



10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Course Overview

Matt Gormley
Lecture 1
Jan. 14, 2019

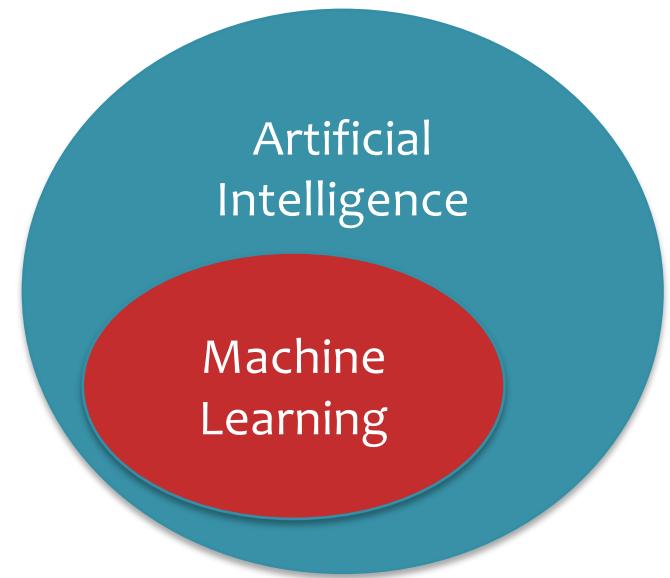
WHAT IS MACHINE LEARNING?

Artificial Intelligence

The basic goal of AI is to develop intelligent machines.

This consists of many sub-goals:

- Perception
- Reasoning
- Control / Motion / Manipulation
- Planning
- Communication
- Creativity
- Learning



What is Machine Learning?

The goal of this course is to provide you with a toolbox:

Machine Learning

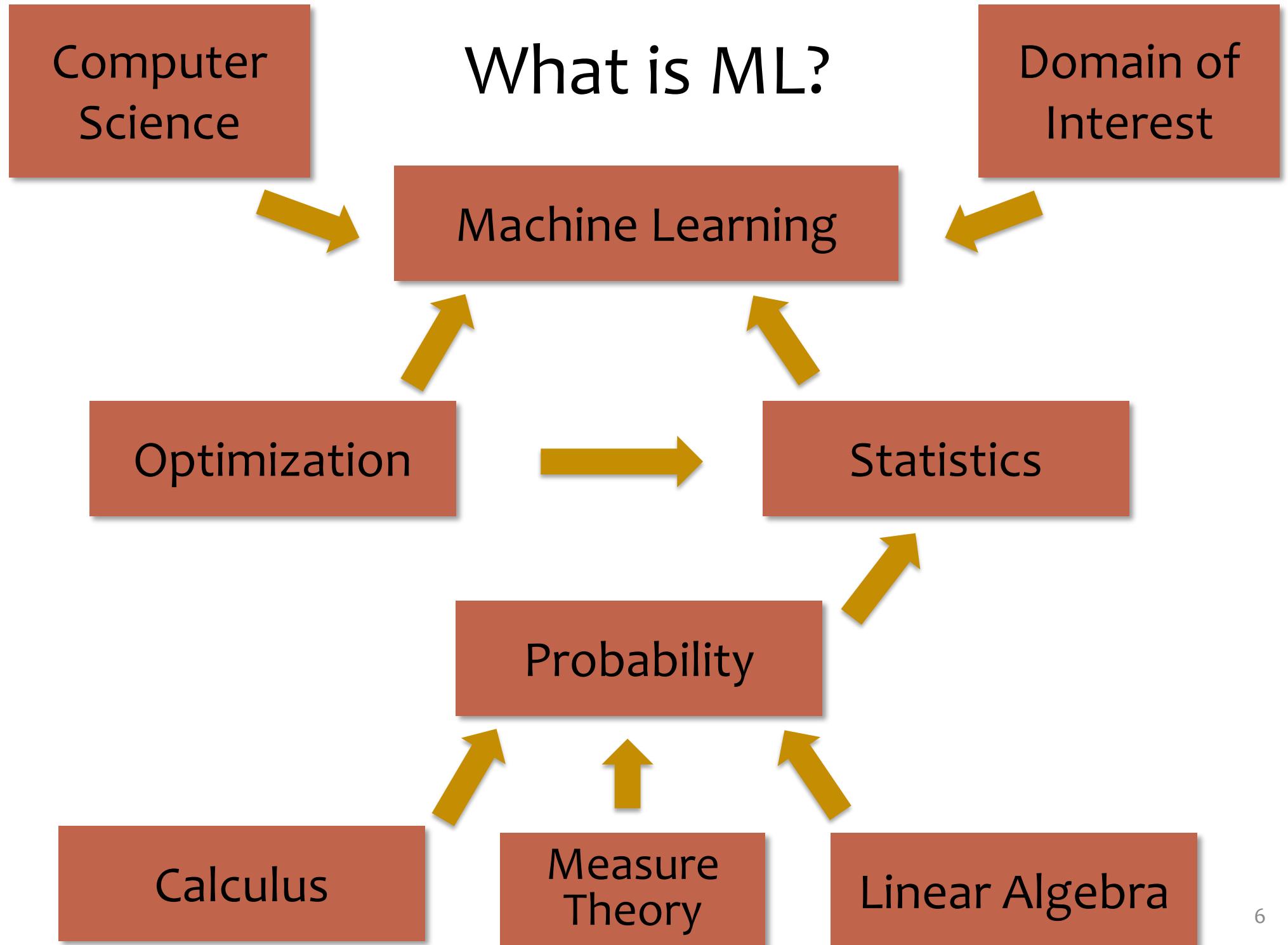
Statistics

Probability

Computer
Science

Optimization





What is ML?

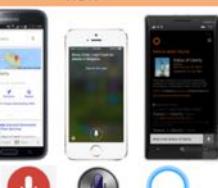
Speech Recognition

1. Learning to recognize spoken words

THEN

“...the SPHINX system (e.g. Lee 1989) learns speaker-specific strategies for recognizing the primitive sounds (phonemes) and words from the observed speech signal...neural network methods...hidden Markov models...”

(Mitchell, 1997)



Source: <https://www.stonetemple.com/great-knowledge-box-showdown/#VoiceStudyResults>

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Robotics

2. Learning to drive an autonomous vehicle

THEN

“...the ALVINN system (Pomerleau 1989) has used its learned strategies to drive unassisted at 70 miles per hour for 90 miles on public highways among other cars...”

(Mitchell, 1997)



waymo.com

9

Games / Reasoning

3. Learning to beat the masters at board games

THEN

“...the world's top computer program for backgammon, TD-GAMMON (Tesauro, 1992, 1995), learned its strategy by playing over one million practice games against itself...”

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10

Computer Vision

4. Learning to recognize images

THEN

“...The recognizer is a convolution network that can be spatially replicated. From the network output, a hidden Markov model produces word scores. The entire system is globally trained to minimize word-level errors....”

(LeCun et al., 1995)



Images from <https://blog.openai.com/generative-models/>

Learning Theory

• 5. In what cases and how well can we learn?

Sample Complexity Results

Definition a.s.: The sample complexity of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. visual to 1).

Four Cases we care about...

