Machine Learning 10-601

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Today:
- Probability
- Bayes Rule
- Estimating parameters
  - maximum likelihood
  - max a posteriori

many of these slides are derived from William Cohen, Andrew Moore, Aarti Singh, Eric Xing, Carlos Guestrin. - Thanks!

Readings:

Probability review
- Bishop Ch. 1 thru 1.2.3
- Bishop, Ch. 2 thru 2.2
- Andrew Moore's online tutorial

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

Random Variables

- Informally, A is a random variable 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

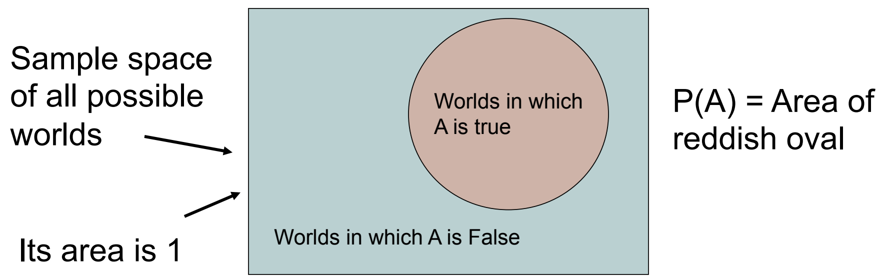
    A: S → {0,1}

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

[di Finetti 1931]:

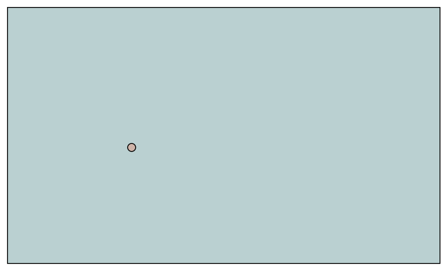
when gambling based on “uncertainty formalism A” you can be exploited by an opponent

iff

your uncertainty formalism A violates these axioms

Interpreting the axioms

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



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

- 0 <= P(A) <= 1
- P(True) = 1
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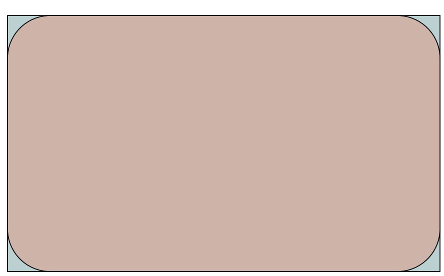


The area of A can't get any bigger than 1

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

Interpreting the axioms

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

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)

  ➔ P(not A) = P(~A) = 1-P(A)

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)

➔ P(not A) = P(~A) = 1-P(A)

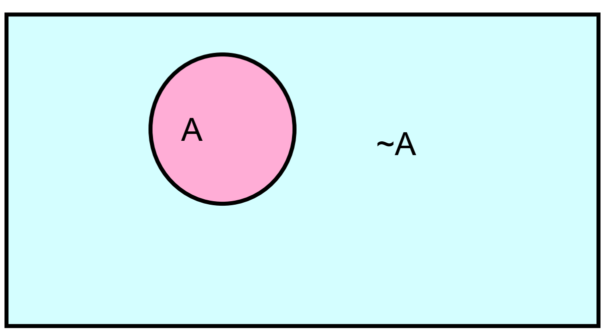
P(A or ~A) = 1   P(A and ~A) = 0

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

1   = P(A) + P(~A) + 0

Elementary Probability in Pictures

- P(~A) + P(A) = 1



Another useful theorem

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

➔ P(A) = P(A ^ B) + P(A ^ ~B)

