Machine Learning 10-601

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Today:
- Probabilistic learning
- Joint probabilities
- Estimating parameters
  - MLE
  - MAP

Readings:
- Estimating Probabilities [Mitchell]

Probability reviews:
- Goodfellow, Ch 3-3.9
- Bishop Ch. 1 thru 1.2.3
- Bishop, Ch. 2 thru 2.2

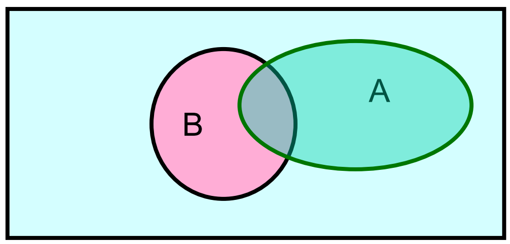
some of these slides are derived from William Cohen, Andrew Moore, Aarti Singh, Eric Xing, Carlos Guestrin. - Thanks!

probabilistic function approximation:

instead of F: X →Y,
learn P(Y | X)

Definition of Conditional Probability

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



Definition of Conditional Probability

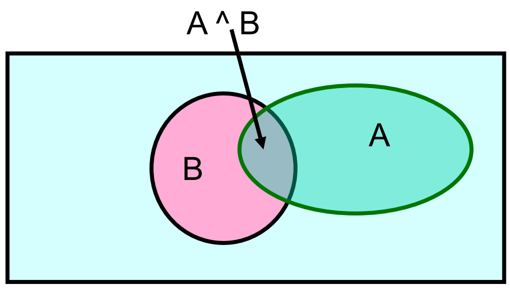
$$P(A|B) = \frac{P(A \wedge B)}{P(B)}$$

Corollary: The Chain Rule

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

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**

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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

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

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

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)?

The Awesome
Joint Probability Distribution
$P(X_1, X_2, \ldots X_N)$

from which we can calculate
$P(X_1|X_2 \ldots X_N)$,
and every other probability we desire
over subsets of $X_1 \ldots X_N$

The Joint Distribution

Example: Boolean variables A, B, C

Recipe for making a joint distribution of M variables:

The Joint Distribution

Example: Boolean variables A, B, C

Recipe for making a joint distribution of M variables:

1. Make a 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
0	0	0
0	0	1
0	1	0
0	1	1
1	0	0
1	0	1
1	1	0
1	1	1

The Joint Distribution

Example: Boolean variables A, B, C

Recipe for making a joint distribution of M variables:

1. Make a 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.

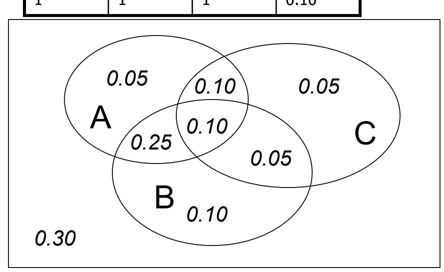
A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10

The Joint Distribution

Recipe for making a joint distribution of M variables:

1. Make a 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



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

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

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

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

P(Poor Male) = 0.4654

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

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

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
		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

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

$\boxed{\text{P(Male | Poor) = 0.4654 / 0.7604 = 0.612}}$

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-) =

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

Are we done?

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

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?
# of people on earth?

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, conditional independencies

1. Be smart about how we estimate probabilities

Estimating Probability of Heads

X=1 X=0

- I show you the above coin X, and ask 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 $\hat{\theta} = \hat{P}(X = 1)$ is …?

Estimating Probability of Heads

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- I show you the above coin X, and ask 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

Algorithm 1 (MLE): $\hat{\theta} = \hat{P}(X = 1) = \frac{\alpha_1}{\alpha_1 + \alpha_0}$

Estimating θ = P(X=1)

X=1 X=0

Test A:

100 flips: 51 Heads, 49 Tails

Test B:

3 flips: 2 Heads, 1 Tails

Estimating Probability of Heads

X=1 X=0

When data sparse, might bring in prior assumptions to bias our estimate

- e.g., represent priors by “hallucinating” γ_1 heads, and γ_0 tails, to complement sparse observed α_1, α_0

Alg 2 (MAP): $\hat{\theta} = \hat{P}(X=1) = \frac{(\alpha_1 + \gamma_1)}{(\alpha_1 + \gamma_1) + (\alpha_0 + \gamma_0)}$

