CSCI 5090/7090- Machine Learning

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Basic Probability

(slides borrowed from Andrew Moore of CMU and Google, http://www.cs.cmu.edu/~awm/tutorials, Tom Mitchell, Barnabás Póczos & Aarti Singh

Probability Overview

- Events
  - discrete random variables, continuous random variables, compound events
- Axioms of probability
  - What defines a reasonable theory of uncertainty
- Independent events
- Conditional probabilities
- Bayes rule and beliefs
- Joint probability distribution
- Expectations
- Independence, Conditional independence
- MLE
- MAP

Discrete Random Variables

- Informally, A is a <u>random variable</u> if
  - A denotes something about which we are uncertain
  - perhaps the outcome of a randomized experiment

- Examples
  - A = True if a randomly drawn person from our class is female
  - A = The hometown of a randomly drawn person from our class
  - A = True if two randomly drawn persons from our class have same birthday

- Define P(A) as "the fraction of possible worlds in which A is true" or "the fraction of times A holds, in repeated runs of the random experiment"
  - the set of possible worlds is called the sample space, S
  - A random variable A is a function defined over S

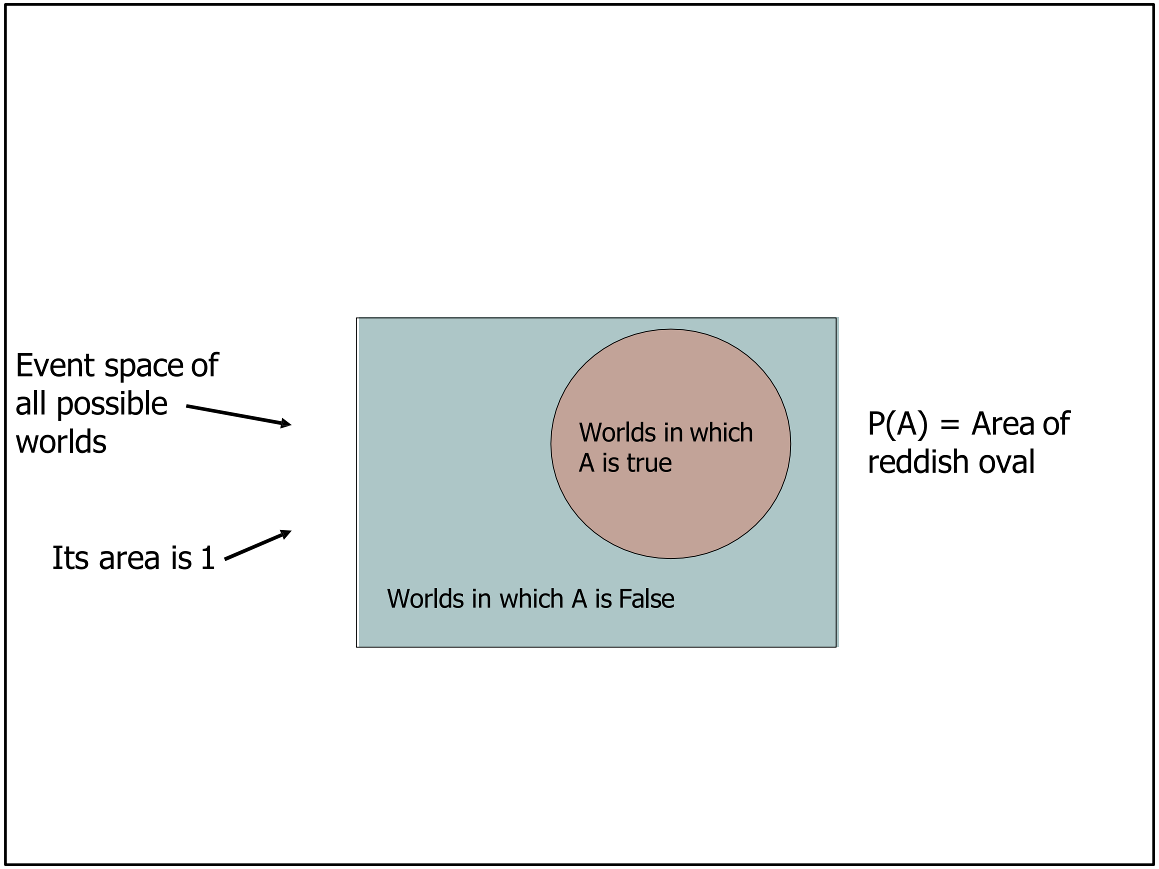
$$A: S \rightarrow \{0,1\}$$

A little Formalism

- More formally, we have
- a sample space S (e.g., set of students in our class)
- – aka the set of possible worlds

- a random variable is a function defined over the sample space
  - Gender: S → { m, f }
  - Height: S → Reals
- an event is a subset of S
  - e.g., the subset of S for which Gender=f
  - e.g., the subset of S for which (Gender=m) AND (eyeColor=blue)
- we're often interested in probabilities of specific events
- and of specific events conditioned on other specific events

Visualizing A



The Axioms of Probability

- $0 <= P(A) <= 1$
- $P(True) = 1$
- $P(False) = 0$
- $P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$

