Caltech

Machine Learning & Data Mining

CS/CNS/EE 155

Lecture 17:

Survey of Advanced Topics

What We Covered

Topic Overview

Supervised Learning

Linear Models

Overfitting

Loss Functions

Non-Linear Models

Learning Algorithms & Optimization

Probabilistic Modeling

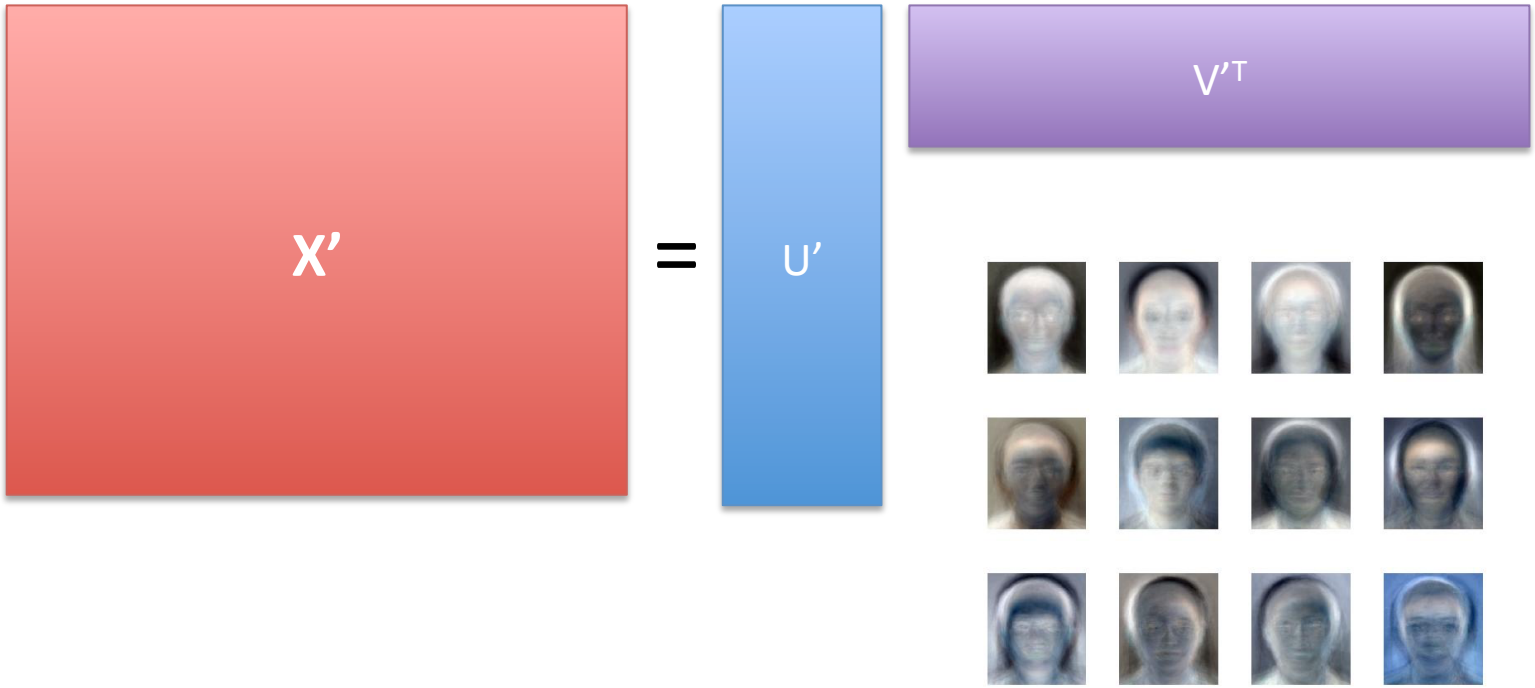
Unsupervised Learning

Basic Supervised Learning

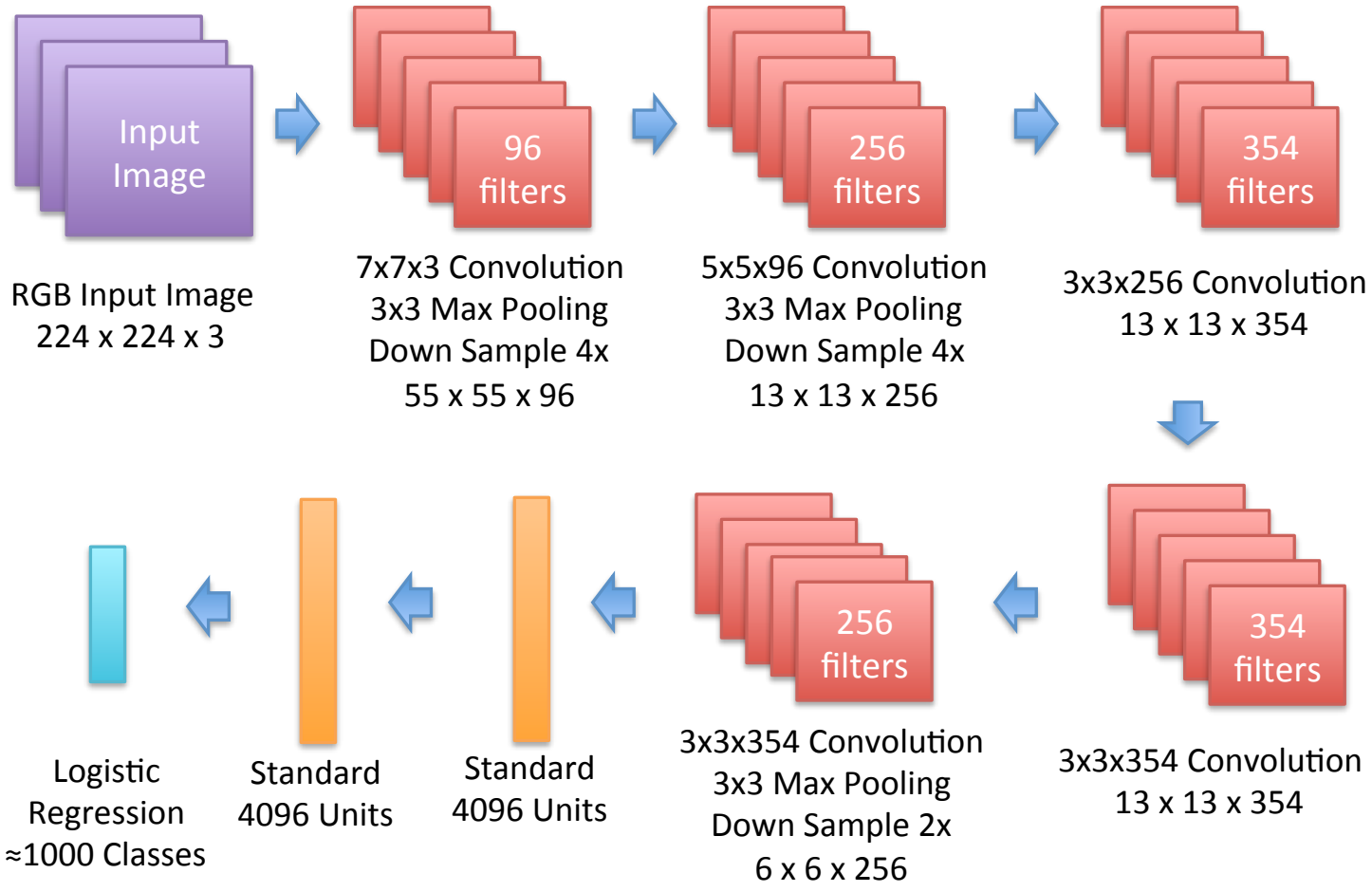
- Training Data: $S = \{(x_i, y_i)\}_{i=1}^{N}$ $x \in R^D$ $y \in \{-1, +1\}$
- Model Class: $f(x \mid w, b) = w^T x - b$ **Linear Models**
- Loss Function: $L(a, b) = (a - b)^2$ **Squared Loss**
- Learning Objective: $\underset{w,b}{\operatorname{argmin}} \sum_{i=1}^{N} L\left(y_i, f(x_i \mid w, b)\right)$

Optimization Problem

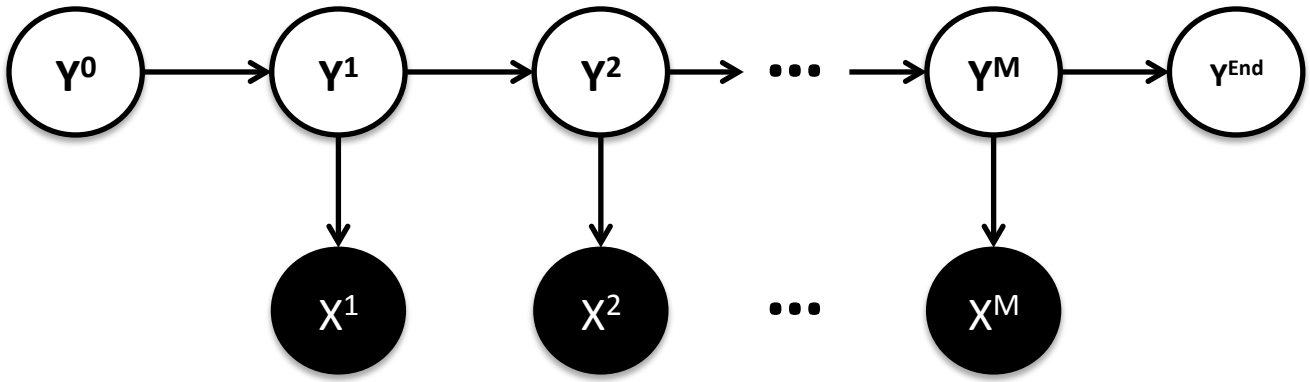
Basic Unsupervised Learning



Deep Learning



Sequence Prediction



Simple Optimization Algorithms

- Stochastic Gradient Descent

- EM algorithm (for HMMs)

