CSE 312 Foundations of Computing II

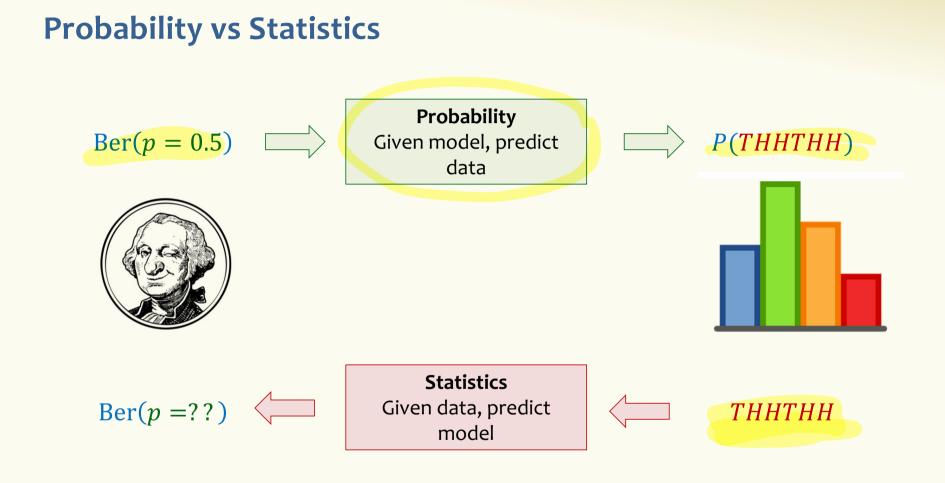
22: Maximum Likelihood Estimation (MLE)

CSE 422

www.slido.com/1692973

Agenda

- Idea: Estimation <
- Maximum Likelihood Estimation (example: mystery coin)
- Continuous MLE



Recap Formalizing Polls

We assume that poll answers $X_1, ..., X_n \sim \text{Ber}(p)$ i.i.d. for <u>unknown</u> p

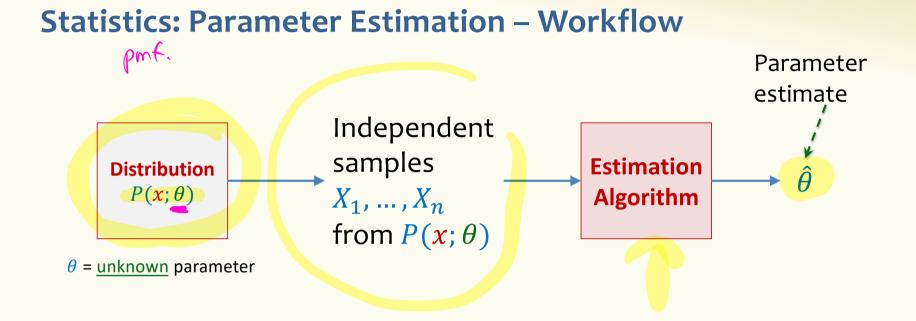
Goal: Estimate *p*

We did this by computing $\hat{p} = \frac{1}{n} \sum_{i=1}^{n} X_i$

Recap More generally ...

In estimation we often

- Assume: we know the type of the random variable that we are observing independent samples from
 - We just don't know the parameters, e.g.
 - the bias p of a random coin Bernoulli(p)
 - The arrival rate λ for the Poisson(λ) or Exponential(λ)
 - The mean μ and variance σ of a normal $\mathcal{N}(\mu, \sigma)$
- Goal: find the "best" parameters to fit the data



Example: coin flip distribution with unknown θ = probability of heads

Goal: Estimate

Example

Suppose we have a mystery coin with some probability p of coming up heads. We flip the coin 8 times, independent of other flips, and see the following sequence of flips

TTHTHTTH

Given this data, what would you estimate *p* is?

Poll: www.slido.com/1692973

a. 1/2
b. 5/8
c. 3/8
d. 1/4

How can you argue "objectively" that this your estimate is the best estimate?

Agenda

- Idea: Estimation
- Maximum Likelihood Estimation (example: mystery coin)
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Say we see outcome *HHTHH*.

You tell me your best guess about the value of the unknown parameter θ (a.k.a. p) is 4/5. Is there some way that you can argue "objectively" that this is the best estimate?

