http://www.cs.cmu.edu/~guestrin/Class/10701/

What's learning? Point Estimation

Machine Learning – 10701/15781
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What is Machine Learning ?

Machine Learning

Study of algorithms that

- improve their performance
- at some task
- with experience

Object detection

(Prof. H. Schneiderman)

Example training images
for each orientation

Text classification

Company home page

vs

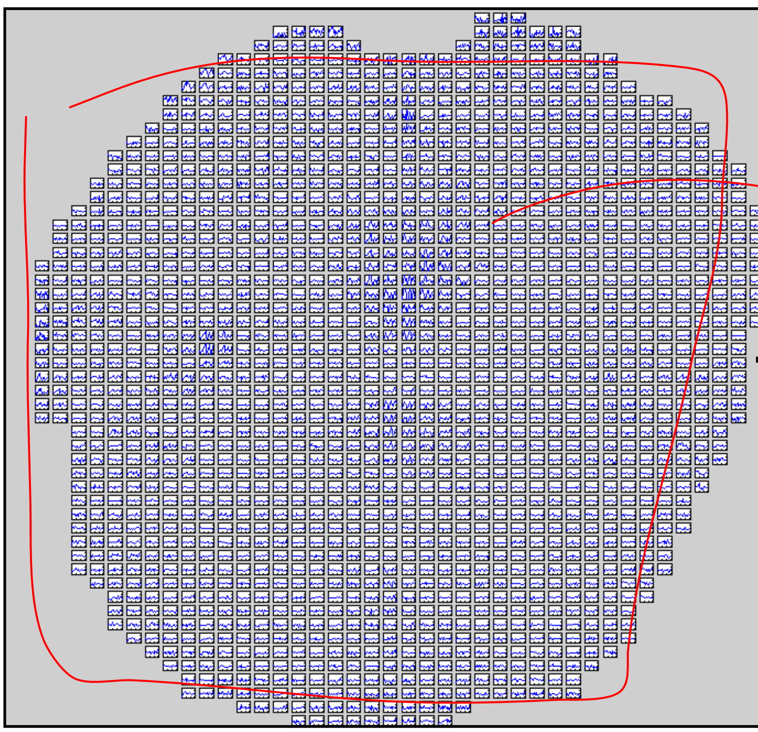
Personal home page

vs

Univeristy home page

vs

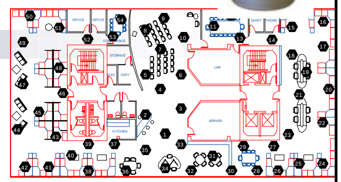
…

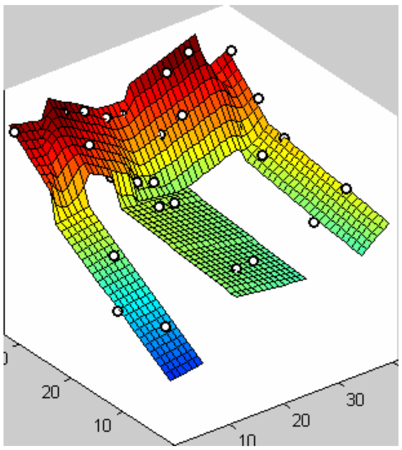


Reading a noun (vs verb)

[Rustandi et al., 2005]

Modeling sensor data





- Measure temperatures at some locations
- Predict temperatures throughout the environment

[Guestrin et al. '04]

Learning to act

- Reinforcement learning
- An agent
  - Makes sensor observations
  - Must select action
  - Receives rewards
    - positive for "good" states
    - negative for "bad" states

[Ng eat al. '05]

Growth of Machine Learning

- 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
  - 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:
  - Naïve Bayes, logistic regression, nearest-neighbor, decision trees, boosting, neural nets, overfitting, regularization, dimensionality reduction, PCA, error bounds, VC dimension, SVMs, kernels, margin bounds, K-means, EM, mixture models, semi-supervised learning, HMMs, graphical models, active learning, reinforcement learning…
- Covers algorithms, theory and applications
- **It's going to be fun and hard work ☺**

Prerequisites

- Probabilities
  - Distributions, densities, marginalization…
- Basic statistics
  - Moments, typical distributions, regression…
- Algorithms
  - Dynamic programming, basic data structures, complexity…
- Programming
  - Mostly your choice of language, but Matlab will be very useful
- We provide some background, but the class will be fast paced
- Ability to deal with "abstract mathematical concepts"

Recitations

- Very useful!
  - Review material
  - Present background
  - Answer questions
- Thursdays, 5:00-6:20 in Wean Hall 5409
- Special recitation 1:
  - **tomorrow, Wean 5409, 5:00-6:20**
  - Review of probabilities
- Special recitation 2 on Matlab
  - Tuesday, Sept. 18th 4:30-5:50pm NSH 3002

