

# **Maximum Likelihood Estimation & Maximum A Posteriori Probability Estimation**

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

We update  $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t)y_t x_t$

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

We update  $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t)y_t x_t$

Theorem:  
if there exists  $w^*$  with  $\|w^*\|_2 = 1$ , such that  
 $y_t(x_t^\top w^*) \geq \gamma > 0, \forall t$ ,  
then:

$$\sum_{t=0}^{\infty} \mathbf{1}(\hat{y}_t \neq y_t) \leq 1/\gamma^2$$

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

We update  $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t)y_t x_t$

Theorem:  
if there exists  $w^*$  with  $\|w^*\|_2 = 1$ , such that  
 $y_t(x_t^\top w^*) \geq \gamma > 0, \forall t$ ,  
then:

$$\sum_{t=0}^{\infty} \mathbf{1}(\hat{y}_t \neq y_t) \leq 1/\gamma^2$$

Q: does the data need to be i.i.d?

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

We update  $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t)y_t x_t$

Theorem:  
if there exists  $w^*$  with  $\|w^*\|_2 = 1$ , such that  
 $y_t(x_t^\top w^*) \geq \gamma > 0, \forall t$ ,  
then:

$$\sum_{t=0}^{\infty} \mathbf{1}(\hat{y}_t \neq y_t) \leq 1/\gamma^2$$

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

We update  $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t)y_t x_t$

Theorem:  
if there exists  $w^*$  with  $\|w^*\|_2 = 1$ , such that  
 $y_t(x_t^\top w^*) \geq \gamma > 0, \forall t$ ,

then:

$$\sum_{t=0}^{\infty} \mathbf{1}(\hat{y}_t \neq y_t) \leq 1/\gamma^2$$

No i.i.d assumption, and indeed data  $\{x_1, y_1, \dots, x_T, y_T\}$  can be selected by an **Adversary** (as long as it is separable)!!!

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

We update  $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t)y_t x_t$

Theorem:  
if there exists  $w^*$  with  $\|w^*\|_2 = 1$ , such that  
 $y_t(x_t^\top w^*) \geq \gamma > 0, \forall t$ ,  
then:

$$\sum_{t=0}^{\infty} \mathbf{1}(\hat{y}_t \neq y_t) \leq 1/\gamma^2$$

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

We update  $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t)y_t x_t$

Theorem:  
if there exists  $w^*$  with  $\|w^*\|_2 = 1$ , such that  
 $y_t(x_t^\top w^*) \geq \gamma > 0, \forall t$ ,  
then:

$$\sum_{t=0}^{\infty} \mathbf{1}(\hat{y}_t \neq y_t) \leq 1/\gamma^2$$

Q: Can this be applied to infinite dimension space ( $d \rightarrow \infty$ )

# Recap on Perceptron

Binary classifier:  $\text{sign}(w^\top x)$

## The Perceptron Alg:

Initialize  $w_0 = 0$

For  $t = 0 \rightarrow \infty$

User comes with feature  $x_t$

We make a prediction  $\hat{y}_t = \text{sign}(w_t^\top x_t)$

User reveals the real label  $y_t$

We update  $w_{t+1} = w_t + \mathbf{1}(\hat{y}_t \neq y_t)y_t x_t$

Theorem:  
if there exists  $w^*$  with  $\|w^*\|_2 = 1$ , such that  
 $y_t(x_t^\top w^*) \geq \gamma > 0, \forall t$ ,  
then:

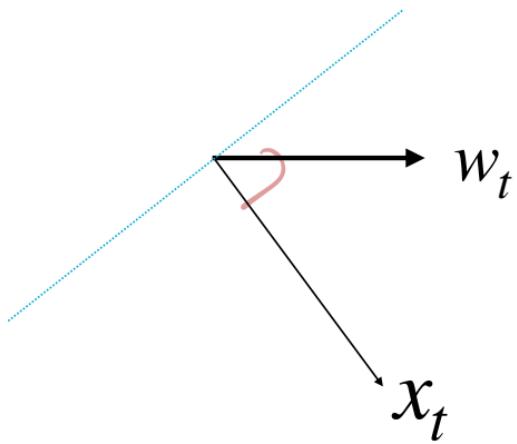
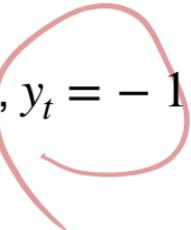
$$\sum_{t=0}^{\infty} \mathbf{1}(\hat{y}_t \neq y_t) \leq 1/\gamma^2$$

Q: Can this be applied to infinite dimension space ( $d \rightarrow \infty$ )

Yes! As long as margin exists!

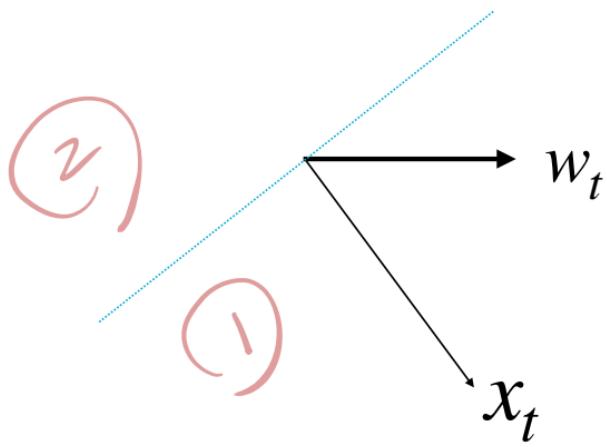
## Recap on Perceptron

When we make a mistake, i.e.,  $y_t(w_t^\top x_t) < 0$  (e.g.,  $y_t = -1$ ,  $w_t^\top x_t > 0$ )



## Recap on Perceptron

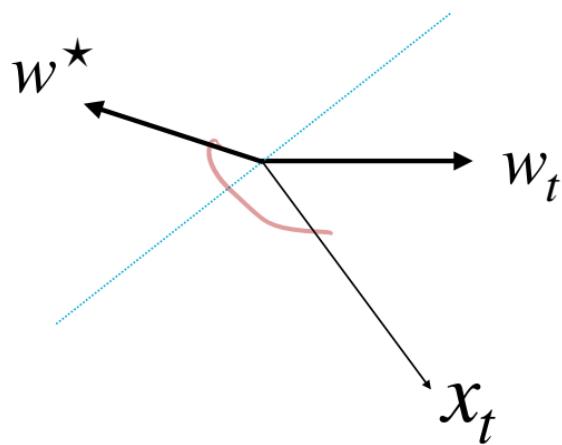
When we make a mistake, i.e.,  $y_t(w_t^\top x_t) < 0$  (e.g.,  $y_t = -1$ ,  $w_t^\top x_t > 0$ )



Q: What does  $w^*$  look like?