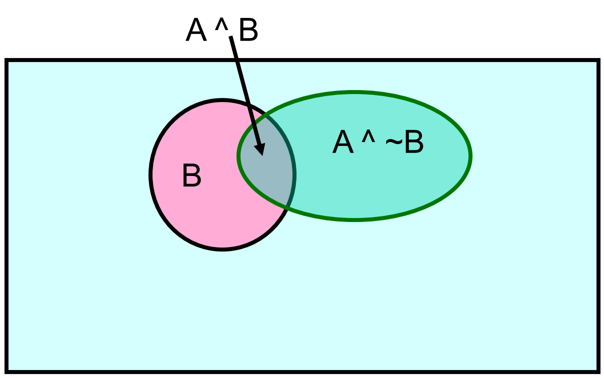
A = [A and (B or ~B)] = [(A and B) or (A and ~B)]

P(A) = P(A and B) + P(A and ~B) – P((A and B) and (A and ~B))

P(A) = P(A and B) + P(A and ~B) – P(A and B and A and ~B)

Elementary Probability in Pictures

- P(A) = P(A ^ B) + P(A ^ ~B)



Multivalued Discrete Random Variables

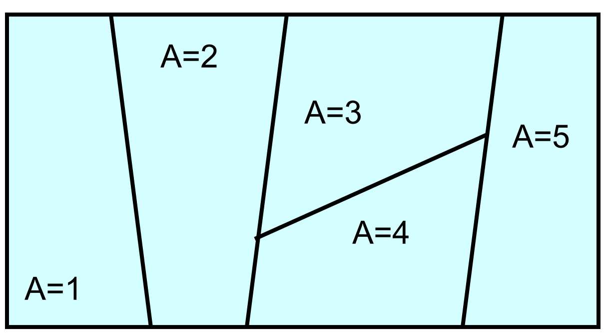
- Suppose A can take on more than 2 values
- A is a random variable with arity k if it can take on exactly one value out of $\{v_1, v_2, \ldots v_k\}$
- Thus…

$$P(A = v_i \wedge A = v_j) = 0 \text{ if } i \neq j$$

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

Elementary Probability in Pictures

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



Definition of Conditional Probability

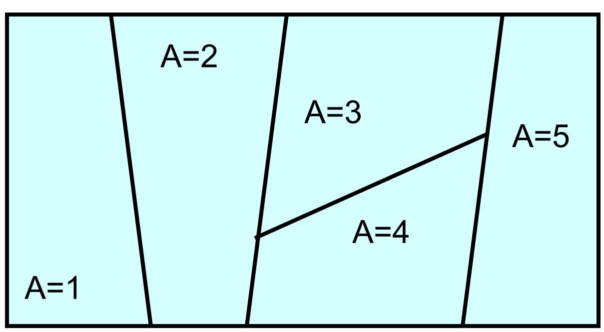
$$P(A|B) = \frac{P(A \wedge B)}{P(B)}$$

Corollary: The Chain Rule

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

Conditional Probability in Pictures

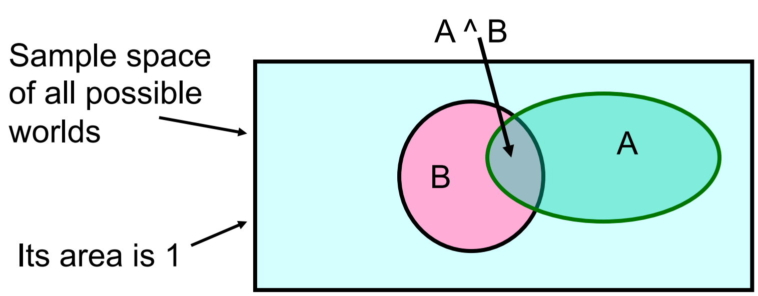
picture: P(B|A=2)



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)

Visualizing Probabilities



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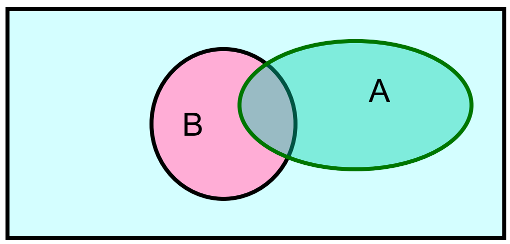
$$P(A|B) = \frac{P(A \wedge B)}{P(B)}$$