Staff

- Four Great TAs: Great resource for learning, interact with them!
  - **Joseph Gonzalez**, Wean 5117, x8-3046, jegonzal@cs, Office hours: Tuesdays 7-9pm
  - **Steve Hanneke**, Doherty 4301H, x8-7375, shanneke@cs, Office hours: Fridays 1-3pm
  - **Jingrui He**, Wean 8102, x8-1299, jingruih@cs, Office hours: Wednesdays 11-1pm
  - **Sue Ann Hong,** Wean 4112, x8-3047, sahong@cs, Office hours: Tuesdays 3-5pm
- Administrative Assistant
  - Monica Hopes, x8-5527, meh@cs

First Point of Contact for HWs

- To facilitate interaction, a TA will be assigned to each homework question – This will be your "first point of contact" for this question
  - But, you can always ask any of us
- For e-mailing instructors, always use:
  - 10701-instructors@cs.cmu.edu
- For announcements, subscribe to:
  - 10701-announce@cs
  - https://mailman.srv.cs.cmu.edu/mailman/listinfo/10701-announce

Text Books

- Required Textbook:
  - Pattern Recognition and Machine Learning; Chris Bishop
- Optional Books:
  - Machine Learning; Tom Mitchell
  - The Elements of Statistical Learning: Data Mining, Inference, and Prediction; Trevor Hastie, Robert Tibshirani, Jerome Friedman
  - Information Theory, Inference, and Learning Algorithms; David MacKay

Grading

- 5 homeworks (35%)
  - First one goes out 9/12
    - Start early, Start early, Start early, Start early, Start early, Start early, Start early, Start early, Start early, Start early
- Final project (25%)
  - Details out around Oct. 1st
  - Projects done individually, or groups of two students
- Midterm (15%)
  - Thu., Oct 25 5-6:30pm
  - location: MM A14
- Final (25%)
  - TBD by registrar

Homeworks

- Homeworks are hard, start early ☺
- Due in the beginning of class
- 3 late days for the semester
- After late days are used up:
  - Half credit within 48 hours
  - Zero credit after 48 hours
- All homeworks **must be handed in**, even for zero credit
- Late homeworks handed in to Monica Hopes, WEH 4619

- Collaboration
  - You may **discuss** the questions
  - Each student writes their own answers
  - Write on your homework anyone with whom you collaborate
  - Each student must write their own code for the programming part
  - **Please don't search for answers on the web, Google, previous years' homeworks, etc.**
    - please ask us if you are not sure if you can use a particular reference

Sitting in & Auditing the Class

- Due to new departmental rules, every student who wants to sit in the class (not take it for credit), must register officially for auditing
- To satisfy the auditing requirement, you must either:
  - Do *two* homeworks, and get at least 75% of the points in each; or
  - Take the final, and get at least 50% of the points; or
  - Do a class project and do *one* homework, and get at least 75% of the points in the homework;
    - Only need to submit project proposal and present poster, and get at least 80% points in the poster.
- Please, send us an email saying that you will be auditing the class and what you plan to do.
- If you are not a student and want to sit in the class, please get authorization from the instructor

Enjoy!

- ML is becoming ubiquitous in science, engineering and beyond
- This class should give you the basic foundation for applying ML and developing new methods
- The fun begins…

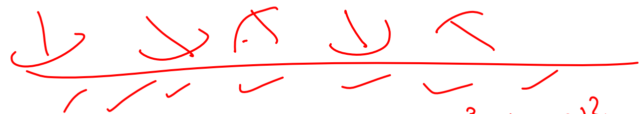
Your first consulting job

- A billionaire from the suburbs of Seattle asks you a question:
  - He says: I have thumbtack, if I flip it, what's the probability it will fall with the nail up?
  - You say: Please flip it a few times:

  - You say: The probability is: $\frac{3}{5}$
  - **He says: Why???**
  - You say: Because…

Thumbtack – Binomial Distribution

- P(Heads) = θ, P(Tails) = 1-θ



$P(HHTHT) = \theta^3 (1-\theta)^2 = \theta\theta(1-\theta)\theta(1-\theta)$

- Flips are i.i.d.:
  - Independent events
  - Identically distributed according to Binomial distribution
- Sequence *D* of α_H Heads and α_T Tails

$$P(\overset{HHTHT}{\mathcal{D}} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

MLE

Maximum Likelihood Estimation

- **Data:** Observed set *D* of α_H Heads and α_T Tails
- **Hypothesis:** Binomial distribution
- Learning θ is an optimization problem
  - What's the objective function?