## Recap on Perceptron

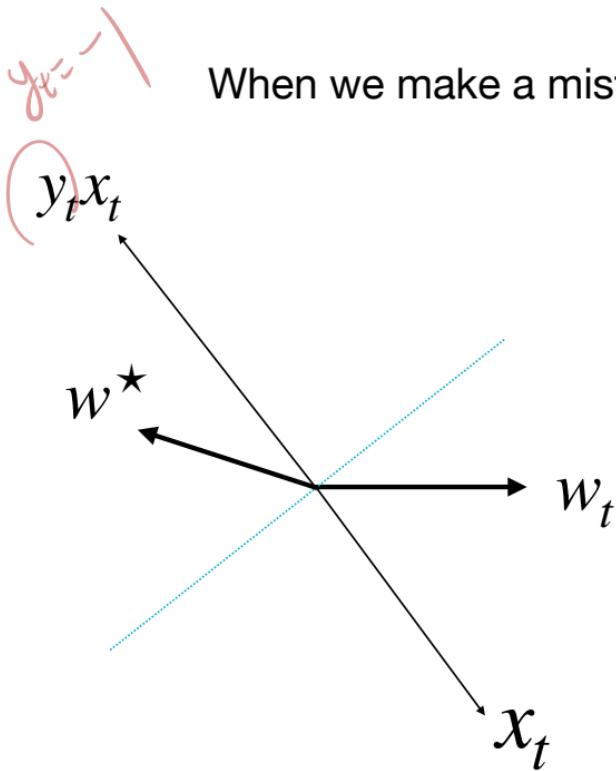
When we make a mistake, i.e.,  $y_t(w_t^\top x_t) < 0$  (e.g.,  $y_t = -1$ ,  $w_t^\top x_t > 0$ )



Q: What does  $w^*$  look like?

## Recap on Perceptron

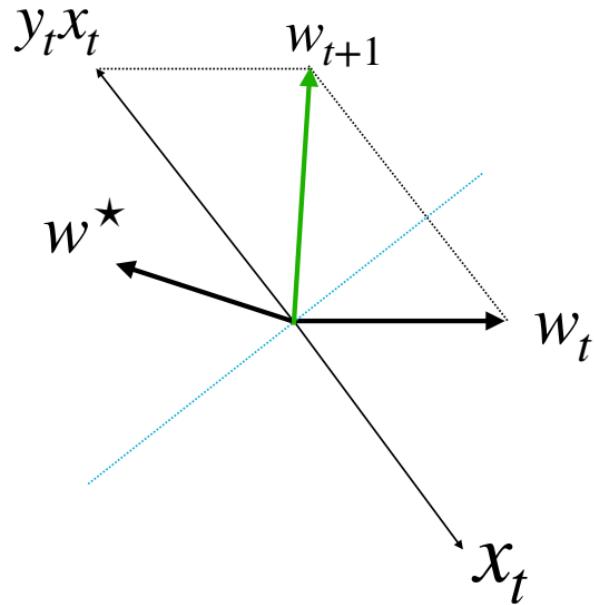
When we make a mistake, i.e.,  $y_t(w_t^\top x_t) < 0$  (e.g.,  $y_t = -1$ ,  $w_t^\top x_t > 0$ )



Q: What does  $w^*$  look like?

## Recap on Perceptron

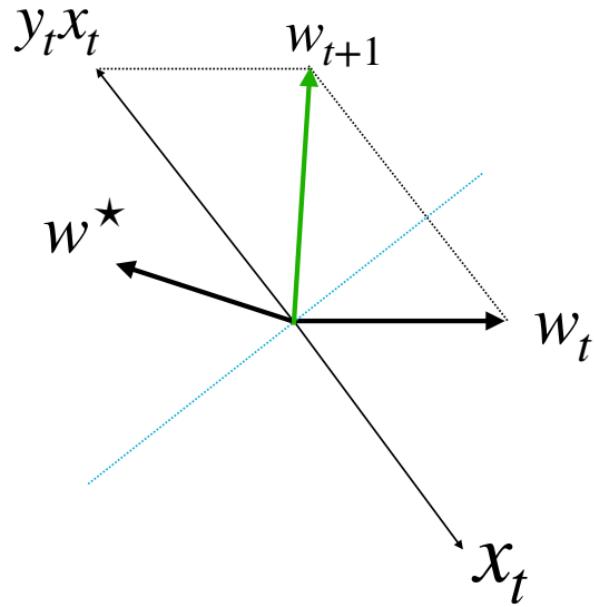
When we make a mistake, i.e.,  $y_t(w_t^\top x_t) < 0$  (e.g.,  $y_t = -1$ ,  $w_t^\top x_t > 0$ )



Q: What does  $w^*$  look like?

## Recap on Perceptron

When we make a mistake, i.e.,  $y_t(w_t^\top x_t) < 0$  (e.g.,  $y_t = -1$ ,  $w_t^\top x_t > 0$ )



We should track how the  $\cos(\theta_t)$  is changing:

$$\cos(\theta_t) = \frac{w_t^\top w^*}{\|w_t\|_2}$$

Q: What does  $w^*$  look like?

## **Outline for today:**

1. Maximum Likelihood estimation (MLE)
2. Maximum a posteriori probability (MAP)
3. Example: MLE and MAP for classification

## Ex 1: Estimating the probability of a coin flip

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

## Ex 1: Estimating the probability of a coin flip

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

Q: assume  $y_i \sim \text{Bernoulli}(\theta^*)$ , how to estimate  $\theta^*$  given  $\mathcal{D}$ ?

$$\begin{cases} +1 & \text{wp } \theta^* \\ -1 & \text{wp } 1-\theta^* \end{cases}$$

## Ex 1: Estimating the probability of a coin flip

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

Q: assume  $y_i \sim \text{Bernoulli}(\theta^*)$ , how to estimate  $\theta^*$  given  $\mathcal{D}$ ?

$$\hat{\theta} \approx \frac{\sum_{i=1}^n \mathbf{1}(y_i = 1)}{n}$$

# of heads

$\hat{\theta} \rightarrow \theta^*, n \rightarrow \infty$

## Ex 1: Estimating the probability of a coin flip

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

Q: assume  $y_i \sim \text{Bernoulli}(\theta^*)$ , how to estimate  $\theta^*$  given  $\mathcal{D}$ ?

$$\hat{\theta} \approx \frac{\sum_{i=1}^n \mathbf{1}(y_i = 1)}{n}$$

Let's make this rigorous!

# Maximum Likelihood Estimation

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

# Maximum Likelihood Estimation

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

If the probability of getting head is  $\theta \in [0,1]$ , what is the probability of observing the data  $\mathcal{D}$  (likelihood)?

$$\mathcal{D} = \{+1, +1, -1, +1, -1\}$$

$$\uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow$$

$$\theta \quad \theta \quad 1-\theta \quad \theta \quad 1-\theta$$

# Maximum Likelihood Estimation

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

If the probability of getting head is  $\theta \in [0,1]$ , what is the probability of observing the data  $\mathcal{D}$  (likelihood)?

$$P(\mathcal{D} | \theta) = \theta^{n_1}(1 - \theta)^{n-n_1}$$

$$n_1 = \# \text{ of } (+1)$$

# Maximum Likelihood Estimation

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

If the probability of getting head is  $\theta \in [0,1]$ , what is the probability of observing the data  $\mathcal{D}$  (likelihood)?

$$P(\mathcal{D} | \theta) = \theta^{n_1}(1 - \theta)^{n-n_1}$$

MLE Principle: Find  $\theta$  that **maximizes the likelihood** of the data:

# Maximum Likelihood Estimation

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

If the probability of getting head is  $\theta \in [0,1]$ , what is the probability of observing the data  $\mathcal{D}$  (likelihood)?

