

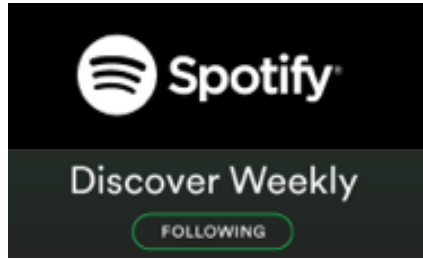


Machine Learning CSE546

Kevin Jamieson

University of Washington

September 28, 2017

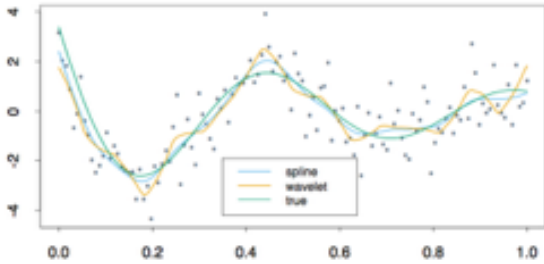


You may also like...

ML uses past data to make personalized predictions

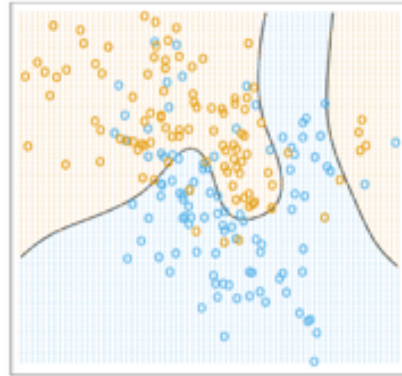


Flavors of ML



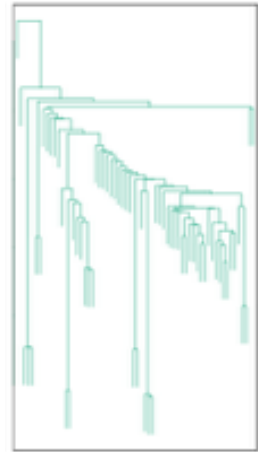
Regression

Predict continuous value:
ex: stock market, credit score,
temperature, Netflix rating



Classification

Predict categorical value:
loan or not? spam or not?
what disease is this?



Unsupervised Learning

Predict structure:
tree of life from DNA,
find similar images,
community detection

Mix of statistics (theory) and algorithms (programming)

Machine Learning Ingredients

- **Data:** past observations
- **Hypotheses/Models:** devised to capture the patterns in data
 - Does not have to be correct, just close enough to be useful
- **Prediction:** apply model to forecast future observations

Why is Machine Learning so popular, now?

- **“Big” Data:** the proliferation of the internet and smart phones has created consumer opportunities that *scale* (\$\$\$\$\$)
- **Computing:** powerful, reliable, commoditized resources
- **Capitalism:** gives companies an edge (e.g., hedge funds)

Growth of Machine Learning

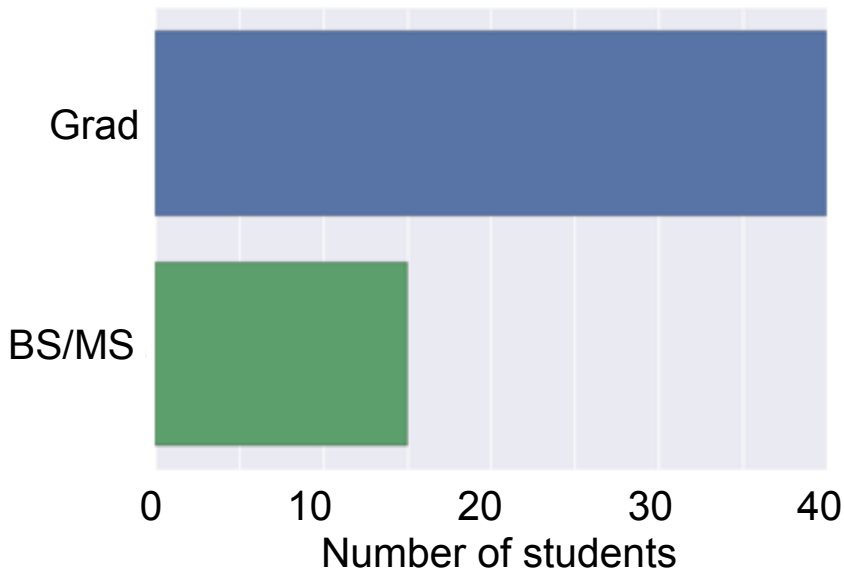
One of the most sought for specialties in industry today.

