

10-315 Introduction to Machine Learning (SCS Majors)

Lecture 4: Estimating Probabilities

Leila Wehbe
Carnegie Mellon University
Machine Learning Department

Function approximation

Problem Setting:

- Set of possible instances X
- Unknown target function $f : X \rightarrow Y$
- Set of function hypotheses $H = \{h | h : X \rightarrow Y\}$

Input:

- Training examples $\{(x^{(i)}, y^{(i)})\}$ of unknown target function f

Output:

- Hypothesis $h \in H$ that best approximates target function f

Probabilistic function approximation:

Instead of $f : X \rightarrow Y$,
learn $P(Y|X)$

Conditional probability

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

Conditional probability

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

Corrollary: The Chain Rule:

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

(Very) Quick recap

Random Variables and probability tables

Example:

- Experiment: flipping a coin
- Universe: {0 = Tails, 1 = Heads}
- Events: 0 (Tails) and 1 (Heads).
- A: random variable indicating that the coin is heads.

A	$P(A)$
0	0.8
1	0.2

Joint distribution

We can have multiple random variables in the same experiment.

The universe corresponds to the set of all joint settings of the variables.

For example, if we throw the same coin three times, we can define:

- A : random variable that indicates that the first flip is heads.
- B : random variable that indicates that the second flip is heads.
- C : random variable that indicates that the third flip is heads.

One example of an event is: $A = 0 \wedge B = 1 \wedge C = 0$,.

We can write a probability table listing all the configuration of values for the variables:

<i>A</i>	<i>B</i>	<i>C</i>	<i>P</i>
0	0	0	0.512
0	0	1	0.128
0	1	0	0.128
0	1	1	0.032
1	0	0	0.128
1	0	1	0.032
1	1	0	0.032
1	1	1	0.008

We can write a probability table listing all the configuration of values for the variables:

<i>A</i>	<i>B</i>	<i>C</i>	<i>P</i>
0	0	0	0.512
0	0	1	0.128
0	1	0	0.128
0	1	1	0.032
1	0	0	0.128
1	0	1	0.032
1	1	0	0.032
1	1	1	0.008

In this coin example, the variables are independent from each other

(you can see for yourself that $P(A|B, C) = P(A)$).

We can consider another example: we select a day at random:

- *A*: the sky is cloudy.
- *B*: the temperature is cold.
- *C*: it rains.

Joint distribution

<i>A</i> – cloudy	<i>B</i> – cold	<i>C</i> – rain	<i>P</i>
0	0	0	0.3
0	0	1	0.1
0	1	0	0.15
0	1	1	0.05
1	0	0	0.05
1	0	1	0.1
1	1	0	0.1
1	1	1	0.15

We can use the joint distribution to compute the probability of any compound event:

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

Joint distribution

$A - \text{cloudy}$	$B - \text{cold}$	$C - \text{rain}$	P
0	0	0	0.3
0	0	1	0.1
0	1	0	0.15
0	1	1	0.05
1	0	0	0.05
1	0	1	0.1
1	1	0	0.1
1	1	1	0.15

We can use the joint distribution to compute the probability of any compound event:

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

What is the probability of the day being not cloudy and cold?

We can use the joint probability table to marginalize variables out

$A - \text{cloudy}$	$B - \text{cold}$	$C - \text{rain}$	P
0	0	0	0.3
0	0	1	0.1
0	1	0	0.15
0	1	1	0.05
1	0	0	0.05
1	0	1	0.1
1	1	0	0.1
1	1	1	0.15

We can use the joint probability table to marginalize variables out

$A - \text{cloudy}$	$B - \text{cold}$	$C - \text{rain}$	P
0	0	0	0.3
0	0	1	0.1
0	1	0	0.15
0	1	1	0.05
1	0	0	0.05
1	0	1	0.1
1	1	0	0.1
1	1	1	0.15

We can use the joint probability table to compute conditional probabilities

A – cloudy	B – cold	C – rain	P
0	0	0	0.3
0	0	1	0.1
0	1	0	0.15
0	1	1	0.05
1	0	0	0.05
1	0	1	0.1
1	1	0	0.1
1	1	1	0.15

What is $P(C = 1|A = 0, B = 1)$?

Recall

Can we just estimate $P(Y|X)$ in this fashion and be done?