Definition of Conditional Probability

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

Corollary: The Chain Rule

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

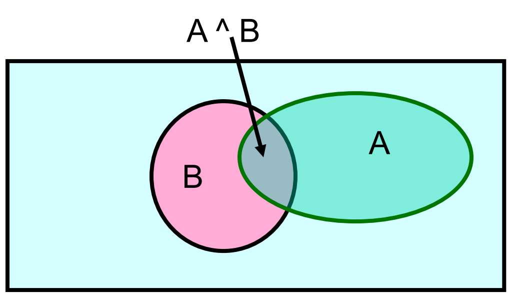
$P(C \wedge A \wedge B) = P(C|A \wedge B)\, P(A|B)\, P(B)$

Independent Events

- Definition: two events A and B are *independent* if   P(A ^ B)=P(A)*P(B)
- Intuition: knowing A tells us nothing about the value of B (and vice versa)

Bayes Rule

- let's write 2 expressions for P(A ^ B)



$$P(A|B) = \frac{P(B|A) * P(A)}{P(B)}$$ Bayes' rule

we call P(A) the "prior"

and P(A|B) the "posterior"

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**

…by no means merely a curious speculation in the doctrine of chances, but necessary to be solved in order to a sure foundation for all our reasonings concerning past facts, and what is likely to be hereafter…. necessary to be considered by any that would give a clear account of the strength of *analogical* or *inductive reasoning*…

Other Forms of Bayes Rule

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

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

Applying Bayes Rule

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

A = you have the flu,   B = you just coughed

Assume:
P(A) = 0.05
P(B|A) = 0.80
P(B| ~A) = 0.2

what is P(flu | cough) = P(A|B)?

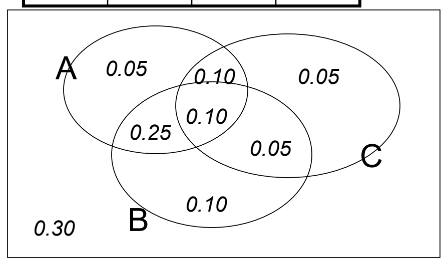
what does all this have to do with function approximation?

The Joint Distribution

Example: Boolean variables A, B, C

Recipe for making a joint distribution of M variables:

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



[A. Moore]

The Joint Distribution

Example: Boolean variables A, B, C

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).

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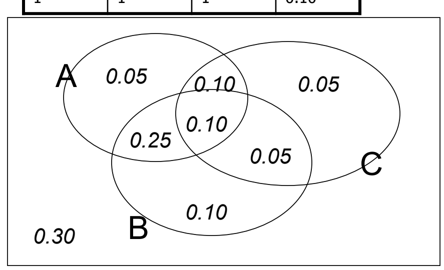

[A. Moore]

The Joint Distribution

Example: Boolean variables A, B, C

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.

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0	1	1	0.05
1	0	0	0.05
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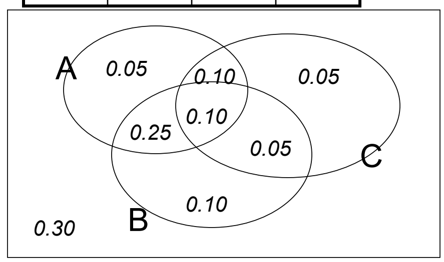


[A. Moore]

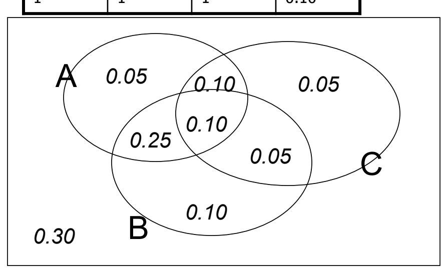
The Joint Distribution

Example: Boolean variables A, B, C

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.