Other Basic Concepts

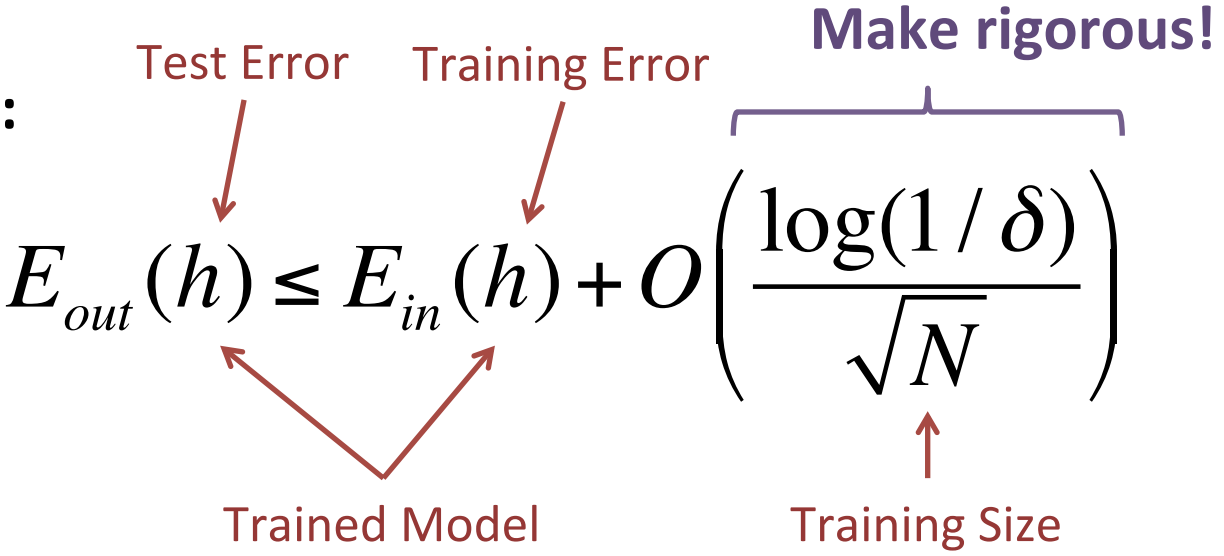
- Cross Validation
- Overfitting
- Bias-Variance Tradeoff

Learning Theory

Generalization Bounds

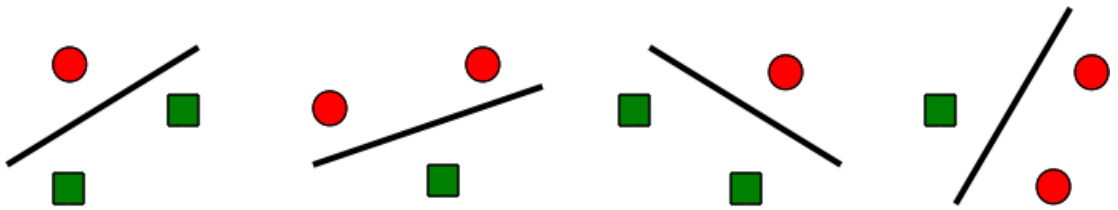
- Formal characterization of overfitting
- Example result:

With Prob. ≥ 1-δ :



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.

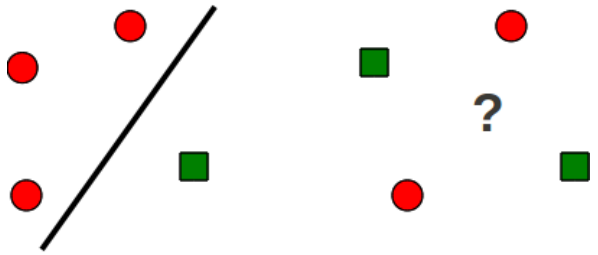


In 2D, any 3 points can always be shattered by linear models!

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. ≥ 1-δ :

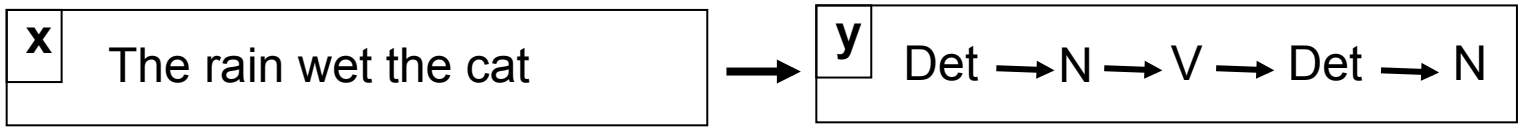
$$E_{out}(h) \leq E_{in}(h) + O\left(\sqrt{\frac{VC(H)\log\left(\frac{2N}{VC(H)}+1\right)+\log\left(\frac{1}{\delta}\right)}{N}}\right)$$

Structured Prediction

Topic of CS159

Examples of Complex Output Spaces

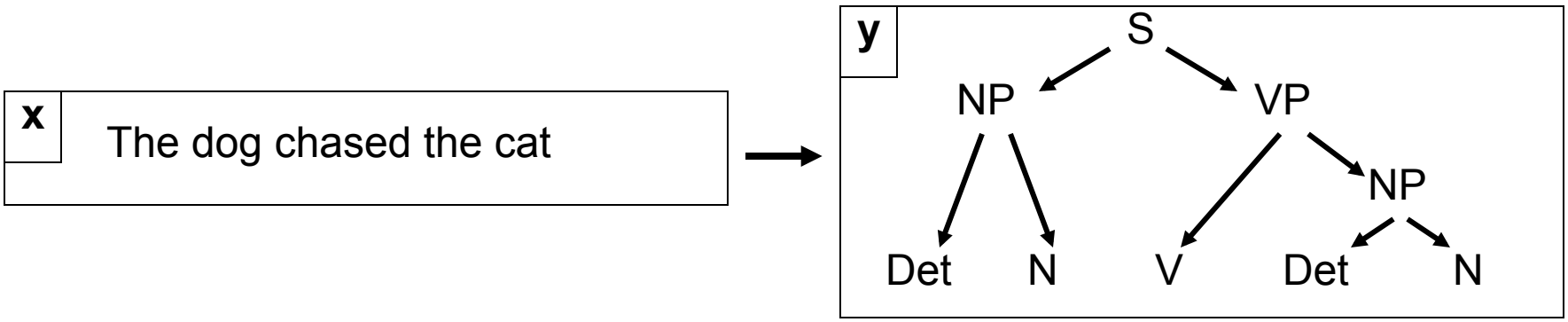
- Part-of-Speech Tagging
  - Given a sequence of words *x*, predict sequence of tags *y*.
  - Dependencies from tag-tag transitions in Markov model.



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

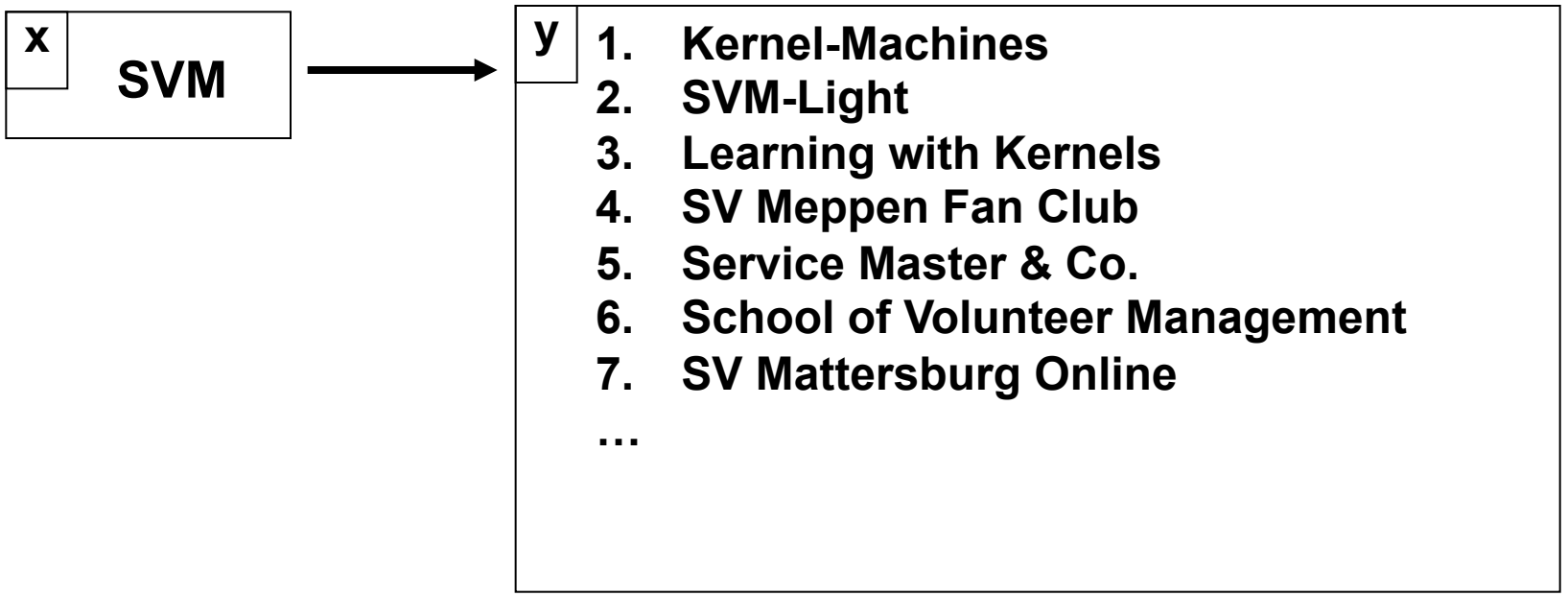
Examples of Complex Output Spaces

- 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.