We might not have enough data. For example consider having 100 attributes of people:

- how many rows will we have?
- how many people on earth?

Can we just estimate $P(Y|X)$ in this fashion and be done?

We might not have enough data. For example consider having 100 attributes of people:

- how many rows will we have? $2^{100} > 10^{30}$
- how many people on earth? 10^{10}
- 99.99\% of rows will not have training examples!

Solution:

1- Be smart about how to estimate probabilities from sparse data

- maximum likelihood estimates
- maximum a posteriori estimates
- Be smart about how to represent joint distributions
- Bayes networks, graphical models, conditional independencies

Estimating probabilities

Assume you throw a thumbtack 10 times and it lands 3 times on its back and 7 times on its side.



What is the probability of this thumbtack falling on its side?

Estimating Probabilities

We model the thumbtack falling on its side as a random variable X .

Each flip of the returns a Boolean value for X , that follows a Bernouilli distribution with parameter θ :

$$X \sim \text{Bernouilli}(\theta)$$

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

$$P(X = 0) = 1 - \theta$$

We have observed the thumbtack falling on its side ($X=1$) 7 times and the thumbtack falling on its back ($X=0$) 3 times.

How can we estimate θ (the probability of the thumbtack falling on its side.)

Maximum Likelihood Estimation

The first principle we will use is the principle of Maximum Likelihood Estimation (MLE).

MLE chooses the parameter $\hat{\theta}$ that **maximize the probability of the observed data**
 $P(\text{data}|\hat{\theta})$

Maximum Likelihood Estimation for Bernoulli Variables

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

$$P(X = 0) = 1 - \theta$$

We refer to observed data as $D : \{1, 0, 1, 0, 0, \dots, 1\}$

Throwing the thumbtack produces data D with α_1 side falls ($X=1$) and α_0 back falls ($X=0$).

Throws are Independently Identically Distributed (IID).

What is $P(D|\theta)$?

Maximum Likelihood Estimation for Bernoulli Variables

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

$$P(X = 0) = 1 - \theta$$

We refer to observed data as $D : \{1, 0, 1, 0, 0, \dots, 1\}$

Throwing the thumbtack produces data D with α_1 side falls ($X=1$) and α_0 back falls ($X=0$).

Throws are Independently Identically Distributed (IID).

$$\begin{aligned} P(D|\theta) &= \theta(1 - \theta) \dots \theta \\ &= \theta^{\alpha_1} (1 - \theta)^{\alpha_0} \end{aligned}$$

MLE chooses the parameter $\hat{\theta}$ that maximize the likelihood of the observed data $P(D|\hat{\theta})$

Maximum Likelihood Estimation for Bernoulli Variables

MLE chooses the parameter $\hat{\theta}_{\text{MLE}}$ that maximize the likelihood of the observed data $P(D|\hat{\theta})$

$$\hat{\theta}_{\text{MLE}} = \operatorname{argmax}_{\theta} P(D|\theta)$$

$$\hat{\theta}_{\text{MLE}} = \operatorname{argmax}_{\theta} \theta^{\alpha_1} (1 - \theta)^{\alpha_0}$$

How to find $\hat{\theta}_{\text{MLE}}$?

Maximum Likelihood Estimation for Bernoulli Variables

MLE chooses the parameter $\hat{\theta}_{\text{MLE}}$ that maximize the likelihood of the observed data $P(D|\hat{\theta})$

$$\hat{\theta}_{\text{MLE}} = \operatorname{argmax}_{\theta} P(D|\theta)$$

$$\hat{\theta}_{\text{MLE}} = \operatorname{argmax}_{\theta} \ln P(D|\theta)$$

Maximum Likelihood Estimation for Bernoulli Variables

MLE chooses the parameter $\hat{\theta}_{\text{MLE}}$ that maximize the **log** likelihood of the observed data $P(D|\hat{\theta})$

$$\begin{aligned}\hat{\theta}_{\text{MLE}} &= \operatorname{argmax}_{\theta} \ln P(D|\theta) \\ &= \operatorname{argmax}_{\theta} \ln \left(\theta^{\alpha_1} (1 - \theta)^{\alpha_0} \right)\end{aligned}$$

