Maximum Likelihood Estimation

Your first consulting job

- *Billionaire*: I have special coin, if I flip it, what's the probability it will be heads?
- *You*: Please flip it a few times:

flip $n=5$ times

HHTHT

- *You*: The probability is: $3/5$

$$\frac{k=3 \text{ heads}}{n=5 \text{ flips}}$$

- *Billionaire:* Why?

Independent, yani P(Xs=b)'nin P(Xt=a) üzerinde etkisi yok.

Coin – Binomial Distribution

- **Data**: sequence *D= (HHTHT ...)*, **k heads** out of **n flips**

Observed

- **Hypothesis:** P(Heads) = θ, P(Tails) = 1-θ
  - Flips are i.i.d.: If $X_t \in \{0,1\}$ denoting tth flip
    - Independent events $\mathbb{P}(X_t = a, X_s = b) = \mathbb{P}(X_t = a)\,\mathbb{P}(X_s = b)$
    - Identically distributed according to Binomial distribution

$$\mathbb{P}(X_t = 0) = \mathbb{P}(X_s = 0) = 1 - \theta$$

$$\mathbb{P}(X_t = 1) = \theta$$

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

$$= P(H|\theta)P(H|\theta)P(T|\theta)P(H|\theta)P(T|\theta)$$

$$= \theta^3(1-\theta)^2$$

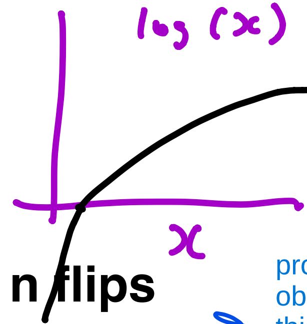
In general,

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

true prob., we don't know that value.

Maximum Likelihood Estimation

$\mathbb{P}(\text{head}) = \theta^*$



- **Data**: sequence *D= (HHTHT…)*, **k heads** out of **n flips**
- **Hypothesis:** P(Heads) = θ, P(Tails) = 1-θ

prob. of observing this data given that theta is true is this expression.

likelihood

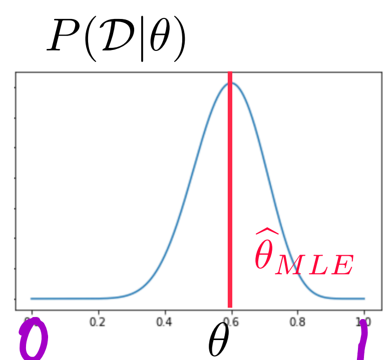
$$\boxed{P(\mathcal{D}|\theta) = \theta^k (1-\theta)^{n-k}}$$

- Maximum likelihood estimation (MLE): Choose θ that maximizes the probability of observed data:

$$\widehat{\theta}_{MLE} = \arg\max_{\theta} \; P(\mathcal{D}|\theta)$$

just scaling

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



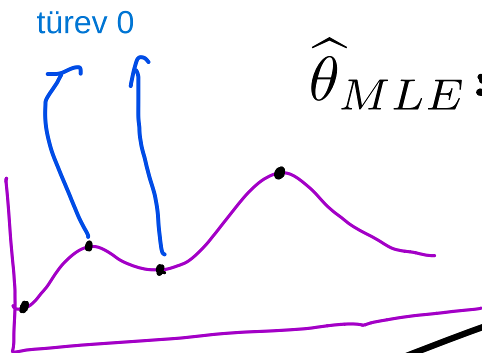
think of this as a function of theta and choose the theta that maximize this func.

BECAUSE LOG FUNCTION IS MONOTONICALLY INCREASING, MAXIMIZING THE LOG OF SOMETHING IS THE SAME AS MAXIMIZING ITSELF.