Finite (N)	Resilient	Agnostic
$N = \frac{1}{\delta} \ln(\frac{2}{\alpha}) + \log(\frac{2}{\beta})$ where $\delta > 0$, $\alpha > 0$, $\beta > 0$. δ is the target error, α is the confidence level, β is the failure probability.	$N = \frac{1}{\delta^2} \ln(\frac{2}{\alpha}) + \log(\frac{2}{\beta})$ where $\delta > 0$, $\alpha > 0$, $\beta > 0$. δ is the target error, $\alpha > 0$, $\beta > 0$.	
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$$\begin{aligned} \text{Time} &\propto \delta^{-3} \text{Error}^{-1} \\ \text{① Train Error} &= \text{Expected } R(\hat{w}) \text{ (aka. Generalization Error)} \\ R(\hat{w}) &\times P_{\text{train}}(s_i \in \text{train} | \hat{w}(s_i)) \xrightarrow{\text{only relevant}} \\ \text{② Train Error} &= \text{Expected } R(\hat{w}) \\ R(\hat{w}) &= P_{\text{train}}(s_i \in \text{train} | \hat{w}(s_i)) \times \text{Expected } R(\hat{w}(s_i)) \\ &= \frac{1}{N} \sum_{i=1}^N P_{\text{train}}(s_i \in \text{train} | \hat{w}(s_i)) \times R(\hat{w}(s_i)) \\ &= \frac{1}{N} \sum_{i=1}^N \left[\frac{1}{N} \# \{s_j \in \text{train} | s_j \neq s_i \} \right] \times R(\hat{w}(s_i)) \end{aligned}$$

- How many examples do we need to learn?
- How do we quantify our ability to generalize to unseen data?
- Which algorithms are better suited to specific learning settings?

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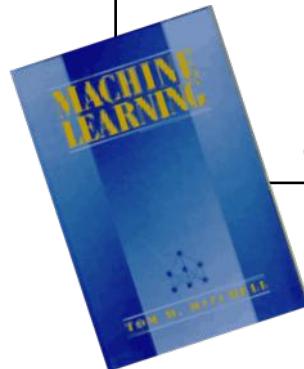
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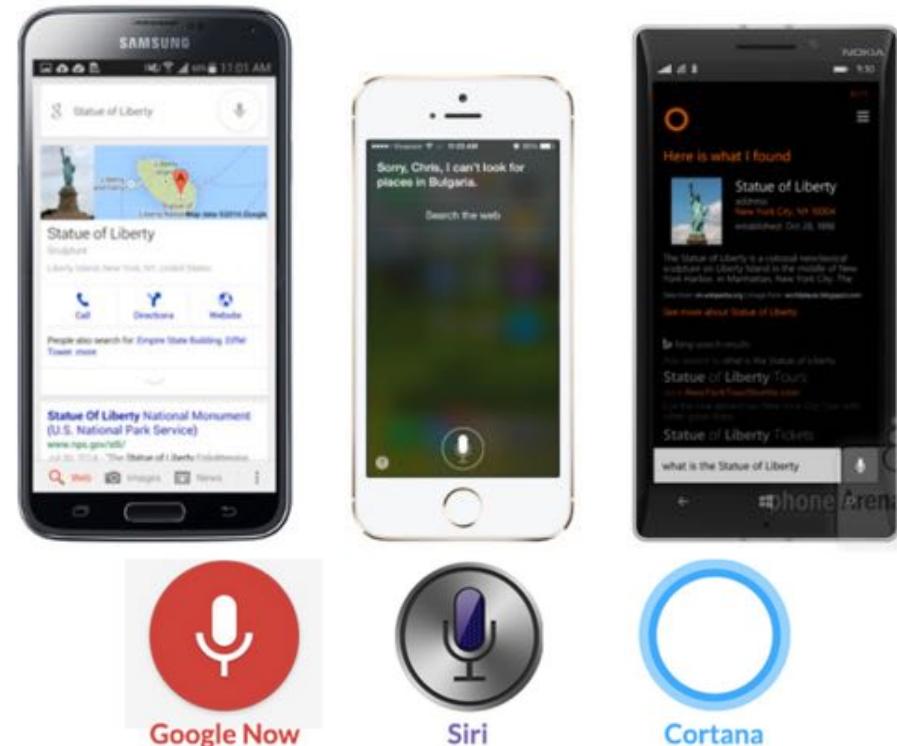
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Robotics

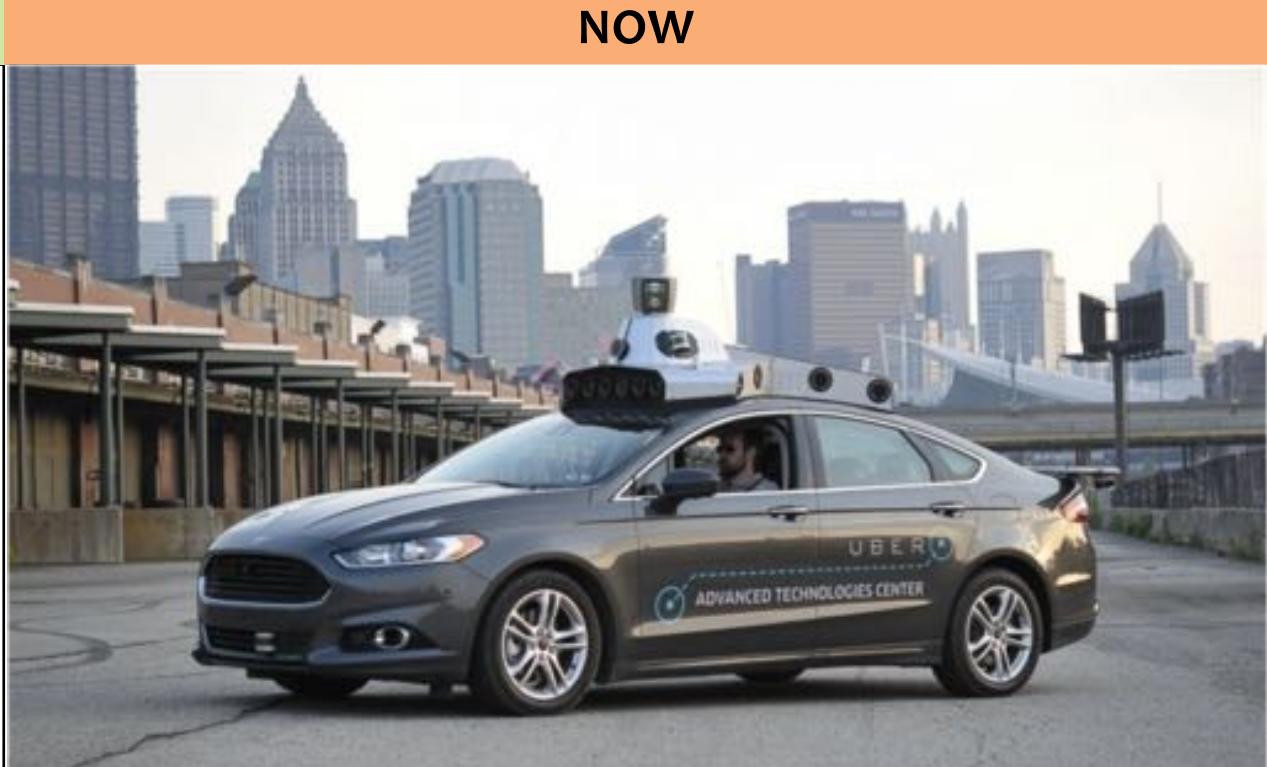
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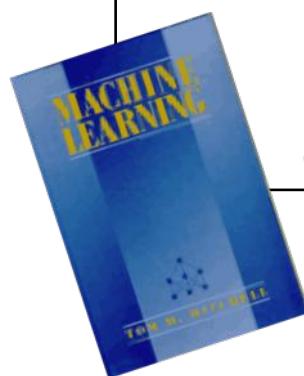
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<https://www.geek.com/wp-content/uploads/2016/03/uber.jpg>