- Machine learning is preferred approach to
 - Speech recognition, Natural language processing
 - Computer vision
 - Medical outcomes analysis
 - Robot control
 - Computational biology
 - Sensor networks
 - ...
- This trend is accelerating, especially with **Big Data**
 - Improved machine learning algorithms
 - Improved data capture, networking, faster computers
 - Software too complex to write by hand
 - New sensors / IO devices
 - Demand for self-customization to user, environment

Syllabus

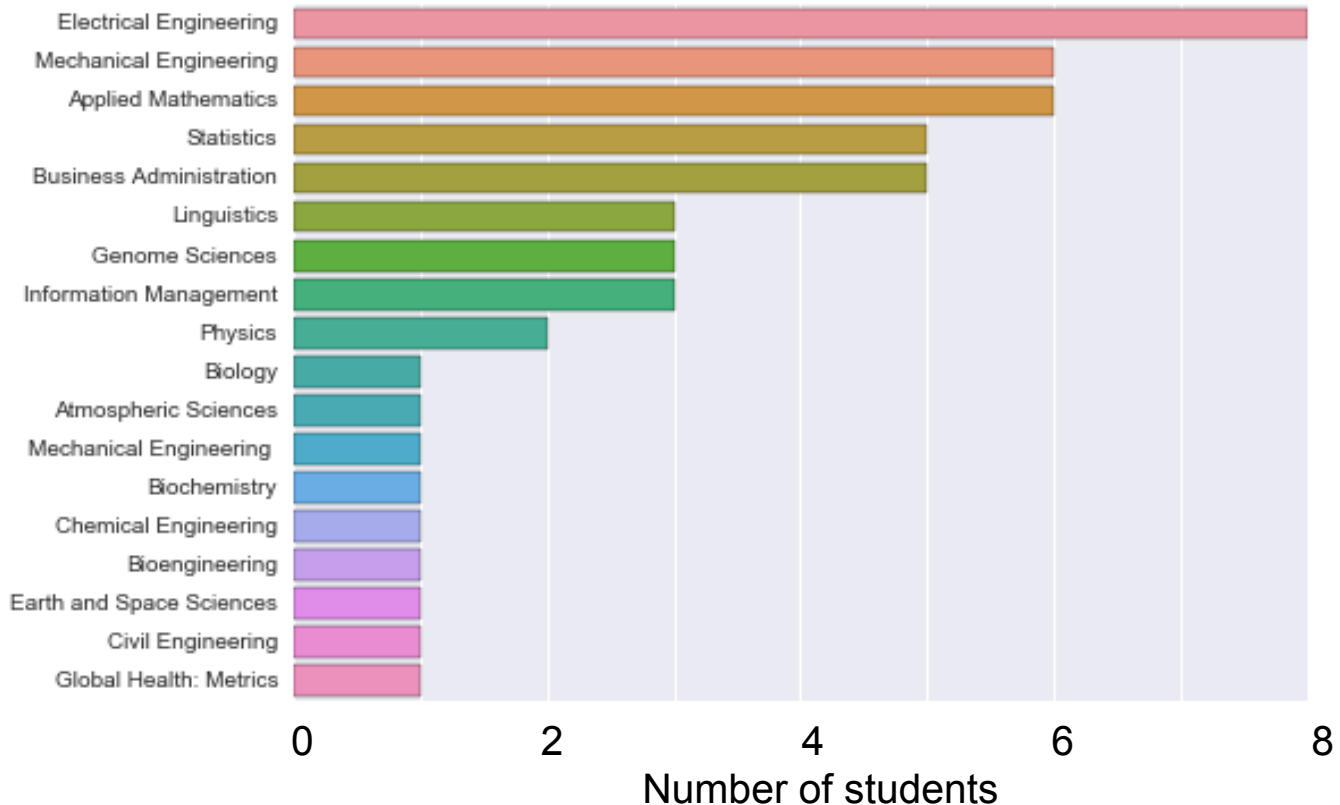
- Covers a wide range of Machine Learning techniques – from basic to state-of-the-art
- You will learn about the methods you heard about:
 - Point estimation, regression, logistic regression, optimization, nearest-neighbor, decision trees, boosting, perceptron, overfitting, regularization, dimensionality reduction, PCA, error bounds, SVMs, kernels, margin bounds, K-means, EM, mixture models, HMMs, graphical models, deep learning, reinforcement learning...
- Covers algorithms, theory and applications
- **It's going to be fun and hard work.**

Student makeup: CSE 55%



About 55 CSE students
(total expected class size)

Student makeup: Non-CSE 45%



Welcome. You may also consider CSE 416 offered in the Spring.