6 maximizes What value of this fn? 50

10

6"(1-6)

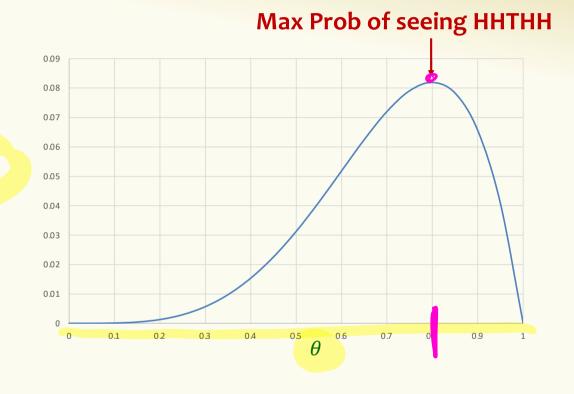
Likelihood

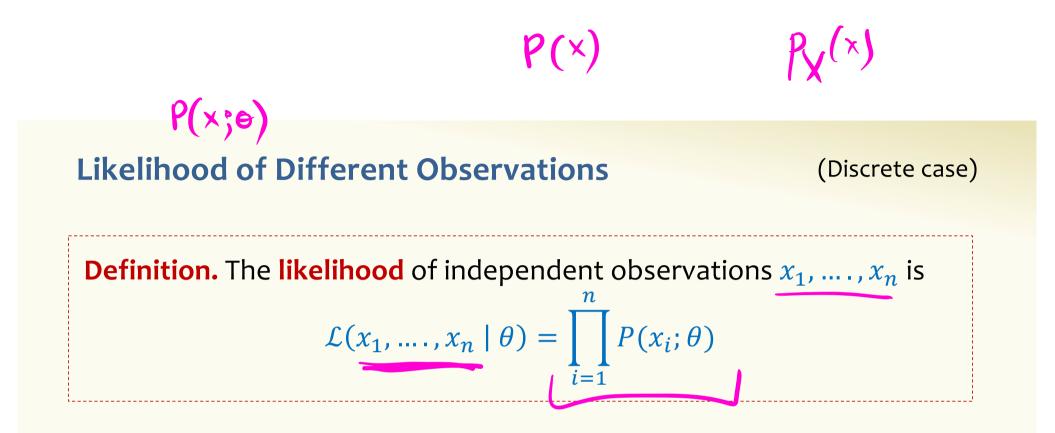
Say we see outcome *HHTHH*.

 $\mathcal{L}(HHTHH \mid \theta) = \theta^4(1-\theta)$

Probability of observing the outcome *HHTHH* if θ = prob. of heads.

For a fixed outcome HHTHH, this is a function of θ .





Example: Say we see outcome *HHTHH*.

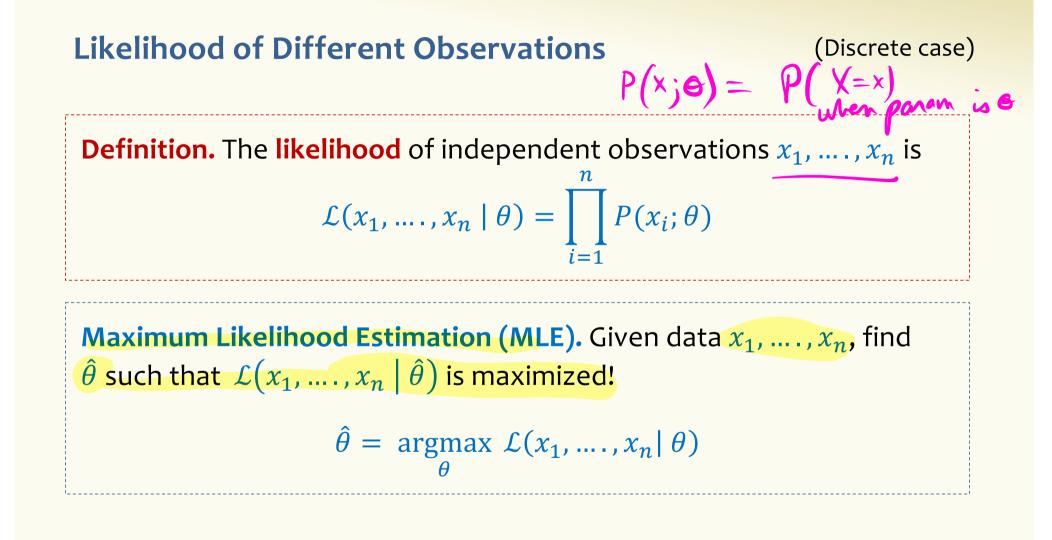
 $\mathcal{L}(HHTHH \mid \theta) = P(H;\theta) \cdot P(H;\theta) \cdot P(T;\theta) \cdot P(H;\theta) \cdot P(H;\theta) = \theta^{4}(1-\theta)$