Your first learning algorithm

$$\log(ab) = \log(a) + \log(b)$$

for any $a, b > 0$



$$\widehat{\theta}_{MLE} := \arg\max_{\theta} \log\left(P(\mathcal{D}|\theta)\right)$$

$$= \arg\max_{\theta} \log\left(\theta^k (1-\theta)^{n-k}\right)$$

$$= \arg\max_{\theta} \; k\log(\theta) + (n-k)\log(1-\theta)$$

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

$$\frac{\partial}{\partial\theta}[\,\cdot\,] = \frac{k}{\theta} + \frac{n-k}{1-\theta}\cdot(-1) = 0$$

(multiply $\theta(1-\theta)$ on both sides)

$$\rightarrow (1-\theta)k - \theta(n-k) = 0 \implies \hat{\theta}_{MLE} = k/n$$

How many flips do I need?

$$\widehat{\theta}_{MLE} = \frac{k}{n}$$

- *You*: flip the coin 5 times. *Billionaire*: I got 3 heads.

$$\widehat{\theta}_{MLE} = 3/5$$

- *You*: flip the coin 50 times. *Billionaire*: I got 20 heads.

$$\widehat{\theta}_{MLE} = 20/50 = 2/5$$

trust that answer a little bit more. Because 50 > 5

- *Billionaire:* Which one is right? Why?

Quantifying Uncertainty

- For **n flips** and **k heads** the MLE is **unbiased** for true θ^*:

$$\widehat{\theta}_{MLE} = \frac{k}{n} \qquad \mathbb{E}[\widehat{\theta}_{MLE}] = \theta^*$$

- **Expectation** describes how the estimator behaves *on average.*

$$\underbrace{\hat{\theta}_{MLE} = \frac{1}{n}\sum_{t=1}^{n} \mathbb{1}\{X_t = H\}}$$

$X_t \in \{H, T\}$

$$\mathbb{1}\{\Omega\} = \begin{cases} 1 & \text{if } \Omega = \text{true} \\ 0 & \text{o.w.} \end{cases}$$

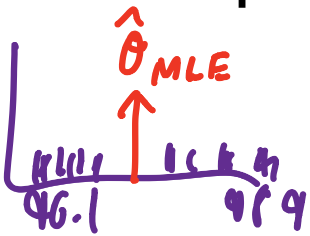
By assumption, $\exists\, \theta^* : \mathbb{P}(X_t = H) = \theta^*$

$= \mathbb{E}[\mathbb{1}\{X_t = H\}]$ = P(Xt=H) * I(Xt=H) + P(Xt=T) * I(Xt=H)

$$\mathbb{E}[\hat{\theta}_{MLE}] = \frac{1}{n}\sum_{t=1}^{n} \mathbb{E}[\mathbb{1}\{X_t = H\}] = \frac{1}{n}\sum_{t} \theta^* = \theta^*$$

Quantifying Uncertainty

- For **n flips** and **k heads** the MLE is **unbiased** for true θ*:



$$\underbrace{\widehat{\theta}_{MLE} = \frac{k}{n}}_{\text{Random}} \qquad \underbrace{\mathbb{E}[\widehat{\theta}_{MLE}] = \theta^*}_{\text{Deterministic}}$$

- **Expectation** describes how the estimator behaves *on average.*
- The **Variance** is the expected squared deviation from the mean:

$$\text{Variance}(\widehat{\theta}_{MLE}) := \mathbb{E}\left[\left(\widehat{\theta}_{MLE} - \mathbb{E}[\widehat{\theta}_{MLE}]\right)^2\right]$$

- As a rule of thumb:

$$\widehat{\theta}_{MLE} \approx \mathbb{E}[\widehat{\theta}_{MLE}] \pm \sqrt{\text{Variance}(\widehat{\theta}_{MLE})}$$

- **Exercise**: compute the $\text{Variance}(\widehat{\theta}_{MLE})$

Expectation versus High Probability

- For **n flips** and **k heads** the MLE is **unbiased** for true θ^*:

$$\widehat{\theta}_{MLE} = \frac{k}{n} \qquad \mathbb{E}[\widehat{\theta}_{MLE}] = \theta^*$$

- Expectation describes how the estimator behaves *on average.*
- For any $\varepsilon>0$ can we bound $\mathbb{P}(|\widehat{\theta}_{MLE} - \mathbb{E}[\widehat{\theta}_{MLE}]| \geq \epsilon)$?