Prerequisites

- Formally:
 - STAT 341, STAT 391, or equivalent
- Probability + statistics
 - Distributions, densities, marginalization, moments
- Math
 - Linear algebra, multivariate calculus
- Algorithms
 - Basic data structures, complexity
- Programming
 - Python
 - LaTeX
- Quick poll...

- **See website for review materials!**

Staff



- Four Great TAs: They are great resources in addition to the discussion board
 - **Nancy Wang:** Monday 4:00-5:00 PM, CSE 220
 - **Yao Lu:** Tuesday 2:30-3:30 PM, CSE 220
 - **Aravind Rajeswaran:** Wednesday 3:00-4:00 PM, CSE 220
 - **Dae Hyun Lee:** Thursday 1:30-2:30 PM, CSE 007
- Check Canvas Discussion board for exceptions/updates

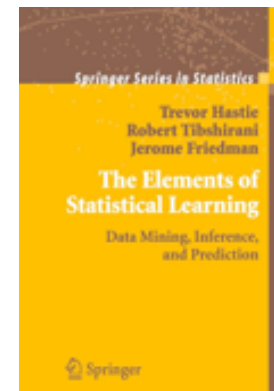
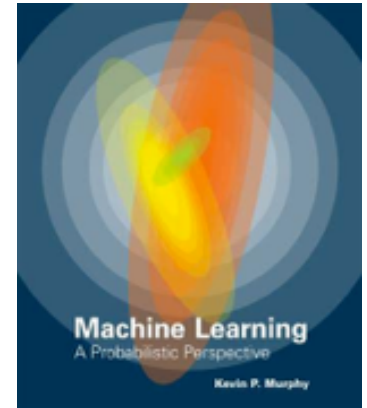
Communication Channels

- **Canvas Discussion board**
 - Announcements (e.g., office hours, due dates, etc.)
 - Questions (logistical or homework) - please participate and help others
 - All non-personal questions should go here
- For e-mailing instructors about personal issues and grading use:
 - cse546-instructors@cs.washington.edu
- Office hours limited to knowledge based questions. Use email for all grading questions.

Text Books

- Required Textbook:
 - ***Machine Learning: a Probabilistic Perspective;***
Kevin Murphy

- Optional Books (free PDF):
 - *The Elements of Statistical Learning: Data Mining, Inference, and Prediction;* Trevor Hastie, Robert Tibshirani, Jerome Friedman



Grading

- 5 homeworks (65%)
 - Each contains both theoretical questions and will have programming
 - Collaboration okay. You must write, submit, and understand your answers and code (which we may run)
 - Do not Google for answers.
- Final project (35%)
 - An ML project of your choice that uses real data
 - 1. Code must be written in Python**
 - 2. Written work must be typeset using LaTeX**

See website for tutorials... otherwise Google it.

Homeworks

- HW 0 is out (10 points, **Due next Thursday**)
 - Short and easy, gets you using Python and LaTeX
- HW 1,2,3,4 (25 points each)
 - They are not easy or short. Start early.
- Grade is minimum of the summed points and 100 points.
- **There is no credit for late work, receives 0 points.**
- **You must turn in all 5 assignments (even if late for 0 points) or else you will not pass.**

Projects (35%)

- An opportunity/intro for research in machine learning
- Grading:
 - We seek some novel exploration.
 - If you write your own code, great. We takes this into account for grading.
 - You may use ML toolkits (e.g. TensorFlow, etc), then we expect more ambitious project (in terms of scope, data, etc).
 - If you use simpler/smaller datasets, then we expect a more involved analysis.
- Individually or groups of two or three.
 - If in a group, the expectation are much
- Must involve real data
 - Must be data that you have available to you by the time of the project proposals
- It's encouraged to be related to your research, but must be something new you did this quarter
 - Not a project you worked on during the summer, last year, etc.
 - You also must have the data right now.