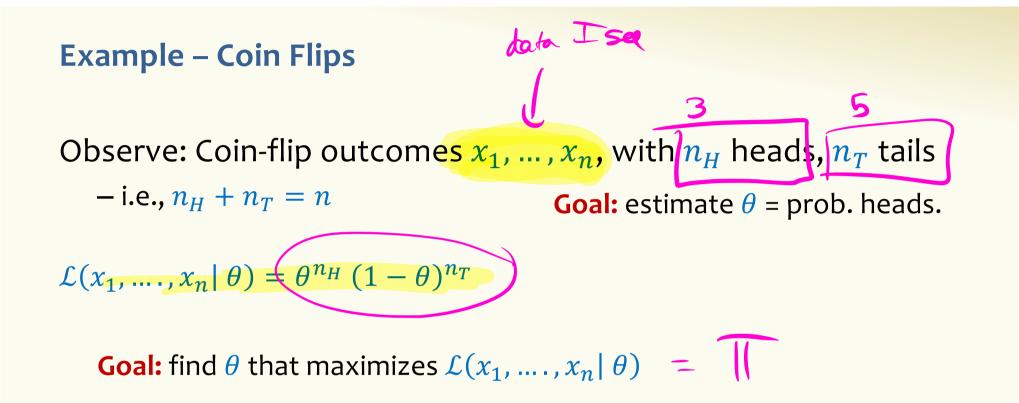
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- Fixed θ : probability $\prod_{i=1}^{n} P(x_i; \theta)$ that dataset x_1, \dots, x_n is sampled by distribution with parameter θ – A function of x_1, \dots, x_n
- Fixed $x_1, ..., x_n$: likelihood $\mathcal{L}(x_1, ..., x_n \mid \theta)$ that parameter θ explains dataset $x_1, ..., x_n$.
 - A function of θ

Likelihood vs. Probability

These notions are the same number if we fix <u>both</u> x_1, \dots, x_n and θ , but different role/interpretation





Example – Coin Flips

Observe: Coin-flip outcomes $x_1, ..., x_n$, with n_H heads, n_T tails - i.e., $n_H + n_T = n$ Goal: estimate θ = prob. heads.

$$\mathcal{L}(x_1,\ldots,x_n|\theta) = \theta^{n_H} (1-\theta)^{n_T}$$

$$\frac{\partial}{\partial \theta} \mathcal{L}(x_1, \dots, x_n | \theta) = ???$$

While it is possible to compute this derivative, it's not always nice since we are working with products.

Log-Likelihood

We can save some work if we use the **log-likelihood** instead of the likelihood directly.

Definition. The **log-likelihood** of independent observations x_1, \dots, x_n is $\ln \mathcal{L}(x_1, \dots, x_n | \theta) = \ln \prod_{i=1}^n P(x_i; \theta) = \sum_{i=1}^n \ln P(x_i; \theta)$

Useful log properties

 $\frac{\ln(ab) = \ln(a) + \ln(b)}{\ln(a/b) = \ln(a) - \ln(b)}$ $\ln(a^b) = b \cdot \ln(a)$

Example – Coin Flips

 $\ln(ab) = \ln(a) + \ln(b)$ $\ln(a/b) = \ln(a) - \ln(b)$ $\ln(a^b) = b \cdot \ln(a)$

Observe: Coin-flip outcomes $x_1, ..., x_n$, with n_H heads, n_T tails - i.e., $n_H + n_T = n$ Goal: estimate θ = prob. heads.