$$P(\mathcal{D} | \theta) = \theta^{n_1}(1 - \theta)^{n-n_1}$$

MLE Principle: Find  $\theta$  that **maximizes the likelihood** of the data:

$$\hat{\theta}_{mle} = \arg \max_{\theta \in [0,1]} P(\mathcal{D} | \theta)$$

*Likelihood*

# Maximum Likelihood Estimation

We have  $n$  patients, we give each the new drug, we record whether or not it's effective

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\}$$

*y<sub>i</sub> = 1 means effective on patient i, -1 otherwise*

*↑ tail → head*

MLE Principle: Find  $\theta$  that maximizes the likelihood of the data:

$$\hat{\theta}_{mle} = \arg \max_{\theta \in [0,1]} P(\mathcal{D} | \theta)$$

# Maximum Likelihood Estimation

We have  $n$  patients, we give each the new drug, we record whether or not it's effective

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_1 = 1 \text{ means effective on patient } i, -1 \text{ otherwise})$$

$\uparrow$  tail       $\uparrow$  head

MLE Principle: Find  $\theta$  that maximizes the likelihood of the data:

$$\hat{\theta}_{mle} = \arg \max_{\theta \in [0,1]} P(\mathcal{D} | \theta) = \arg \max_{\theta \in [0,1]} \theta^{n_1} (1 - \theta)^{n - n_1}$$

$n_1 = \# \text{ of } +1 \text{ (heads)}$

# Maximum Likelihood Estimation

We have  $n$  patients, we give each the new drug, we record whether or not it's effective

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (\text{$y_i = 1$ means effective on patient $i$, -1 otherwise})$$

MLE Principle: Find  $\theta$  that maximizes the likelihood of the data:

$$\begin{aligned}\hat{\theta}_{mle} &= \arg \max_{\theta \in [0,1]} P(\mathcal{D} | \theta) = \arg \max_{\theta \in [0,1]} \theta^{n_1} (1 - \theta)^{n-n_1} \\ &= \arg \max_{\theta \in [0,1]} \ln(\theta^{n_1} (1 - \theta)^{n-n_1})\end{aligned}$$

$\theta = 0.01$

$n_1 = 100$

# Maximum Likelihood Estimation

We have  $n$  patients, we give each the new drug, we record whether or not it's effective

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (\text{$y_1 = 1$ means effective on patient $i$, -1 otherwise})$$

MLE Principle: Find  $\theta$  that maximizes the likelihood of the data:

$$\hat{\theta}_{mle} = \arg \max_{\theta \in [0,1]} P(\mathcal{D} | \theta) = \arg \max_{\theta \in [0,1]} \theta^{n_1} (1 - \theta)^{n - n_1}$$

$$= \arg \max_{\theta \in [0,1]} \ln(\theta^{n_1} (1 - \theta)^{n - n_1})$$

$$= \arg \max_{\theta \in [0,1]} n_1 \ln(\theta) + (n - n_1) \ln(1 - \theta)$$

# Maximum Likelihood Estimation

We have  $n$  patients, we give each the new drug, we record whether or not it's effective

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_1 = 1 \text{ means effective on patient } i, -1 \text{ otherwise})$$

MLE Principle: Find  $\theta$  that maximizes the likelihood of the data:

$$\hat{\theta}_{mle} = \arg \max_{\theta \in [0,1]} P(\mathcal{D} | \theta) = \arg \max_{\theta \in [0,1]} \theta^{n_1} (1 - \theta)^{n-n_1}$$

$$= \arg \max_{\theta \in [0,1]} \ln(\theta^{n_1} (1 - \theta)^{n-n_1})$$

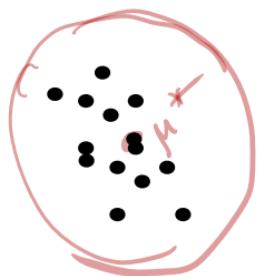
$$= \arg \max_{\theta \in [0,1]} n_1 \ln(\theta) + (n - n_1) \ln(1 - \theta) \quad \textcircled{=} \quad \frac{n_1}{n}$$

$$\frac{n_1}{\theta} - \frac{n-n_1}{1-\theta} = 0$$

solve for  $\theta$

## Ex 2: Estimate the mean

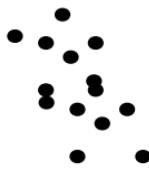
$$\mathcal{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}^d$$



Assume data is from  $\mathcal{N}(\mu^*, I)$ , want to estimate  $\mu^*$  from the data  $\mathcal{D}$

## Ex 2: Estimate the mean

$$\mathcal{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}^d$$



Assume data is from  $\mathcal{N}(\mu^*, I)$ , want to estimate  $\mu^*$  from the data  $\mathcal{D}$

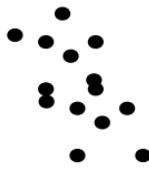
Let's apply the MLE Principle:

$$\text{Step 1: } P(\mathcal{D} | \mu) = \prod_{i=1}^n \frac{1}{\sqrt{(2\pi)^d}} \exp \left( -\frac{1}{2} (x_i - \mu)^\top (x_i - \mu) \right)$$

likelihood of  $x_i$  from  
 $\mathcal{N}(\mu, I)$

## Ex 2: Estimate the mean

$$\mathcal{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}^d$$



Assume data is from  $\mathcal{N}(\mu^*, I)$ , want to estimate  $\mu^*$  from the data  $\mathcal{D}$

Let's apply the MLE Principle:

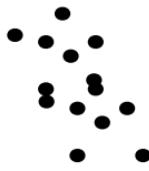
Step 1:  $P(\mathcal{D} | \mu) = \prod_{i=1}^n \frac{1}{\sqrt{(2\pi)^d}} \exp\left(-\frac{1}{2}(x_i - \mu)^\top(x_i - \mu)\right)$

Step 2: apply log and maximize the log-likelihood:

$$\arg \max_{\mu} \underbrace{\sum_{i=1}^n - (x_i - \mu)^\top(x_i - \mu)}$$

## Ex 2: Estimate the mean

$$\mathcal{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}^d$$



Assume data is from  $\mathcal{N}(\mu^\star, I)$ , want to estimate  $\mu^\star$  from the data  $\mathcal{D}$

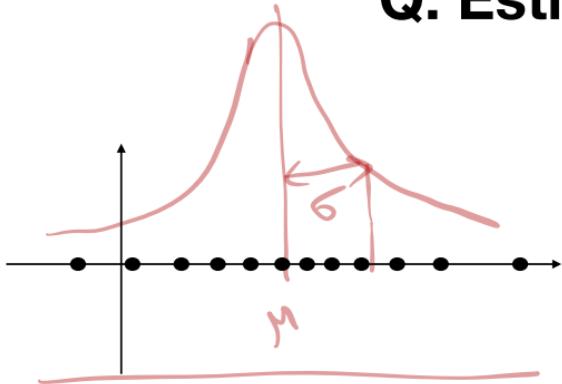
Let's apply the MLE Principle:

$$\text{Step 1: } P(\mathcal{D} | \mu) = \prod_{i=1}^n \frac{1}{\sqrt{(2\pi)^d}} \exp\left(-\frac{1}{2}(x_i - \mu)^\top(x_i - \mu)\right)$$