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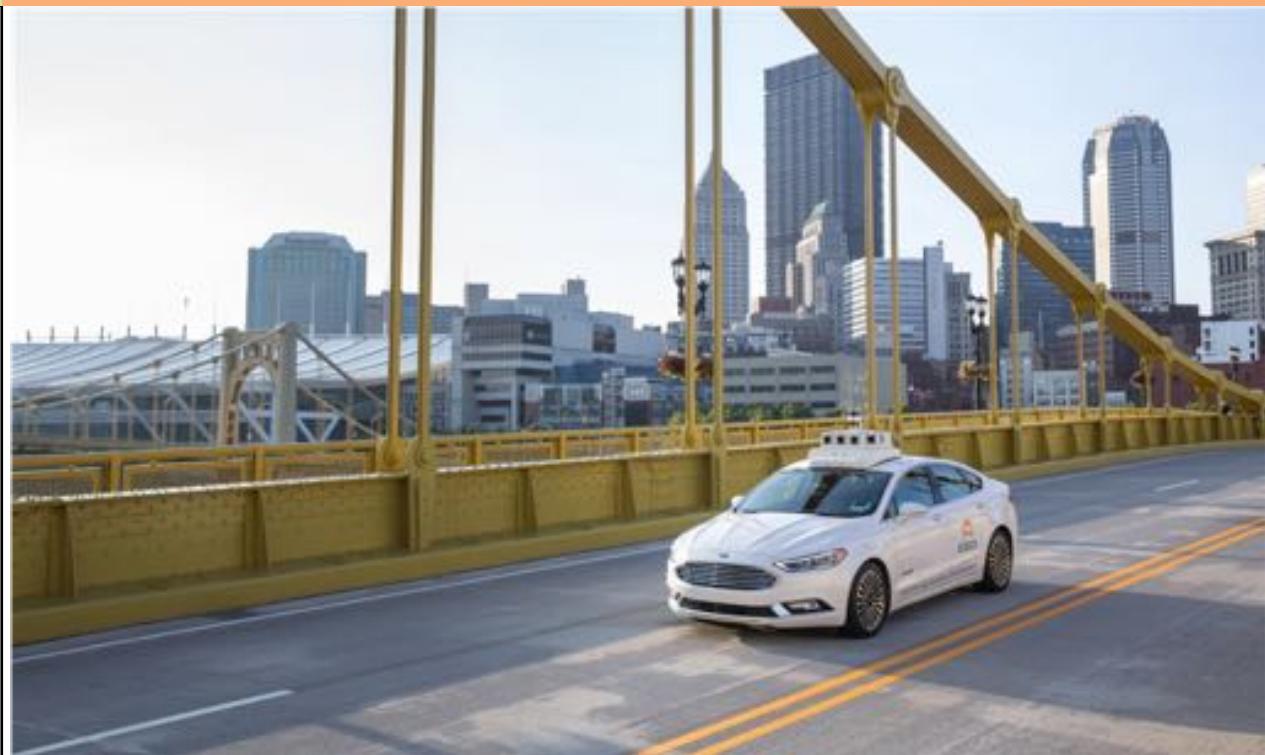
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<https://www.argo.ai/>

Games / Reasoning

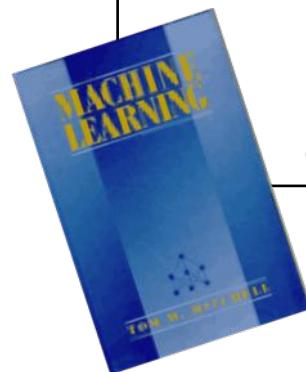
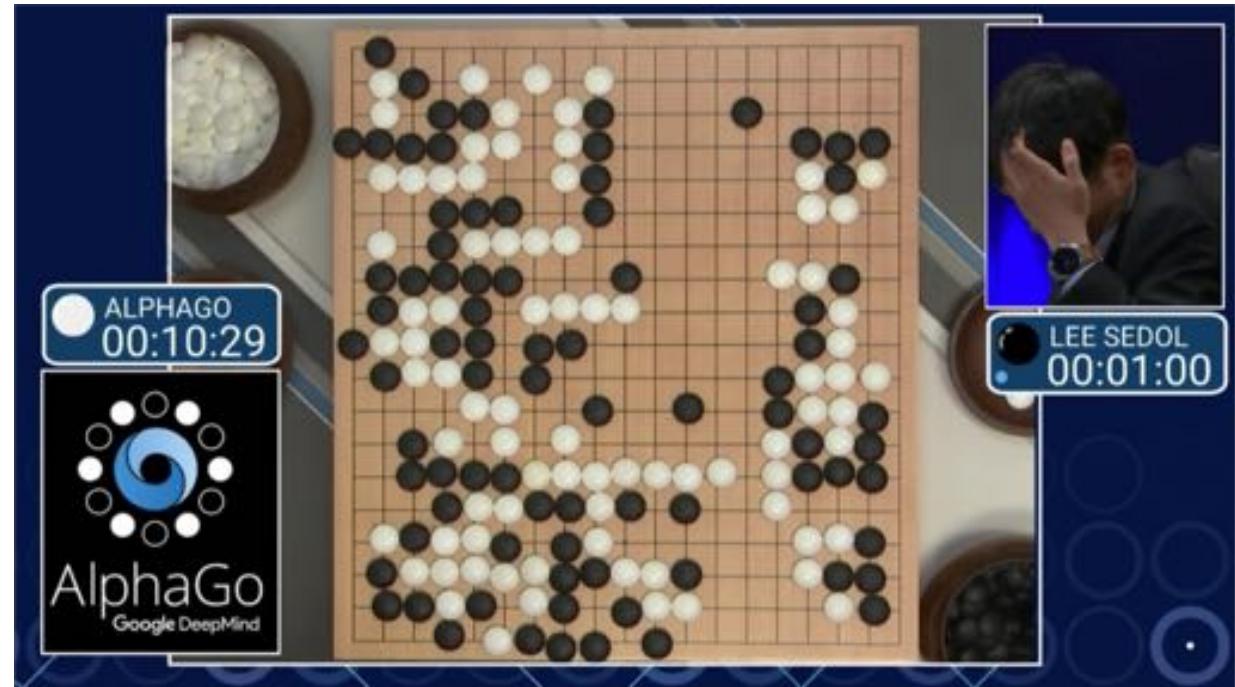
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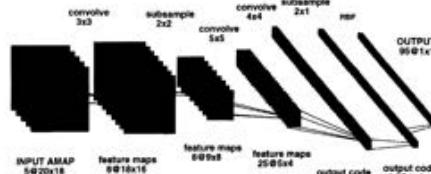