Example – Coin Flips

Observe: Coin-flip outcomes $x_1, ..., x_n$, with n_H heads, n_T tails - i.e., $n_H + n_T = n$ Goal: estimate θ = prob. heads.

$$\mathcal{L}(x_{1}, \dots, x_{n} | \theta) = \theta^{n_{H}} (1 - \theta)^{n_{T}}$$

$$\ln \mathcal{L}(x_{1}, \dots, x_{n} | \theta) = n_{H} \ln \theta + n_{T} \ln(1 - \theta)$$

$$\frac{\partial}{\partial \theta} \ln \mathcal{L}(x_{1}, \dots, x_{n} | \theta) = n_{H} \cdot \frac{1}{\theta} - n_{T} \cdot \frac{1}{1 - \theta}$$
Want value $\hat{\theta}$ of θ s.t. $\frac{\partial}{\partial \theta} \ln \mathcal{L}(x_{1}, \dots, x_{n} | \theta) = 0$
So we need $n_{H} \cdot \frac{1}{\theta} - n_{T} \cdot \frac{1}{1 - \theta} = 0$

$$\int_{10}^{10} \theta^{n_{H}} = 0$$

General Recipe

1. Input Given *n* i.i.d. samples $x_1, ..., x_n$ from parametric model with parameter θ .

Ben (O) Poissa (O)

- 2. Likelihood Define your likelihood $\mathcal{L}(x_1, \dots, x_n | \theta)$.
 - For discrete $\mathcal{L}(x_1, \dots, x_n | \theta) = \prod_{i=1}^n P(x_i; \theta)$
- 3. Log Compute $\ln \mathcal{L}(x_1, \dots, x_n | \theta)$
- 4. **Differentiate** Compute $\frac{\partial}{\partial \theta} \ln \mathcal{L}(x_1, \dots, x_n | \theta)$
- 5. Solve for $\hat{\theta}$ by setting derivative to 0 and solving for max.

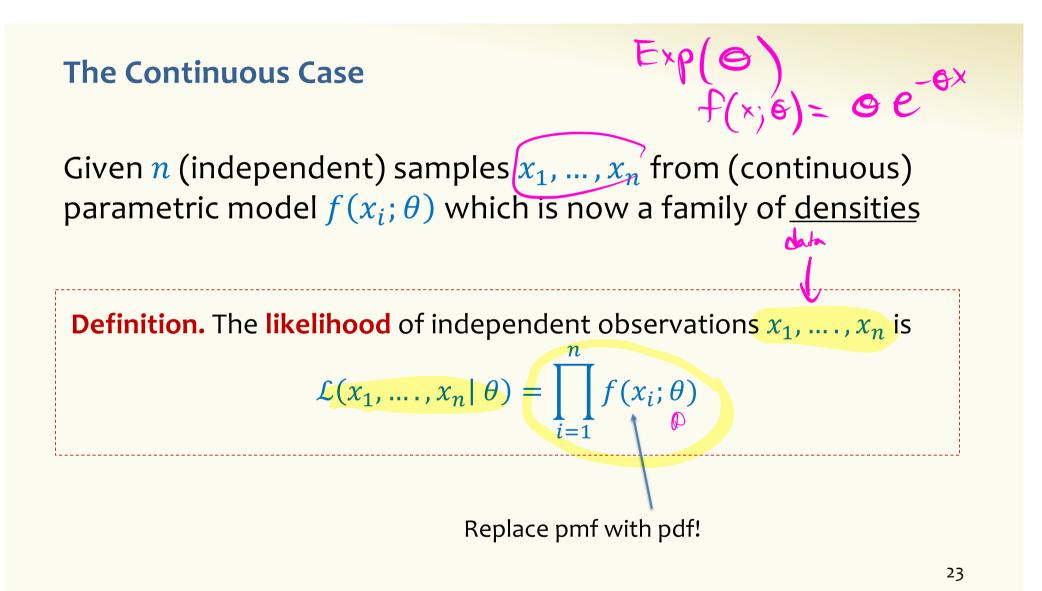
Generally, you need to do a second derivative test to verify it is a maximum, but we won't ask you to do that in CSE 312.

Brain Break



Agenda

- Idea: Estimation
- Maximum Likelihood Estimation (example: mystery coin)
- Continuous MLE 🗲



Why density?