Interpreting the axioms

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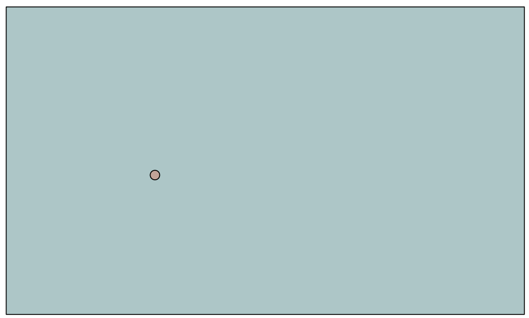

The area of A can't get any smaller than 0

And a zero area would mean no world could ever have A true

Interpreting the axioms

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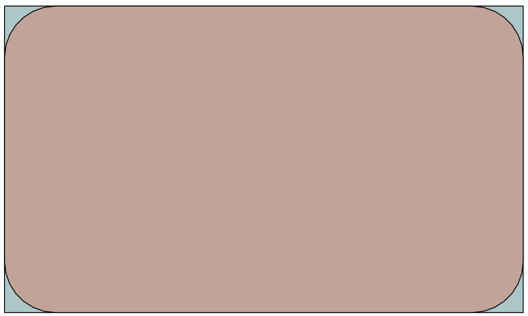

The area of A can't get any bigger than 1

And an area of 1 would mean all worlds will have A true

Interpreting the axioms

- 0 <= P(A) <= 1
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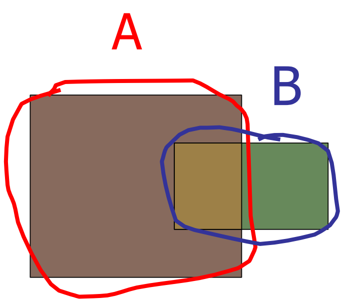
- P(A or B) = P(A) + P(B) - P(A and B)



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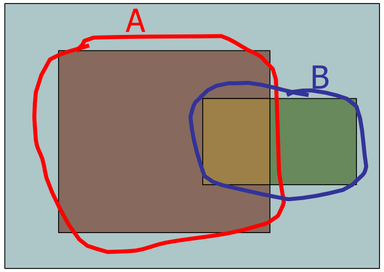
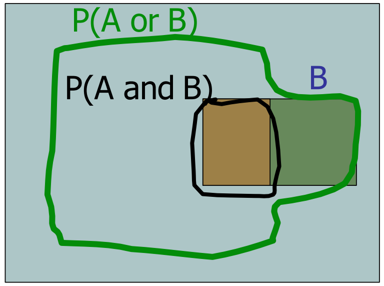




Simple addition and subtraction

Theorems from the Axioms

- 0 <= P(A) <= 1, P(True) = 1, P(False) = 0
- P(A or B) = P(A) + P(B) - P(A and B)

From these we can prove:

P(not A) = P(~A) = 1-P(A)

- How?

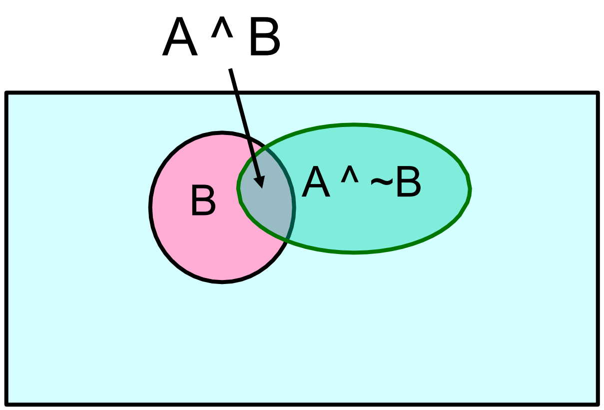
Another important theorem

- $0 <= P(A) <= 1$, $P(True) = 1$, $P(False) = 0$
- $P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$

From these we can prove:

$P(A) = P(A \wedge B) + P(A \wedge \sim B)$

- How?



Notation Digression

Binary valued variables

- P(A) is shorthand for P(A=true)
- P(~A) or P(Ā) is shorthand for P(A=false)
- For binary variables that aren't true/false: P(Gender=M), P(Gender=F)

Multivalued variables

- P(Major=history), P(Age=19), P(Q<13.75)

Notation Digression

Note: upper case letters/names for *variables*, lower case letters/names for *values*

- P(X) vs P(x)
- For multivalued RVs, P(Q) is shorthand for P(Q=q) for some unknown q

Conjunctions

- P(X, Y) equivalent to $P(X \wedge Y)$

Multivalued Random Variables

- Suppose A can take on more than 2 values
- A is a random variable with arity k if it can take on exactly one value out of $\{v_1, v_2, .. v_k\}$
- Thus…

$$P(A = v_i \wedge A = v_j) = 0 \text{ if } i \neq j$$
$$P(A = v_1 \vee A = v_2 \vee \ldots \vee A = v_k) = 1$$

An easy fact about Multivalued Random Variables:

- Using the axioms of probability…

  0 <= P(A) <= 1, P(True) = 1, P(False) = 0

  P(A or B) = P(A) + P(B) - P(A and B)