Step 2: apply log and maximize the log-likelihood:

$$\arg \max_{\mu} \sum_{i=1}^n -(x_i - \mu)^\top(x_i - \mu) \Rightarrow \hat{\mu}_{mle} = \sum_{i=1}^n x_i/n$$

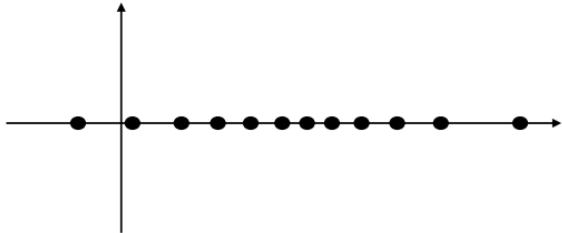
## Q: Estimate the mean and variance



$$\mathcal{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}$$

Assume data is from  $\mathcal{N}(\mu^*, \sigma^2)$ , want to estimate  
 $\mu^*, \sigma$  from the data  $\mathcal{D}$

## Q: Estimate the mean and variance



$$\mathcal{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}$$

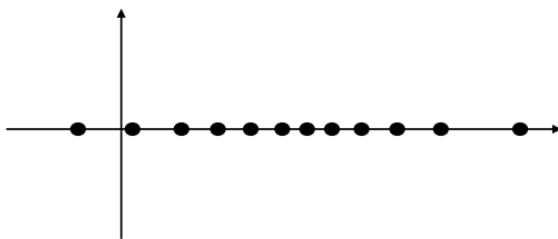
Assume data is from  $\mathcal{N}(\mu^*, \sigma^2)$ , want to estimate  $\mu^*, \sigma$  from the data  $\mathcal{D}$

Let's apply the MLE Principle:

$$\text{Step 1: } P(\mathcal{D} | \mu, \sigma) = \prod_{i=1}^n \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{1}{2}(x_i - \mu)^2 / \sigma^2\right)$$

Likelihood of  $x_i \sim \mathcal{N}(\mu, \sigma^2)$

## Q: Estimate the mean and variance



$$\mathcal{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}$$

Assume data is from  $\mathcal{N}(\mu^*, \sigma^2)$ , want to estimate  $\mu^*, \sigma$  from the data  $\mathcal{D}$

Let's apply the MLE Principle:

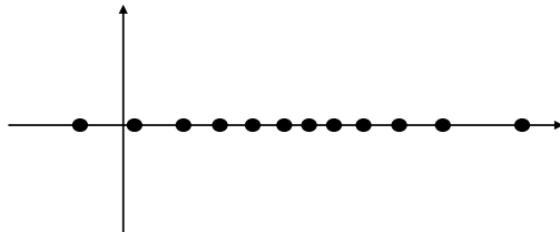
$$\begin{aligned} & \ln P(\mathcal{D} | \mu, \sigma) \\ &= \sum_{i=1}^n \left[ \ln \left( \frac{1}{\sigma \sqrt{2\pi}} \right) \right. \\ &\quad \left. + \ln \exp \left( -\frac{1}{2} \frac{(x_i - \mu)^2}{\sigma^2} \right) \right] \end{aligned}$$

Step 1:  $P(\mathcal{D} | \mu, \sigma) = \prod_{i=1}^n \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{1}{2} (x_i - \mu)^2 / \sigma^2 \right)$

Step 2: apply log and maximize the log-likelihood:

$$\arg \max_{\mu, \sigma > 0} \sum_{i=1}^n \left( - (x_i - \mu)^2 / \sigma^2 - \ln(\sigma) \right)$$

## Q: Estimate the mean and variance



$$\mathcal{D} = \{x_i\}_{i=1}^n, x_i \in \mathbb{R}$$

Assume data is from  $\mathcal{N}(\mu^*, \sigma^2)$ , want to estimate  $\mu^*, \sigma$  from the data  $\mathcal{D}$

Let's apply the MLE Principle:

Step 1:  $P(\mathcal{D} | \mu, \sigma) = \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}(x_i - \mu)^2/\sigma^2\right)$

Step 2: apply log and maximize the log-likelihood:

$$\arg \max_{\mu, \sigma > 0} \sum_{i=1}^n (- (x_i - \mu)^2 / \sigma^2 - \ln(\sigma)) = ??$$

## Summary of MLE

1. MLE is consistent: if our model assumption is correct (e.g., coin flip follows some Bernoulli distribution), then  $\hat{\theta}_{mle} \rightarrow \theta^*$ , as  $n \rightarrow \infty$

$$\left| \hat{\theta}_{mle} - \theta^* \right| \leq \frac{1}{\sqrt{n}}$$

## Summary of MLE

1. MLE is consistent: if our model assumption is correct (e.g., coin flip follows some Bernoulli distribution), then  $\hat{\theta}_{mle} \rightarrow \theta^*$ , as  $n \rightarrow \infty$
2. When our model assumption is wrong (e.g., we use Gaussian to model data which is from some more complicated distribution), then MLE loses such guarantee

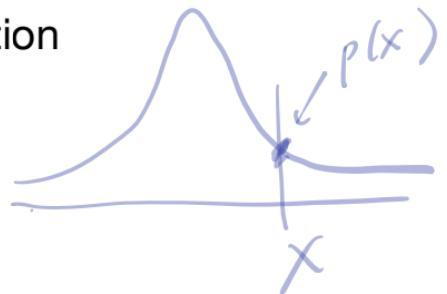
## Outline for today:

1. Maximum Likelihood estimation (MLE)

2. Maximum a Posteriori Probability (MAP)

3. Example: MLE and MAP for classification

$$\int p(x) = 1$$



## Ex: Estimating the probability of a coin flip

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

## Ex: Estimating the probability of a coin flip

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

A Bayesian Statistician will treat the optimal parameter  $\theta^*$  being a random variable:

$$\theta^* \sim P(\theta)$$

$T$   
prob of head

## Ex: Estimating the probability of a coin flip

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

A Bayesian Statistician will treat the optimal parameter  $\theta^*$  being a random variable:

$$\theta^* \sim P(\theta) \text{ prior-post}$$

Example:  $P(\theta)$  being a Beta distribution:

$$P(\theta) = \theta^{\alpha-1}(1-\theta)^{\beta-1}/Z,$$

where  $Z = \int_{\theta \in [0,1]} \theta^{\alpha-1}(1-\theta)^{\beta-1} d\theta$

$\rightarrow \int_{\theta \in [0,1]} P(\theta) d\theta = 1$

# Ex: Estimating the probability of a coin flip

We toss a coin  $n$  times (independently), we observe the following outcomes:

$$\mathcal{D} = \{y_i\}_{i=1}^n, y_i \in \{-1, 1\} \quad (y_i = 1 \text{ means head in } i\text{'s trial, } -1 \text{ means tail})$$