Computer Vision

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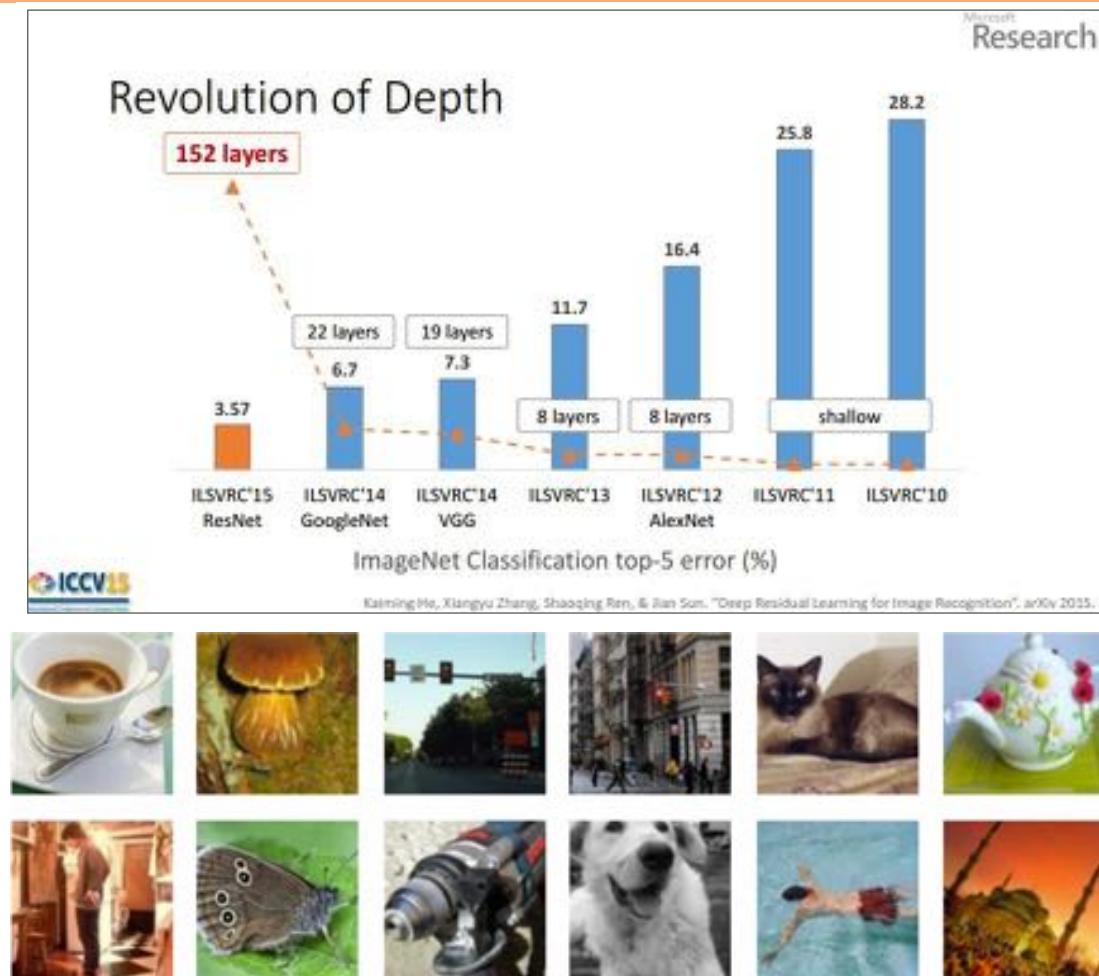
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“...The recognizer is a convolution network that can be spatially replicated. From the network output, a hidden Markov model produces word scores. The entire system is globally trained to minimize word-level errors....”



(LeCun et al., 1995)

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Learning Theory

• 5. In what cases and how well can we learn?

Sample Complexity Results

Definition 0.1. The **sample complexity** of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. close to 1).

Four Cases we care about...

	Realizable	Agnostic
Finite $ \mathcal{H} $	$N \geq \frac{1}{\epsilon} [\log(\mathcal{H}) + \log(\frac{1}{\delta})]$ labeled examples are sufficient so that with probability $(1 - \delta)$ all $h \in \mathcal{H}$ with $R(h) \geq \epsilon$ have $\hat{R}(h) > 0$.	$N \geq \frac{1}{2\epsilon^2} [\log(\mathcal{H}) + \log(\frac{2}{\delta})]$ labeled examples are sufficient so that with probability $(1 - \delta)$ for all $h \in \mathcal{H}$ we have that $ R(h) - \hat{R}(h) < \epsilon$.
Infinite $ \mathcal{H} $	$N = O(\frac{1}{\epsilon} [\text{VC}(\mathcal{H}) \log(\frac{1}{\epsilon}) + \log(\frac{1}{\delta})])$ labeled examples are sufficient so that with probability $(1 - \delta)$ all $h \in \mathcal{H}$ with $R(h) \geq \epsilon$ have $\hat{R}(h) > 0$.	$N = O(\frac{1}{\epsilon^2} [\text{VC}(\mathcal{H}) + \log(\frac{1}{\delta})])$ labeled examples are sufficient so that with probability $(1 - \delta)$ for all $h \in \mathcal{H}$ we have that $ R(h) - \hat{R}(h) \leq \epsilon$.

Two Types of Error

① True Error (aka. expected risk) (aka. Generalization Error)

$$R(h) = P_{x \sim p^*(x)} (c^*(x) \neq h(x)) \quad \leftarrow \text{always unknown.}$$

② Train Error (aka. empirical risk)

$$\begin{aligned} \hat{R}(h) &= P_{x \sim S} (c^*(x) \neq h(x)) \quad \leftarrow S = \{x^{(1)}, \dots, x^{(n)}\} \\ &= \frac{1}{N} \sum_{i=1}^N \mathbb{I}(c^*(x^{(i)}) \neq h(x^{(i)})) \\ &= \frac{1}{N} \sum_{i=1}^N \mathbb{I}(y^{(i)} \neq h(x^{(i)})) \quad \text{known, computable} \end{aligned}$$

PAC Learning

Q: Can we bound $R(h)$ in terms of $\hat{R}(h)$?
A: Yes!

PAC stands for Probably Approximately Correct

PAC learner yields hypothesis h , which is approximately correct with high probability

$R(h) \approx 0$
 $\Pr(R(h) \approx 0) \approx 1$

Def = PAC Criterion

$$\Pr(\forall h, |R(h) - \hat{R}(h)| \leq \epsilon) \geq 1 - \delta$$

1. How many examples do we need to learn?
2. How do we quantify our ability to generalize to unseen data?
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What is ML?

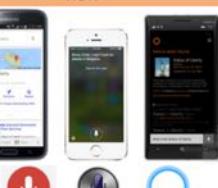
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$$\begin{aligned} \text{Training Error} \\ \text{① Train Error (aka expected risk)} &= R(\hat{w}) = P_{\hat{w}}[c(\hat{w}, s) \neq c(w^*, s)] \\ &= R(0) \times P_{\hat{w}}[c(0, s) \neq c(w^*, s)] \quad \text{only relevant} \\ \text{② Train Error (aka empirical risk)} &= R(\hat{w}) = P_{\hat{w}}[c(\hat{w}, s) \neq c(w^*, s)] \\ &= \frac{1}{N} \sum_{i=1}^N I(c(\hat{w}, s_i) \neq c(w^*, s_i)) \\ &= \frac{1}{N} \sum_{i=1}^N I(\hat{w}(s_i) \neq w^*(s_i)) \quad \text{known compatible} \\ \text{Inference Error} \\ \text{③ Inference Error} &= R(w^*) = P_{w^*}[c(w^*, s) \neq c(w^*, s)] \\ &= P_{w^*}[c(w^*, s) \neq c(\hat{w}, s)] \\ &= P_{w^*}[c(w^*, s) \neq c(\hat{w}, s)] \quad \text{known compatible} \\ \text{④ PAC Lower Bound} \\ \text{Q: Can we bound } R(w^*) \text{ in terms of } R(\hat{w})? \\ \text{A: Yes!} \\ \text{PAC stands for Probably Approximately Correct} \\ \text{PAC Lower Bound: } R(w^*) \geq R(\hat{w}) + \text{Approximate error with high probability} \\ \text{Approximate error with high probability: } R(\hat{w}) + O(\epsilon) \end{aligned}$$

- How many examples do we need to learn?
- How do we quantify our ability to generalize to unseen data?
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What is Machine Learning?