Enjoy!



- ML is becoming ubiquitous in science, engineering and beyond
- It's one of the hottest topics in industry today
- This class should give you the basic foundation for applying ML and developing new methods
- The fun begins...



Maximum Likelihood Estimation

Machine Learning – CSE546

Kevin Jamieson

University of Washington

September 28, 2017

Your first consulting job

- *Billionaire*: I have special coin, if I flip it, what's the probability it will be heads?
- *You*: Please flip it a few times:

HH T HT

- *You*: The probability is: $\frac{3}{5}$
- *Billionaire*: Why?

Maximum Likelihood Estimation

- **Data:** sequence $D = (HHTHT\dots)$, **k heads** out of **n flips**
- **Hypothesis:** $P(\text{Heads}) = \theta$, $P(\text{Tails}) = 1 - \theta$

$$P(\mathcal{D}|\theta) = \theta^k (1 - \theta)^{n-k}$$

- Maximum likelihood estimation (MLE): Choose θ that maximizes the probability of observed data:

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} P(\mathcal{D}|\theta) \\ &= \arg \max_{\theta} \log P(\mathcal{D}|\theta)\end{aligned}$$

Your first learning algorithm

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} \log P(\mathcal{D}|\theta) \\ &= \arg \max_{\theta} \log \theta^k (1 - \theta)^{n-k}\end{aligned}$$

- Set derivative to zero:

$$\frac{d}{d\theta} \log P(\mathcal{D}|\theta) = 0$$

$$\frac{2}{20} [k \log(\theta) + (n-k) \log(1-\theta)]$$

$$= \frac{k}{\theta} - \frac{n-k}{1-\theta} = 0$$

$$k(1-\theta) - (n-k)\theta = 0$$

$$k - \theta n = 0 \quad \hat{\theta}_{MLE} = k/n$$

How many flips do I need?

$$\hat{\theta}_{MLE} = \frac{k}{n}$$

- *You*: flip the coin 5 times. *Billionaire*: I got 3 heads.

$$\hat{\theta}_{MLE} = 3/5$$

- *You*: flip the coin 50 times. *Billionaire*: I got 20 heads.

$$\hat{\theta}_{MLE} = 20/50 = 2/5$$

- *Billionaire*: Which one is right? Why?

Simple bound *If R.V. X has density $f(x)$ then* (based on Hoeffding's inequality) $\mathbb{E}[g(x)]$ *$= \int g(x)f(x)dx$*

- For n flips and k heads the MLE is unbiased for true θ^* :

$$\hat{\theta}_{MLE} = \frac{k}{n} \quad \mathbb{E}[\hat{\theta}_{MLE}] = \theta^*$$

- Hoeffding's inequality says that for any $\epsilon > 0$:

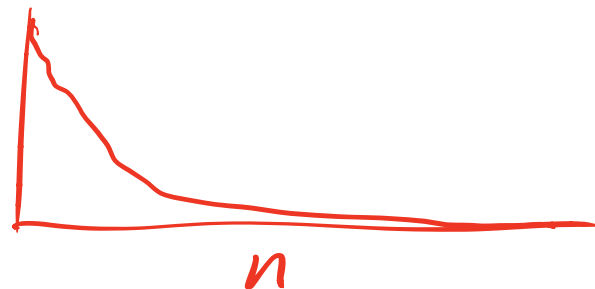
$$P(|\hat{\theta}_{MLE} - \theta^*| \geq \epsilon) \leq 2e^{-2n\epsilon^2}$$

$n=5$
 $\frac{2}{5}$

$n=50$
 $\frac{3}{5}$

$\epsilon=0.05$

$P(\cdot)$



PAC Learning

- PAC: Probably Approximate Correct
- *Billionaire*: I want to know the parameter θ^* , within $\epsilon = 0.1$, with probability at least $1 - \delta = 0.95$. How many flips?

$$P(|\hat{\theta}_{MLE} - \theta^*| \geq \epsilon) \leq 2e^{-2n\epsilon^2} = \delta$$

$$\epsilon = \sqrt{\frac{\log(2/\delta)}{2n}}$$

Solve for epsilon

$$\text{w.p.} \geq 1 - \delta$$

$$|\hat{\theta}_{MLE} - \theta^*| \leq \sqrt{\frac{\log(2/\delta)}{2n}} = 0.1$$

What about continuous variables?