Maximum Likelihood Estimation for Bernoulli Variables

MLE chooses the parameter $\hat{\theta}_{\text{MLE}}$ that maximize the log likelihood of the observed data $P(D|\hat{\theta})$

$$\begin{aligned}\hat{\theta}_{\text{MLE}} &= \operatorname{argmax}_{\theta} \ln P(D|\theta) \\ &= \operatorname{argmax}_{\theta} \ln \left(\theta^{\alpha_1} (1 - \theta)^{\alpha_0} \right) = \operatorname{argmax}_{\theta} [\alpha_1 \ln \theta + \alpha_0 \ln(1 - \theta)]\end{aligned}$$

Maximum Likelihood Estimation for Bernoulli Variables

$$\hat{\theta}_{\text{MLE}} = \underset{\theta}{\operatorname{argmax}} [\alpha_1 \ln \theta + \alpha_0 \ln(1 - \theta)]$$

Take the derivative and set it to 0:

$$\frac{d}{d\theta} \ln P(D|\theta) = \frac{d}{d\theta} [\alpha_1 \ln \theta + \alpha_0 \ln(1 - \theta)] = 0$$

Maximum Likelihood Estimation for Bernoulli Variables

$$\hat{\theta}_{\text{MLE}} = \underset{\theta}{\operatorname{argmax}} [\alpha_1 \ln \theta + \alpha_0 \ln(1 - \theta)]$$

Take the derivative and set it to 0:

$$\frac{d}{d\theta} \ln P(D|\theta) = \frac{d}{d\theta} [\alpha_1 \ln \theta + \alpha_0 \ln(1 - \theta)] = 0$$

Recall

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

$$\frac{d}{d\theta} f(g(\theta)) = g'(\theta) f'(g(\theta))$$

Maximum Likelihood Estimation for Bernoulli Variables

$$\hat{\theta}_{\text{MLE}} = \operatorname{argmax}_{\theta} [\alpha_1 \ln \theta + \alpha_0 \ln(1 - \theta)]$$

Take the derivative and set it to 0:

$$\begin{aligned} \frac{d}{d\theta} \ln P(D|\theta) &= \frac{d}{d\theta} [\alpha_1 \ln \theta + \alpha_0 \ln(1 - \theta)] \\ &= \frac{\alpha_1}{\theta} - \frac{\alpha_0}{(1 - \theta)} \end{aligned}$$

Maximum Likelihood Estimation for Bernoulli Variables

Summary:

Random Variable $X \sim \text{Bernoulli}(\theta)$, i.e. $P(X = 1) = \theta$ and $P(X = 0) = 1 - \theta$.

We can write $P(X) = \theta^X (1 - \theta)^{1-X}$

We observe data D . We observe $X = 1$ α_1 times and $X = 0$ α_0 times.

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

We can estimate:

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

Probability Bound

In our example, we estimate $\hat{\theta}_{\text{MLE}} = 7/10$. We only threw the thumbtack 10 times.

How much can we trust this estimate?

Use Hoeffding Inequality

Given $X \sim \text{Bernoulli}(\theta)$, and D consisting of n IID samples where $X = 1$ is observed α_1 times and $X = 0$ is observed α_0 times, we have the guarantee:

$$\text{For any } \epsilon > 0, \quad P(|\hat{\theta}_{\text{MLE}} - \theta| \geq \epsilon) \leq 2e^{-2n\epsilon^2}$$

In [82]: `import numpy as np`

```
epsilon = 0.1  
n = 1000
```

```
p_mistake = 2*np.exp(-2*n*epsilon**2)
```

```
print("the probability of making a mistake greater than {} is less than {}".format(  
    epsilon, p_mistake))
```

```
print("the probability of making a mistake at most {} is more than {}".format(epsil  
    on, 1- p_mistake))
```

```
the probability of making a mistake greater than 0.1 is less than 4.1223072448  
77101e-09
```

```
the probability of making a mistake at most 0.1 is more than 0.999999995877692
```


Hoeffding Inequality

For any $\epsilon > 0$, $P(|\hat{\theta}_{\text{MLE}} - \theta| \geq \epsilon) \leq 2e^{-2n\epsilon^2}$

High Probability Bound

If we want to know how many flips we need to estimate parameter θ with error at most ϵ with a probability of $1 - \delta$.

For example: estimate parameter θ with error at most 0.01 with a probability of 0.99.

$$\text{For any } \epsilon > 0, \quad P(|\hat{\theta}_{\text{MLE}} - \theta| \geq \epsilon) \leq 2e^{-2n\epsilon^2} \leq \delta$$

How many flips do we need?