The goal of this course is to provide you with a toolbox:

Machine Learning

Statistics

Probability

Computer
Science

Optimization

To solve all the problems above and more



Topics

- Foundations
 - Probability
 - MLE, MAP
 - Optimization
- Classifiers
 - KNN
 - Naïve Bayes
 - Logistic Regression
 - Perceptron
 - SVM
- Regression
 - Linear Regression
- Important Concepts
 - Kernels
 - Regularization and Overfitting
 - Experimental Design
- Unsupervised Learning
 - K-means / Lloyd's method
 - PCA
 - EM / GMMs
- Neural Networks
 - Feedforward Neural Nets
 - Basic architectures
 - Backpropagation
 - CNNs, LSTMs
- Graphical Models
 - Bayesian Networks
 - HMMs
 - Learning and Inference
- Learning Theory
 - Statistical Estimation (covered right before midterm)
 - PAC Learning
- Other Learning Paradigms
 - Matrix Factorization
 - Reinforcement Learning
 - Information Theory

ML Big Picture

Learning Paradigms:

What data is available and when? What form of prediction?

- supervised learning
- unsupervised learning
- semi-supervised learning
- reinforcement learning
- active learning
- imitation learning
- domain adaptation
- online learning
- density estimation
- recommender systems
- feature learning
- manifold learning
- dimensionality reduction
- ensemble learning
- distant supervision
- hyperparameter optimization

Theoretical Foundations:

What principles guide learning?

- probabilistic
- information theoretic
- evolutionary search
- ML as optimization

Problem Formulation:

What is the structure of our output prediction?

boolean	Binary Classification
categorical	Multiclass Classification
ordinal	Ordinal Classification
real	Regression
ordering	Ranking
multiple discrete	Structured Prediction
multiple continuous	(e.g. dynamical systems)
both discrete & cont.	(e.g. mixed graphical models)

Application Areas

Key challenges?

NLP, Speech, Computer Vision, Robotics, Medicine, Search

Facets of Building ML Systems:

How to build systems that are robust, efficient, adaptive, effective?

1. Data prep
2. Model selection
3. Training (optimization / search)
4. Hyperparameter tuning on validation data
5. (Blind) Assessment on test data

Big Ideas in ML:

Which are the ideas driving development of the field?

- inductive bias
- generalization / overfitting
- bias-variance decomposition
- generative vs. discriminative
- deep nets, graphical models
- PAC learning
- distant rewards

DEFINING LEARNING PROBLEMS

Well-Posed Learning Problems

Three components $\langle T, P, E \rangle$:

1. Task, T
2. Performance measure, P
3. Experience, E

Definition of learning:

A computer program **learns** if its performance at tasks in T , as measured by P , improves with experience E .

Example Learning Problems

3. Learning to beat the masters at **chess**
 1. Task, T :
 2. Performance measure, P :
 3. Experience, E :

Example Learning Problems

4. Learning to **respond to voice commands (Siri)**
 1. Task, T :
 2. Performance measure, P :
 3. Experience, E :

Capturing the Knowledge of Experts



Solution #1: Expert Systems

- Over 20 years ago, we had rule based systems
- Ask the expert to
 1. Obtain a PhD in Linguistics
 2. Introspect about the structure of their native language
 3. Write down the rules they devise

Give me directions to Starbucks

If: "give me directions to X"
Then: directions (here, nearest (X))

How do I get to Starbucks?

If: "how do i get to X"
Then: directions (here, nearest (X))

Where is the nearest Starbucks?

If: "where is the nearest X"
Then: directions (here, nearest (X))

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I need directions to Starbucks

If: "I need directions to X"
Then: directions(here, nearest(X))

Starbucks directions

If: "X directions"
Then: directions(here, nearest(X))

Is there a Starbucks nearby?

If: "Is there an X nearby"
Then: directions(here, nearest(X))

Capturing the Knowledge of Experts



Solution #2: Annotate Data and Learn

- Experts:
 - Very good at answering questions about specific cases
 - Not very good at telling **HOW** they do it
- 1990s: So why not just have them tell you what they do on **SPECIFIC CASES** and then let **MACHINE LEARNING** tell you how to come to the same decisions that they did

Capturing the Knowledge of Experts



Solution #2: Annotate Data and Learn

1. Collect raw sentences $\{x_1, \dots, x_n\}$
2. Experts annotate their meaning $\{y_1, \dots, y_n\}$

x_1 : How do I get to Starbucks?

y_1 : directions(here,
nearest(Starbucks))

x_2 : Show me the closest Starbucks

y_2 : map(nearest(Starbucks))

x_3 : Send a text to John that I'll be late

y_3 : txtmsg(John, I'll be late)

x_4 : Set an alarm for seven in the
morning

y_4 : setalarm(7:00AM)

Example Learning Problems

4. Learning to **respond to voice commands (Siri)**

1. Task, T :
predicting action from speech
2. Performance measure, P :
percent of correct actions taken in user pilot study
3. Experience, E :
examples of (speech, action) pairs

Problem Formulation

- Often, the same task can be formulated in more than one way:
- Ex: Loan applications
 - creditworthiness/score (regression)
 - probability of default (density estimation)
 - loan decision (classification)

Problem Formulation:

What is the structure of our output prediction?

boolean	Binary Classification
categorical	Multiclass Classification
ordinal	Ordinal Classification
real	Regression
ordering	Ranking
multiple discrete	Structured Prediction
multiple continuous	(e.g. dynamical systems)
both discrete & cont.	(e.g. mixed graphical models)

Well-posed Learning Problems

In-Class Exercise

1. Select a **task**, T
2. Identify **performance measure**, P
3. Identify **experience**, E
4. Report ideas back to rest of class

Example Tasks

- Identify objects in an image
- Translate from one human language to another
- Recognize speech
- Assess risk (e.g. in loan application)
- Make decisions (e.g. in loan application)
- Assess potential (e.g. in admission decisions)
- Categorize a complex situation (e.g. medical diagnosis)
- Predict outcome (e.g. medical prognosis, stock prices, inflation, temperature)
- Predict events (default on loans, quitting school, war)
- Plan ahead under perfect knowledge (chess)
- Plan ahead under partial knowledge (Poker, Bridge)

Machine Learning & Ethics

What ethical responsibilities do we have as machine learning experts?

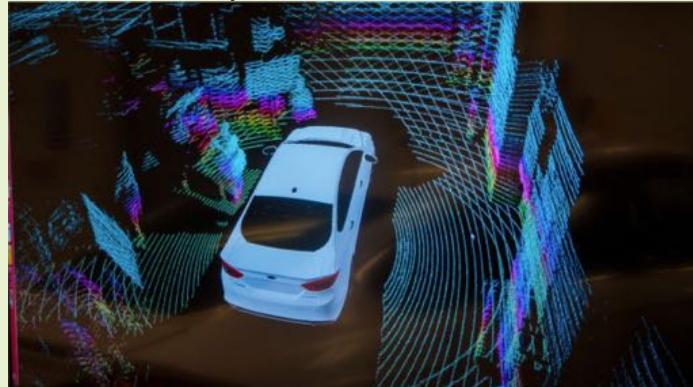
Some topics that we won't cover are probably deserve an entire course

If our search results for news are optimized for ad revenue, might they reflect gender / racial / socio-economic biases?



