Machine Learning: Bayesian Approach

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UMBC CMSC 478

Today:
- Bayes Rule
- Estimating parameters
  - MLE
  - MAP

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

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

we call P(A) the "prior"

and P(A|B) the "posterior"

…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

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

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

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

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

$= 0.17$

$P(A|B) = \frac{.8 \cdot .05}{.8 \cdot .05 + 0.2 \; 0.95}$

Assume:
P(A) = 0.05
P(B|A) = 0.80
P(B| ~A) = 0.20

$P(A) = 1 - P(\neg A)$

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

What does all this have to do with function approximation?

instead of $h: X \rightarrow Y$,
learn $P(Y \mid X)$

Discriminative vs Generative Models

Goal is same

Calculate posterior distribution

Probability of Data, $\boldsymbol{P(y|X)}$

Discriminative Models	Generative Models
Find the decision boundary that separates the classes	Say, you have two classes – y_1 and y_2, with features X_1 and X_2
Only knows the differences between classes	First, looking at examples of y_1, build a model of what y_1 looks like/ distribution of y_1's features
To classify a new example, see which side of the decision boundary it falls	Then, looking at examples of y_2, build a model of what y_2 looks like/ distribution of y_2's features
	To classify a new example, match the new example with model of each class, to see whether the new example looks more like y_1 or more like y_2 we had seen in the training set

Discriminative vs Generative Models

Goal is same

Calculate $\boldsymbol{P(y|X)}$

$$\hat{\boldsymbol{y}} = \underset{\boldsymbol{y}}{\mathbf{argmax}}\, \boldsymbol{P(y|X)}$$

Discriminative Models	**Generative Models**
Find the decision boundary that separates the classes	Say, you have two classes – y_1 and y_2, with features X_1 and X_2
Only knows the differences between classes	First, looking at examples of y_1, build a model of what y_1 looks like/ distribution of y_1's features
To classify a new example, see which side of the decision boundary it falls	Then, looking at examples of y_2, build a model of what y_2 looks like/ distribution of y_2's features
	To classify a new example, match the new example with model of each class, to see whether the new example looks more like y_1 or more like y_2 we had seen in the training set

Discriminative vs Generative Models

Discriminative Models	Generative Models
Directly learn the function mapping $$\boldsymbol{h}:\ \boldsymbol{X}\ \rightarrow\ \boldsymbol{y}$$ **or,** Calculate likelihood $$\boldsymbol{P}(\boldsymbol{y}\vert\boldsymbol{X})$$	Calculate $$\boldsymbol{P}(\boldsymbol{y}\vert\boldsymbol{X})$$ **HOW?**
1. Assume some functional form for $\boldsymbol{P}(\boldsymbol{y}\vert\boldsymbol{X})$ 2. Estimate parameters of $\boldsymbol{P}(\boldsymbol{y}\vert\boldsymbol{X})$ directly from training data	

Discriminative vs Generative Models

<table>
<tr><th>Discriminative Models</th><th>Generative Models</th></tr>
<tr><td>Directly learn the function mapping
$$h: X \rightarrow y$$
or, Calculate likelihood
$$P(y|X)$$</td><td>Calculate
$$P(y|X)$$
from $P(X|y)$ and $P(y)$