Markov's inequality

For any $t > 0$ and non-negative random variable X

$$\mathbb{P}(X \geq t) \leq \frac{\mathbb{E}[X]}{t}$$

- **Exercise**: Apply Markov's inequality to obtain bound.
  (Hint: set $X = |\widehat{\theta}_{MLE} - \theta^*|^2$)

Maximum Likelihood Estimation

Each X_i is iid from $f(x;\theta)$ pmf

Observe $X_1, X_2, \ldots, X_n$ drawn IID from $f(x;\theta)$ for some "true" $\theta = \theta_*$

Likelihood function $L_n(\theta) = \prod_{i=1}^{n} f(X_i;\theta)$

Log-Likelihood function $l_n(\theta) = \log(L_n(\theta)) = \sum_{i=1}^{n} \log(f(X_i;\theta))$

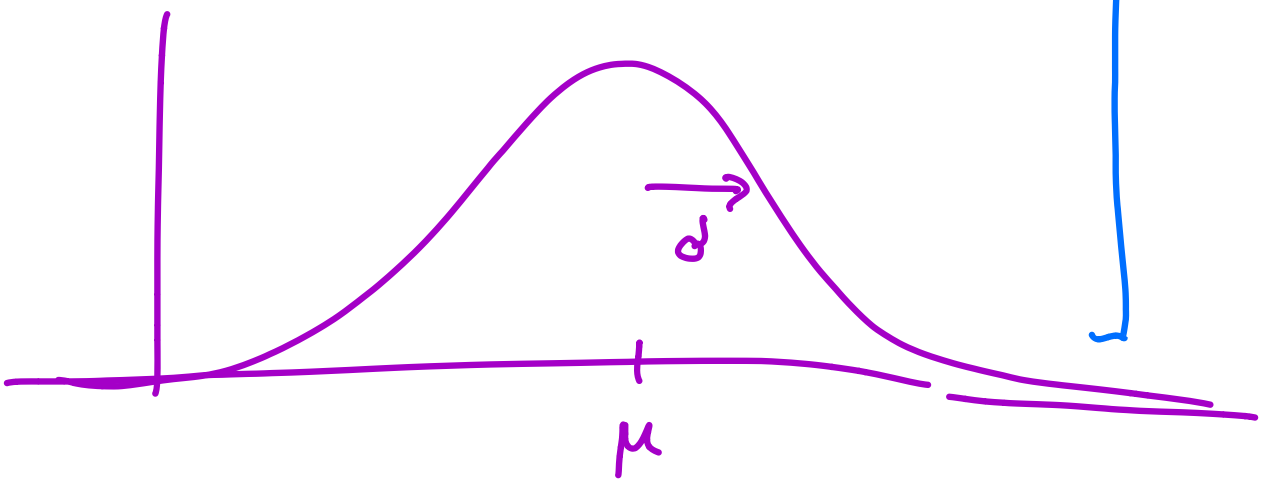
Maximum Likelihood Estimator (MLE) $\widehat{\theta}_{MLE} = \underline{\arg\max_{\theta} L_n(\theta)}$

Set d/dx (log(Ln(theta))) to ZERO. $\rightarrow$ for closed-form solutions

What about continuous variables?

- *Billionaire*: What if I am measuring a **continuous variable**?
- ***You*: Let me tell you about Gaussians…**

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



Some properties of Gaussians

- affine transformation (multiplying by scalar and adding a constant)
  - X ~ $N(\mu,\sigma^2)$
  - Y = aX + b ➔ Y ~ $N(a\mu+b,a^2\sigma^2)$

- Sum of Gaussians
  - X ~ $N(\mu_X,\sigma^2_X)$
  - Y ~ $N(\mu_Y,\sigma^2_Y)$
  - Z = X+Y ➔ Z ~ $N(\mu_X+\mu_Y, \sigma^2_X+\sigma^2_Y)$

MLE for Gaussian

- Prob. of i.i.d. samples $D=\{x_1,\ldots,x_n\}$ (e.g., temperature):

$$P(\mathcal{D}|\mu,\sigma) = P(x_1,\ldots,x_n|\mu,\sigma) = \prod_{i=1}^{n} P(x_i|\mu,\sigma)$$

$$= \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \prod_{i=1}^{n} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

We can draw different distributions by trying different (mu,sigma) tuples.