- *Billionaire*: What if I am measuring a **continuous variable**?
- **You**: Let me tell you about **Gaussians...**

$$X \stackrel{iid}{\sim} P(x | \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$X \sim \mathcal{N}(\mu, \sigma)$$

Some properties of Gaussians

- affine transformation (multiplying by scalar and adding a constant)
 - $X \sim N(\mu, \sigma^2)$
 - $Y = aX + b \rightarrow Y \sim N(a\mu + b, a^2\sigma^2)$

- Sum of Gaussians
 - $X \sim N(\mu_X, \sigma_X^2)$
 - $Y \sim N(\mu_Y, \sigma_Y^2)$
 - $Z = X + Y \rightarrow Z \sim N(\mu_X + \mu_Y, \sigma_X^2 + \sigma_Y^2)$

MLE for Gaussian

- Prob. of i.i.d. samples $D=\{x_1, \dots, x_N\}$ (e.g., exam scores):

$$\begin{aligned} P(D|\mu, \sigma) &= P(x_1, \dots, x_n|\mu, \sigma) = \prod_{i=1}^n \left(\frac{1}{\sqrt{2\pi}\sigma} \right) e^{-\frac{(x_i - \mu)^2}{2\sigma^2}} \\ &= \left(\frac{1}{\sigma\sqrt{2\pi}} \right)^n \prod_{i=1}^n e^{-\frac{(x_i - \mu)^2}{2\sigma^2}} \end{aligned}$$

- Log-likelihood of data:

$$\log P(D|\mu, \sigma) = -n \log(\sigma\sqrt{2\pi}) - \sum_{i=1}^n \frac{(x_i - \mu)^2}{2\sigma^2}$$

Your second learning algorithm: MLE for mean of a Gaussian

- What's MLE for mean?

$$\frac{d}{d\mu} \log P(\mathcal{D}|\mu, \sigma) = \frac{d}{d\mu} \left[\underbrace{-n \log(\sigma\sqrt{2\pi})}_{\text{constant}} - \sum_{i=1}^n \frac{(x_i - \mu)^2}{2\sigma^2} \right]$$

$$= - \sum_{i=1}^n \frac{d}{d\mu} \frac{(x_i - \mu)^2}{2\sigma^2}$$

$$= + \sum_{i=1}^n \frac{(x_i - \mu)}{\sigma^2} \rightarrow 0$$

$$\frac{1}{n} \sum_{i=1}^n (x_i - \mu) = 0$$
$$\hat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^n x_i$$

MLE for variance

$$\log(ab) = \log(a) + \log(b)$$

- Again, set derivative to zero:

$$\frac{d}{d\sigma} \log P(D|\mu, \sigma) = \frac{d}{d\sigma} \left[-n \log(\sigma\sqrt{2\pi}) - \sum_{i=1}^n \frac{(x_i - \mu)^2}{2\sigma^2} \right]$$

$$= -\frac{n}{\sigma} + \sum_{i=1}^n \frac{(x_i - \mu)^2}{\sigma^3} = 0$$

both sides
mult by $\frac{\sigma^3}{n}$

$$-n\sigma^2 + \sum_i (x_i - \mu)^2 = 0$$

$$\hat{\sigma}_{MLE}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu}_{MLE})^2$$

Learning Gaussian parameters

MLE:

$$\hat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^n x_i \quad \mathbb{E}[\hat{\mu}_{MLE}] = \mu$$

$$\hat{\sigma}^2_{MLE} = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu}_{MLE})^2$$

- MLE for the variance of a Gaussian is **biased**

$$\mathbb{E}[\hat{\sigma}^2_{MLE}] \neq \sigma^2$$

- Unbiased variance estimator:

$$\hat{\sigma}^2_{unbiased} = \frac{1}{n-1} \sum_{i=1}^n (x_i - \hat{\mu}_{MLE})^2$$

Recap

- Learning is...
 - Collect some data
 - E.g., coin flips
 - Choose a hypothesis class or model
 - E.g., binomial
 - Choose a loss function
 - E.g., data likelihood
 - Choose an optimization procedure
 - E.g., set derivative to zero to obtain MLE
 - Justifying the accuracy of the estimate
 - E.g., Hoeffding's inequality