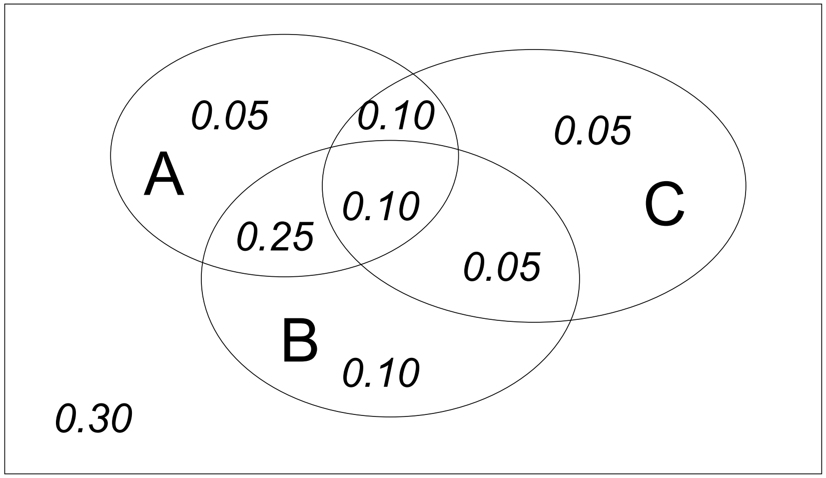
But Joint Distribution
$$P(X, y) = P(X|y)\,P(y)$$</td></tr>
<tr><td>1. Assume some functional form for $P(y|X)$
2. Estimate parameters of $P(y|X)$ directly from training data</td><td>1. Assume some functional form for $P(y), P(X|y)$
2. Estimate parameters of $P(X|y), P(y)$ directly from training data
3. Use Bayes rule to calculate $P(y\ |X)$</td></tr>
</table>

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 (M Boolean variables → 2^M rows).

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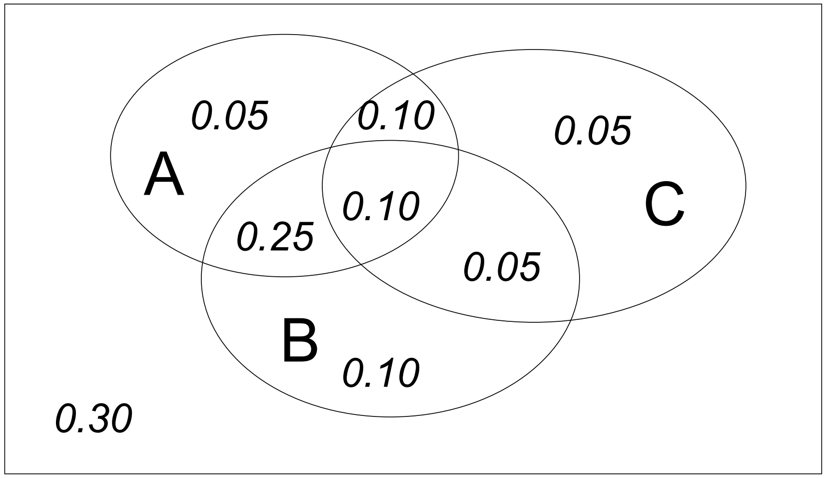

[A. Moore]

The Joint Distribution

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

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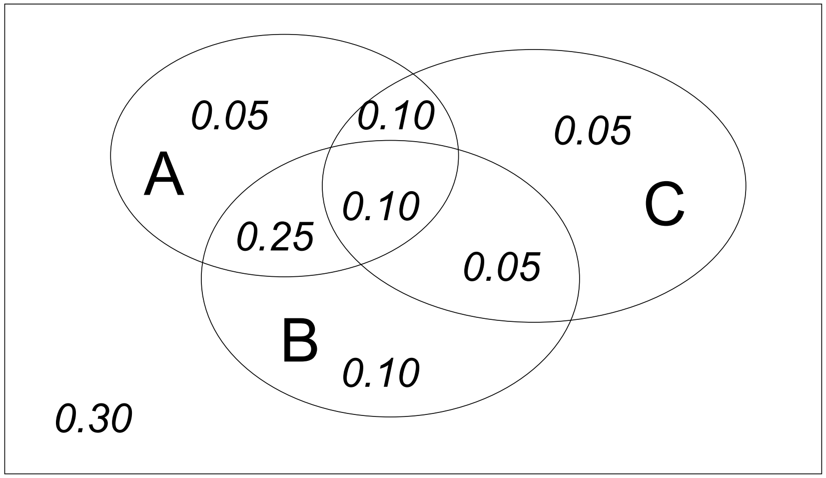


[A. Moore]