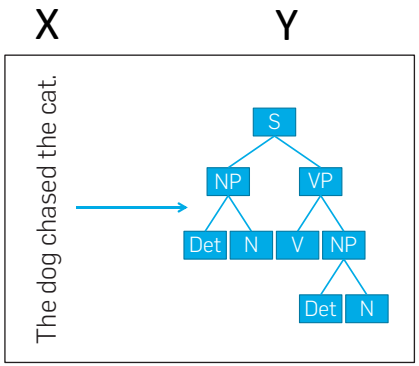


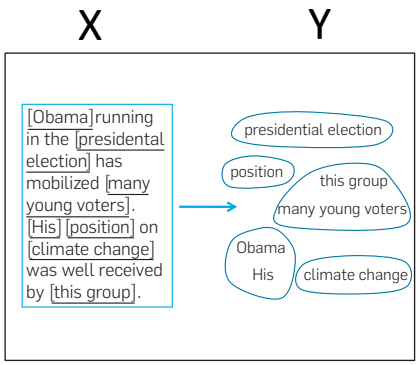
Examples of Complex Output Spaces

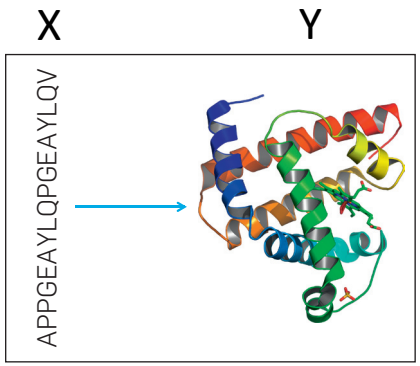
- Information Retrieval
  - Given a query x, predict a ranking *y*.
  - Dependencies between results (e.g. avoid redundant hits)
  - Loss function over rankings (e.g. Average Precision)

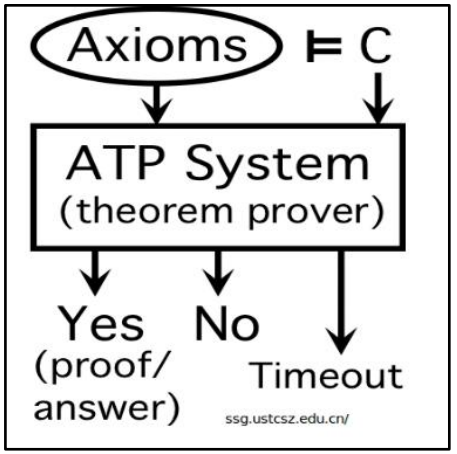


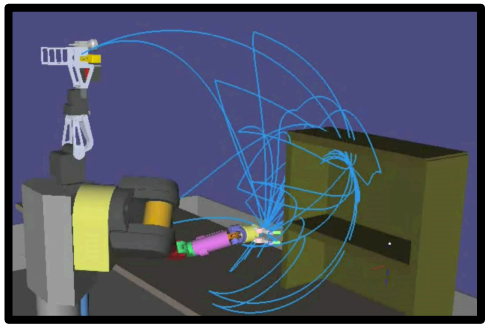
Structured Prediction

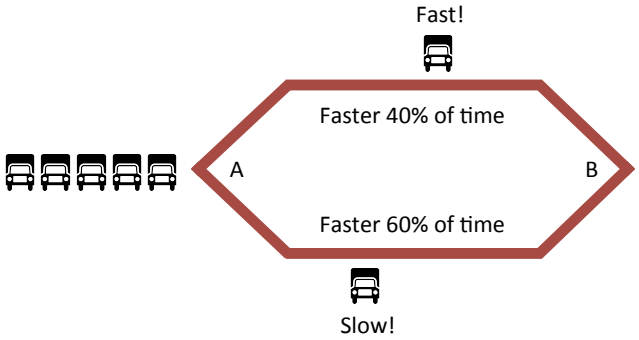


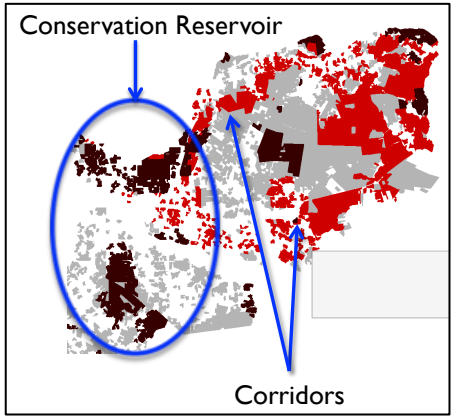












General Formula
(Linear Models)

- 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:

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

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

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

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

Examples

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

1st Order Sequences:

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

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

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

Solve using Viterbi!

Examples

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

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

Integer Linear Program:

$Y(\mathbf{x})$ = Feasible settings of **y**

Each $y^j \in \{0,1\}$

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

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

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

Structured Prediction Learning Problem

- **Efficient Inference/Prediction**

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

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

- **Efficient Learning/Training**
  - Learn parameters *w* from training data $\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1..N}$
  - Structural SVM: Hinge Loss Minimization
  - Conditional Random Fields: Log Loss Minimization
  - Structured Perceptron, etc…

Perceptron Learning Algorithm

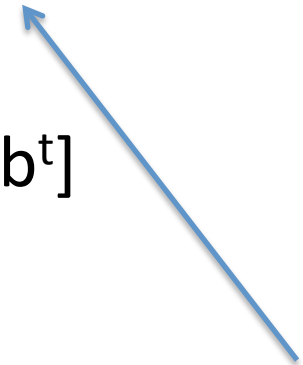
- $w^1 = 0, b^1 = 0$
- For t = 1 ….
  - Receive example (x,y)
  - If $h(x|w^t) = y$
    - $[w^{t+1}, b^{t+1}] = [w^t, b^t]$
  - Else
    - $w^{t+1} = w^t + yx$
    - $b^{t+1} = b^t + y$

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

Training Set:

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

$$y \in \{+1, -1\}$$



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

Structured Perceptron

- $w^1 = 0$
- For t = 1 ….
  - Receive example (x,y)
  - If $h(x|w^t) = y$
    - $w^{t+1} = w^t$
  - Else
    - $w^{t+1} = w^t + \Psi(x,y)$

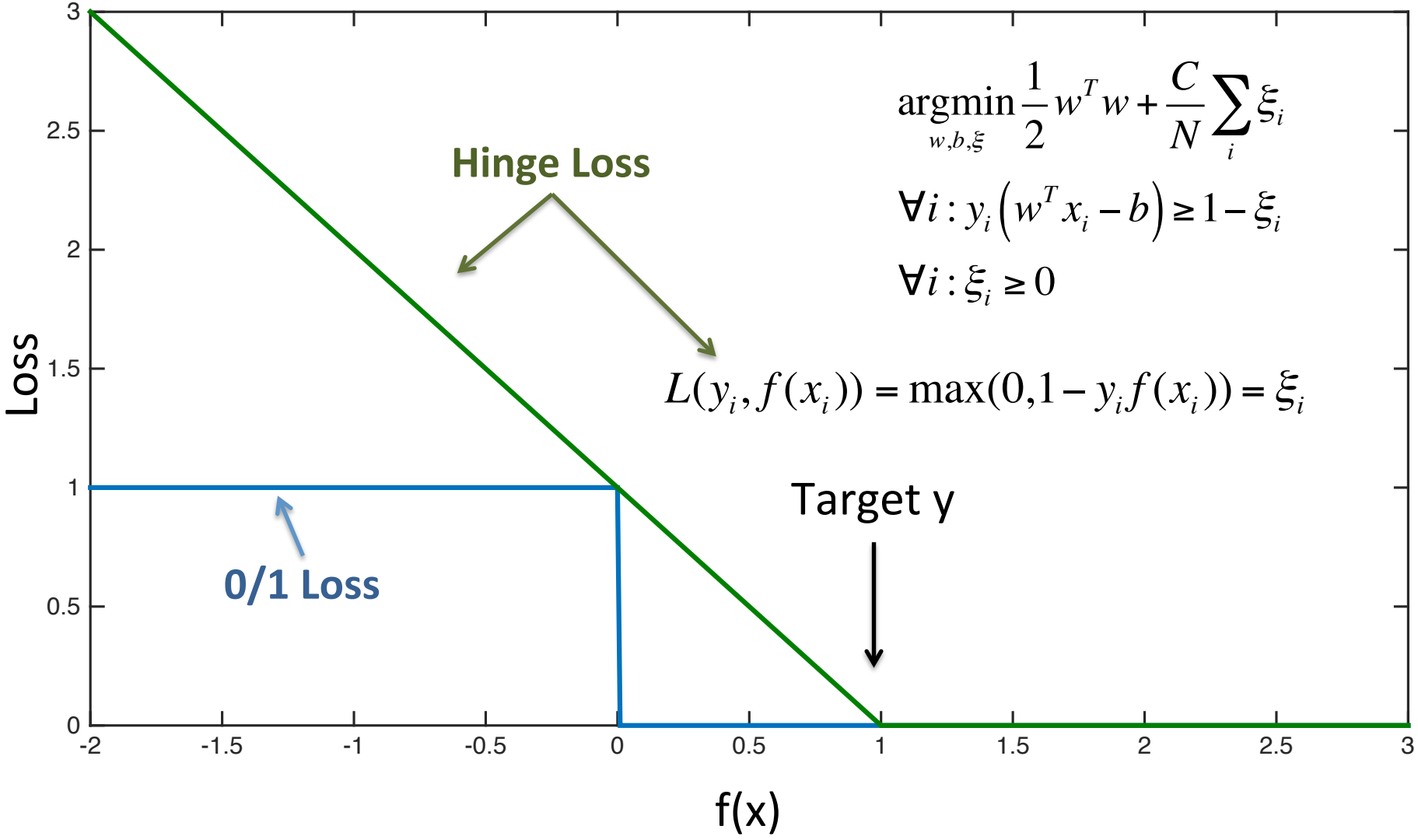
$$h(x \mid w) = \underset{y'}{\operatorname{argmax}}\, w^T \Psi(x, y')$$

Training Set:

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

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

Conventional SVMs



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**.

$$\forall i, \forall \mathbf{y}' \neq \mathbf{y}^{(i)} : \quad w^T \Psi(\mathbf{y}^{(i)}, \mathbf{x}^{(i)}) \geq w^T \Psi(\mathbf{y}', \mathbf{x}^{(i)}) + \Delta_i(\mathbf{y}') - \xi_i$$

Score(y$^{(i)}$) Score(y') Loss(y') Slack

http://www.cs.cornell.edu/People/tj/svm_light/svm_struct.html

Interpreting Constraints

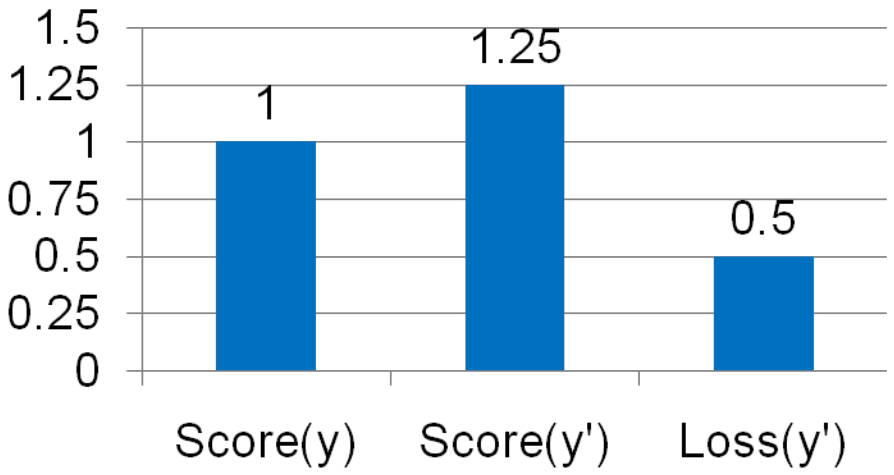
$$\frac{1}{2}w^2 + \frac{C}{N}\sum_i \xi_i$$

$$\forall i, \forall \mathbf{y}' \neq \mathbf{y}^{(i)}: \quad w^T\Psi(\mathbf{y}^{(i)}, \mathbf{x}^{(i)}) \geq w^T\Psi(\mathbf{y}', \mathbf{x}^{(i)}) + \Delta_i(\mathbf{y}') - \xi_i$$

Score($y^{(i)}$) Score(y') Loss(y') Slack

Suppose for incorrect **y'** :

Then: $\xi_i \geq 0.75 \geq \Delta(\mathbf{y}')$



http://www.cs.cornell.edu/People/tj/svm_light/svm_struct.html

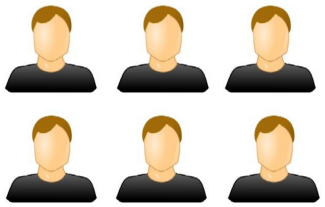
Sample Research Questions

- Scale
  - Predicting over millions of variables
- Structured Representation Learning
  - Deep learning for structured outputs?
- Cost of labeling

Crowdsourcing

Acquiring Labels from Annotators

amazon mechanical turk beta



How Reliable are Annotators?

