10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Course Overview

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Lecture 1
January 17, 2018

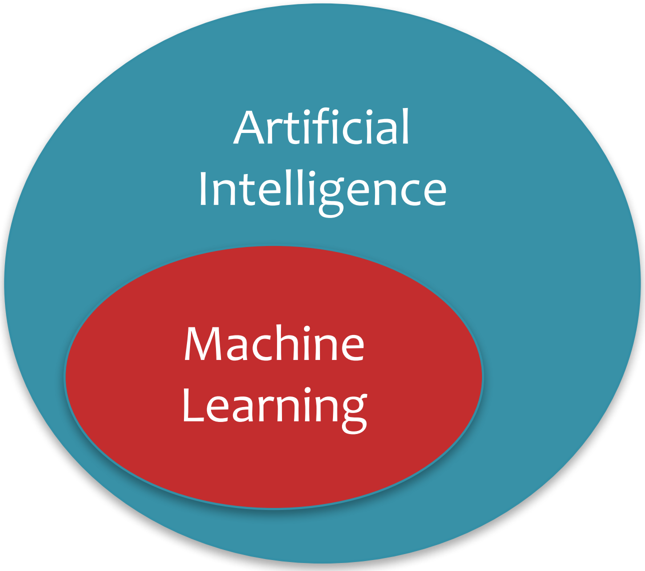
WHAT IS MACHINE LEARNING?