<http://bing.com/>

<http://arstechnica.com/>



How do autonomous vehicles make decisions when all of the outcomes are likely to be negative?

Should restrictions be placed on intelligent agents that are capable of interacting with the world?



<http://vizdoom.cs.put.edu.pl/>

SYLLABUS HIGHLIGHTS

Syllabus Highlights

The syllabus is located on the course webpage:

<http://www.cs.cmu.edu/~mgormley/courses/10601>

The **course policies** are **required** reading.

Syllabus Highlights

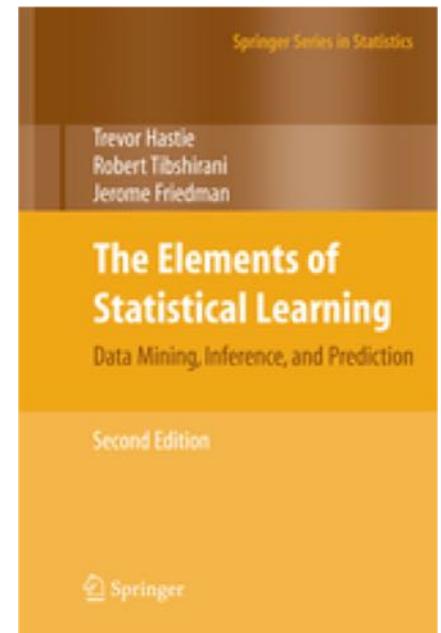
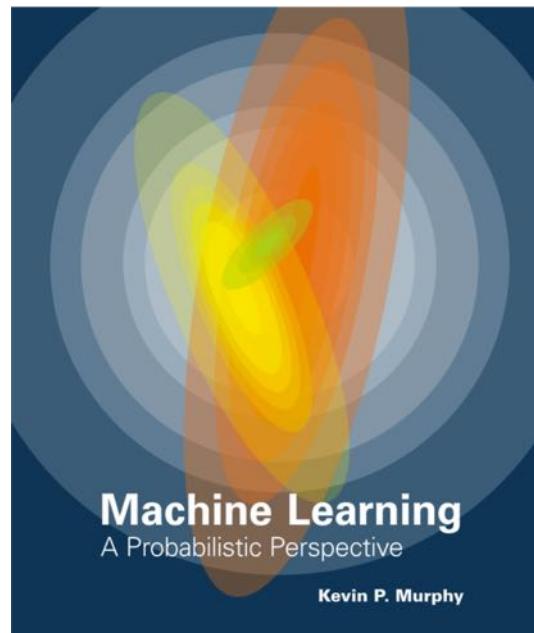
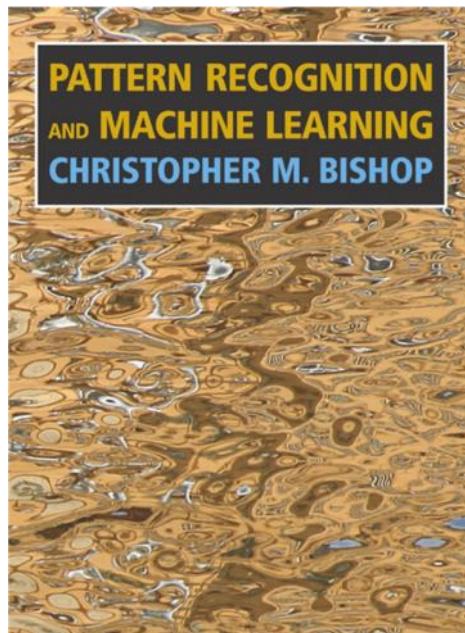
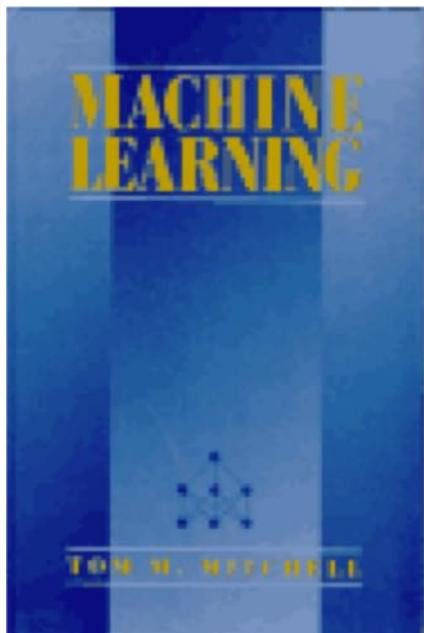
- **Grading:** 40% homework, 15% exam 1, 15% exam 2, 25% final exam, 5% participation
- **Midterm Exam 1:** evening exam, Thu, Feb. 21
- **Midterm Exam 2:** evening exam, Thu, Apr. 04
- **Final Exam:** final exam week, date TBD
- **Homework:** ~4 written and ~5 programming
 - 6 grace days for homework assignments
 - Late submissions: 80% day 1, 60% day 2, 40% day 3, 20% day 4
 - No submissions accepted after 4 days w/o extension
 - Extension requests: see syllabus
- **Recitations:** Fridays, same time/place as lecture (optional, interactive sessions)
- **Readings:** required, online PDFs, recommended for after lecture
- **Technologies:** Piazza (discussion), Autolab (programming), Canvas (quiz-style), Gradescope (open-ended)
- **Academic Integrity:**
 - Collaboration encouraged, but must be documented
 - Solutions must always be written independently
 - No re-use of found code / past assignments
 - Severe penalties (i.e.. failure)
- **Office Hours:** posted on Google Calendar on “People” page

Lectures

- You should ask lots of questions
 - Interrupting (by raising a hand) to ask your question is strongly encouraged
 - Asking questions later (or in real time) on Piazza is also great
- When I ask a question...
 - I want you to answer
 - Even if you don't answer, think it through as though I'm about to call on you
- Interaction improves learning (both in-class and at my office hours)

Textbooks

You are not *required* to read a textbook, but it will help immensely!



PREREQUISITES

Prerequisites

What they are:

- Significant programming experience (15-122)
 - Written programs of 100s of lines of code
 - Comfortable learning a new language
- Probability and statistics (36-217, 36-225, etc.)
- Mathematical maturity: discrete mathematics (21-127, 15-151), linear algebra, and calculus

Prerequisites

What if you need additional review?

- Consider first taking 10-606/607: Mathematical/Computational Foundations for Machine Learning
- More details here:
<http://bit.ly/math4ml>

How to describe 606/607 to a friend

606/607 is...

a **formal** presentation of **mathematics** and **computer science**...