Estimating Probability of Heads

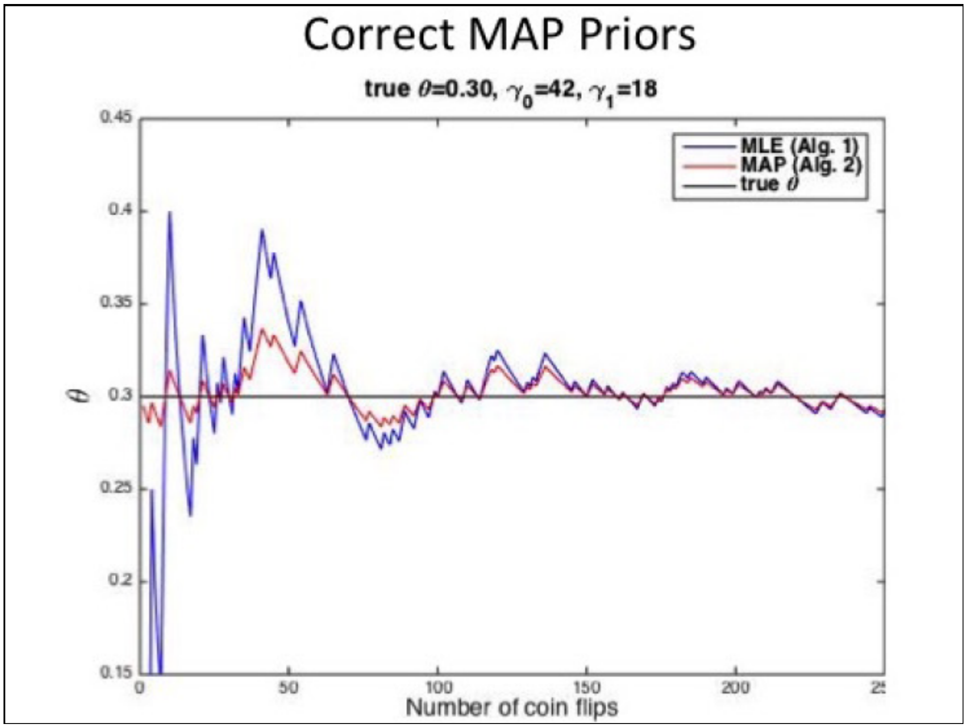
X=1 X=0

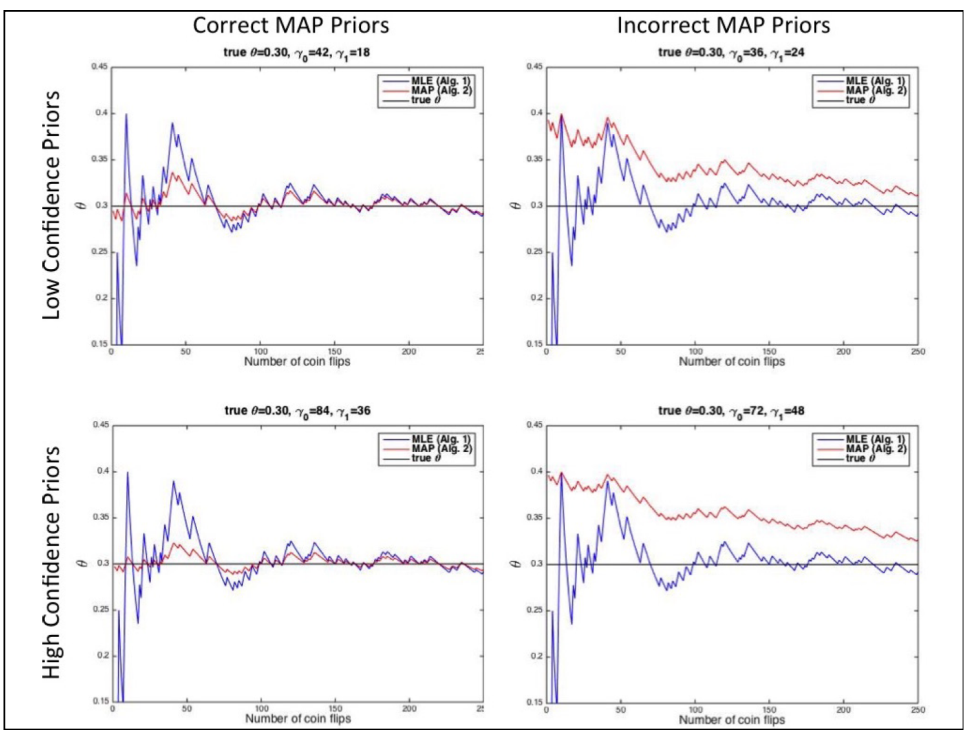
When data sparse, might bring in prior assumptions to bias our estimate

- e.g., represent priors by “hallucinating” γ_1 heads, and γ_0 tails, to complement sparse observed α_1, α_0

Alg 2 (MAP): $\hat{\theta} = \hat{P}(X=1) = \frac{(\alpha_1 + \gamma_1)}{(\alpha_1 + \gamma_1) + (\alpha_0 + \gamma_0)}$

Consider $\gamma_1 = 1 \quad \gamma_0 = 1$
versus $\gamma_1 = 1000 \quad \gamma_0 = 1000$
versus $\gamma_1 = 500 \quad \gamma_0 = 1500$