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

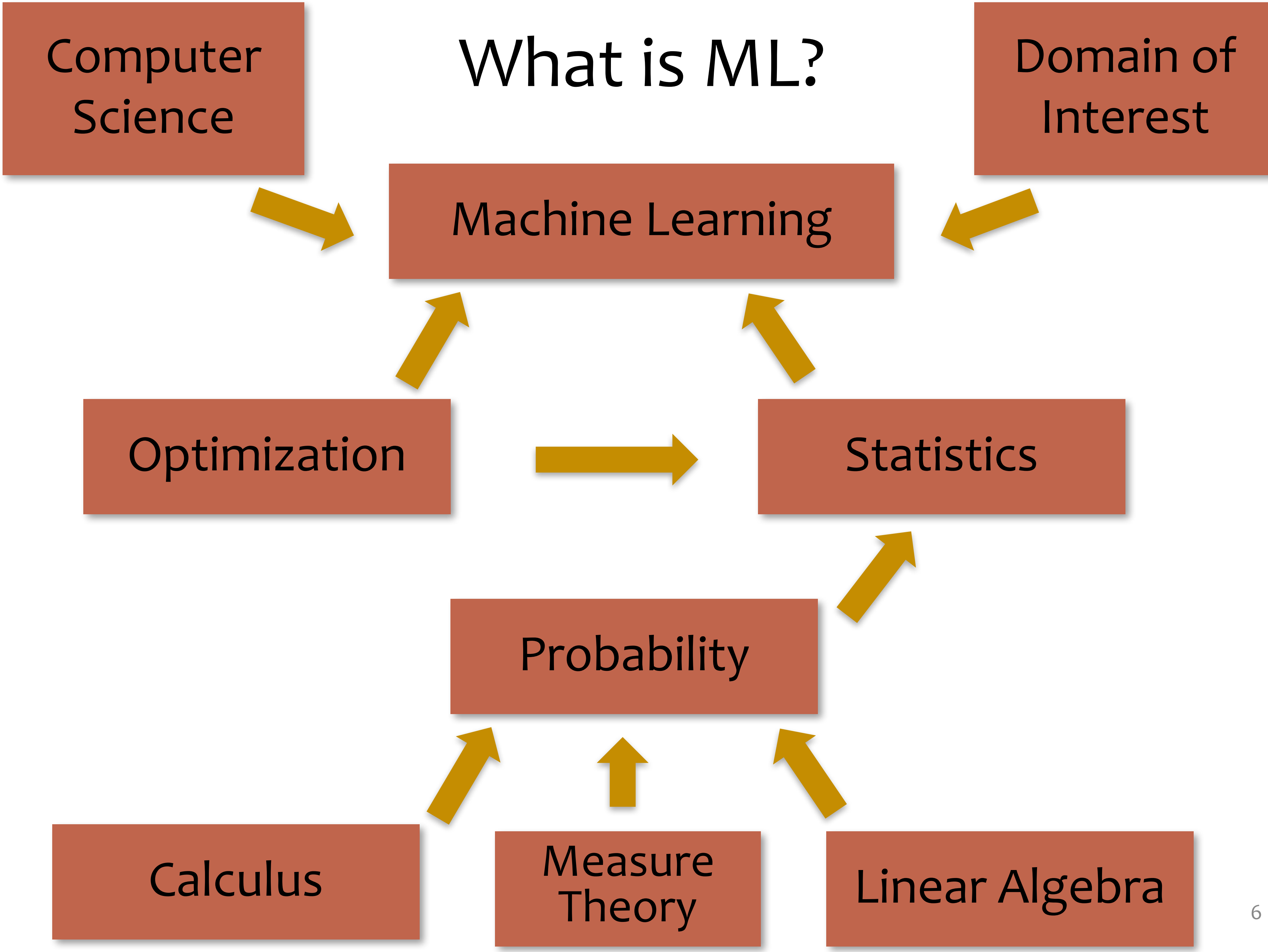
Statistics

Probability

Computer Science

Optimization

What is ML?


Computer Science
Domain of Interest
Machine Learning
Optimization
Statistics
Probability
Calculus
Measure Theory
Linear Algebra

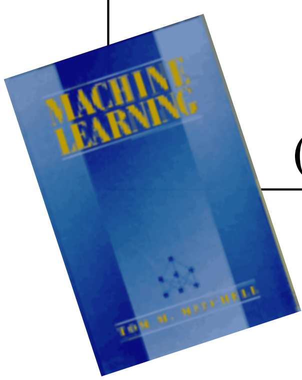
Speech Recognition

1. Learning to recognize spoken words

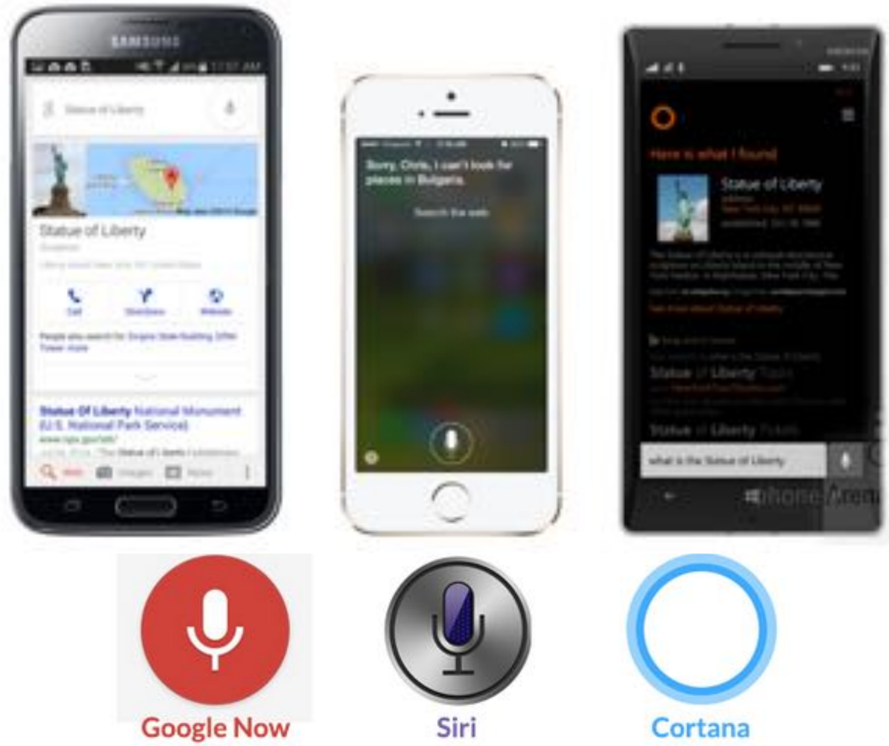
THEN

"…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)



NOW

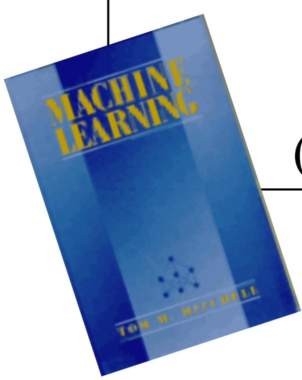


Source: https://www.stonetemple.com/great-knowledge-box-showdown/#VoiceStudyResults