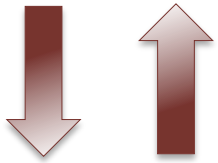
- If we knew what the labels were
  - Can judge workers on label quality
- If we knew who the good workers were
  - Can create labels from their annotations
- **Chicken and egg problem!**

Worker Reliability as Latent Variable

- Let z_m denote the reliability of worker m

Estimated label

$$y_i = \frac{1}{\sum_m z_m} \sum_m y_{im} z_m$$



$$z_m = \frac{1}{N} \sum_i L(y_i, y_{im})$$

Differing Ambiguities Across Tasks

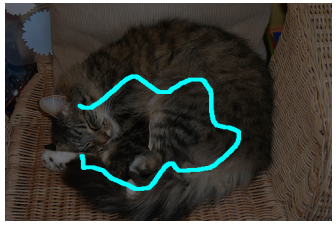
- Often collecting annotations for many tasks
- Some tasks are harder than others
- How many labels to collect for each task?

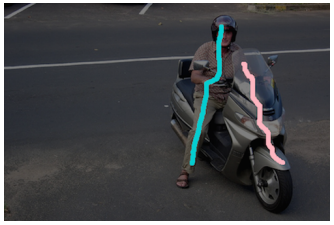
Structured Annotations

Full supervision

Image-level supervision

Point-level supervision

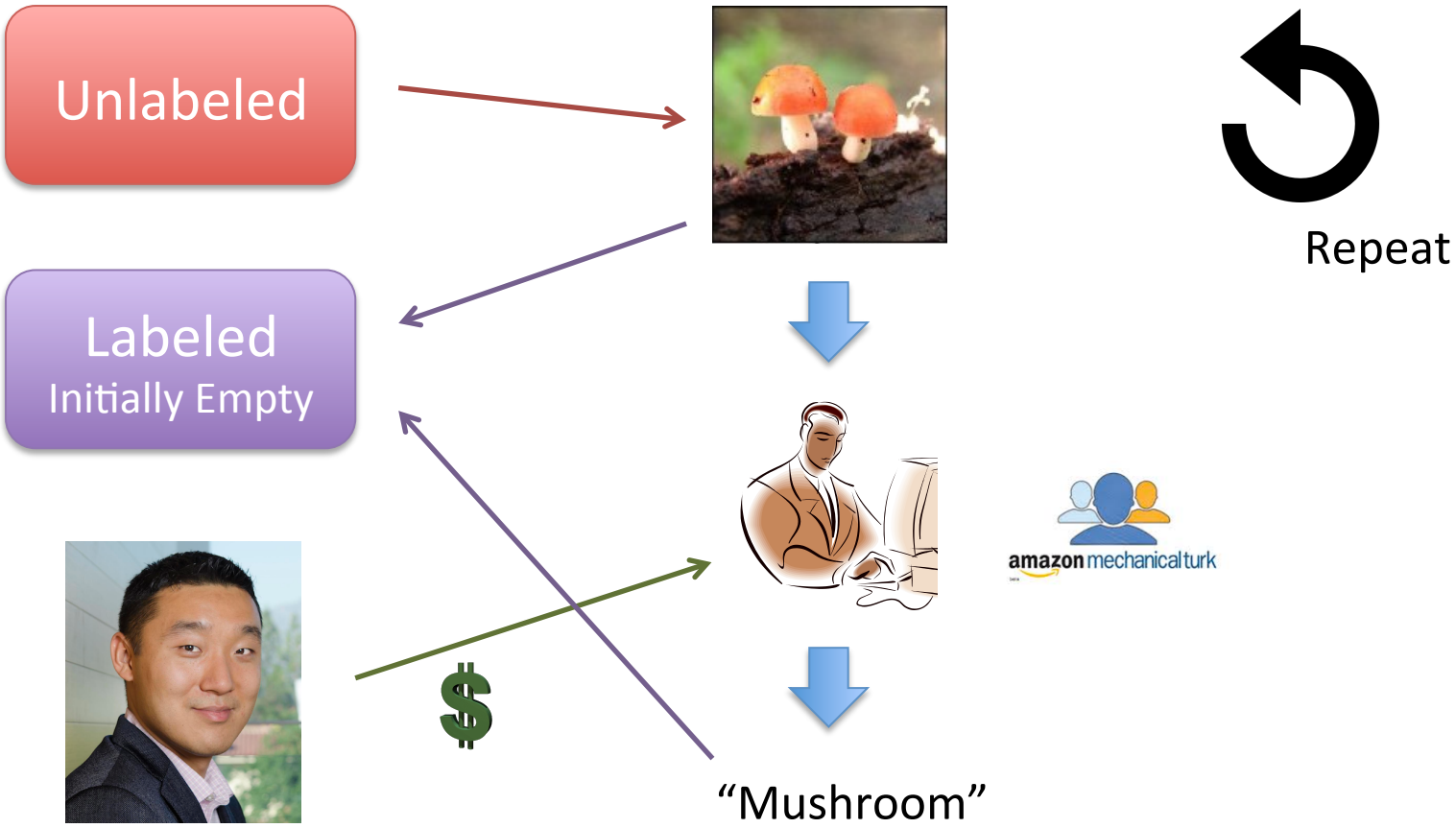




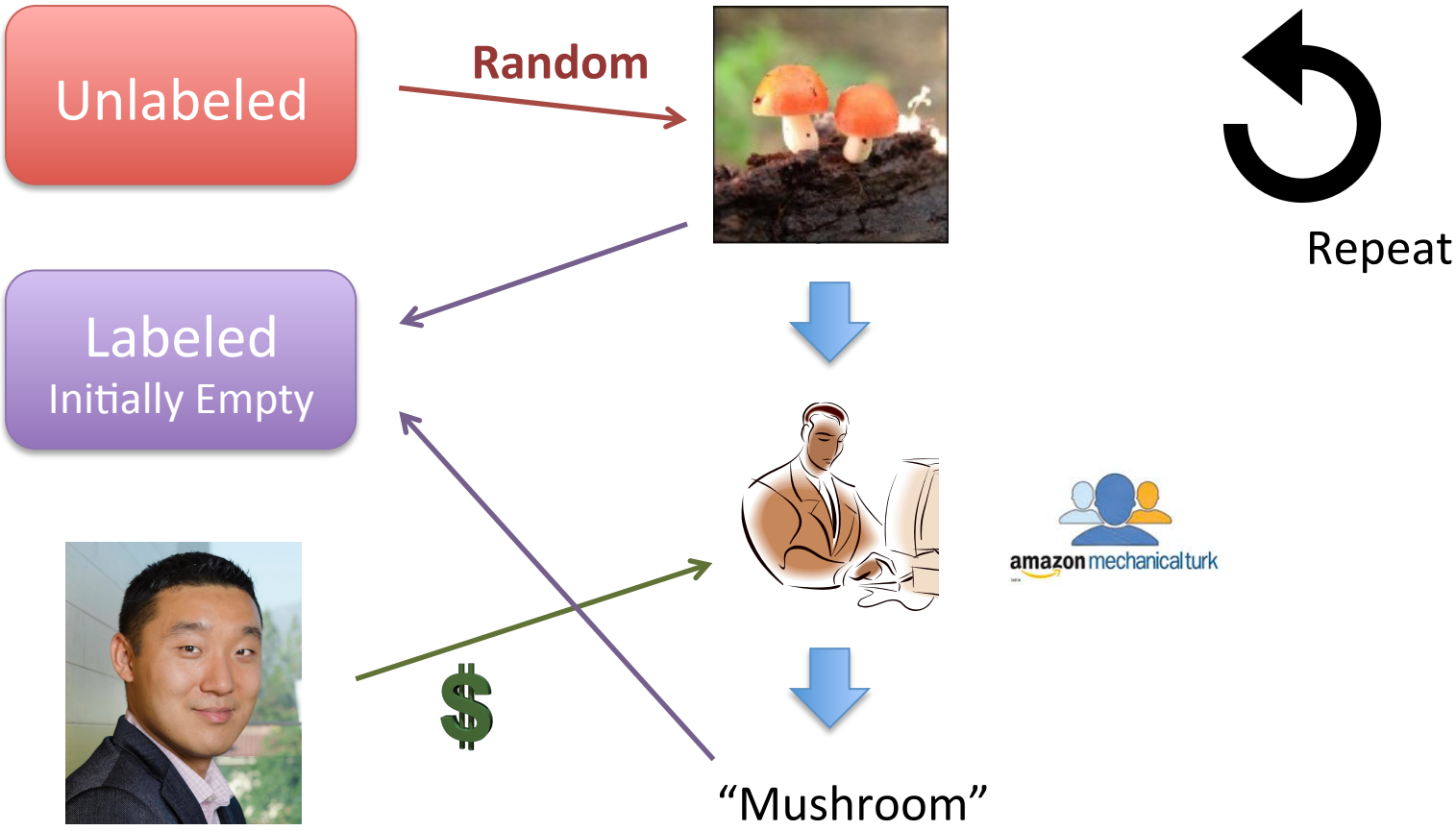
http://arxiv.org/pdf/1506.02106v4.pdf

Active Learning

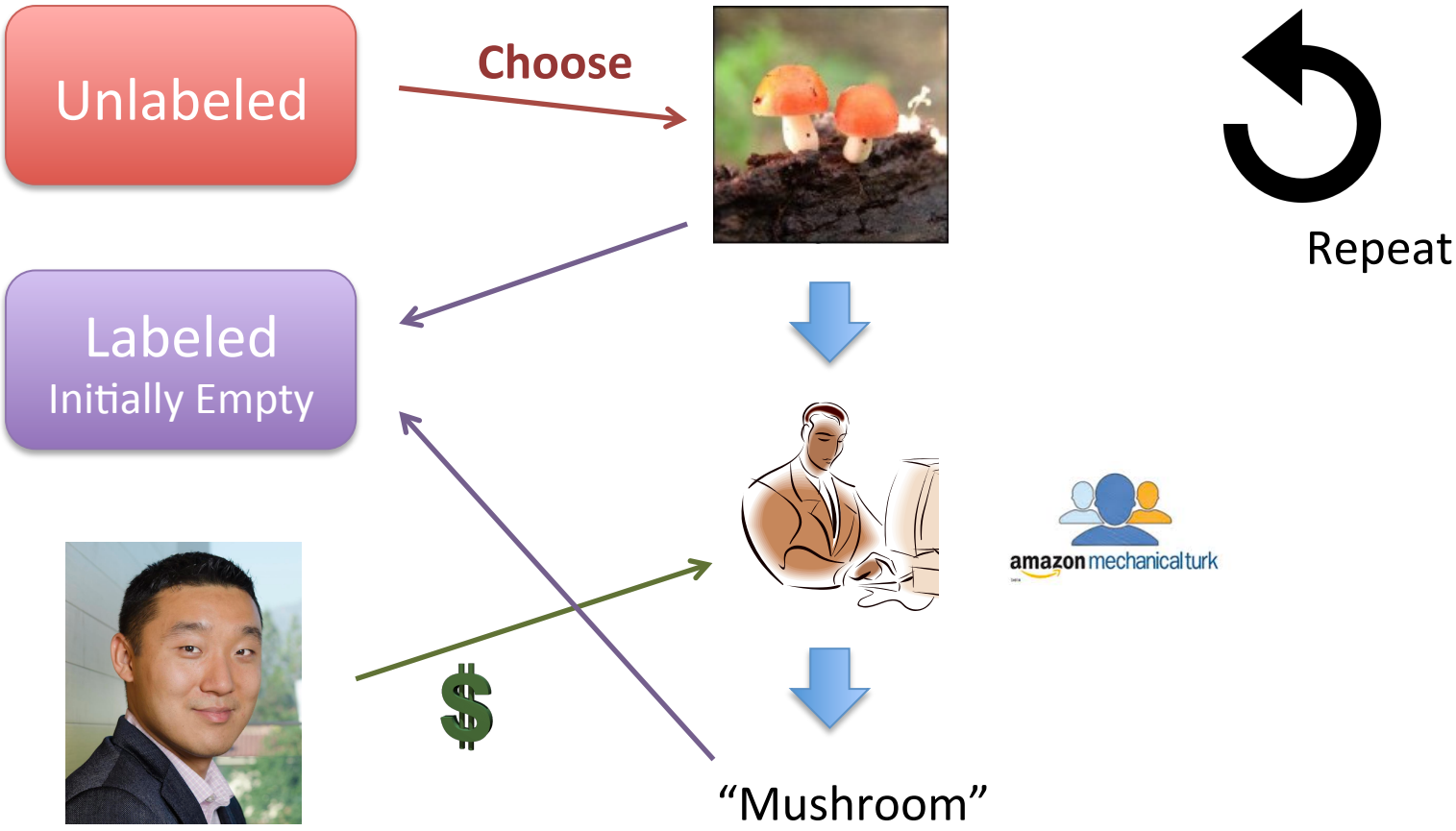
Crowdsourcing



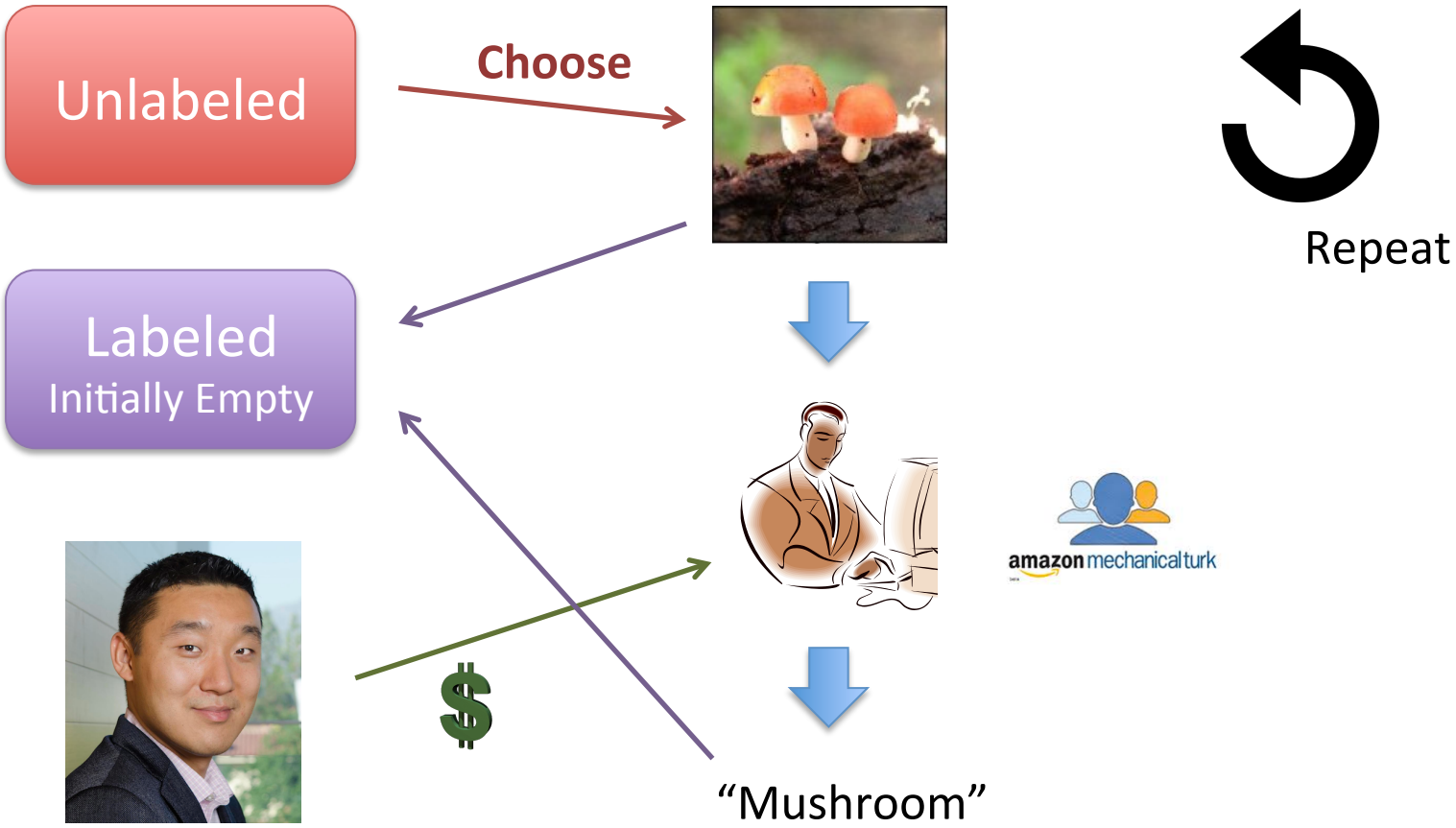
Passive Learning



Active Learning



Goal: Maximize Accuracy with Minimal Cost



Comparison with Passive Learning

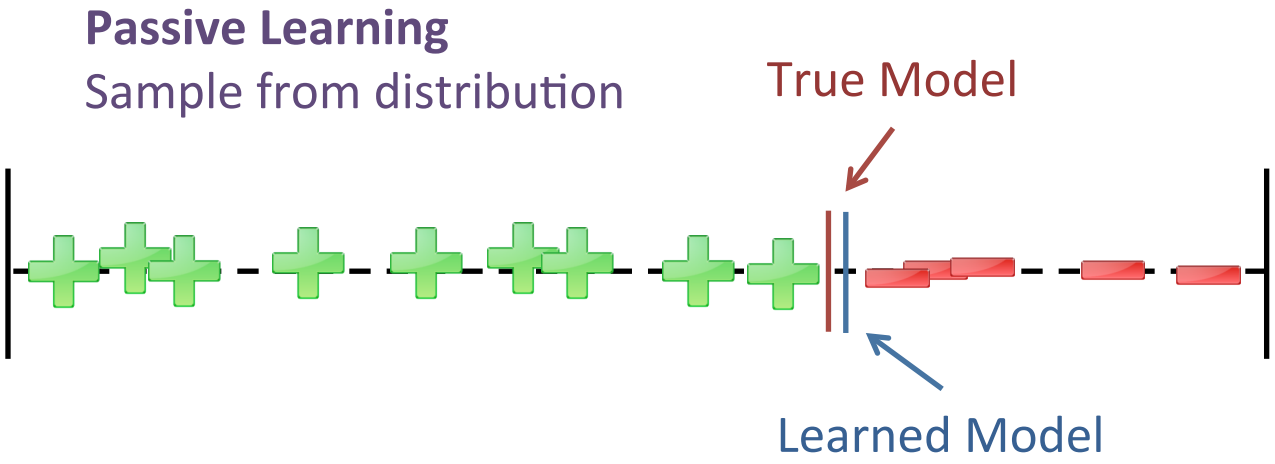
- Conventional Supervised Learning is considered "Passive" Learning

