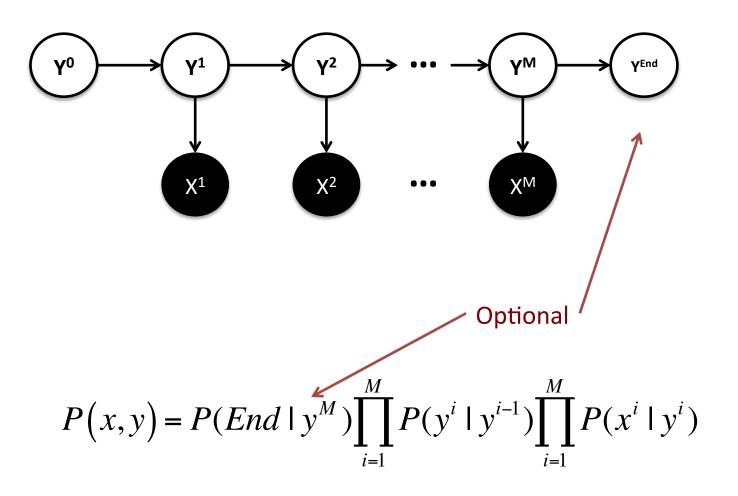
#### Action at current state impacts future states!

#### Much harder to do exploration!

http://www.nature.com/nature/journal/v518/n7540/pdf/nature14236.pdf

## **Non-Convex Optimization**

### **Recall: Hidden Markov Models**



# **Recall: EM Algorithm for HMMs**

- If we had y's → max likelihood.
- If we had (A,O) → predict y's
- 1. Initialize A and O arbitrarily

**Chicken vs Egg!** 

**Expectation Step** 

- 2. Predict prob. of y's for each training x
- 3. Use y's to estimate new (A,O) Maximization Step

4. Repeat back to Step 1 until convergence

http://en.wikipedia.org/wiki/Baum%E2%80%93Welch algorithm

Non-Convex Optimization Problem! Converges to local optimum.

- If we had y's → max likelihood.
- If we had (A,O) → predict y's
- 1. Initialize A and O arbitrarily

Chicken vs Egg!

**Expectation Step** 



http://en.wikipedia.org/wiki/Baum%E2%80%93Welch\_algorithm

Inspiration from Dimensionality Reduction

• Find best rank K approximation to Y:

$$\underset{U \in \mathbb{R}^{NxK}, V \in \mathbb{R}^{MxK}}{\operatorname{argmin}} \left\| Y - UV^T \right\|_2^2$$

- Non-convex optimization problem!
   Due to non-convex feasible region
- But optimally solved via SVD!

# Spectral Learning of HMMs

Want to Estimate:

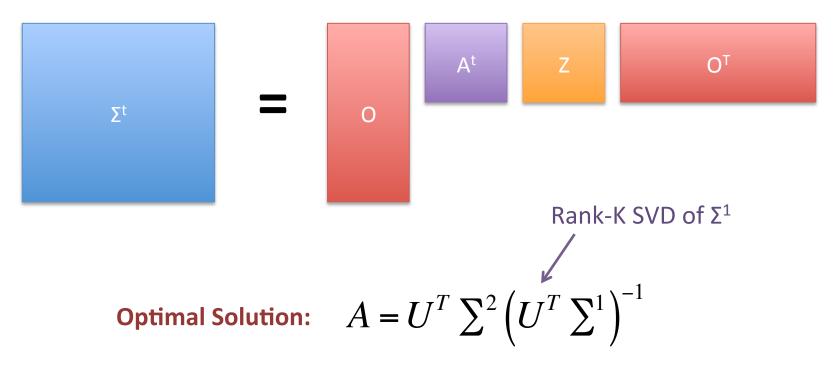
$$P(y^{j} | y^{j-1}) = A$$
  $P(x^{j} | y^{j}) = O$ 

Treat each x<sup>j</sup> and y<sup>j</sup> as indicator vector

$$\sum^{t} = E\left[x^{j+t}\left(x^{j}\right)^{T}\right] = E\left[E\left[x^{j+t}\left(x^{j}\right)^{T}\middle|y^{j}\right]\right]$$
$$= E\left[E\left[x^{j+t}\middle|y^{j}\right]E\left[\left(x^{j}\right)^{T}\middle|y^{j}\right]\right]$$
and y<sup>j</sup>  
ector
$$= E\left[\left(OA^{t}ky^{j}\right)\left(Oy^{j}\right)^{T}\right]$$
$$= OA^{t}E\left[y^{j}\left(y^{j}\right)^{T}\right]O^{T}$$
$$= OA^{t}ZO^{T}$$

http://www.cs.cmu.edu/~ggordon/spectral-learning/

# Spectral Learning of HMMs



(requires a lot of data)

http://www.cs.cmu.edu/~ggordon/spectral-learning/

# ...and many more topics!

- Probabilistic Models
- Representation Learning
  - Deep learning is the most visible example
- Causal Reasoning
- ML + Game Theory
- ML + Systems
  - Large Scale Machine Learning
- Etc ...

# CS 159

- Special Topics in Machine Learning
  - Taught Every Spring Term
  - Topics Rotate

### • Next Term:

- "Online Learning, Interactive Machine Learning, and Learning from Human Feedback"
- Paper Reading & Presenting + Final Project

- Graded on participation and final project