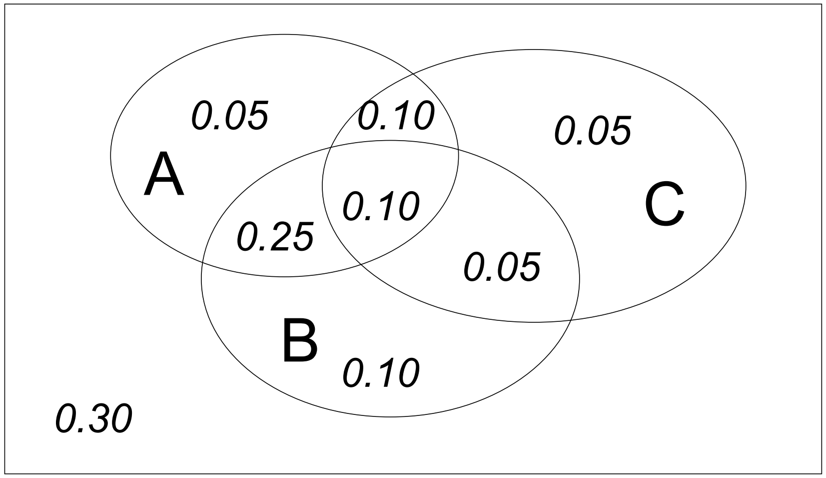
The Joint Distribution

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 (M Boolean variables → 2^M rows).
2. For each combination of values, say how probable it is.
3. If you subscribe to the axioms of probability, those probabilities 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 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

One you have the JD you can ask for the probability of **any** logical expression involving these variables

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

[A. Moore]

Using the Joint

gender	hours_worked	wealth	
Female	v0:40.5-	poor	0.253122
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	v1:40.5+	poor	0.0421768
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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 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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		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 $h: X \rightarrow Y$, or $P(Y \mid X)$.

Are we done?

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

$2^{10} = 1024$

Main problem: learning P(Y|X) can require more data than we have

consider learning Joint Dist. with 100 attributes

# of rows in this table? $2^{100} \gtrsim 1000^{10} = 10^{30}$

# of people on earth?

fraction of rows with 0 training examples? 0.9999

What to do?

1. Be smart about how we estimate probabilities from sparse data
   - maximum likelihood estimates
   - maximum a posteriori estimates

2. Be smart about how to represent joint distributions
   - Bayes networks, graphical models

1. Be smart about how we estimate probabilities

Estimating Probability of Heads

X=1 X=0

- I show you the above coin X, and hire you to estimate the probability that it will turn up heads ($X = 1$) or tails ($X = 0$)
- You flip it repeatedly, observing
  - it turns up heads α_1 times
  - it turns up tails α_0 times
- Your estimate for $P(X = 1)$ is....?

Estimating θ = P(X=1)

X=1 X=0

Test A:

100 flips: 51 Heads (X=1), 49 Tails (X=0)

α_1 α_0

$$\frac{\alpha_1}{\alpha_1 + \alpha_0} = \frac{51}{100} \rightarrow \hat{P}(X=1) = 0.51$$

Test B:

3 flips: 2 Heads (X=1), 1 Tails (X=0)

α_1 α_0

$$= \frac{2}{2+1} = 0.666$$

Estimating $\theta = P(X=1)$

X=1 X=0

Case C: (online learning)

- keep flipping, want single learning algorithm that gives reasonable estimate after each flip

α_1 = # obs. heads $(x=1)$

α_0 = # obs $x=0$

β_1 = # hallucinated $x=1$'s

β_0 = # hallucinated $x=0$'s

$n = \alpha_1 + \alpha_0$

$$\frac{\alpha_1 + 10}{(\alpha_1 + 10) + (\alpha_0 + 10)} \rightarrow \frac{(\alpha_1 + \beta_1)}{(\alpha_1 + \beta_1) + (\alpha_0 + \beta_0)}$$

Principles for Estimating Probabilities

Principle 1 (maximum likelihood):