- Unlabeled training set sampled according to test distribution

- So we label it at random
  - **Very Expensive!**

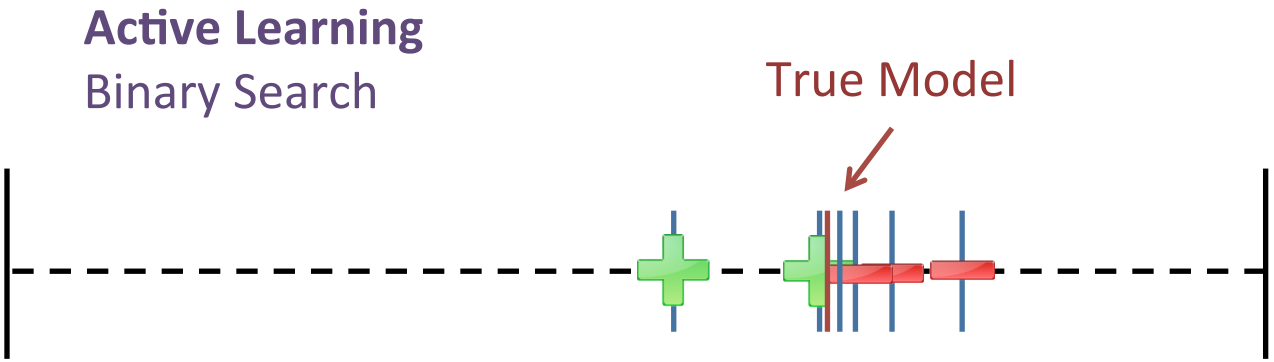
Simple Example

- 1 feature
- Learn threshold function



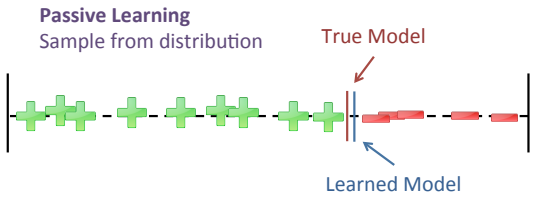
Simple Example

- 1 feature
- Learn threshold function

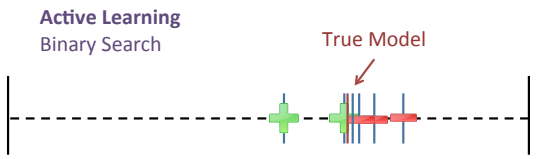


Comparison with Passive Learning

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



- Active Learning: $O\left(\log\frac{1}{\varepsilon}\right)$

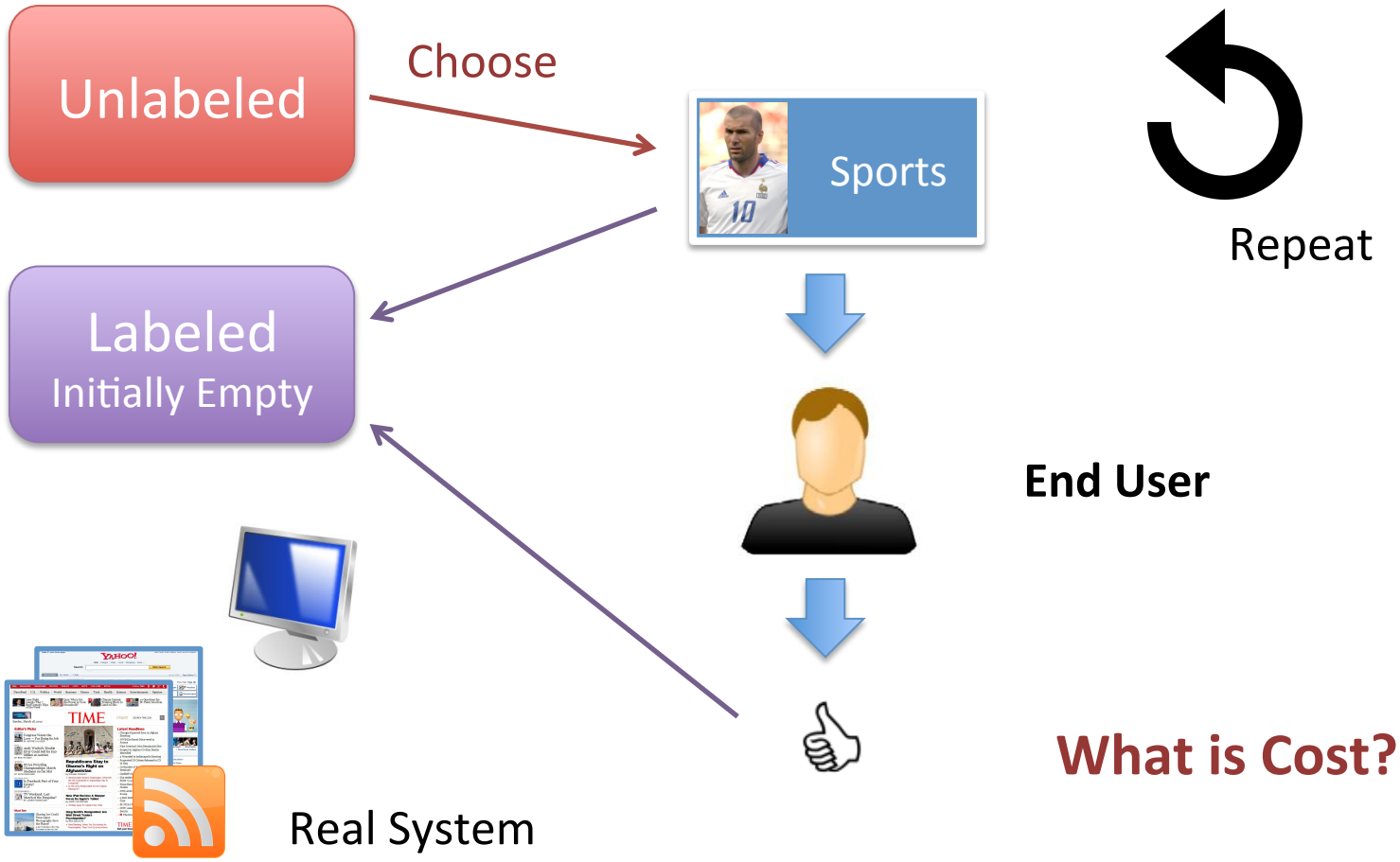


Multi-Armed Bandits

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

- K actions/classes
- Each action has an average reward: μ_k
  - Unknown to us
  - Assume WLOG that u_1 is largest

Basic Setting
K classes
No features

- For t = 1…T
  - Algorithm chooses action a(t)
  - Receives random reward y(t)
    - Expectation $\mu_{a(t)}$

Algorithm Simultaneously
Predicts & Receives Labels

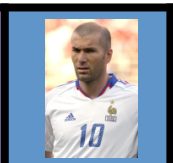
- **Goal:** minimize $Tu_1 - (\mu_{a(1)} + \mu_{a(2)} + \ldots + \mu_{a(T)})$

If we had perfect information to start

Expected Reward of Algorithm

Interactive Personalization

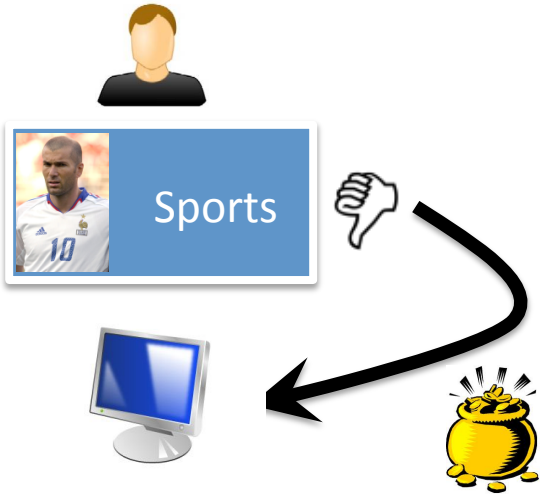
(5 Classes, No features)

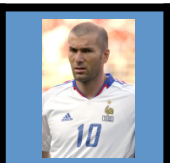
					
Average Likes	--	--	--	--	--
# Shown	0	0	0	1	0

 : 0

Interactive Personalization

(5 Classes, No features)



					
Average Likes	--	--	--	0	--
# Shown	0	0	0	1	0

Interactive Personalization

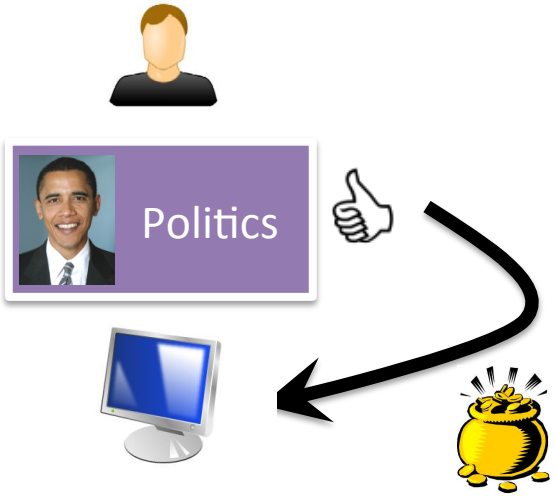
(5 Classes, No features)

					
Average Likes	--	--	--	0	--
# Shown	0	0	1	1	0

 : 0

Interactive Personalization

(5 Classes, No features)



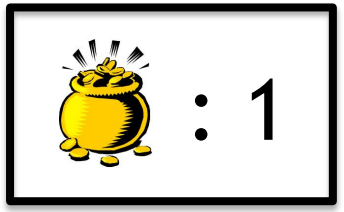
					
Average Likes	--	--	1	0	--
# Shown	0	0	1	1	0

 : 1

Interactive Personalization

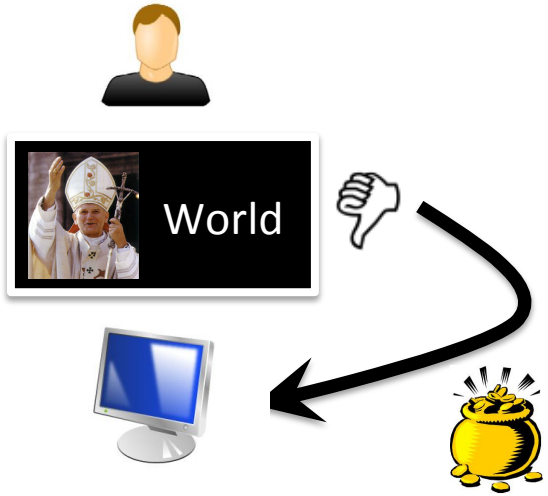
(5 Classes, No features)

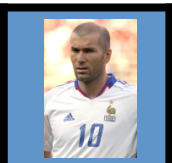
					
Average Likes	--	--	1	0	--
# Shown	0	0	1	1	1



Interactive Personalization

(5 Classes, No features)