θ that make $P(D = \{HHTHT\} \mid \theta)$ as likely as possible

- MLE: Choose θ that maximizes the probability of observed data:

$$\begin{aligned} \hat{\theta} &= \arg\max_{\theta} \; P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \; \ln P(\mathcal{D} \mid \theta) \end{aligned}$$

ln is monotonic

log likelihood

Your first learning algorithm

$\log a \cdot b = \log a + \log b$

$\log a^b = b \log a$

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} \ \ln P(\mathcal{D} \mid \theta)$$
$$= \arg\max_{\theta} \ \ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

$\frac{d}{d\theta} \ln \theta = \frac{1}{\theta}$

$\frac{d}{d\theta} \cdot \ln(1-\theta) = \frac{-1}{1-\theta}$

- Set derivative to zero: $\boxed{\frac{d}{d\theta} \ln P(\mathcal{D} \mid \theta) = 0}$

$\frac{d}{d\theta}\left[\ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\right]$

$= \frac{d}{d\theta}\left[\alpha_H \ln\theta + \alpha_T \log(1-\theta)\right]$

$= \alpha_H \frac{d}{d\theta}\ln\theta + \alpha_T \frac{d\ln(1-\theta)}{d\theta}$

$\frac{\alpha_H}{\theta} - \frac{\alpha_T}{1-\theta} = 0$

$\Rightarrow \alpha_H - \theta\alpha_H = \theta\alpha_T$

$\hat{\theta} = \frac{\alpha_H}{\alpha_H + \alpha_T}$

$\alpha_H = 3$

$\alpha_T = 2$

$\theta = \frac{3}{2+3}$

How many flips do I need?

$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

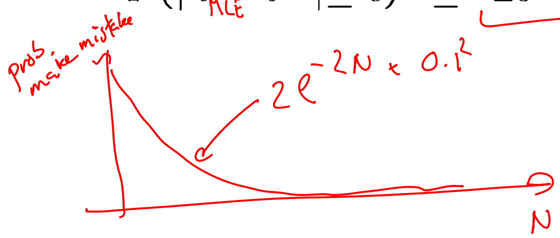
- Billionaire says: I flipped 3 heads and 2 tails.
- You say: θ = 3/5, I can prove it!
- He says: What if I flipped 30 heads and 20 tails?
- You say: Same answer, I can prove it!
- **He says: What's better?**
- You say: Humm… The more the merrier???
- He says: Is this why I am paying you the big bucks???

Simple bound (based on Hoeffding's inequality)

- For $N = \alpha_H + \alpha_T$, and $\widehat{\theta}_{MLE} = \dfrac{\alpha_H}{\alpha_H + \alpha_T}$
- Let θ^* be the true parameter, for any $\epsilon > 0$: 0.1

prob. make mistake

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



PAC Learning

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

$$P(|\widehat{\theta} - \theta^*| \geq \epsilon) \leq 2e^{-2N\epsilon^2}$$

$\delta \geq 2e^{-2N\varepsilon^2}$

$\ln \frac{\delta}{2} \geq -2N\varepsilon^2$

$\Rightarrow N \geq \dfrac{\ln \frac{2}{\delta}}{2\varepsilon^2}$

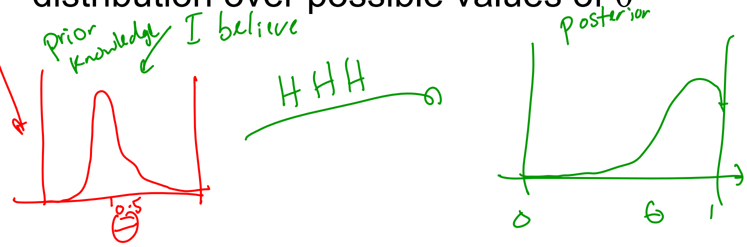
slowly with δ because of ln

grow fast with ε

$N \geq \dfrac{\ln \frac{2}{0.05}}{2 \times 0.1^2}$

What about prior

- Billionaire says: Wait, I know that the thumbtack is "close" to 50-50. What can you do for me now?
- **You say: I can learn it the Bayesian way…**
- Rather than estimating a single θ, we obtain a distribution over possible values of θ

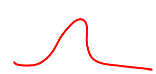


Bayesian Learning

- Use Bayes rule:

HHH

$$P(\theta \mid \mathcal{D}) = \frac{P(\mathcal{D} \mid \theta)P(\theta)}{P(\mathcal{D})}$$



- Or equivalently:

observations likelihood fn. prior

$$P(\theta \mid \mathcal{D}) \propto \underbrace{P(\mathcal{D} \mid \theta)}_{\theta^{\alpha_H}(1-\theta)^{\alpha_T}} P(\theta)$$

posterior distribution

Bayesian Learning for Thumbtack

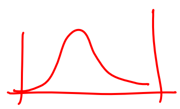
posterior $\quad$ likelihood $\quad$ prior

$$P(\theta \mid \mathcal{D}) \;\propto\; P(\mathcal{D} \mid \theta) P(\theta)$$

- Likelihood function is simply Binomial:

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- What about prior?
  - Represent expert knowledge
  - Simple posterior form



- Conjugate priors:
  - Closed-form representation of posterior
  - **For Binomial, conjugate prior is Beta distribution**

Beta prior distribution – P(θ)

most likely parameter value

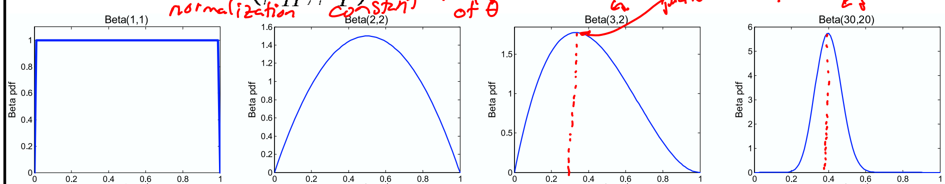
Mean: $E[\theta] = \frac{\beta_H}{\beta_H + \beta_T}$

Mode: $\frac{\beta_H - 1}{\beta_H + \beta_T - 2}$

$$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$

normalization constant independent of θ

peak



- Likelihood function: $P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$
- Posterior: $P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta) P(\theta)$

$\theta^{\alpha_H}(1-\theta)^{\alpha_T}$ $\quad$ $\leftarrow Beta(\beta_H, \beta_T)$

$P(\theta|D) \propto$

$$\theta^{\alpha_H}(1-\theta)^{\alpha_T} \cdot \theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1} = \theta^{\alpha_H + \beta_H - 1}(1-\theta)^{\alpha_T + \beta_T - 1}$$

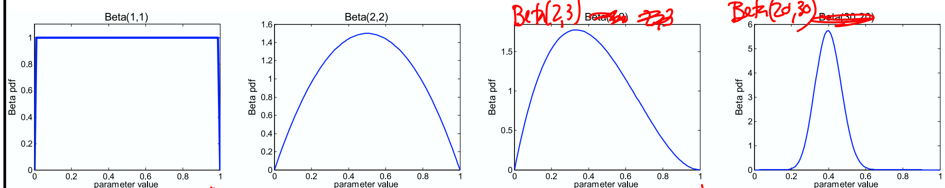
posterior $\sim Beta(\alpha_H + \beta_H, \alpha_T + \beta_T)$

Posterior distribution

- Prior: $Beta(\beta_H, \beta_T)$
- Data: α_H heads and α_T tails   Binomial
- Posterior distribution:

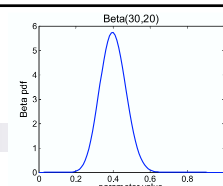
$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

Beta(2,3)   Beta(20,30)



prior Beta(1,1) $P(\theta \mid H,T)$ $P(\theta \mid H,T,T)$ one more T   19 - H, 29 - T

Using Bayesian posterior



- Posterior distribution:

$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

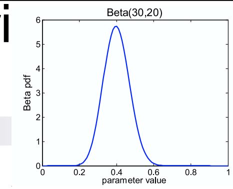
- Bayesian inference:
  - No longer single parameter: bets returns

$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta \mid \mathcal{D}) d\theta$$

expected return

  - Integral is often hard to compute

MAP: Maximum a posteriori approximation



$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta \mid \mathcal{D}) d\theta$$

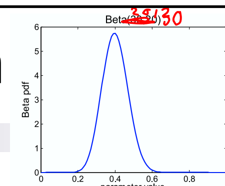
- As more data is observed, Beta is more certain
- MAP: use most likely parameter:

$$\widehat{\theta}_{MAP} = \arg\max_{\theta} P(\theta \mid \mathcal{D}) \qquad E[f(\theta)] \approx f(\widehat{\theta}_{MAP})$$

$$\hat{\theta}_{MAP} = \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2}$$

MAP for Beta distribution

$$E[\theta] = \text{mean} = \frac{\beta_H}{\beta_H + \beta_T}$$



$$P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_H + \alpha_H - 1}(1-\theta)^{\beta_T + \alpha_T - 1}}{B(\beta_H + \alpha_H, \beta_T + \alpha_T)} \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

- MAP: use most likely parameter:

$$\widehat{\theta} = \arg\max_{\theta} P(\theta \mid \mathcal{D}) = \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2}$$

- Beta prior equivalent to extra thumbtack flips
- As $N \rightarrow \infty$, prior is "forgotten"
- **But, for small sample size, prior is important!**

What you need to know

- Go to the recitation on intro to probabilities
  - And, other recitations too
- Point estimation:
  - MLE Theory.
  - D ~~Learning~~
  - Bayesian learning
  - MAP