- choose parameters θ that maximize **P(data | θ)**
- e.g., $$\hat{\theta}^{MLE} = \frac{\alpha_1}{\alpha_1 + \alpha_0}$$

$$\frac{P(data|\theta)P(\theta)}{P(data)}$$

$=$

Principle 2 (maximum a posteriori prob.):

- choose parameters θ that maximize **P(θ | data)**
- e.g.

$$\hat{\theta}^{MAP} = \frac{\alpha_1 + \#\text{hallucinated\_1s}}{(\alpha_1 + \#\text{hallucinated\_1s}) + (\alpha_0 + \#\text{hallucinated\_0s})}$$

Maximum Likelihood Estimation

X=1 X=0

$\boxed{P(X=1) = \theta}$ $P(X=0) = (1-\theta)$

Data D: $= \{1 \quad 0 \quad 0 \quad 1\} \quad 1$

$P(D|\theta) = \theta \cdot (1-\theta) \cdot (1-\theta) \cdot \theta \cdot \theta = \theta^{\alpha_1}(1-\theta)^{\alpha_0}$

Flips produce data D with $\boxed{\alpha_1 \text{ heads, } \alpha_0 \text{ tails}}$

- flips are independent, identically distributed 1's and 0's (Bernoulli)
- α_1 and α_0 are counts that sum these outcomes (Binomial)

$$P(D|\theta) = P(\alpha_1, \alpha_0|\theta) = \theta^{\alpha_1}(1-\theta)^{\alpha_0}$$

Maximum Likelihood Estimate for Θ

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

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

[C. Guestrin]

$$\hat{\theta} = \arg\max_{\theta} \ \ln P(D|\theta)$$
$$= \arg\max_{\theta} \ \ln \left[\theta^{\alpha_1}(1-\theta)^{\alpha_0}\right]$$

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

hint: $\dfrac{\partial \ln \theta}{\partial \theta} = \dfrac{1}{\theta}$

$$\frac{\partial}{\partial \theta} \alpha_1 \ln \theta + \alpha_0 \ln(1-\theta)$$

$$\alpha_1 \frac{1}{\theta} + \alpha_0 \underbrace{\frac{\partial \ln(1-\theta)}{\partial \theta}}$$

$$\underbrace{\frac{\partial \ln(1-\theta)}{\partial (1-\theta)}}_{\frac{1}{1-\theta}} \cdot \underbrace{\frac{\partial (1-\theta)}{\partial \theta}}_{-1}$$

$$\boxed{0 = \alpha_1 \frac{1}{\theta} - \frac{\alpha_0}{1-\theta}}$$

$$\theta = \frac{\alpha_1}{\alpha_1 + \alpha_0}$$

Summary:
Maximum Likelihood Estimate

X=1 X=0

P(X=1) = θ
P(X=0) = 1-θ
(Bernoulli)

- Each flip yields boolean value for X

$$X \sim \text{Bernoulli: } P(X) = \theta^X(1-\theta)^{(1-X)}$$

- Data set D of independent, identically distributed (iid) flips produces α_1 ones, α_0 zeros (Binomial)

$$P(D|\theta) = P(\alpha_1, \alpha_0|\theta) = \theta^{\alpha_1}(1-\theta)^{\alpha_0}$$

$$\hat{\theta}^{MLE} = \text{argmax}_\theta\, P(D|\theta) = \frac{\alpha_1}{\alpha_1+\alpha_0}$$

Principles for Estimating Probabilities

Principle 1 (maximum likelihood):

- choose parameters θ that maximize $P(\text{data} \mid \theta)$

Principle 2 (maximum a posteriori prob.):

- choose parameters θ that maximize

$$P(\theta \mid \text{data}) = \frac{P(\text{data} \mid \theta)\, P(\theta)}{P(\text{data})}$$

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

Beta prior distribution – P(θ)