Robotics

2. Learning to drive an autonomous vehicle

THEN	NOW
"…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



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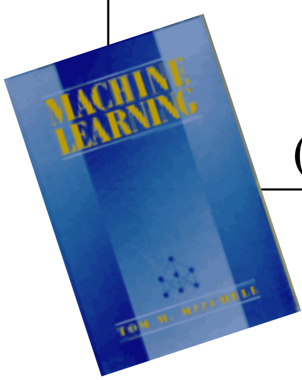


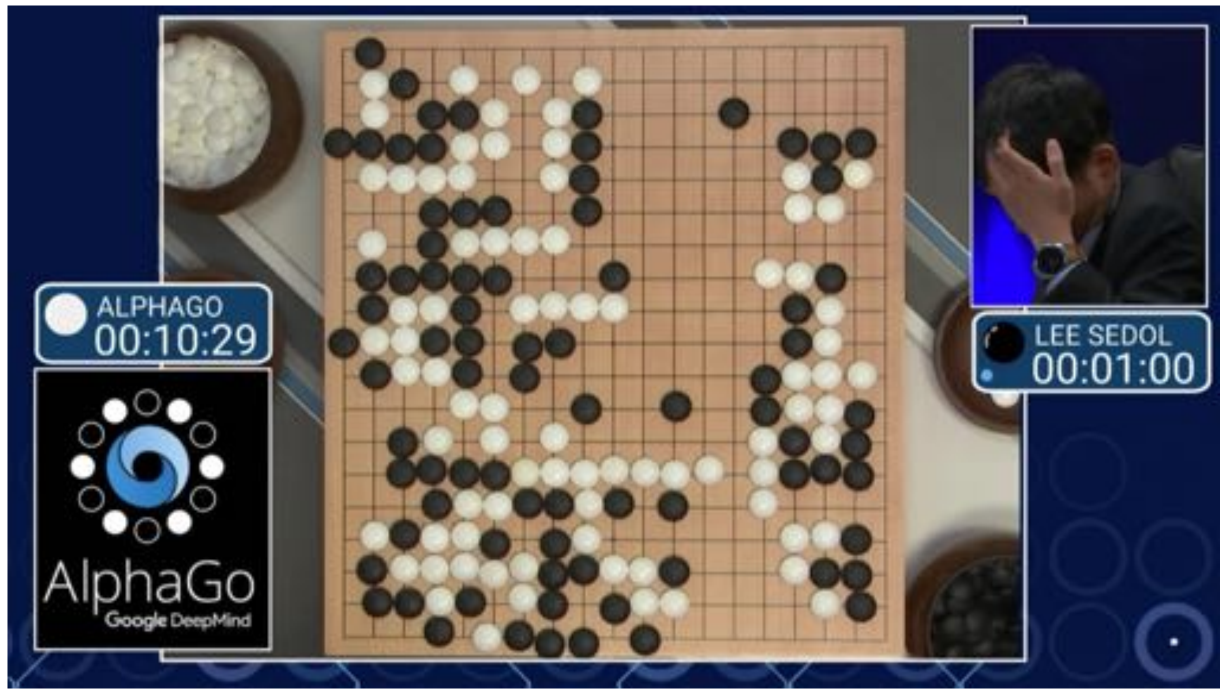
(Mitchell, 1997)

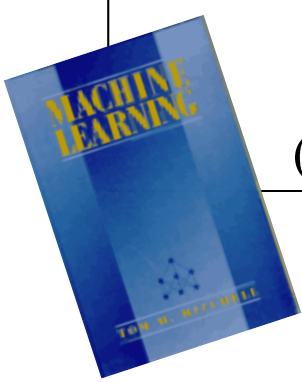
NOW

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

Games / Reasoning

3. Learning to beat the masters at board games

THEN	NOW
"…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…" (Mitchell, 1997)	