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



[A. Moore]

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

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

[A. Moore]

Using the Joint

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

P(Poor Male) = 0.4654

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

[A. Moore]

Using the Joint

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

P(Poor) = 0.7604

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

[A. Moore]

Inference with 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

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

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

[A. Moore]

Learning and the Joint Distribution

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

Suppose we want to learn the function f: <G, H> → W

Equivalently, P(W | G, H)

Solution: learn joint distribution from data, calculate P(W | G, H)

e.g., P(W=rich | G = female, H = 40.5-) =

[A. Moore]

sounds like the solution to
learning F: X →Y,
or P(Y | X).

Are we done?

Your first consulting job

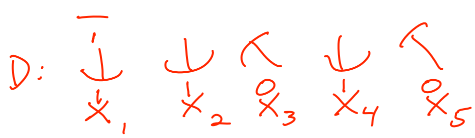
- A billionaire from the suburbs of Seattle asks you a question:
  - He says: I have thumbtack, if I flip it, what's the probability it will fall with the nail up?
  - You say: Please flip it a few times:

  - You say: The probability is:
  - **He says: Why???**
  - You say: Because…

[C. Guestrin]

Thumbtack – Binomial Distribution

- P(Heads) = θ, P(Tails) = 1-θ



Flips produce data set D with α_H heads and α_T tails

- Flips are independent, identically distributed 1's and 0's (Bernoulli)
- α_H and α_T are counts that sum these outcomes (Binomial)

$$P(D|\theta) = P(\alpha_H, \alpha_T|\theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

[C. Guestrin]

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

$$\hat{\theta} = \arg\max_{\theta} P(\mathcal{D} \mid \theta) = \arg\max_{\theta} \ln P(\mathcal{D} \mid \theta)$$

[C. Guestrin]

Maximum Likelihood Estimate for Θ

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

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

[C. Guestrin]

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

$$\begin{aligned} \widehat{\theta} &= \arg\max_{\theta} \ \ln P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \ \ln \theta^{\alpha_H}(1-\theta)^{\alpha_T} \end{aligned}$$

[C. Guestrin]

How many flips do I need?

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

[C. Guestrin]

Bayesian Learning

- Use Bayes rule:

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

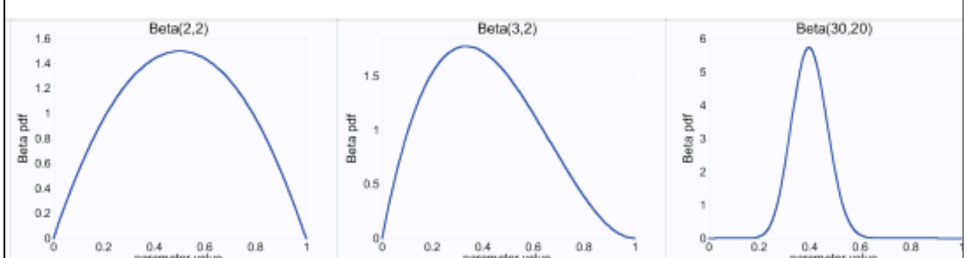
- Or equivalently:

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

[C. Guestrin]

Beta prior distribution – P(θ)

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



[C. Guestrin]

Beta prior distribution – P(θ)

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

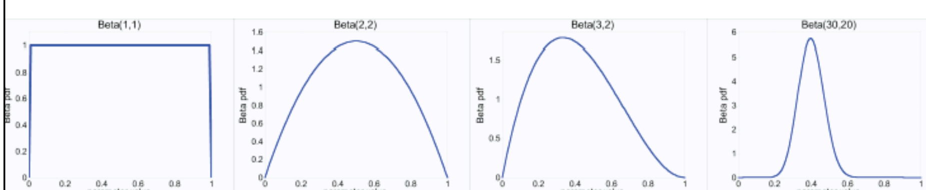
- Likelihood function: $P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$
- Posterior: $P(\theta \mid \mathcal{D}) \;\propto\; P(\mathcal{D} \mid \theta) P(\theta)$