- And assuming that A obeys…

$$P(A=v_i \wedge A=v_j) = 0 \text{ if } i \neq j$$
$$P(A=v_1 \vee A=v_2 \vee \ldots \vee A=v_k) = 1$$

- It's easy to prove that
  - $P(A=v_1 \vee A=v_2 \vee \ldots \vee A=v_k) = \sum_{j=1}^{j=k} P(A=v_j)$

Another fact about Multivalued Random Variables:

- Using the axioms of probability…

  0 <= P(A) <= 1, P(True) = 1, P(False) = 0

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- It's easy to prove that

$$P(B \wedge [A = v_1 \vee A = v_2 \vee A = v_i]) = \sum_{j=1}^{k} P(B \wedge A = v_j)$$

Another fact about Multivalued Random Variables:

- Using the axioms of probability…

  0 <= P(A) <= 1, P(True) = 1, P(False) = 0

  P(A or B) = P(A) + P(B) - P(A and B)

- And assuming that A obeys…

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  $$P(A = v_1 \vee A = v_2 \vee A = v_k) = 1$$

- It's easy to prove that

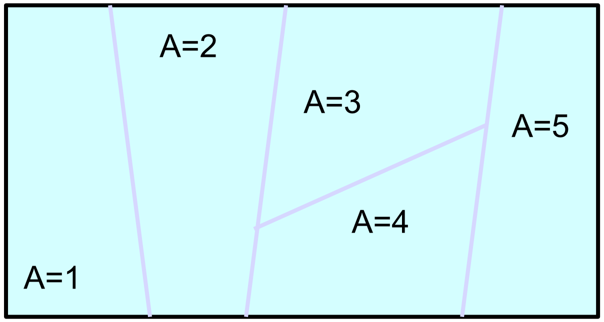
$$P(B \wedge [A = v_1 \vee A = v_2 \vee A = v_i]) = \sum_{j=1} P(B \wedge A = v_j)$$

- And thus we can prove

$$P(B) = \sum_{j=1}^{k} P(B \wedge A = v_j)$$

Elementary Probability in Pictures

- P(~A) + P(A) = 1
- P(B) = P(B ^ A) + P(B ^ ~A)
- $$\sum_{j=1}^{k} P(A = v_j) = 1$$
- $$P(B) = \sum P(B \wedge A = v_j)$$



Independent Events

- Definition: two events A and B are *independent* if Pr(A and B)=Pr(A)*Pr(B)

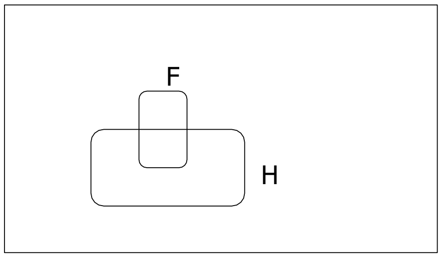
- Intuition: knowing A tells us nothing about the value of B (and vice versa)

Conditional Probability

- P(A|B) = Fraction of worlds in which B is true that also have A true

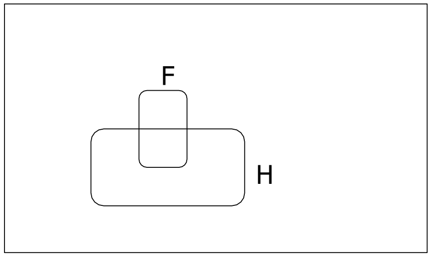
H = "Have a headache"
F = "Coming down with Flu"

P(H) = 1/10
P(F) = 1/40
P(H|F) = 1/2



"Headaches are rare and flu is rarer, but if you're coming down with 'flu there's a 50-50 chance you'll have a headache."

Conditional Probability



H = "Have a headache"
F = "Coming down with Flu"

P(H) = 1/10
P(F) = 1/40
P(H|F) = 1/2

P(H | F) = Fraction of flu-inflicted worlds in which you have a headache

$$= \frac{\#\text{worlds with flu and headache}}{\#\text{worlds with flu}}$$

$$= \frac{\text{Area of "H and F" region}}{\text{Area of "F" region}}$$

$$= \frac{P(H \wedge F)}{P(F)}$$

Definition of Conditional Probability

$$P(A|B) = \frac{P(A \wedge B)}{P(B)}$$

Corollary: The Chain Rule

$$P(A \wedge B) = P(A|B)\, P(B)$$

What we just did…

$$P(B|A) = \frac{P(A \wedge B)}{P(A)} = \frac{P(A|B)\,P(B)}{P(A)}$$

This is Bayes Rule

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. Philosophical Transactions of the Royal Society of London, **53:370-418**

More General Forms of Bayes Rule

$$P(A|B) = \frac{P(B|A)P(A)}{P(B|A)P(A) + P(B|\sim A)P(\sim A)}$$

$$P(A|B \wedge X) = \frac{P(B|A \wedge X)P(A \wedge X)}{P(B \wedge X)}$$

$$P(A = a_1 | B) = \frac{P(B | A = a_1)P(A = a_1)}{\sum_i P(B | A = a_i)P(A = a_i)}$$