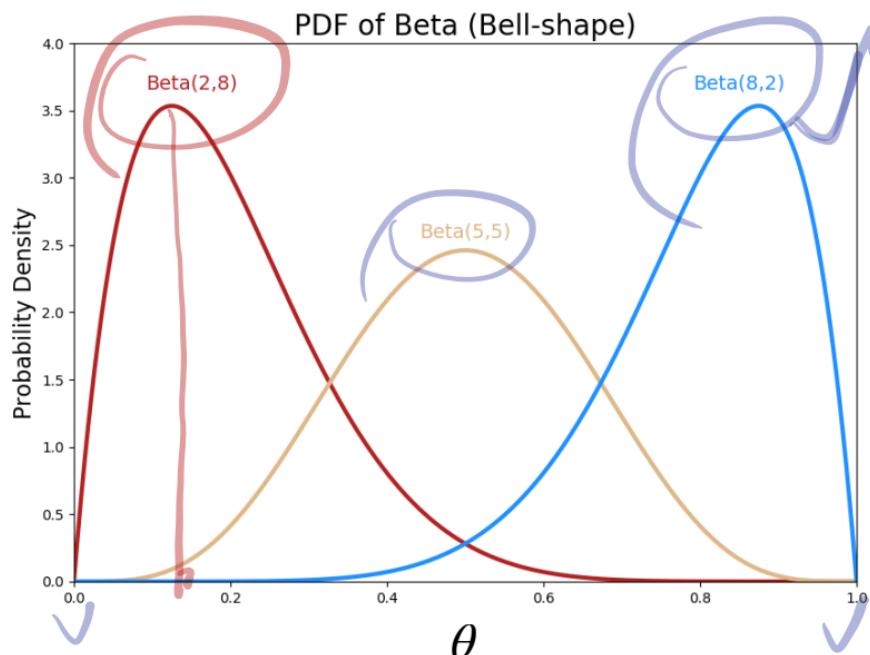
A Bayesian Statistician will treat the optimal parameter  $\theta^*$  being a random variable:

$$\theta^* \sim P(\theta)$$

Example:  $P(\theta)$  being a Beta distribution:

$$P(\theta) = \theta^{\alpha-1}(1-\theta)^{\beta-1}/Z,$$

$$\text{where } Z = \int_{\theta \in [0,1]} \theta^{\alpha-1}(1-\theta)^{\beta-1} d\theta$$



## The Posterior distribution over $\theta$

Now, we have a prior  $P(\theta)$ , and we have a

dataset  $\mathcal{D} = \{y_i\}_{i=1}^n$ , define **posterior  
distribution**:

$$\underline{P(\theta | \mathcal{D})}$$

## The Posterior distribution over $\theta$

Now, we have a prior  $P(\theta)$ , and we have a

dataset  $\mathcal{D} = \{y_i\}_{i=1}^n$ , define **posterior distribution**:

$$P(\theta | \mathcal{D})$$

$$P(a, b)$$

Using Bayes rule, we get:

$$= P(a) P(b|a)$$

$$P(\theta | \mathcal{D}) = P(\theta) P(\mathcal{D} | \theta) / P(\mathcal{D}) = P(b) P(a|b)$$

# The Posterior distribution over $\theta$

Now, we have a prior  $P(\theta)$ , and we have a

dataset  $\mathcal{D} = \{y_i\}_{i=1}^n$ , define **posterior distribution**:

$$P(\theta | \mathcal{D})$$

Using Bayes rule, we get:

$$P(\theta | \mathcal{D}) = P(\theta)P(\mathcal{D} | \theta) / P(\mathcal{D})$$

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

$P(\mathcal{D})$  is independent of  $\theta$

# The Posterior distribution over $\theta$

Now, we have a prior  $P(\theta)$ , and we have a

dataset  $\mathcal{D} = \{y_i\}_{i=1}^n$ , define **posterior distribution**:

$$P(\theta | \mathcal{D})$$

Using Bayes rule, we get:

$$P(\theta | \mathcal{D}) = P(\theta)P(\mathcal{D} | \theta)/P(\mathcal{D})$$

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

Data likelihood

Prior  $\propto$  Posterior  $\propto$  Likelihood

# The Posterior distribution over $\theta$

Now, we have a prior  $P(\theta)$ , and we have a

dataset  $\mathcal{D} = \{y_i\}_{i=1}^n$ , define **posterior distribution**:

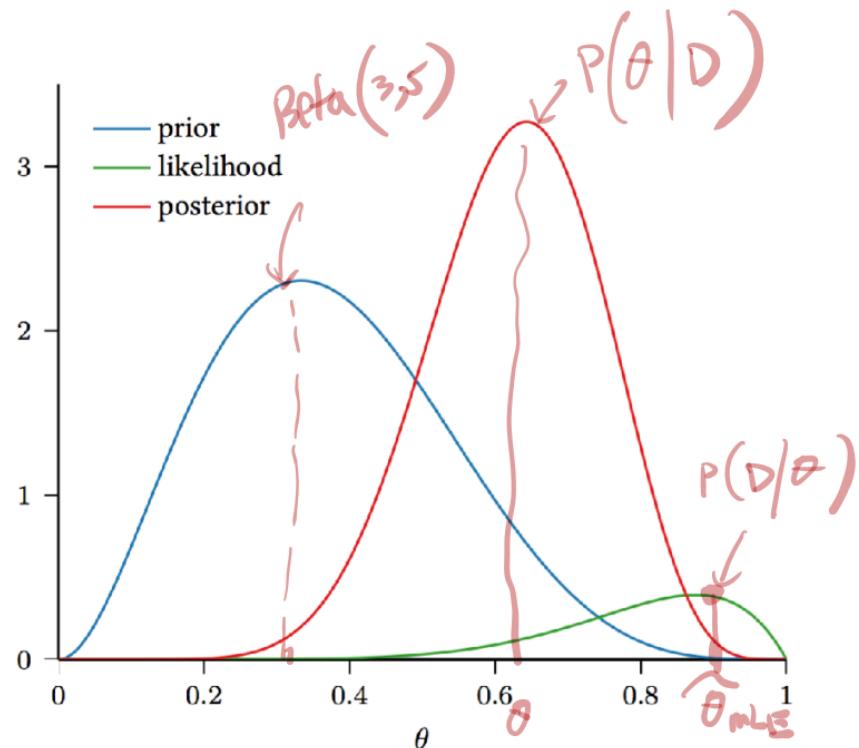
$$P(\theta | \mathcal{D})$$

Using Bayes rule, we get:

$$P(\theta | \mathcal{D}) = P(\theta)P(\mathcal{D} | \theta)/P(\mathcal{D})$$

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

Posterior  $\propto$  Prior  $\times$  Likelihood



# The Posterior distribution over $\theta$

Now, we have a prior  $P(\theta)$ , and we have a

dataset  $\mathcal{D} = \{y_i\}_{i=1}^n$ , define **posterior distribution**:

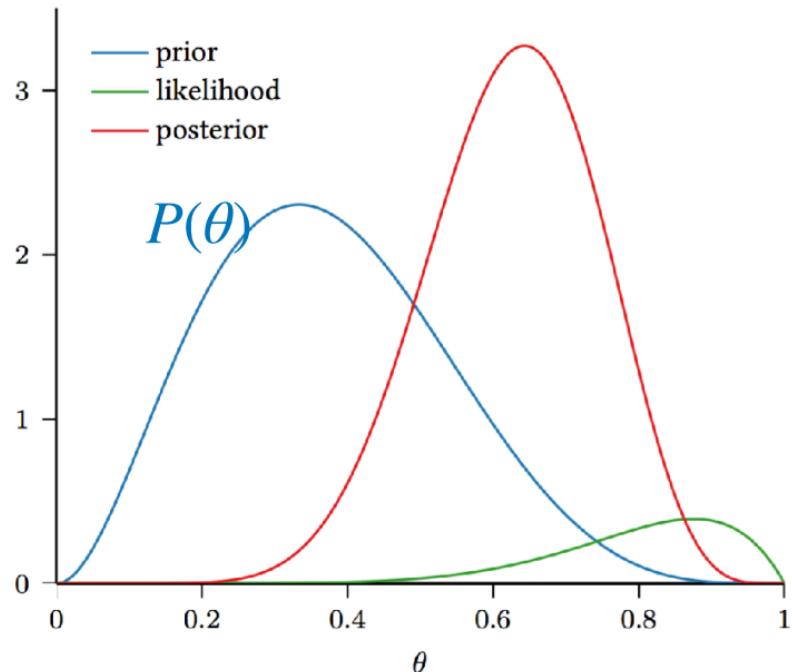
$$P(\theta | \mathcal{D})$$

Using Bayes rule, we get:

$$P(\theta | \mathcal{D}) = P(\theta)P(\mathcal{D} | \theta)/P(\mathcal{D})$$

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

Posterior  $\propto$  Prior  $\times$  Likelihood



# The Posterior distribution over $\theta$

Now, we have a prior  $P(\theta)$ , and we have a

dataset  $\mathcal{D} = \{y_i\}_{i=1}^n$ , define **posterior distribution**:

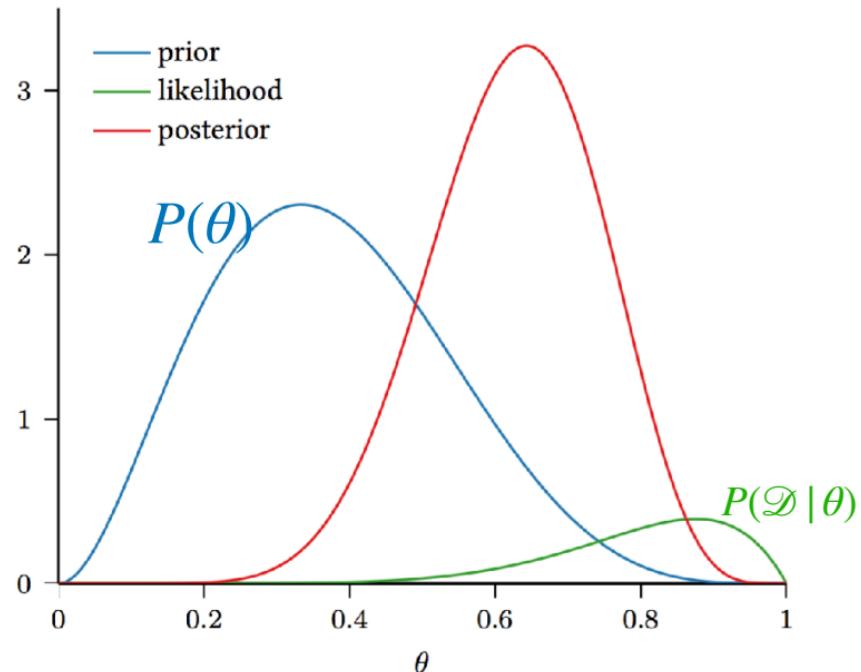
$$P(\theta | \mathcal{D})$$

Using Bayes rule, we get:

$$P(\theta | \mathcal{D}) = P(\theta)P(\mathcal{D} | \theta)/P(\mathcal{D})$$

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

Posterior  $\propto$  Prior  $\times$  Likelihood



# The Posterior distribution over $\theta$

Now, we have a prior  $P(\theta)$ , and we have a

dataset  $\mathcal{D} = \{y_i\}_{i=1}^n$ , define **posterior distribution**:

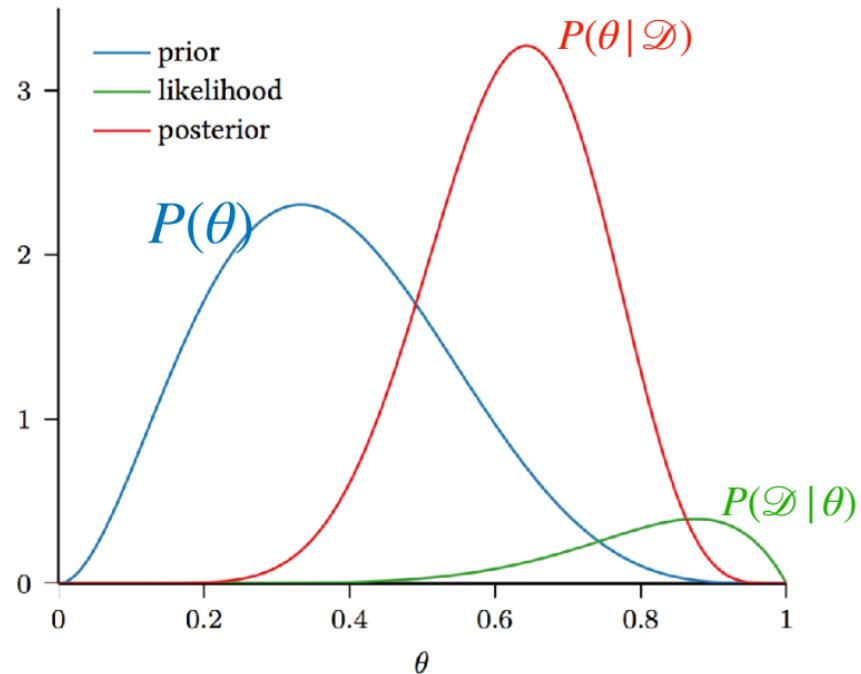
$$P(\theta | \mathcal{D})$$

Using Bayes rule, we get:

$$P(\theta | \mathcal{D}) = P(\theta)P(\mathcal{D} | \theta)/P(\mathcal{D})$$

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

Posterior  $\propto$  Prior  $\times$  Likelihood



# Maximum A Posteriori Probability estimation (MAP)

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

## Maximum A Posteriori Probability estimation (MAP)

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

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} P(\theta | \mathcal{D}) = \arg \max_{\theta \in [0,1]} P(\theta)P(\mathcal{D} | \theta)$$

## Maximum A Posteriori Probability estimation (MAP)

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

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} P(\theta | \mathcal{D}) = \arg \max_{\theta \in [0,1]} P(\theta)P(\mathcal{D} | \theta)$$