Hoeffding Inequality

For any $\epsilon > 0$, $P(|\hat{\theta}_{\text{MLE}} - \theta| \geq \epsilon) \leq 2e^{-2n\epsilon^2}$

High Probability Bound

If we want to know how many flips we need to estimate parameter θ with error at most ϵ with a probability of $1 - \delta$.

For example: estimate parameter θ with error at most 0.05 with a probability of 0.95.

For any $\epsilon > 0$, $P(|\hat{\theta}_{\text{MLE}} - \theta| \geq \epsilon) \leq 2e^{-2n\epsilon^2} \leq \delta$

How many flips do we need?

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

```
In [87]: epsilon = 0.05
delta = 0.1
minimum_n = int(np.ceil(np.log(2/delta)/(2*epsilon**2)))
print("the minimum number of flips is {}".format(minimum_n))
```

the minimum number of flips is 600

Estimating Probabilities

Let's go back to the original example. We threw the thumbtack 10 times, it landed 7 times on its head and 3 times on its back.

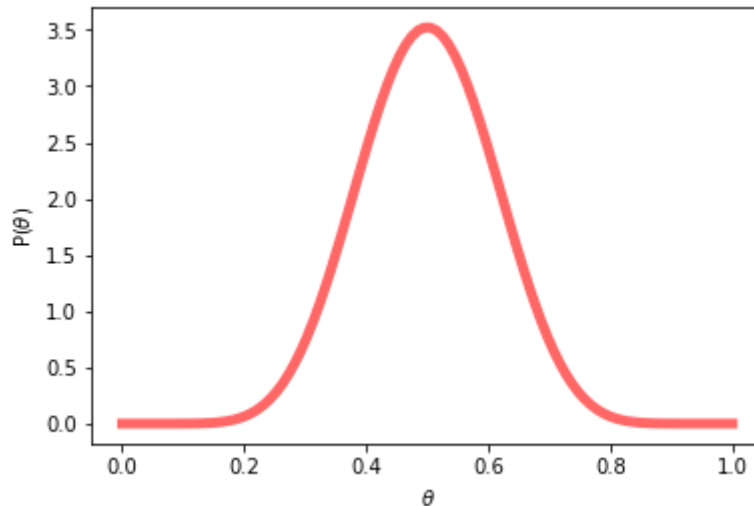
What if instead I told you that you take a coin from your pocket, you flip it lands 7 times on heads and 3 times on tails.

What is θ , the probability of heads?

Estimating Probabilities

You have a strong prior belief for the coin being fair. As an example of your prior distribution:

```
In [90]: import matplotlib.pyplot as plt
from scipy.stats import beta
beta1 = 10
beta0 = 10
x = np.linspace(0,1, 100)
plt.plot(x, beta.pdf(x, beta1,beta0), 'r-', lw=5, alpha=0.6, label='beta pdf')
plt.xlabel(r'$\theta$');plt.ylabel(r'$P(\theta)$');
```



Bayes Rule

Recall $P(A, B) = P(A|B)P(B) = P(B|A)P(A)$

We use this to state:

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

In our context:

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

Bayes Rule

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

$P(D|\theta)$ is the **likelihood** of the data, $P(\theta)$ is the **prior** probability and $P(\theta|D)$ is the **posterior** probability of the parameter θ .

Because $P(D)$ is constant for different values of θ , it is often omitted. In that case we don't compute the exact value of the posterior but we can compare it for different values of θ :

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

MAP estimation

The second principle we will use is the principle of Maximum A-posteriori Probability (MAP) Estimation.

MAP estimation chooses the parameter $\hat{\theta}_{\text{MAP}}$ that **maximize the posterior probability** $P(\hat{\theta}|\text{data})$

$$\hat{\theta}_{\text{MAP}} = \operatorname{argmax}_{\theta} P(\theta|D) = \operatorname{argmax}_{\theta} P(D|\theta)P(\theta)$$

Compare this with MLE, which chooses the parameter $\hat{\theta}_{\text{MLE}}$ that **maximize the likelihood of the observed data** $P(D|\hat{\theta})$

$$\hat{\theta}_{\text{MLE}} = \operatorname{argmax}_{\theta} P(D|\theta)$$

How to choose a prior?