More General Forms of Bayes Rule

$$P(A=v_i|B) = \frac{P(B|A=v_i)P(A=v_i)}{\sum_{k=1}^{n_A} P(B|A=v_k)P(A=v_k)}$$

Useful Easy-to-prove facts

$$P(A \mid B) + P(\neg A \mid B) = 1$$

$$\sum_{k=1}^{n_A} P(A = v_k \mid B) = 1$$

You Should Know

- Events
  - discrete random variables, continuous random variables, compound events
- Axioms of probability
  - What defines a reasonable theory of uncertainty
- Independent events
- Conditional probabilities
- Bayes rule

what does all this have to do with function approximation?

learn

$f: X \rightarrow Y$

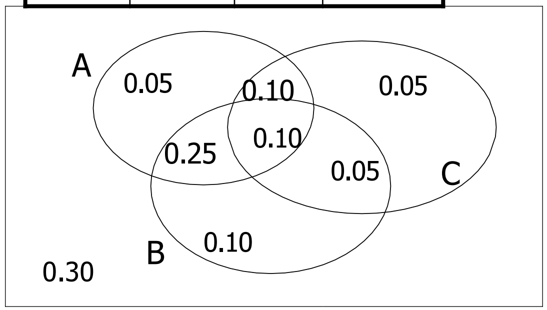
$P(Y|X)$

The Joint Distribution

Recipe for making a joint distribution of M variables:

Example: Boolean variables A, B, C

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10



The Joint Distribution

Recipe for making a joint distribution of M variables:

1. Make a truth table listing all combinations of values of your variables (if there are M Boolean variables then the table will have 2^M rows).

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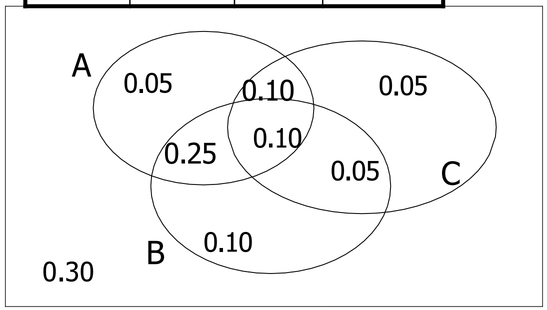

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1	1	0	0.25
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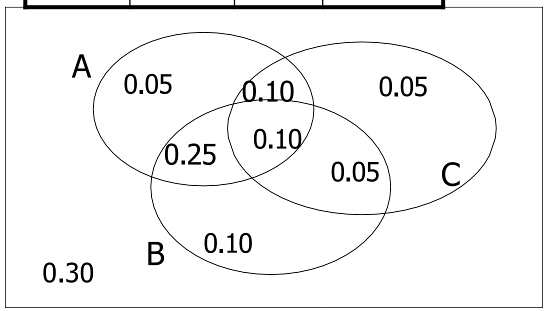

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Recipe for making a joint distribution of M variables:

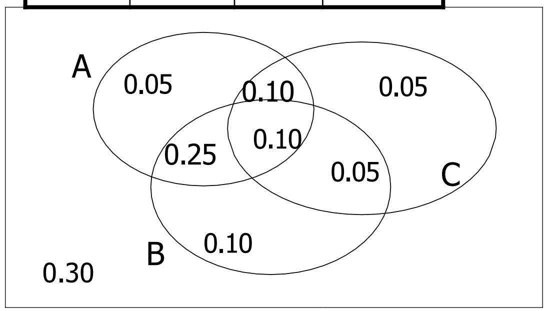
1. Make a truth table listing all combinations of values of your variables (if there are M Boolean variables then the table will have 2^M rows).

2. For each combination of values, say how probable it is.

3. If you subscribe to the axioms of probability, those numbers must sum to 1.

Example: Boolean variables A, B, C

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10



Learning a joint distribution

Build a JD table for your attributes in which the probabilities are unspecified

A	B	C	Prob
0	0	0	?
0	0	1	?
0	1	0	?
0	1	1	?
1	0	0	?
1	0	1	?
1	1	0	?
1	1	1	?

Then fill in each row with

$$\hat{P}(\text{row}) = \frac{\text{records matching row}}{\text{total number of records}}$$

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	**0.25**
1	1	1	0.10

Fraction of all records in which A and B are True but C is False

Using the Joint

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
		rich	0.0245895
	v1:40.5+	poor	0.0421768
		rich	0.0116293
Male	v0:40.5-	poor	0.331313
		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

One you have the JD you can ask for the probability of any logical expression involving your attribute

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

Using the Joint

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P(Poor Male) = 0.4654

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

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		rich	0.0971295
	v1:40.5+	poor	0.134106
		rich	0.105933

P(Poor) = 0.7604

$$P(E) = \sum_{\text{rows matching } E} P(\text{row})$$

Inference with the Joint

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
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$$P(E_1 \mid E_2) = \frac{P(E_1 \wedge E_2)}{P(E_2)} = \frac{\sum_{\text{rows matching } E_1 \text{ and } E_2} P(\text{row})}{\sum_{\text{rows matching } E_2} P(\text{row})}$$

Inference with the Joint

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$$P(E_1 \mid E_2) = \frac{P(E_1 \wedge E_2)}{P(E_2)} = \frac{\sum_{\text{rows matching } E_1 \text{ and } E_2} P(\text{row})}{\sum_{\text{rows matching } E_2} P(\text{row})}$$

P(Male | Poor) = 0.4654 / 0.7604 = 0.612

sounds like the solution to learning $F: X \rightarrow Y$, or $P(Y|X)$

Are we done?