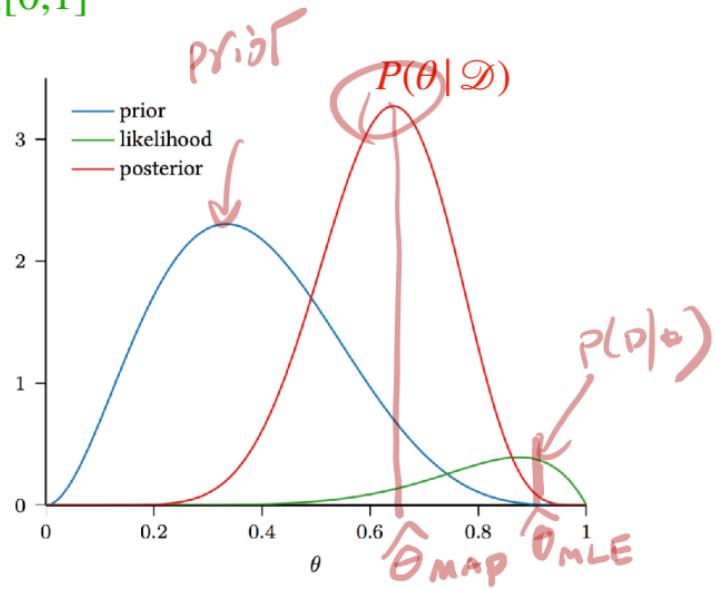
$$= \arg \max_{\theta \in [0,1]} \underbrace{\ln P(\theta) + \ln P(\mathcal{D} | \theta)}$$

# Maximum A Posteriori Probability estimation (MAP)

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

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} P(\theta | \mathcal{D}) = \arg \max_{\theta \in [0,1]} P(\theta)P(\mathcal{D} | \theta)$$

$$= \arg \max_{\theta \in [0,1]} \ln P(\theta) + \ln P(\mathcal{D} | \theta)$$



## MAP for coin flip

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} \ln(P(\theta)P(\mathcal{D} | \theta))$$

## MAP for coin flip

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} \ln(P(\theta)P(\mathcal{D} | \theta))$$

Step 1: specify Prior  $P(\theta) \propto \underline{\theta^{\alpha-1}(1-\theta)^{\beta-1}}$  Beta  $\alpha > 0$   
 $\beta > 0$

## MAP for coin flip

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} \ln(P(\theta)P(\mathcal{D} | \theta))$$

Step 1: specify Prior  $P(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$

Step 2: data likelihood  $P(\mathcal{D} | \theta) = \theta^{n_1}(1-\theta)^{n-n_1}$

✓  $n_1 = \# \text{ of } +1 \text{ (heads)}$

## MAP for coin flip

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} \ln(P(\theta)P(\mathcal{D} | \theta))$$

Step 1: specify Prior  $P(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$

Step 2: data likelihood  $P(\mathcal{D} | \theta) = \theta^{n_1}(1-\theta)^{n-n_1}$

Step 3: Compute posterior  $\underline{P(\theta | \mathcal{D})} \propto \theta^{n_1+\alpha-1}(1-\theta)^{n-n_1+\beta-1}$

## MAP for coin flip

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} \ln(P(\theta)P(\mathcal{D} | \theta))$$

Step 1: specify Prior  $P(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$

Step 2: data likelihood  $P(\mathcal{D} | \theta) = \theta^{n_1}(1-\theta)^{n-n_1}$

Step 3: Compute posterior  $P(\theta | \mathcal{D}) \propto \theta^{n_1+\alpha-1}(1-\theta)^{n-n_1+\beta-1}$

Step 4: Compute MAP  $\hat{\theta}_{map} = \frac{n_1 + \alpha - 1}{n + \alpha + \beta - 2}$

$$(MLE = \frac{n_1}{n})$$

$$\underset{\theta \in [0,1]}{\operatorname{arg\,max}} P(\theta | \mathcal{D})$$

## MAP for coin flip

$$\hat{\theta}_{map} = \arg \max_{\theta \in [0,1]} \ln(P(\theta)P(\mathcal{D} | \theta))$$

Step 1: specify Prior  $P(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$

Step 2: data likelihood  $P(\mathcal{D} | \theta) = \theta^{n_1}(1-\theta)^{n-n_1}$

Step 3: Compute posterior  $P(\theta | \mathcal{D}) \propto \theta^{n_1+\alpha-1}(1-\theta)^{n-n_1+\beta-1}$  # of heads:  $n_1 + \alpha - 1$

Step 4: Compute MAP  $\hat{\theta}_{map} = \frac{n_1 + \alpha - 1}{n + \alpha + \beta - 2}$

# of Exp:  $n + \alpha - 1 + \beta - 1$

$(\alpha - 1, \beta - 1)$  can be understood as some fictitious flips: we had  $\alpha - 1$  hallucinated heads, and  $\beta - 1$  hallucinated tails

## Some considerations on prior distributions

1. In coin flip example, when  $n \rightarrow \infty$ ,  $\hat{\theta}_{map} = \frac{n_1 + \alpha - 1}{n + \alpha + \beta - 2} \rightarrow \frac{n_1}{n}$  (i.e.,  $\hat{\theta}_{mle}$ )

## Some considerations on prior distributions

1. In coin flip example, when  $n \rightarrow \infty$ ,  $\hat{\theta}_{map} = \frac{n_1 + \alpha - 1}{n + \alpha + \beta - 2} \rightarrow \frac{n_1}{n}$  (i.e.,  $\hat{\theta}_{mle}$ )
2. When  $n$  is small and our prior is accurate, MAP can work better than MLE

## Some considerations on prior distributions

1. In coin flip example, when  $n \rightarrow \infty$ ,  $\hat{\theta}_{map} = \frac{n_1 + \alpha - 1}{n + \alpha + \beta - 2} \rightarrow \frac{n_1}{n}$  (i.e.,  $\hat{\theta}_{mle}$ )
2. When  $n$  is small and our prior is accurate, MAP can work better than MLE
3. In general, not so easy to set up a good prior....

## **Outline for today:**

1. Maximum Likelihood estimation (MLE)
2. Maximum a posteriori probability (MAP)
3. Example: MLE and MAP for classification

## Binary Classification

$$x \sim P(x) \quad y \sim P(y|x)$$

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y|x)$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y | x)$

Let us assume the ground truth has the form  $P(y = 1 | x; \theta^\star) = \frac{\exp((\theta^\star)^\top x)}{1 + \exp((\theta^\star)^\top x)}$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y | x)$

Let us assume the ground truth has the form  $P(y = 1 | x; \theta^\star) = \frac{\exp((\theta^\star)^\top x)}{1 + \exp((\theta^\star)^\top x)}$

Goal: estimate  $\theta^\star$  using  $\mathcal{D}$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y | x)$

Start with a parametric form  $P(y = 1 | x; \theta) = \frac{\exp(\theta^\top x)}{1 + \exp(\theta^\top x)}$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y|x)$

Start with a parametric form  $P(y=1|x; \theta) = \frac{\exp(\theta^\top x)}{1 + \exp(\theta^\top x)}$

$P(a,b) = P(a) \cdot P(b|a)$

Using MLE:

$$\arg \max_{\theta} P(\mathcal{D}|\theta) = \arg \max_{\theta} \prod_{i=1}^n P(x_i, y_i | \theta)$$

$\downarrow$

$P(y_i|x_i; \theta) \cdot P(x_i)$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y|x)$

Start with a parametric form  $P(y = 1 | x; \theta) = \frac{\exp(\theta^\top x)}{1 + \exp(\theta^\top x)}$

Using MLE:

$$\arg \max_{\theta} P(\mathcal{D} | \theta) = \arg \max_{\theta} \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max \ln \prod_{i=1}^n P(y_i | x_i; \theta)$$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y|x)$

Start with a parametric form  $P(y = 1 | x; \theta) = \frac{\exp(\theta^\top x)}{1 + \exp(\theta^\top x)}$