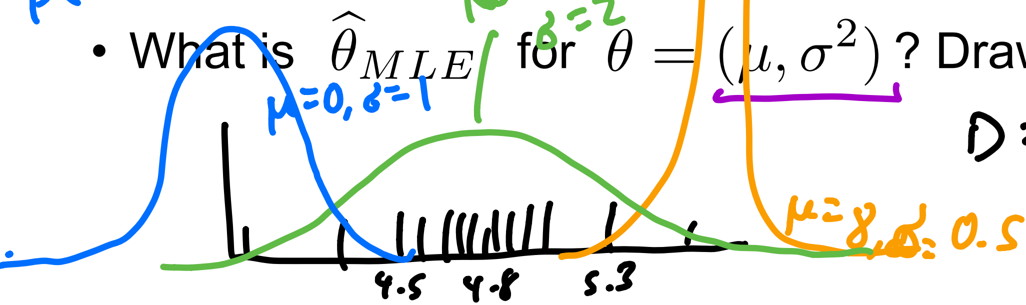
- Log-likelihood of data:

$$\log P(\mathcal{D}|\mu,\sigma) = -n\log(\sigma\sqrt{2\pi}) - \sum_{i=1}^{n}\frac{(x_i-\mu)^2}{2\sigma^2}$$

$p(x|\mu,\sigma^2)$

- What is $\widehat{\theta}_{MLE}$ for $\theta = (\mu,\sigma^2)$? Draw a picture!

$D = \{4.5, 5.3, 4.8, \ldots\ldots\}$



Your second learning algorithm: MLE for mean of a Gaussian

- What's MLE for mean?

$$\frac{d}{d\mu}\log P(\mathcal{D}|\mu,\sigma) = \frac{d}{d\mu}\left[\overset{0}{\cancel{-n\log(\sigma\sqrt{2\pi})}} - \sum_{i=1}^{n}\frac{(x_i-\mu)^2}{2\sigma^2}\right]$$

$$= \sum_{i=1}^{n}\frac{(x_i-\mu)}{\sigma^2} = 0$$

$$\Rightarrow \quad \hat{\mu}_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

MLE for variance

depends on mu

- Again, set derivative to zero:

$$\frac{d}{d\sigma}\log P(\mathcal{D}|\mu,\sigma) = \frac{d}{d\sigma}\left[\underline{-n\log(\sigma\sqrt{2\pi})} - \sum_{i=1}^{n}\frac{(x_i-\mu)^2}{2\sigma^2}\right]$$

$$= -n\cdot\frac{1}{\sigma\sqrt{2\pi}}\cdot\sqrt{2\pi} - \sum_{i=1}^{n}\frac{(x_i-\mu)^2}{2}\cdot(-2)\sigma^{-3} = 0$$

(multiply σ^3 on both sides after setting deriv. $=0$)

$$\rightarrow \quad -n\sigma^2 + \sum_{i=1}^{n}(x_i-\mu)^2 = 0$$

$$\hat{\sigma}^2_{MLE} = \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\hat{\mu}_{MLE})^2$$

Learning Gaussian parameters

- MLE:

$$\left[\begin{array}{l} \widehat{\mu}_{MLE} = \frac{1}{n}\sum_{i=1}^{n} x_i \\ \widehat{\sigma^2}_{MLE} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \widehat{\mu}_{MLE})^2 \end{array}\right.$$

- MLE for the variance of a Gaussian is **biased** (Exercise)

$$\underbrace{\mathbb{E}[\widehat{\sigma^2}_{MLE}]} \neq \underline{\sigma}^2$$

- Unbiased variance estimator:

$$\left[\ \widehat{\sigma^2}_{unbiased} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \widehat{\mu}_{MLE})^2\right.$$

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Maximum Likelihood Estimator (MLE) $\widehat{\theta}_{MLE} = \arg\max_{\theta} L_n(\theta)$

$X_i \sim \exp(\lambda)$

$P(X_i \geq t) = e^{-\lambda t}$

$\hat{\theta}_{MLE}$ is unbiased if

$\mathbb{E}[\hat{\theta}_{MLE}] = \theta^*$

Maximum Likelihood Estimation

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$\sqrt{\text{Sample Variance}}$

Properties (under benign regularity conditions—smoothness, identifiability, etc.):

- Asymptotically consistent and normal: $\frac{\widehat{\theta}_{MLE} - \theta_*}{\widehat{se}} \sim \mathcal{N}(0,1)$
- Asymptotic Optimality, minimum variance (see Cramer-Rao lower bound)

Recap

- Learning is…
  - Collect some data
    - E.g., coin flips
  - Choose a hypothesis class or model
    - E.g., binomial
  - Choose a loss function
    - E.g., data likelihood
  - Choose an optimization procedure
    - E.g., set derivative to zero to obtain MLE
  - Justifying the accuracy of the estimate
    - E.g., Markov’s inequality