Our first machine learning problem:

Parameter estimation:
MLE, MAP

Estimating Probabilities

Flipping a Coin

I have a coin, if I flip it, what's the probability that it will fall with the head up?

Let us flip it a few times to estimate the probability:

The estimated probability is: **3/5** "Frequency of heads"

Flipping a Coin

The estimated probability is: **3/5** "Frequency of heads"

Questions:

(1) Why frequency of heads???

(2) How good is this estimation???

(3) Why is this a machine learning problem???

We are going to answer these questions

Question (1)

Why frequency of heads???

- Frequency of heads is exactly the
  maximum likelihood estimator for this problem

- MLE has nice properties
  (interpretation, statistical guarantees, simple)

Maximum Likelihood Estimation

MLE for Bernoulli distribution

Data, D =

$$D = \{X_i\}_{i=1}^{n}, \;\; X_i \in \{\mathrm{H}, \mathrm{T}\}$$

P(Heads) = θ, *P(Tails)* = 1-θ

Flips are **i.i.d.**:

- **Independent** events
  - **Identically distributed** according to Bernoulli distribution

MLE: Choose θ that maximizes the probability of observed data

Maximum Likelihood Estimation

MLE: Choose θ that maximizes the probability of observed data

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} P(D \mid \theta)$$

$$= \arg\max_{\theta} \prod_{i=1}^{n} P(X_i|\theta)$$

Independent draws

$$= \arg\max_{\theta} \prod_{i:X_i=H} \theta \prod_{i:X_i=T} (1-\theta)$$

Identically distributed

$$= \arg\max_{\theta} \underbrace{\theta^{\alpha_H}(1-\theta)^{\alpha_T}}_{J(\theta)}$$

Maximum Likelihood Estimation

MLE: Choose θ that maximizes the probability of observed data

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} P(D \mid \theta)$$

$$= \arg\max_{\theta} \underbrace{\theta^{\alpha_H}(1-\theta)^{\alpha_T}}_{J(\theta)}$$

$$\frac{\partial J(\theta)}{\partial \theta} = \alpha_H \theta^{\alpha_H - 1}(1-\theta)^{\alpha_T} - \alpha_T \theta^{\alpha_H}(1-\theta)^{\alpha_T - 1}\Big|_{\theta=\hat{\theta}_{\mathrm{MLE}}} = 0$$

$$\alpha_H(1-\theta) - \alpha_T\theta\Big|_{\theta=\hat{\theta}_{\mathrm{MLE}}} = 0$$

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

That's exactly the "Frequency of heads"

Question (2)

How good is this MLE estimation???

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

How many flips do I need?

I flipped the coins 5 times: 3 heads, 2 tails

$$\widehat{\theta}_{MLE} = \frac{3}{5}$$

What if I flipped 30 heads and 20 tails?

$$\widehat{\theta}_{MLE} = \frac{30}{50}$$

- **Which estimator should we trust more?**
- **The more the merrier???**

Simple bound

Let θ^* be the true parameter.

For $n = \alpha_H + \alpha_T$, and $$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

For any $\varepsilon > 0$:

Hoeffding's inequality:

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

Probably Approximate Correct (PAC) Learning

I want to know the coin parameter θ, within ε = 0.1 error with probability at least 1-δ = 0.95.

How many flips do I need?

$$P(|\,\widehat{\theta}-\theta^*\,|\geq\epsilon)\;\;\leq\;\;2e^{-2n\epsilon^2}\leq\delta$$

Sample complexity:

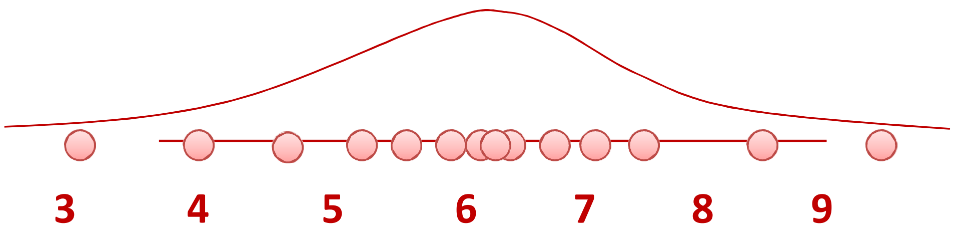
$$n\geq\frac{\ln(2/\delta)}{2\epsilon^2}$$

Question (3)

Why is this a machine learning problem???

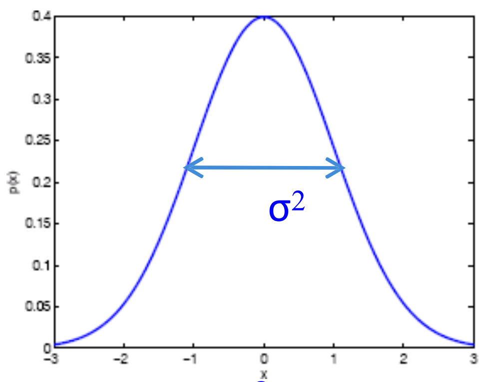
- improve their performance   (accuracy of the predicted prob.)
- at some task (predicting the probability of heads)
- with experience (the more coins we flip the better we are)

What about continuous features?