Correct MAP Priors
true θ=0.30, γ0=42, γ1=18
MLE (Alg. 1)
MAP (Alg. 2)
true θ
θ
Number of coin flips


Correct MAP Priors
Incorrect MAP Priors
Low Confidence Priors
High Confidence Priors
true θ=0.30, γ0=42, γ1=18
true θ=0.30, γ0=36, γ1=24
true θ=0.30, γ0=84, γ1=36
true θ=0.30, γ0=72, γ1=48
MLE (Alg. 1)
MAP (Alg. 2)
true θ
Number of coin flips

Principles for Estimating Probabilities

- 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 observed data

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

Principles for Estimating Probabilities

Principle 1 (maximum likelihood):

- choose parameters θ that maximize **P(data | θ)**
- result in our case: $\hat{\theta}^{MLE} = \frac{\alpha_1}{\alpha_1 + \alpha_0}$

Principle 2 (maximum a posteriori probability):

- choose parameters θ that maximize **P(θ | data)**
- result in our case:

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

Maximum Likelihood Estimation

given data D, choose θ that maximizes P(D | θ)

X=1 X=0

P(X=1) = θ
P(X=0) = 1-θ
(Bernoulli)

Data D:

$P(D|\theta) =$

Maximum Likelihood Estimation

given data D, choose θ that maximizes P(D | θ)

X=1 X=0

P(X=1) = θ
P(X=0) = 1-θ
(Bernoulli)

Data D: < 1 0 0 1 1 >

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

Flips are independent, identically distributed 1's and 0's, producing α_1 1's, and α_0 0's

Now solve for:
$$\hat{\theta}^{MLE} = \arg\max_{\theta} P(D|\theta)$$
$$= \arg\max_{\theta} P(\alpha_1, \alpha_0|\theta)$$
$$= \arg\max_{\theta} \ \theta^{\alpha_1}(1-\theta)^{\alpha_0}$$

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

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

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

Summary: Maximum Likelihood Estimate for Bernoulli random variable

X=1 X=0

P(X=1) = θ
P(X=0) = 1-θ
(Bernoulli)

- Each flip yields boolean value for X

  $X \sim$ 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(data | θ)

Principle 2 (maximum a posteriori prob.):

- choose parameters θ that maximize

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

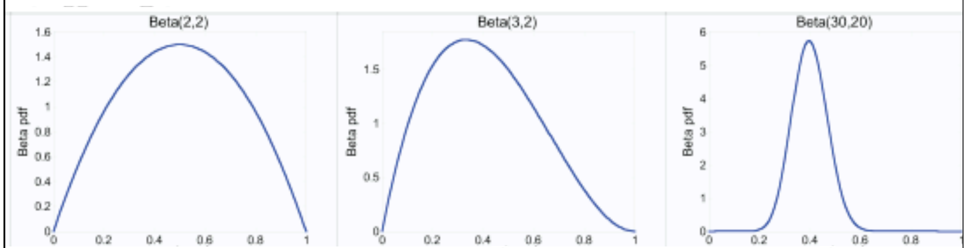
Beta prior distribution : P(θ)

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

- 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)

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



θ θ θ

Summary:
Maximum a Posteriori (MAP) Estimate for Bernoulli random variable

X=1 X=0

P(X=1) = θ
P(X=0) = 1-θ
(Bernoulli)

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

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

and MAP estimate is therefore

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

Maximum a Posteriori (MAP) Estimate for random variable with k possible outcomes

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,

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

Then posterior is Dirichlet distribution

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

and MAP estimate is therefore

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

Some terminology

- Likelihood function: P(data | θ)
- Prior: P(θ)
- Posterior: P(θ | data)

- Conjugate prior: P(θ) is the conjugate prior for likelihood function P(data | θ) if the forms of P(θ) and P(θ | data) are the same.
  - Beta is conjugate prior for Bernoulli, Binomial
  - Dirichlet is conjugate prior for Multinomial

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 – Bernoulli, Binomial, Beta, Dirichlet, …
  - conjugate priors

Extra slides

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)

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=PLAYS_FOOTBALL

or X=GENDER, Y=LEFT_HANDED

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

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

- $P(\theta)$ and $P(\theta|D)$ have the same form

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,

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

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.

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[A. Singh]

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 its conjugate prior

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

Lejeune Dirichlet

Johann Peter Gustav Lejeune Dirichlet

Born	13 February 1805 Düren, French Empire
Died	5 May 1859 (aged 54) Göttingen, Hanover
Residence	Germany
Nationality	German
Fields	Mathematician
Institutions	University of Berlin University of Breslau University of Göttingen
Alma mater	University of Bonn
Doctoral advisor	Simeon Poisson Joseph Fourier
Doctoral students	Ferdinand Eisenstein Leopold Kronecker Rudolf Lipschitz Carl Wilhelm Borchardt
Known for	Dirichlet function Dirichlet eta function