Using MLE:

$$\arg \max_{\theta} P(\mathcal{D} | \theta) = \arg \max_{\theta} \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max \ln \prod_{i=1}^n P(y_i | x_i; \theta)$$

$$= \arg \max_{\theta} \sum_i \ln P(y_i | x_i; \theta)$$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y|x)$

Start with a parametric form  $P(y = 1 | x; \theta) = \frac{\exp(\theta^\top x)}{1 + \exp(\theta^\top x)}$

Using MLE:

$$\arg \max_{\theta} P(\mathcal{D} | \theta) = \arg \max_{\theta} \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max \ln \prod_{i=1}^n P(y_i | x_i; \theta)$$

$$= \arg \max_{\theta} \sum_i \ln P(y_i | x_i; \theta)$$

Using MAP:

$$\arg \max_{\theta} P(\theta | \mathcal{D}) = \arg \max_{\theta} P(\theta) \prod_{i=1}^n P(x_i, y_i | \theta)$$

prior ————— pat<sub>n</sub> likelihood

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y|x)$

Start with a parametric form  $P(y = 1 | x; \theta) = \frac{\exp(\theta^\top x)}{1 + \exp(\theta^\top x)}$

Using MLE:

$$\arg \max_{\theta} P(\mathcal{D} | \theta) = \arg \max_{\theta} \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max \ln \prod_{i=1}^n P(y_i | x_i; \theta)$$

$$= \arg \max_{\theta} \sum_i \ln P(y_i | x_i; \theta)$$

Using MAP:

$$\arg \max_{\theta} P(\theta | \mathcal{D}) = \arg \max_{\theta} P(\theta) \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max_{\theta} \ln(P(\theta)) \prod_{i=1}^n P(y_i | x_i; \theta)$$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y|x)$

Start with a parametric form  $P(y = 1 | x; \theta) = \frac{\exp(\theta^\top x)}{1 + \exp(\theta^\top x)}$

Using MLE:

$$\arg \max_{\theta} P(\mathcal{D} | \theta) = \arg \max_{\theta} \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max \ln \prod_{i=1}^n P(y_i | x_i; \theta)$$

$$= \arg \max_{\theta} \sum_i \ln P(y_i | x_i; \theta)$$

Using MAP:

$$\arg \max_{\theta} P(\theta | \mathcal{D}) = \arg \max_{\theta} P(\theta) \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max_{\theta} \ln(P(\theta)) \prod_{i=1}^n P(y_i | x_i; \theta)$$

$$= \arg \max_{\theta} \ln P(\theta) + \sum_i \ln P(y_i | x_i; \theta)$$

# Binary Classification

Given labeled dataset  $\{x_i, y_i\}_{i=1}^n, x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ , we want to estimate  $P(y|x)$

Start with a parametric form  $P(y = 1 | x; \theta) = \frac{\exp(\theta^\top x)}{1 + \exp(\theta^\top x)}$

Using MLE:

$$\arg \max_{\theta} P(\mathcal{D} | \theta) = \arg \max_{\theta} \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max \ln \prod_{i=1}^n P(y_i | x_i; \theta)$$

$$= \arg \max_{\theta} \sum_i \ln P(y_i | x_i; \theta)$$

Using MAP:

$$\arg \max_{\theta} P(\theta | \mathcal{D}) = \arg \max_{\theta} P(\theta) \prod_{i=1}^n P(x_i, y_i | \theta)$$

$$= \arg \max_{\theta} \ln(P(\theta)) \prod_{i=1}^n P(y_i | x_i; \theta)$$

$$= \arg \max_{\theta} \ln P(\theta) + \sum_i \ln P(y_i | x_i; \theta)$$

Independent of the data

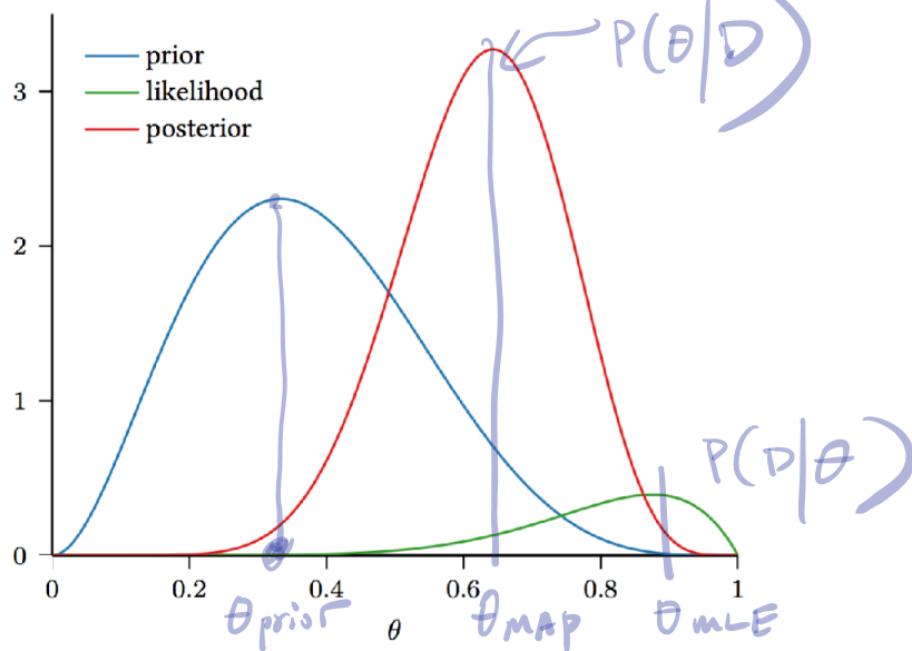
# Binary Classification

MLE:

$$\arg \max_{\theta} \sum_i \ln P(y_i | x_i; \theta)$$

MAP:

$$\arg \max_{\theta} \ln P(\theta) + \sum_i \ln P(y_i | x_i; \theta)$$



# Summary for today

## 1 MLE (frequentist perspective):

The ground truth  $\theta^*$  is unknown but fixed; we search for the parameter that makes the data as likely as possible

# Summary for today

## 1 MLE (frequentist perspective):

The ground truth  $\theta^*$  is unknown but fixed; we search for the parameter that makes the data as likely as possible

$$\arg \max_{\theta} P(\mathcal{D} | \theta)$$

# Summary for today

1 MLE (frequentist perspective):

The ground truth  $\theta^*$  is unknown but fixed; we search for the parameter that makes the data as likely as possible

$$\arg \max_{\theta} P(\mathcal{D} | \theta)$$

2 MAP (Bayesian perspective):

The ground truth  $\theta^*$  treated as a random variable, i.e.,  $\theta^* \sim P(\theta)$ ; we search for the parameter that maximizes the posterior

# Summary for today



## 1 MLE (frequentist perspective):

The ground truth  $\theta^*$  is unknown but fixed; we search for the parameter that makes the data as likely as possible

$$\arg \max_{\theta} P(\mathcal{D} | \theta)$$

## 2 MAP (Bayesian perspective):

The ground truth  $\theta^*$  treated as a random variable, i.e.,  $\theta^* \sim P(\theta)$ ; we search for the parameter that maximizes the posterior

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