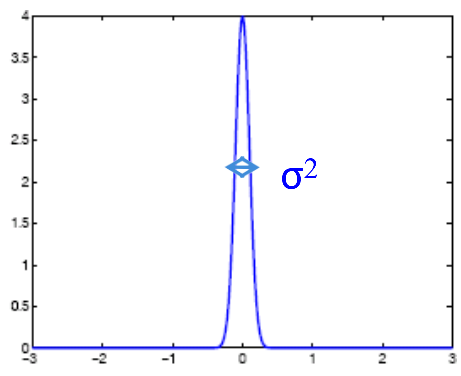


Let us try Gaussians...

$$p(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) = \mathcal{N}_x(\mu, \sigma)$$



∝= 0



∝= 0

MLE for Gaussian mean and variance

Choose θ= (∝,σ²) that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg\max_{\theta} \; P(D \mid \theta)$$

$$= \arg\max_{\theta} \prod_{i=1}^{n} P(X_i|\theta)$$

Independent draws

$$= \arg\max_{\theta} \prod_{i=1}^{n} \frac{1}{2\sigma^2} e^{-(X_i - \mu)^2/2\sigma^2}$$

Identically distributed

$$= \arg \max_{\theta=(\mu,\sigma^2)} \underbrace{\frac{1}{2\sigma^2} e^{-\sum_{i=1}^{n}(X_i-\mu)^2/2\sigma^2}}_{J(\theta)}$$

55

MLE for Gaussian mean and variance

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

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

Note: MLE for the variance of a Gaussian is **biased**

[Expected result of estimation is **not** the true parameter!]

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

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

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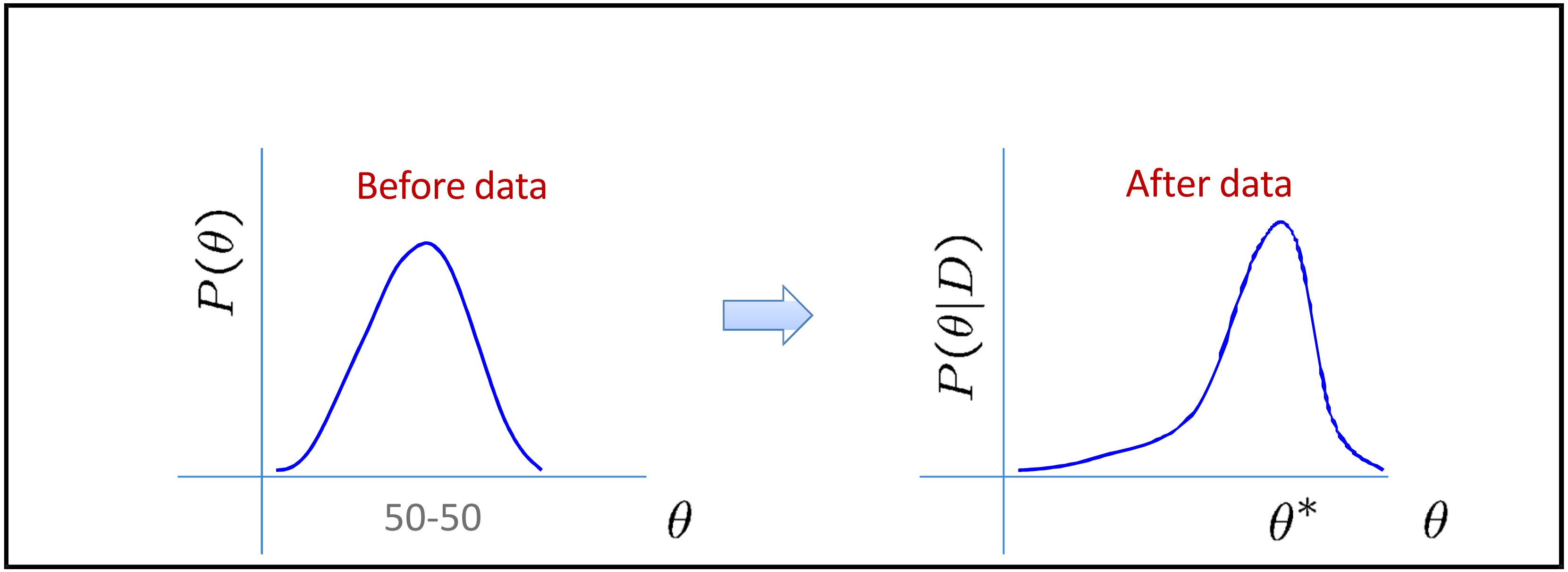
What about prior knowledge?

(MAP Estimation)

What about prior knowledge?