					
Average Likes	--	--	1	0	0
# Shown	0	0	1	1	1

 : 1

Interactive Personalization

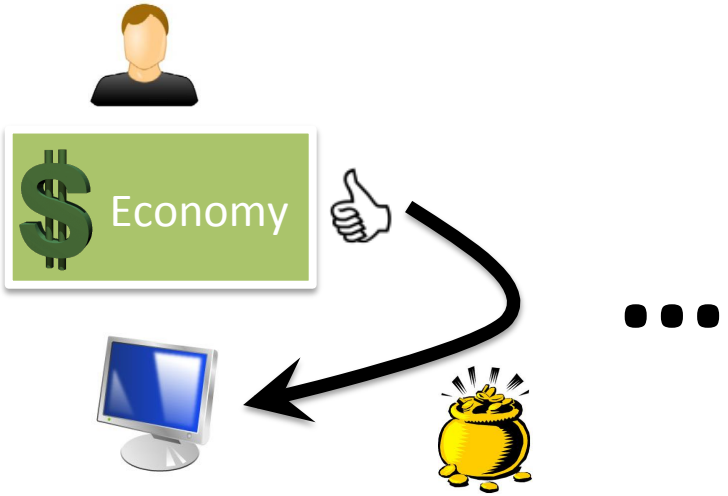
(5 Classes, No features)

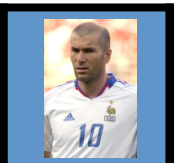
					
Average Likes	--	--	1	0	0
# Shown	0	1	1	1	1

 : 1

Interactive Personalization

(5 Classes, No features)



					
Average Likes	--	1	1	0	0
# Shown	0	1	1	1	1

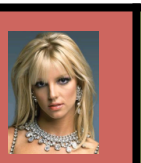
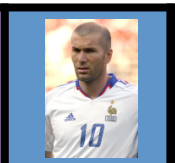
What should Algorithm Recommend?

Exploit:

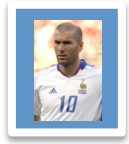
Explore:

Best:

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

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

$(OPT) = ($  $) + ($  $) + ($  $) \ldots$

$(ALG) = ($  $) + ($  $) + ($  $) \ldots$

Time Horizon

Regret: $R(T) = (OPT) - (ALG)$

- Opportunity cost of not knowing preferences
- "**no-regret**" if R(T)/T ➔ 0
  - Efficiency measured by convergence rate

Recap: The Multi-Armed Bandit Problem

- K actions/classes
- Each action has an average reward: μ_k
  - All unknown to us
  - Assume WLOG that u_1 is largest

Basic Setting
K classes
No features

- For t = 1…T
  - Algorithm chooses action a(t)
  - Receives random reward y(t)
    - Expectation $\mu_{a(t)}$

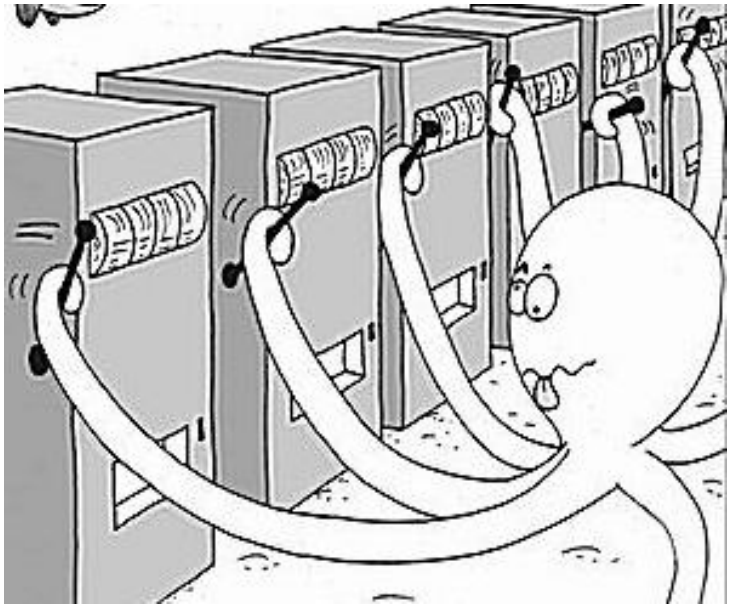
Algorithm Simultaneously
Predicts & Receives Labels

- Goal: minimize $Tu_1 - (\mu_{a(1)} + \mu_{a(2)} + \ldots + \mu_{a(T)})$

Regret

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

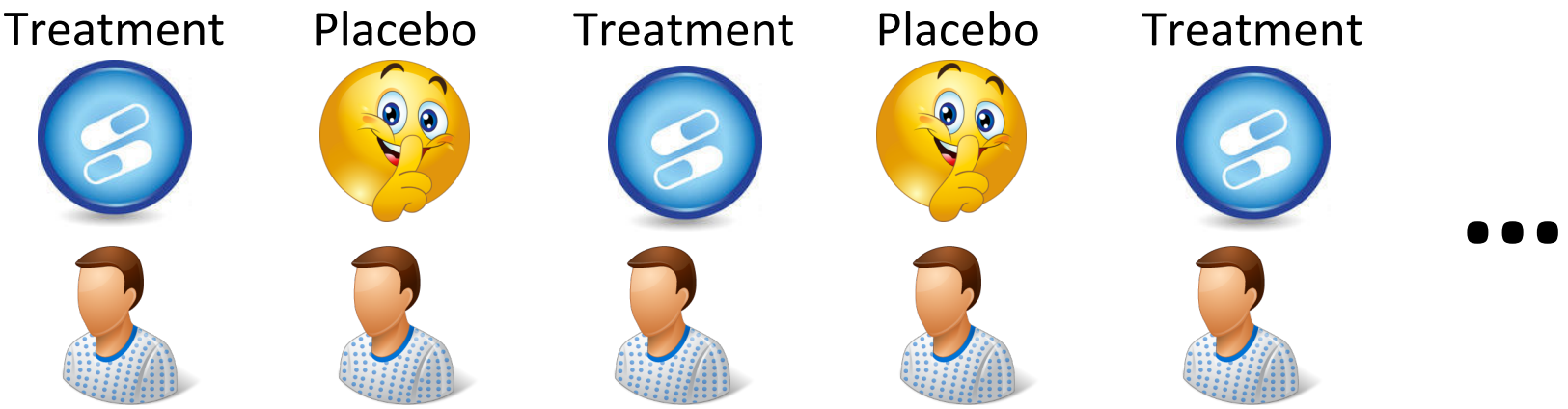
Implications of Regret

Regret: $R(T) = \text{(OPT)} - \text{(ALG)}$

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

Experimental Design

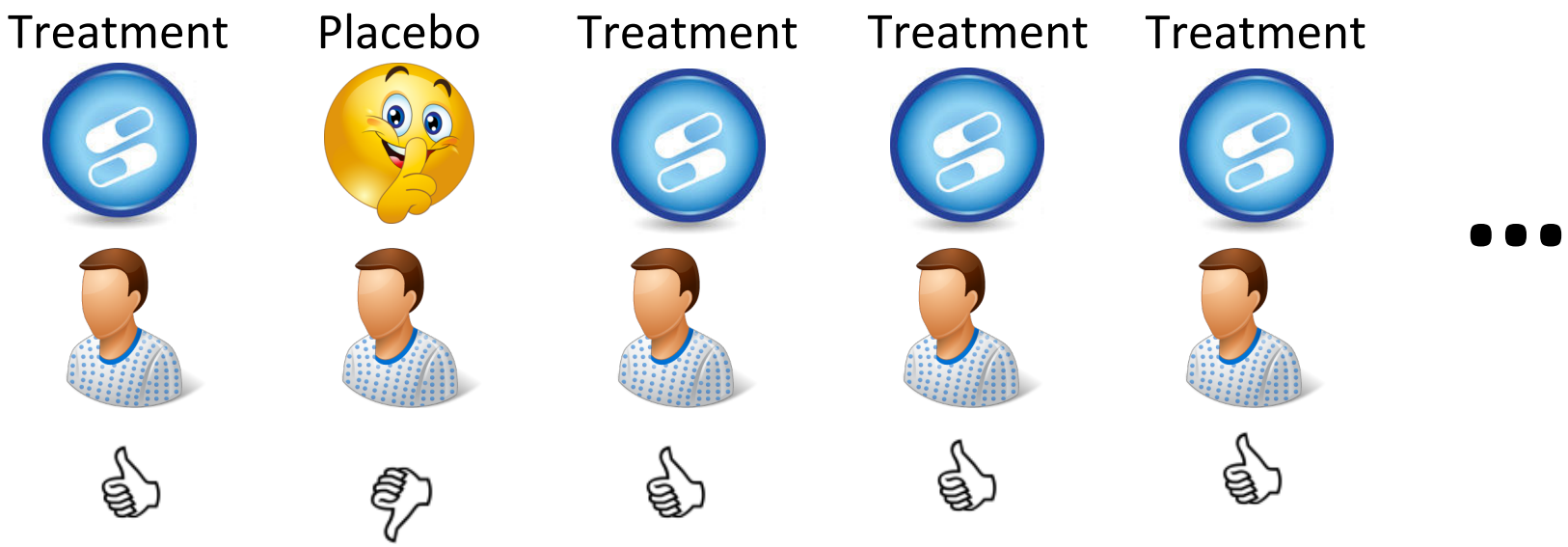
- How to split trials to collect information
- **Static Experimental Design**
  - Standard practice
  - (pre-planned)