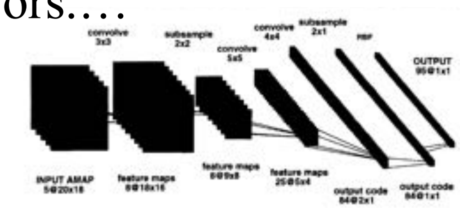
Computer Vision

4. Learning to recognize images

THEN	NOW

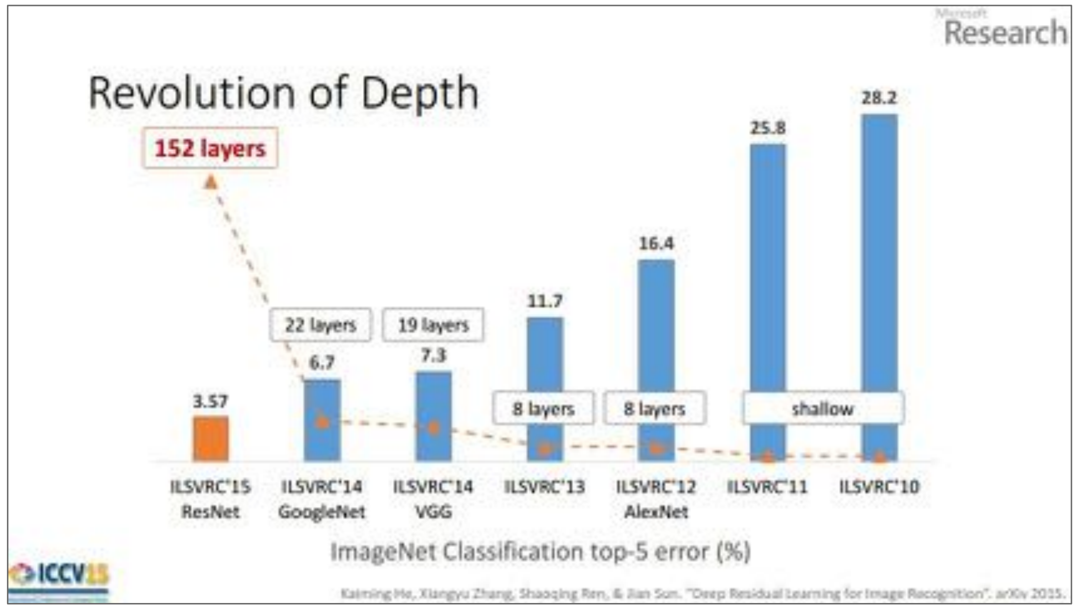
THEN

"…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)

NOW



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

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

Two Types of Error

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

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

② Train Error (aka. empirical risk)

$$\hat{R}(h) = P_{x \sim S}\left(c^*(x) \neq h(x)\right) \qquad S = \{x^{(1)}, \ldots, x^{(N)}\}$$

$$= \frac{1}{N}\sum_{i=1}^{N} \mathbb{1}\left(c^*(x^{(i)}) \neq h(x^{(i)})\right)$$

$$= \frac{1}{N}\sum_{i=1}^{N} \mathbb{1}\left(y^{(i)} \neq h(x^{(i)})\right)$$

known, computable

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 $R(h) \approx 0$ with high probability $Pr(R(h) \approx 0) \approx 1$

Def: PAC Criterion

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

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

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
- 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

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

Theoretical Foundations:

What principles guide learning?

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

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 *<T,P,E>***:**

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*.

Definition from (Mitchell, 1997)

Example Learning Problems

3. Learning to beat the masters at **chess**
   1. Task, *T*:

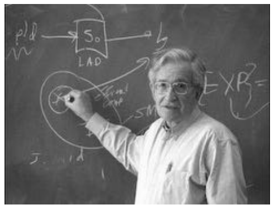
   2. Performance measure, *P*:

   3. Experience, *E*:

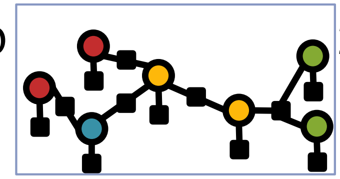
Example Learning Problems

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

Capturing the Knowledge of Experts

1980 

1990 

2000 

2010

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))`

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

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 $\{x_1, \ldots, x_n\}$
2. Experts annotate their meaning $\{y_1, \ldots, y_n\}$

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)

Examples from Roni Rosenfeld

ML as Function Approximation

Chalkboard

- ML as Function Approximation
  - Problem setting
  - Input space
  - Output space
  - Unknown target function
  - Hypothesis space
  - Training examples