- We know the coin is "close" to 50-50. What can we do now?
- **The Bayesian way...**
- Rather than estimating a single θ, we obtain a distribution over possible values of θ



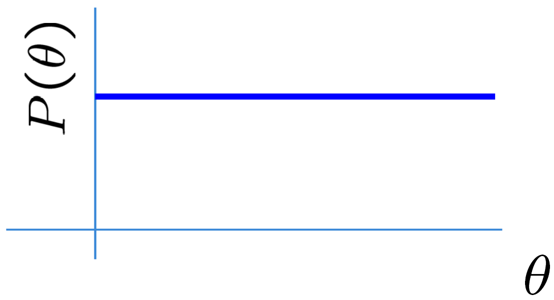
Prior distribution

What prior? What distribution do we want for a prior?

- Represents expert knowledge (philosophical approach)
- Simple posterior form (engineer's approach)

Uninformative priors:

- Uniform distribution



Conjugate priors:

- Closed-form representation of posterior
- P(θ) and P(θ|D) have the same form

In order to proceed we will need:

Bayes Rule

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. *Philosophical Transactions of the Royal Society of London,* **53:370-418**

Chain Rule & Bayes Rule

Chain rule:

$$P(X,Y) = P(X|Y)P(Y) = P(Y|X)P(X)$$

Bayes rule:

$$P(X|Y) = \frac{P(Y|X)P(X)}{P(Y)}$$

Bayes rule is important for reverse conditioning.

Bayesian Learning

- Use Bayes rule:

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

- Or equivalently:

$$\underbrace{P(\theta \mid \mathcal{D})}_{\text{posterior}} \propto \underbrace{P(\mathcal{D} \mid \theta)}_{\text{likelihood}} \underbrace{P(\theta)}_{\text{prior}}$$

MLE vs. MAP

- Maximum Likelihood estimation (MLE)

  Choose value that maximizes the probability of observed data $$\widehat{\theta}_{MLE} = \arg\max_{\theta} P(D|\theta)$$

- Maximum *a posteriori* (MAP) estimation

  Choose value that is most probable given observed data and prior belief $$\begin{aligned}\widehat{\theta}_{MAP} &= \arg\max_{\theta} P(\theta|D) \\ &= \arg\max_{\theta} P(D|\theta)P(\theta)\end{aligned}$$

When is MAP same as MLE?

MAP estimation for Binomial distribution

Coin flip problem: Likelihood is Binomial

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

If the prior is Beta distribution,

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

$\Rightarrow$ posterior is Beta distribution

Beta function: $B(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1}\, dt$

MAP estimation for Binomial distribution

Likelihood is Binomial: $P(\mathcal{D} \mid \theta) = \binom{n}{\alpha_H} \theta^{\alpha_H} (1-\theta)^{\alpha_T}$

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

$\Rightarrow$ posterior is Beta distribution

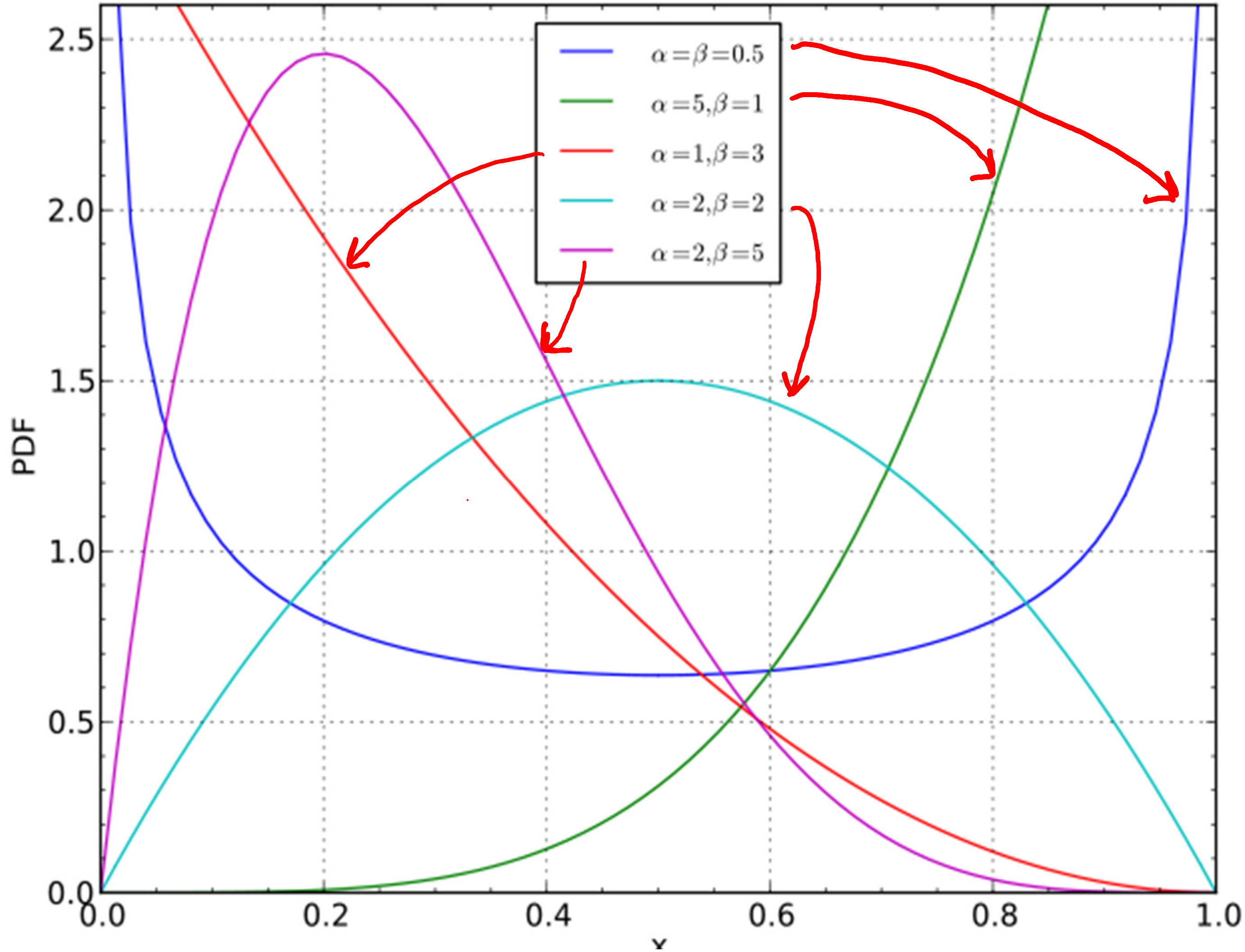
$$P(\theta|D) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