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

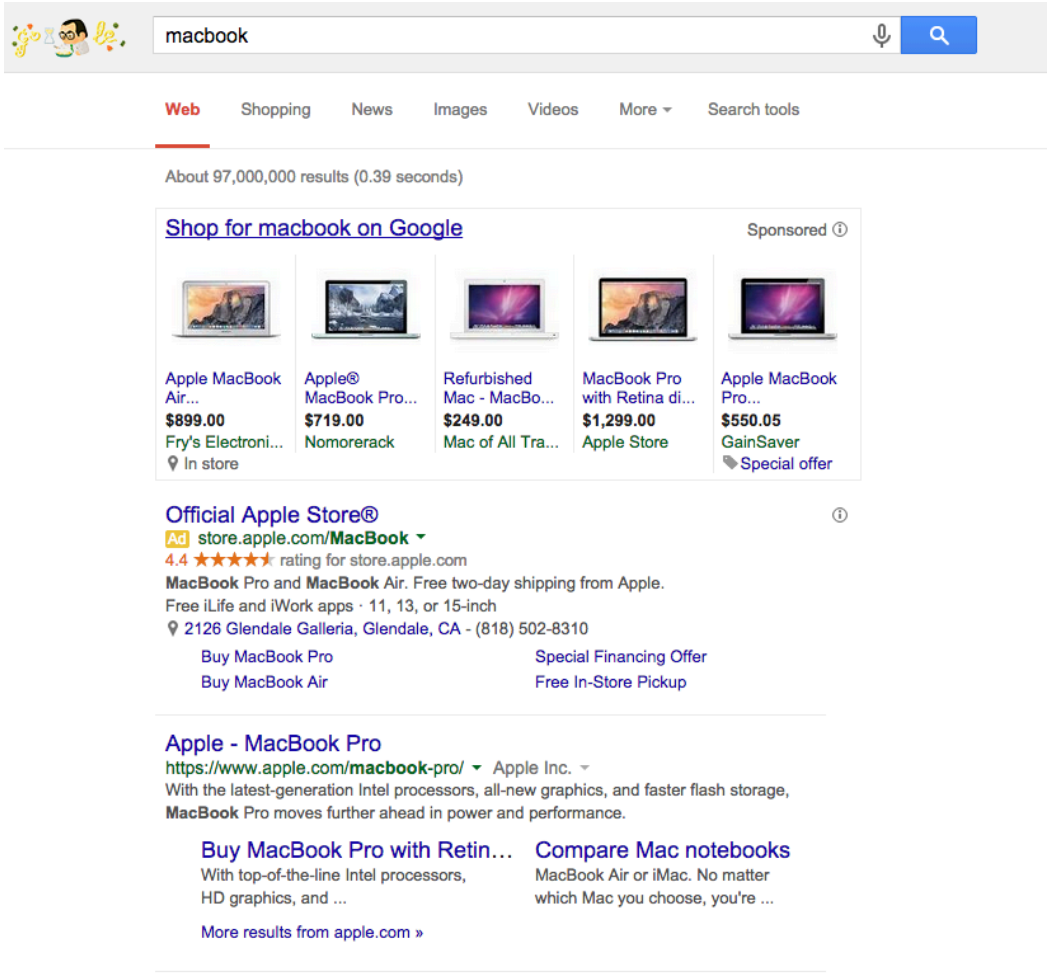
Two Cousins, Two Paths Thomas McLaughlin, left, was given a promising experimental drug to treat his lethal skin cancer in a medical trial; Brandon Ryan had to go without it.

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

Reinforcement Learning

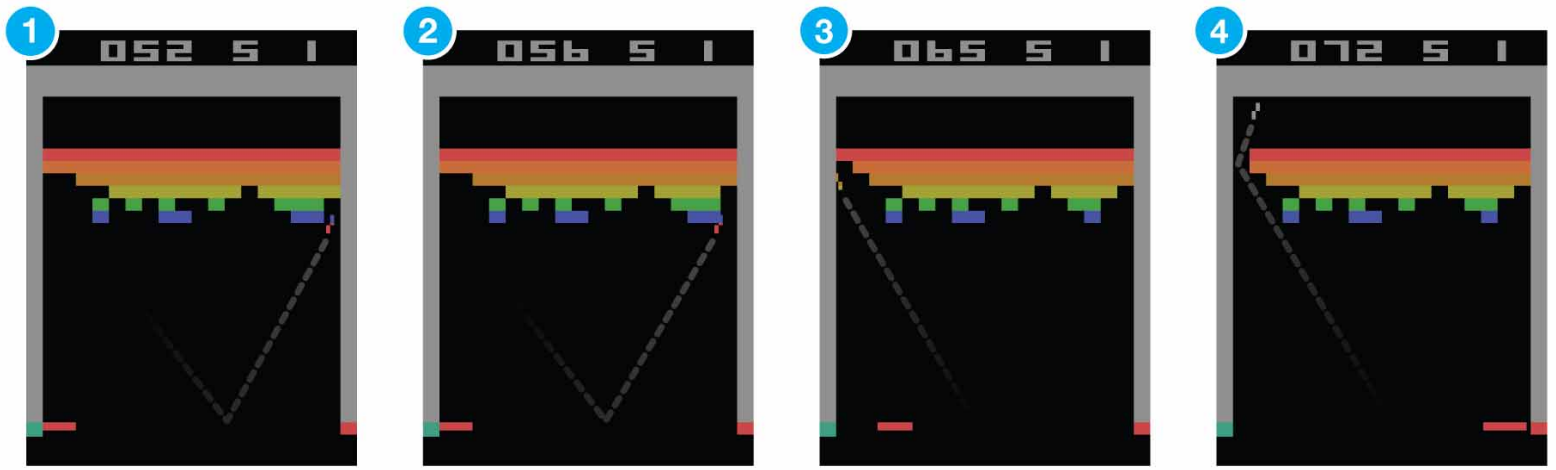
Actions Impact State

- 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!

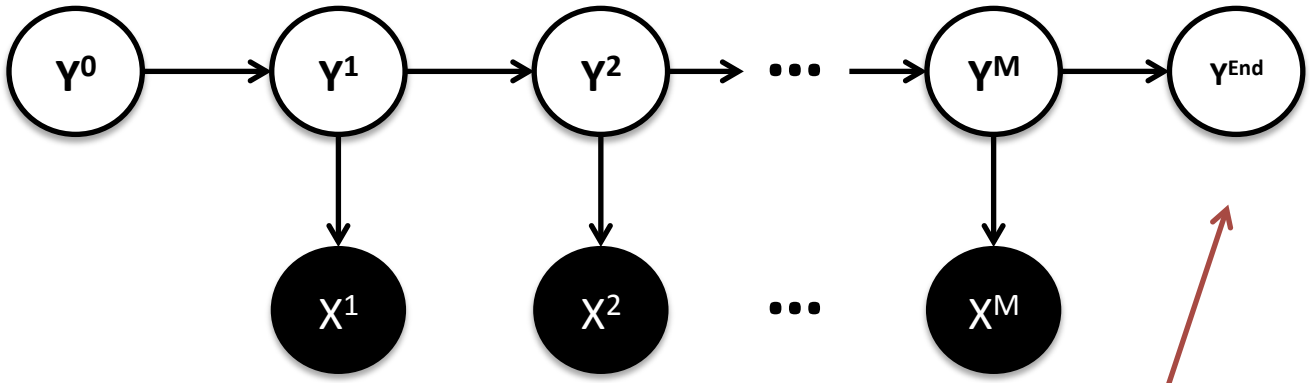
Much harder to do exploration!

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

Non-Convex Optimization

Anima
Anandkumar

Recall: Hidden Markov Models



Optional

$$P(x,y) = P(End \mid y^M) \prod_{i=1}^{M} P(y^i \mid y^{i-1}) \prod_{i=1}^{M} P(x^i \mid y^i)$$

Recall: EM Algorithm for HMMs

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

Chicken vs Egg!

1. Initialize A and O arbitrarily
2. Predict prob. of y's for each training x

Expectation Step

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

Chicken vs Egg!

1. Initialize A and O arbitrarily

Expectation Step

2

3

4

Can We Train HMMs Optimally?

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

Inspiration from Dimensionality Reduction

- Find best rank K approximation to Y:

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

- Non-convex optimization problem!
  - Due to non-convex feasible region

- **But optimally solved via SVD!**

Spectral Learning of HMMs

Want to Estimate: $P(y^j \mid y^{j-1}) = A \qquad P(x^j \mid y^j) = O$

$$\sum^t = E\left[x^{j+t}\left(x^j\right)^T\right] = E\left[E\left[x^{j+t}\left(x^j\right)^T \middle| y^j\right]\right]$$

$$= E\left[E\left[x^{j+t} \middle| y^j\right] E\left[\left(x^j\right)^T \middle| y^j\right]\right]$$

$$= E\left[\left(OA^t k y^j\right)\left(O y^j\right)^T\right]$$

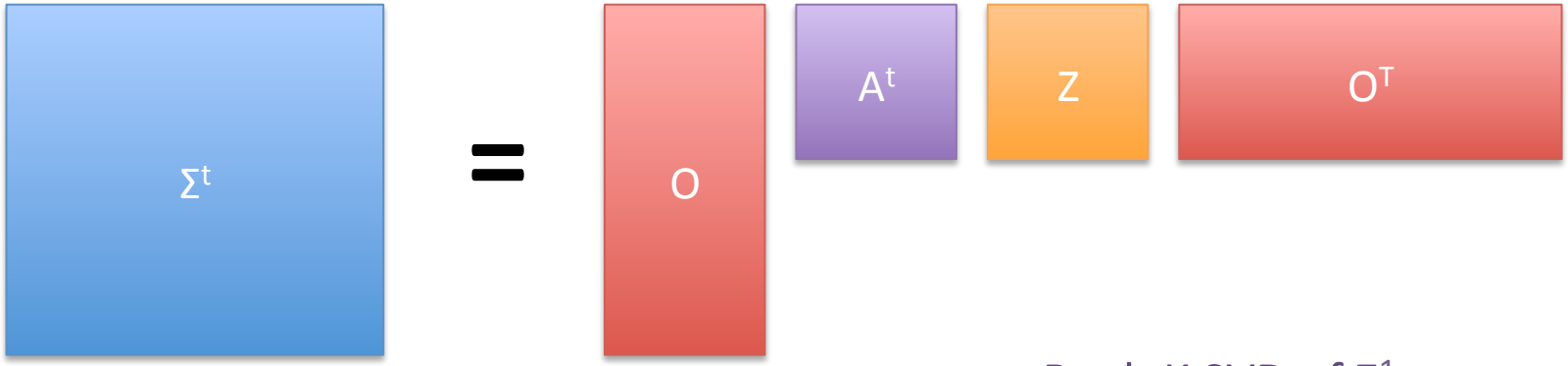
$$= OA^t E\left[y^j\left(y^j\right)^T\right] O^T$$

$$= OA^t Z O^T$$

Treat each x^j and y^j as indicator vector

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

Spectral Learning of HMMs



Rank-K SVD of Σ^1

Optimal Solution: $A = U^T \Sigma^2 \left(U^T \Sigma^1 \right)^{-1}$

(requires a lot of data)

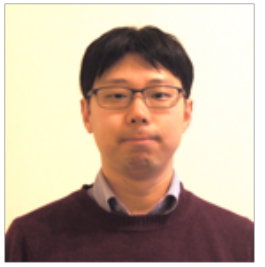
http://www.cs.cmu.edu/~ggordon/spectral-learning/

…and many more topics!

- Probabilistic Models & Bayesian Reasoning
- 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:**
  - "Structured Prediction"



Taehwan Kim

- Paper Reading & Presenting + Final Project
  - Graded on participation and final project