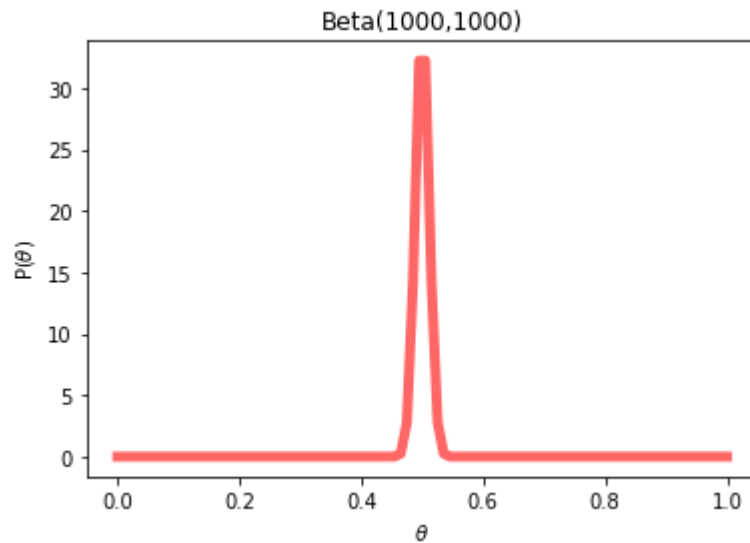
- Uniform / uninformative prior: constant for all values of θ ==> similar to MLE.
- Can represent the prior belief
- Conjugate prior: $P(\theta)$ and $P(\theta|D)$ have same form (will see soon)

For our problem with a binomial likelihood (X is bernouilli and D binomial), the beta distribution is very useful. It has parameters β_H and β_T which can represent the prior probability.

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

```
In [97]: beta_H = 1000
beta_T = 1000

plt.plot(x, beta.pdf(x, beta_H,beta_T), 'r-', lw=5, alpha=0.6, label='beta pdf')
plt.xlabel(r'$\theta$');plt.ylabel(r'$P(\theta)$'), plt.title('Beta({},{})'.format
(beta_H,beta_T));
```



MAP estimation

Assume you observe data D with α_H heads and α_T tails:

$$\begin{aligned} P(\theta|D) &\propto P(D|\theta)P(\theta) \\ &= \theta^{\alpha_H}(1-\theta)^{\alpha_T} \frac{\theta^{\beta_H-1}(1-\theta)^{\beta_T-1}}{B(\beta_H, \beta_T)} \\ &\propto \theta^{\alpha_H+\beta_H-1}(1-\theta)^{\alpha_T+\beta_T-1} \end{aligned}$$

$P(\theta|D)$ is a Beta distribution with parameters $\alpha_H + \beta_H$ and $\alpha_T + \beta_T$.

Both the prior and posterior are of the same family. A binomial likelihood with a Beta prior gives a Beta posterior.

There are many other combinations of prior and likelihood functions that lead to a conjugate prior.

MAP estimation

$$\begin{aligned}\hat{\theta}_{\text{MAP}} &= \underset{\theta}{\operatorname{argmax}} P(\theta|D) \\ &= \underset{\theta}{\operatorname{argmax}} \theta^{\alpha_H + \beta_H - 1} (1 - \theta)^{\alpha_T + \beta_T - 1} \\ &= \underset{\theta}{\operatorname{argmax}} \ln[\underset{\theta}{\operatorname{argmax}} \theta^{\alpha_H + \beta_H - 1} (1 - \theta)^{\alpha_T + \beta_T - 1}]\end{aligned}$$

We already know how to solve this:

$$\underset{\theta}{\operatorname{argmax}} = \frac{\alpha_H + \beta_H - 1}{(\alpha_H + \beta_H - 1) + (\alpha_T + \beta_T - 1)}$$

Notice how the prior acts as additional coin flips:

- prior influences the value of θ_{MAP}
- prior can be strong or weak (high or low β_H and β_T)
- a large amount of data will reduce the effect of the prior