P(θ) and P(θ|D) have the same form! [Conjugate prior]

$$\widehat{\theta}_{MAP} = \arg\max_{\theta} \; P(\theta \mid D) = \arg\max_{\theta} \; P(D \mid \theta) P(\theta)$$

$$= \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2}$$

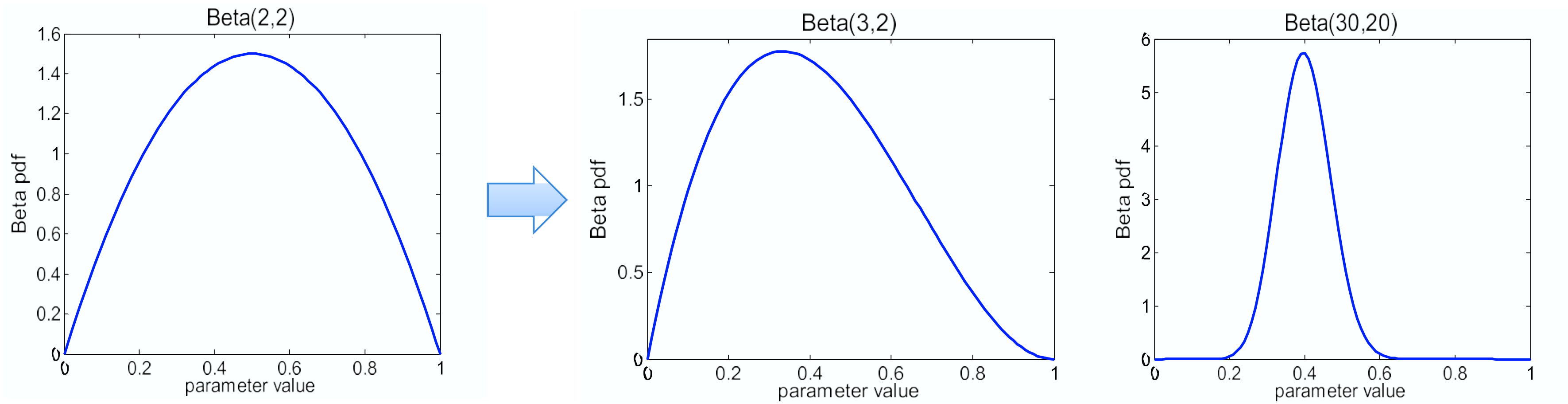
Beta distribution



More concentrated as values of α, β increase

Beta conjugate prior

$$P(\theta) \sim Beta(\beta_H, \beta_T) \qquad P(\theta|D) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$



As $n = \alpha_H + \alpha_T$ increases

As we get more samples, effect of prior is "washed out"

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

From Binomial to Multinomial

Example: Dice roll problem (6 outcomes instead of 2)

Likelihood is ~ Multinomial($\theta = \{\theta_1, \theta_2, \ldots, \theta_k\}$)

$$P(\mathcal{D} \mid \theta) = \theta_1^{\alpha_1} \theta_2^{\alpha_2} \ldots \theta_k^{\alpha_k}$$

If prior is Dirichlet distribution,

$$P(\theta) = \frac{\prod_{i=1}^{k} \theta_i^{\beta_i - 1}}{B(\beta_1, \ldots, \beta_k)} \sim \text{Dirichlet}(\beta_1, \ldots, \beta_k)$$

Then posterior is Dirichlet distribution

$$P(\theta|D) \sim \text{Dirichlet}(\beta_1 + \alpha_1, \ldots, \beta_k + \alpha_k)$$

For Multinomial, conjugate prior is Dirichlet distribution.

http://en.wikipedia.org/wiki/Dirichlet_distribution

You should know

- Probability basics
  - random variables, events, sample space, conditional probs, …
  - independence of random variables
  - Bayes rule
  - Joint probability distributions
  - calculating probabilities from the joint distribution
- Point estimation
  - maximum likelihood estimates
  - maximum a posteriori estimates
  - distributions – binomial, Beta, Dirichlet, …