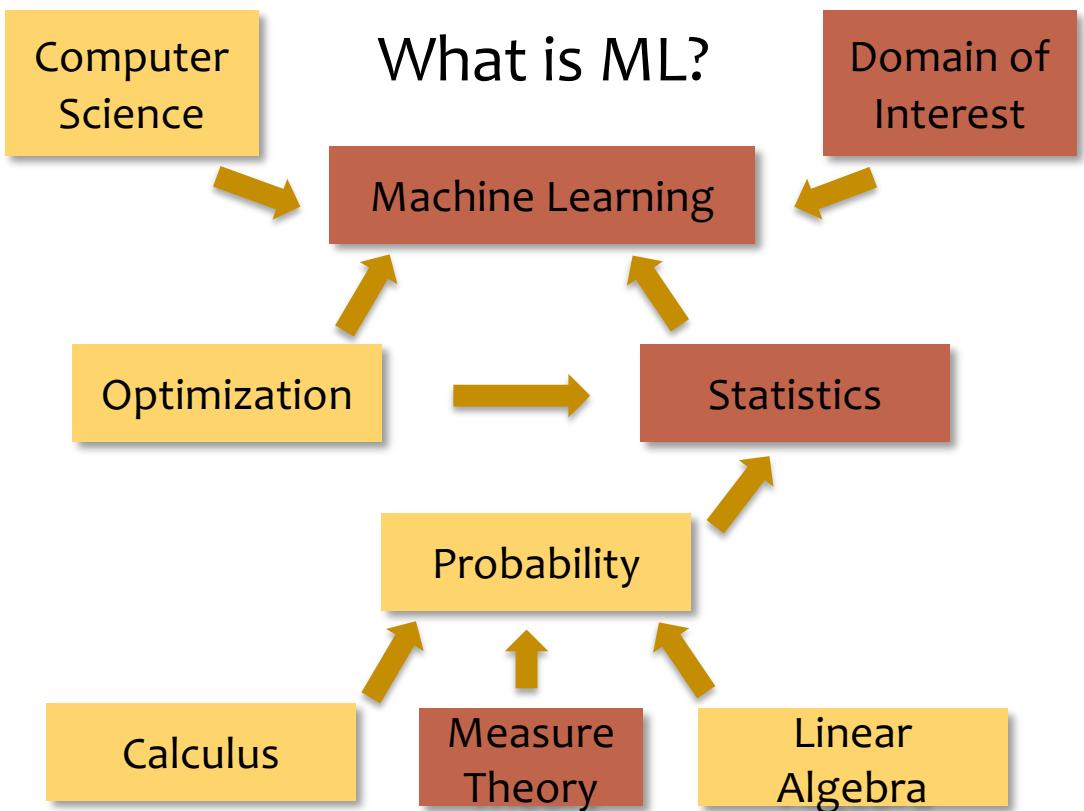
motivated by (carefully chosen) **real-world problems** that arise in **machine learning**...

where the **broader picture** of how those problems arise is treated **somewhat informally**.

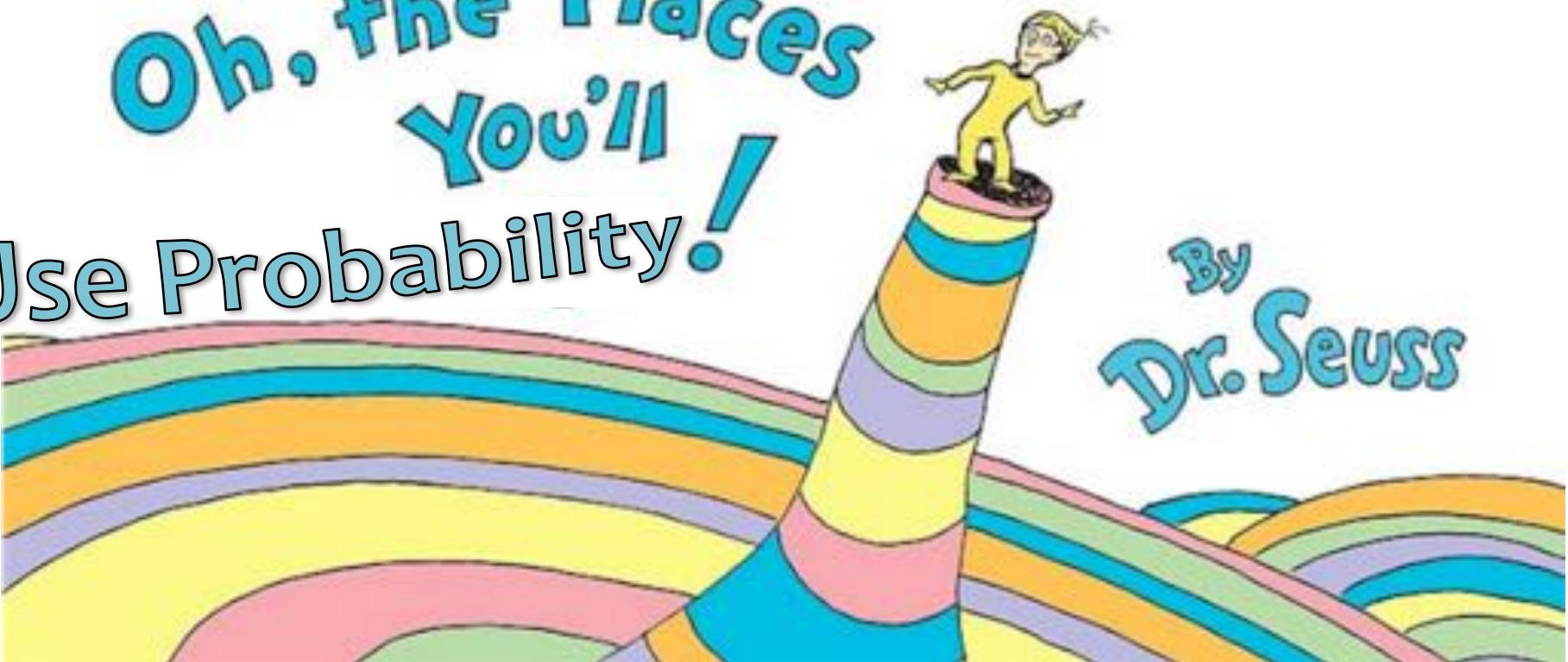
Prerequisites

What if you need additional review?

- Consider first taking 10-606/607: Mathematical/Computational Foundations for Machine Learning
- More details here:
<http://bit.ly/math4ml>



Oh, the Places
You'll
Use Probability!



By
Dr. Seuss

Oh, the Places You'll Use Probability!

Supervised Classification

- Naïve Bayes

$$p(y|x_1, x_2, \dots, x_n) = \frac{1}{Z} p(y) \prod_{i=1}^n p(x_i|y)$$

- Logistic regression

$$\begin{aligned} P(Y = y|X = x; \boldsymbol{\theta}) &= p(y|x; \boldsymbol{\theta}) \\ &= \frac{\exp(\boldsymbol{\theta}_y \cdot \mathbf{f}(x))}{\sum_{y'} \exp(\boldsymbol{\theta}_{y'} \cdot \mathbf{f}(x))} \end{aligned}$$

Note: This is just motivation – we'll cover these topics later!

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ML Theory

(Example: Sample Complexity)

- Goal: h has small error over D .