[C. Guestrin]

Posterior distribution

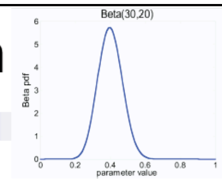
- Prior: $Beta(\beta_H, \beta_T)$
- Data: α_H heads and α_T tails
- Posterior distribution:

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



[C. Guestrin]

MAP for Beta distribution



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

- MAP: use most likely parameter:

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

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

[C. Guestrin]

Conjugate priors

- P(θ) and P(θ|D) have the same form

Eg. 1 Coin flip problem

Likelihood is ~ Binomial

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

If prior is Beta distribution,

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

Then posterior is Beta distribution

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

For Binomial, conjugate prior is Beta distribution.

[A. Singh]

Conjugate priors

- P(θ) and P(θ|D) have the same form

Eg. 2 Dice roll problem (6 outcomes instead of 2)

Likelihood is ~ Multinomial(θ = {θ_1, θ_2, … , θ_k})

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

If prior is Dirichlet distribution,

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

Then posterior is Dirichlet distribution

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

For Multinomial, conjugate prior is Dirichlet distribution.

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[A. Singh]

Estimating Parameters

- Maximum Likelihood Estimate (MLE): choose θ that maximizes probability of observed data $\mathcal{D}$

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

- Maximum a Posteriori (MAP) estimate: choose θ that is most probable given prior probability and the data

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

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

Dirichlet distribution

- number of heads in N flips of a two-sided coin
  - follows a binomial distribution
  - Beta is a good prior (conjugate prior for binomial)

- what it's not two-sided, but k-sided?
  - follows a *multinomial* distribution
  - *Dirichlet* distribution is the conjugate prior

$$P(\theta_1, \theta_2, ...\theta_K) = \frac{1}{B(\alpha)} \prod_{i}^{K} \theta_i^{(\alpha_1 - 1)}$$

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
- Estimating parameters from data
  - maximum likelihood estimates (MLE)
  - maximum a posteriori estimates (MAP)
  - distributions – binomial, Beta, Dirichlet, …
  - conjugate priors

Extra slides

Expected values

Given discrete random variable X, the expected value of X, written E[X] is

$$E[X] = \sum_{x \in \mathcal{X}} x P(X = x)$$

We also can talk about the expected value of functions of X

$$E[f(X)] = \sum_{x \in \mathcal{X}} f(x) P(X = x)$$

Covariance

Given two discrete r.v.'s X and Y, we define the covariance of X and Y as

$$Cov(X,Y) = E[(X - E(X))(Y - E(Y))]$$

e.g., X=gender, Y=playsFootball

or X=gender, Y=leftHanded

Remember: $E[X] = \sum_{x \in \mathcal{X}} x P(X = x)$

Example: Bernoulli model

- Data:
  - We observed N ***iid*** coin tossing: D={1, 0, 1, …, 0}
- Representation:

  Binary r.v: $x_n = \{0,1\}$
- Model: $P(x) = \begin{cases} 1-\theta & \text{for } x = 0 \\ \theta & \text{for } x = 1 \end{cases} \quad \Rightarrow \quad P(x) = \theta^x (1-\theta)^{1-x}$
- How to write the likelihood of a single observation x_i?

  $$P(x_i) = \theta^{x_i}(1-\theta)^{1-x_i}$$
- The likelihood of dataset $D=\{x_1, \ldots, x_N\}$:

  $$P(x_1, x_2, \ldots, x_N \mid \theta) = \prod_{i=1}^{N} P(x_i \mid \theta) = \prod_{i=1}^{N} \left(\theta^{x_i}(1-\theta)^{1-x_i}\right) = \theta^{\sum_{i=1}^{N} x_i}(1-\theta)^{\sum_{i=1}^{N} 1-x_i} = \theta^{\#\text{head}}(1-\theta)^{\#\text{tails}}$$