Machine Learning & Ethics

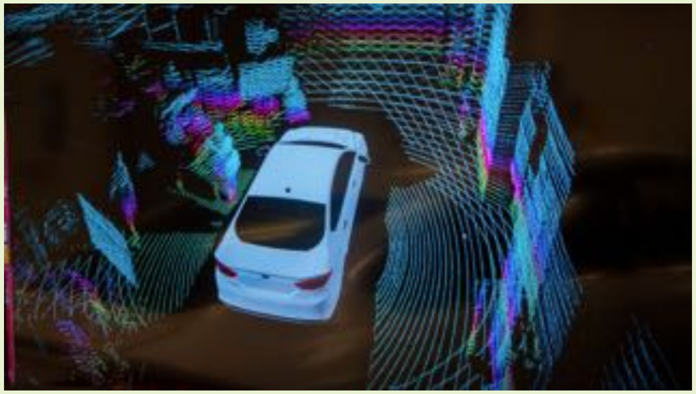
What ethical responsibilities do we have as machine learning experts?

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-s18

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

Syllabus Highlights

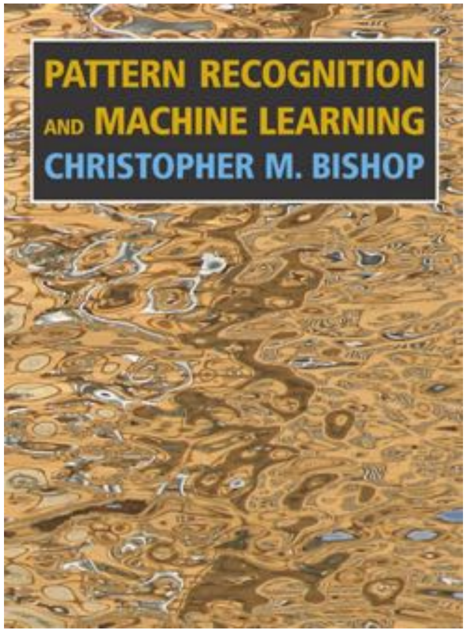
- **Grading**: 45% homework, 25% midterm exam, 30% final exam
- **Midterm Exam**: evening exam, March 22, 2018
- **Final Exam**: final exam week, date TBD
- **Homework**: ~5 written and ~5 programming
  - 4 grace days for programming assignments only
  - Late submissions: 80% day 1, 60% day 2, 40% day 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

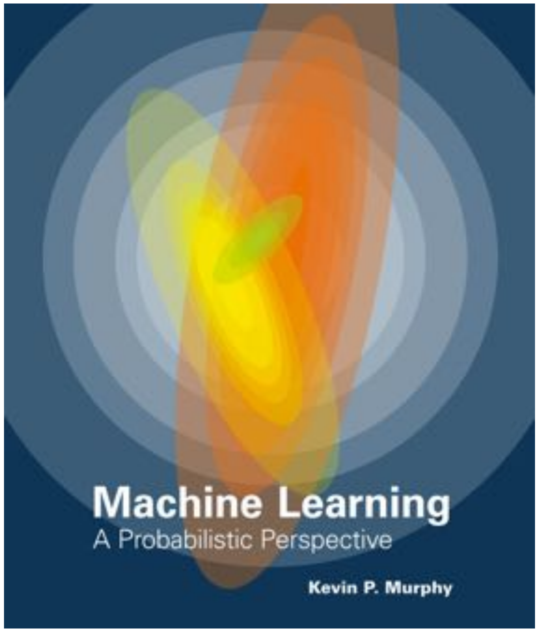
Lectures

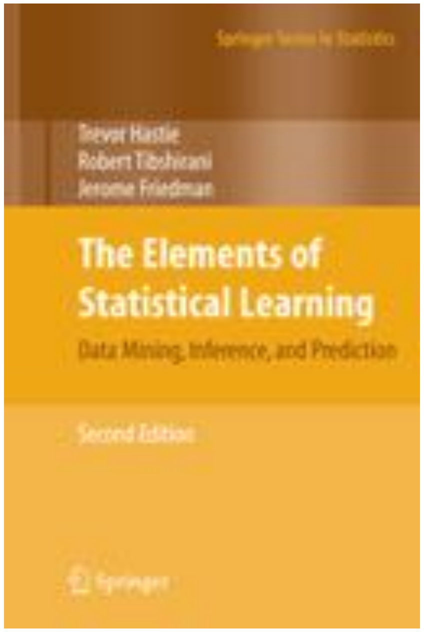
- You should ask lots of questions
  - Interrupting (by raising a hand) to ask your question is strongly encouraged
  - Asking questions later (or in real time) on Piazza is also great
- When I ask a question…
  - I want you to answer
  - Even if you don’t answer, think it through as though I’m about 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