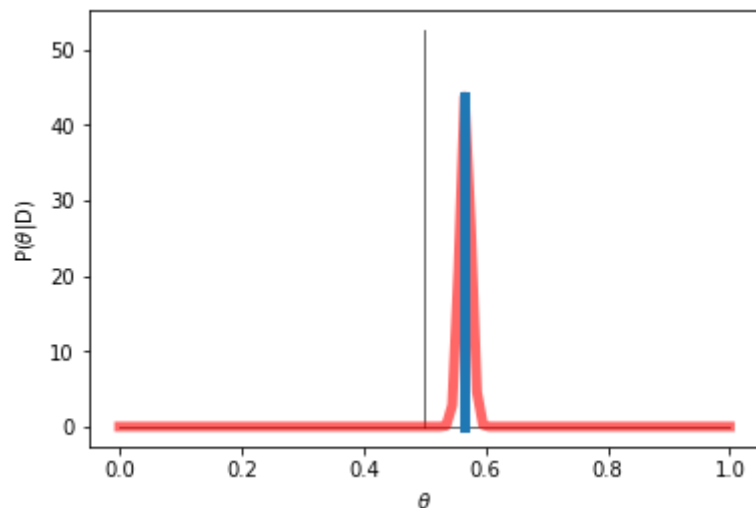
```

In [106]: alpha_H = 700; alpha_T = 300
          beta_H = 1000; beta_T = 1000
          map_pdf = beta.pdf(x, alpha_H + beta_H, alpha_T + beta_T)
          map_value = x[np.argmax(map_pdf)]

          plt.plot([0,1],[0,0], 'k', lw=1, alpha=0.6)
          plt.plot([0.5,0.5],[0,np.max(map_pdf)*1.2], 'k', lw=1, alpha=0.6)
          plt.plot(x, map_pdf, 'r-', lw=5, alpha=0.6, label='beta pdf')
          plt.plot([map_value,map_value],[0,np.max(map_pdf)],lw=5)
          plt.xlabel(r'$\theta$');plt.ylabel(r'$P(\theta|D)$'), #plt.title('Beta({},\{\})'.for
          mat(beta_H,beta_T));

```

Out[106]: (Text(0, 0.5, 'P($\theta|D)$ '),)



MAP estimation for other distributions

Multinomial likelihood and Dirichlet prior distribution:

We roll a dice with 6 sides. The data D we observe consists of counts $\alpha_1, \alpha_2 \dots \alpha_6$ of observing each of the sides respectively.

The data is $\sim \text{Multinomial}(\theta_1, \theta_2, \dots, \theta_k)$. θ is a parameter vector with k entries ($\theta_1, \theta_2, \dots, \theta_k$) (6 in the case of a dice).

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

We choose a Dirichlet prior $\theta \sim \text{Dirichlet}(\beta_1, \dots, \beta_k)$

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

The posterior is also a Dirichlet: $\theta \sim \text{Dirichlet}(\alpha_1 + \beta_1, \dots, \alpha_k + \beta_k)$

For a Multinomial likelihood, the conjugate prior is Dirichlet.

Continuous Variables

Likelihood and prior are normal distributions.

Assume $X \sim N(\mu, \sigma)$

$$p(x|\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{\sigma^2}}$$

MLE estimation for mean of gaussian

You observe n IID samples $D = \{x_1, x_2, \dots, X_n\}$.

$$\begin{aligned} P(D|\mu, \sigma) &= \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x_i - \mu)^2}{\sigma^2}\right) \\ &= \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \exp\left(-\frac{\sum_{i=1}^n (x_i - \mu)^2}{\sigma^2}\right) \end{aligned}$$

We want to find μ_{MLE} :

$$\begin{aligned} \frac{d}{d\mu} \ln P(D|\mu, \sigma) &= \frac{d}{d\mu} \ln \exp\left(-\frac{\sum_{i=1}^n (x_i - \mu)^2}{\sigma^2}\right) = \frac{d}{d\mu} -\frac{\sum_{i=1}^n (x_i - \mu)^2}{\sigma^2} = \\ &= -2 \frac{\sum_{i=1}^n (x_i - \mu)}{\sigma^2} \end{aligned}$$

Setting to 0 and solving gives

$$\mu_{MLE} = \frac{\sum_{i=1}^n x_i}{n}$$

MAP estimation for mean of gaussian

Using a normal prior for μ $N(\mu_0, \sigma_0)$ results in a normal posterior as well.

(Can do it on your own).

What you should know:

- revise concepts of joint / marginal / conditional probability
- bayes rule
- MLE estimation principles
- MAP estimation principles
- Bernoulli, Binomial, Multinomial, Beta, Dirichlet and Normal distributions