True error: $err_D(h) = \Pr_{x \sim D}(h(x) \neq c^*(x))$

How often $h(x) \neq c^*(x)$ over future instances drawn at random from D

- But, can only measure:

Training error: $err_S(h) = \frac{1}{m} \sum_i I(h(x_i) \neq c^*(x_i))$

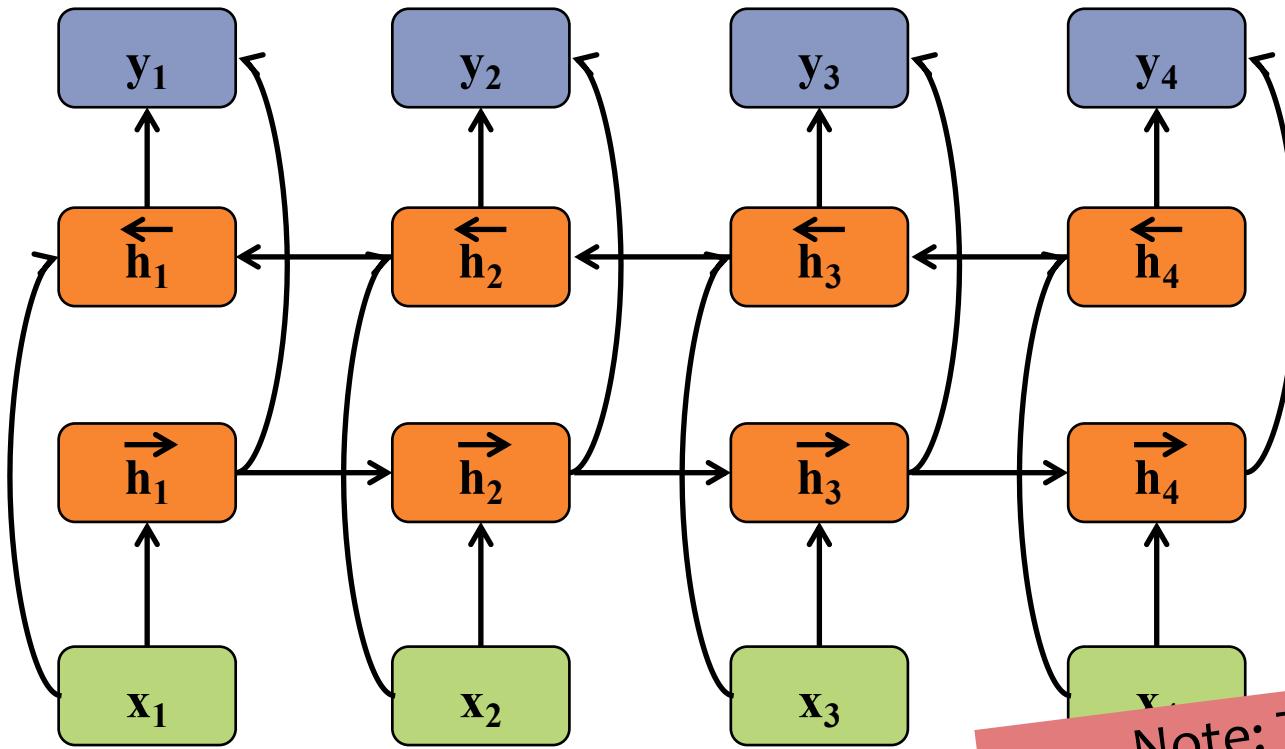
How often $h(x) \neq c^*(x)$ over training instances

Sample complexity: bound $err_D(h)$ in terms of $err_S(h)$

Note: This is just motivation – we'll cover these topics later!

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Deep Learning (Example: Deep Bi-directional RNN)

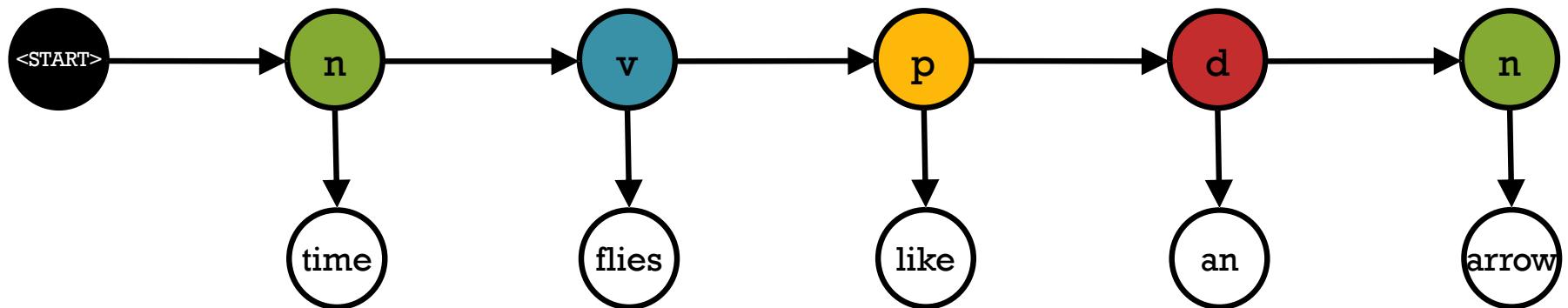


Note: This is just motivation – we'll cover these topics later!

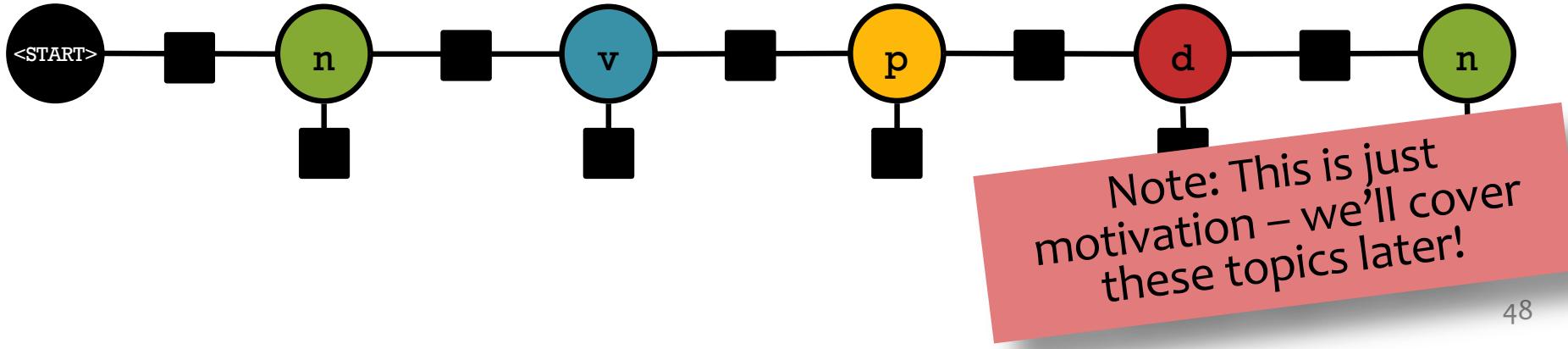
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Graphical Models

- Hidden Markov Model (HMM)



- Conditional Random Field (CRF)



Prerequisites

What if I'm not sure whether I meet them?

- Don't worry: we're not sure either
- However, we've designed a way to assess your background knowledge so that you know what to study!

(see instructions of Canvas portion of HW1)

Reminders

- **Homework 1: Background**
 - Out: Wed, Jan 16 (2nd lecture)
 - Due: Wed, Jan 23 at 11:59pm
 - Two parts:
 1. written part to Gradescope,
 2. programming part to Autolab
 - unique policy for this assignment:
 1. **two submissions** for written (see writeup for details)
 2. **unlimited submissions** for programming (i.e. keep submitting until you get 100%),

Learning Objectives

You should be able to...

1. Formulate a well-posed learning problem for a real-world task by identifying the task, performance measure, and training experience
2. Describe common learning paradigms in terms of the type of data available, when it's available, the form of prediction, and the structure of the output prediction
3. Implement Decision Tree training and prediction (w/simple scoring function)
4. Explain the difference between memorization and generalization [CIML]
5. Identify examples of the ethical responsibilities of an ML expert

Q&A