Oh, the Places
You'll
Use Probability!
By
Dr. Seuss

Oh, the Places You'll Use Probability!

Supervised Classification

- Naïve Bayes

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

- 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!

Oh, the Places You'll Use Probability!

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

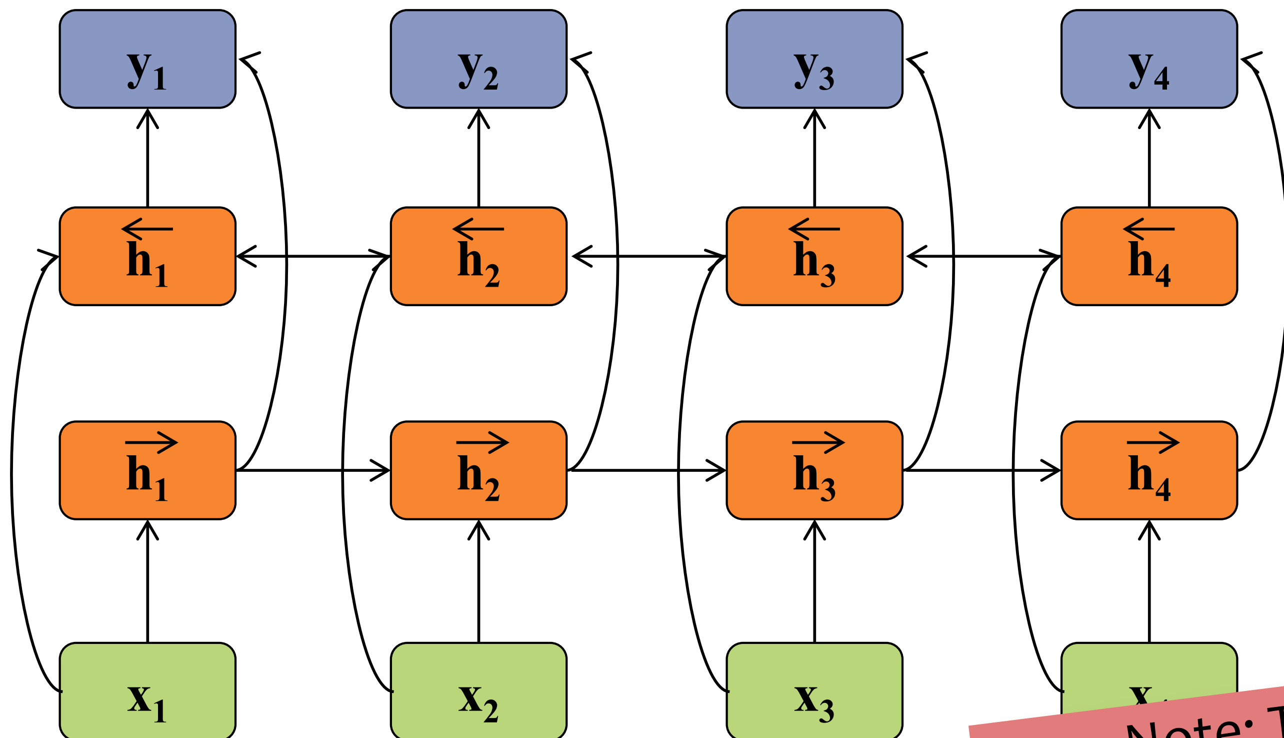
Sample complexity: bound $err_D(h)$ in terms of $err_S(h)$

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

Oh, the Places You'll Use Probability!