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

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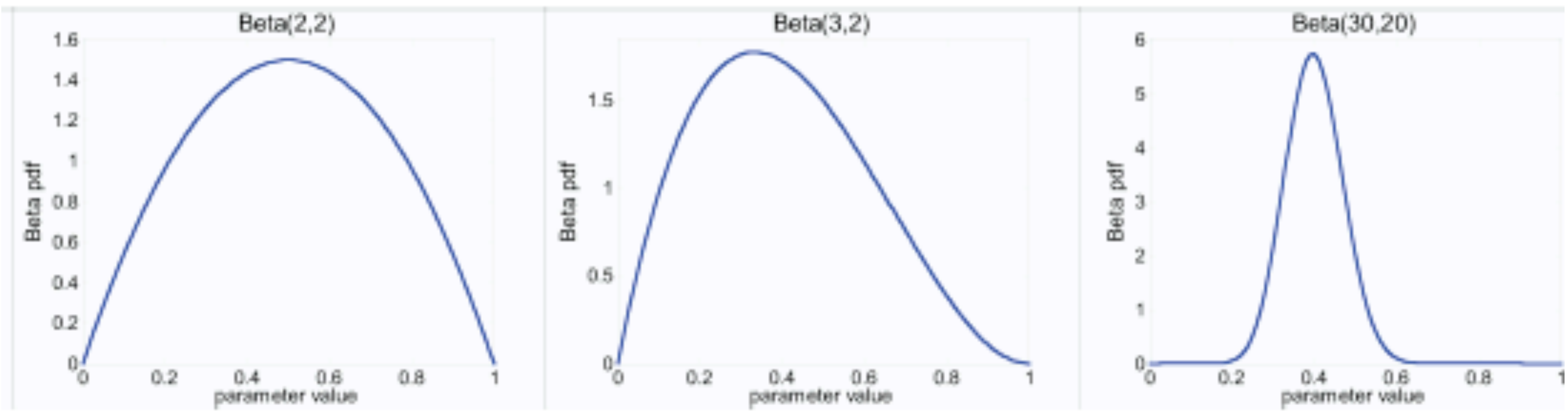
- Posterior: $P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta) P(\theta)$

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

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

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]

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

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

and MAP estimate is therefore

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

Eg. 2 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,

$$P(\theta) = \frac{\theta_1^{\beta_1 - 1}\ \theta_2^{\beta_2 - 1} \ldots \theta_k^{\beta_k - 1}}{B(\beta_1, \ldots, \beta_k)} \sim \mathrm{Dirichlet}(\beta_1, \ldots, \beta_k)$$

Then posterior is Dirichlet distribution

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

and MAP estimate is therefore

$$\hat{\theta}_i^{MAP} = \frac{\alpha_i + \beta_i - 1}{\sum_{j=1}^{k}(\alpha_j + \beta_j - 1)}$$

MLE vs MAP

- Goal is same
  - Calculate posterior distribution
  - Probability of Data, $\boldsymbol{P(y|X)}$
- **MLE**
  - **Does not use prior**
  - Starts with an assumption
- **MAP**
  - Uses Bayes Rule
  - Uses Prior
  - $\boldsymbol{P(y|X) \propto P(X|y)P(y)}$

Some terminology

- Likelihood function: $P(\text{data} \mid \theta)$
- Prior: $P(\theta)$
- Posterior: $P(\theta \mid \text{data})$

- Conjugate prior: $P(\theta)$ is the conjugate prior for likelihood function $P(\text{data} \mid \theta)$ if the forms of $P(\theta)$ and $P(\theta \mid \text{data})$ are the same.

You should know

- Probability basics
  - random variables, conditional probs, …
  - Bayes rule
  - Joint probability distributions
  - calculating probabilities from the joint distribution
- Estimating parameters from data
  - maximum likelihood estimates
  - maximum a posteriori estimates
  - distributions – binomial, Beta, Dirichlet, …
  - conjugate priors

Extra slides

Independent Events

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

Picture "A independent of B"

Expected values

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

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

Example:

X	P(X)
0	0.3
1	0.2
2	0.5

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