Deep Learning

(Example: Deep Bi-directional RNN)



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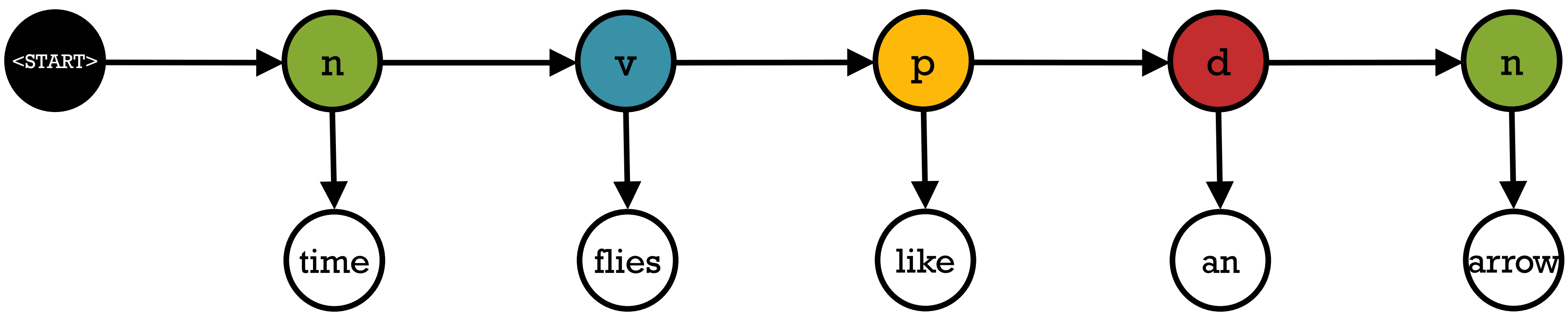
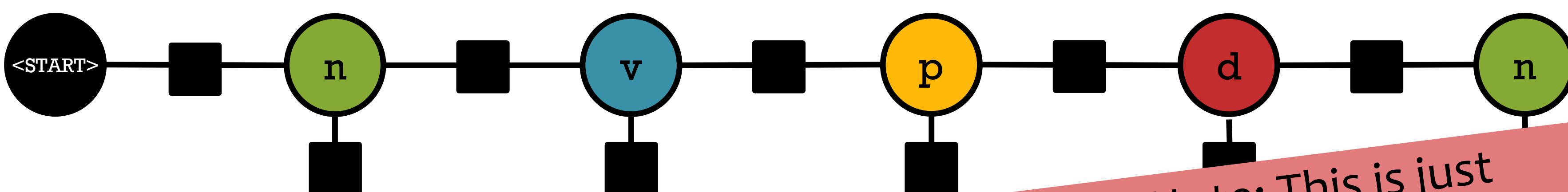
Oh, the Places You’ll Use Probability!

Graphical Models

- Hidden Markov Model (HMM)



- Conditional Random Field (CRF)



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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 17 (today)**
  - **Due: Wed, Jan 24 at 11:59pm**
  - Two parts: written part on Canvas, programming part on Autolab
  - unique policy for this assignment: **unlimited submissions** (i.e. keep submitting until you get 100%)

DECISION TREES

Decision Trees

Chalkboard

- Example: Medical Diagnosis
- Does memorization = learning?
- Decision Tree as a hypothesis
- Function approximation for DTs
- Decision Tree Learning

Tree to Predict C-Section Risk

Learned from medical records of 1000 women (Sims et al., 2000)

Negative examples are C-sections

```
[833+,167-] .83+ .17-
Fetal_Presentation = 1: [822+,116-] .88+ .12-
| Previous_Csection = 0: [767+,81-] .90+ .10-
| | Primiparous = 0: [399+,13-] .97+ .03-
| | Primiparous = 1: [368+,68-] .84+ .16-
| | | Fetal_Distress = 0: [334+,47-] .88+ .12-
| | | | Birth_Weight < 3349: [201+,10.6-] .95+ .
| | | | Birth_Weight >= 3349: [133+,36.4-] .78+
| | | Fetal_Distress = 1: [34+,21-] .62+ .38-
| Previous_Csection = 1: [55+,35-] .61+ .39-
Fetal_Presentation = 2: [3+,29-] .11+ .89-
Fetal_Presentation = 3: [8+,22-] .27+ .73-
```

Figure from Tom Mitchell

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
5. Identify examples of the ethical responsibilities of an ML expert