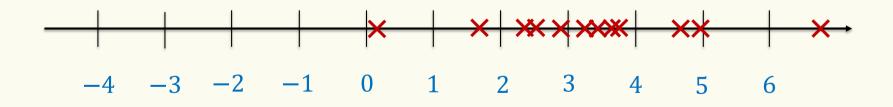
- Density ≠ probability, but:
 - For maximizing likelihood, we really only care about relative likelihoods, and density captures that
 - has desired property that likelihood increases with better fit to the model

$f(x \in [x;,x;+dx]) \not\approx f(x;)dx$

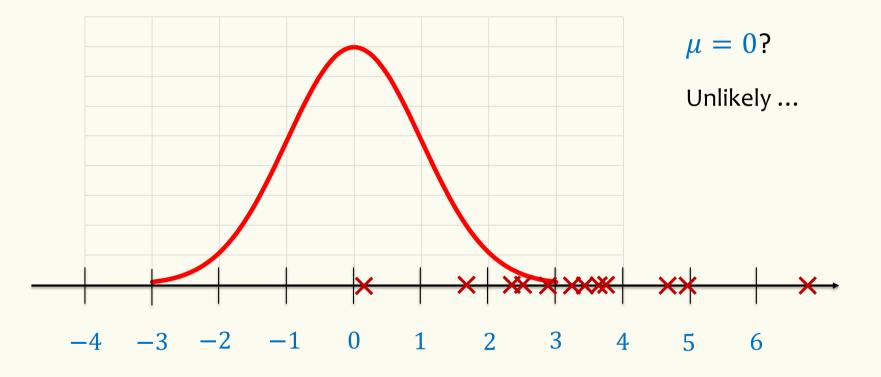
Agenda

- MLE for Normal Distribution
- Unbiased and Consistent Estimators
- Odds and ends

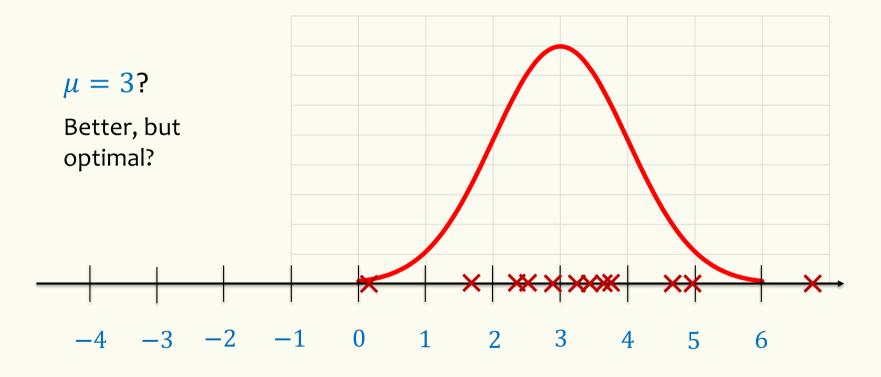
n samples $x_1, ..., x_n \in \mathbb{R}$ from Gaussian $\mathcal{N}(\mu, 1)$. Most likely μ ? [i.e., we are given the promise that the variance is 1]



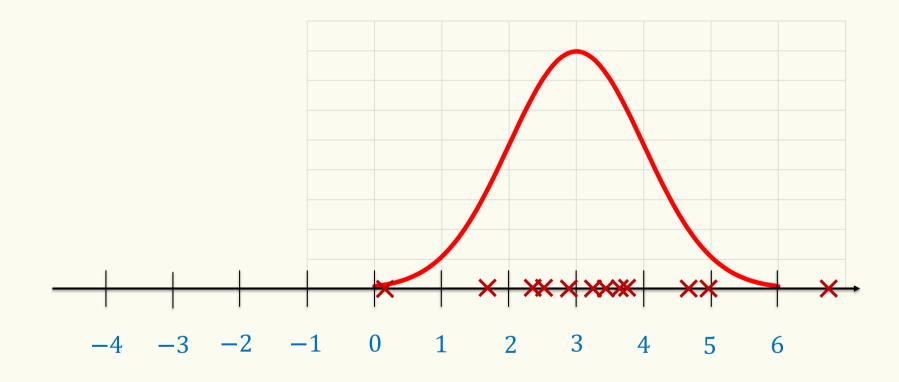
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1 12



 $+(x_{i}) = \frac{1}{\sqrt{2\pi}}$

 $\ln(ab) = \ln(a) + \ln(b)$ $\ln(a/b) = \ln(a) - \ln(b)$ **Example – Gaussian Parameters** $\ln(a^b) = b \cdot \ln(a)$ Normal outcomes $x_1, ..., x_n$, known variance $\sigma^2 = 1$ **Goal:** estimate θ , the expectation $\mathcal{L}(x_1, \dots, x_n | \theta) = \prod_{i=1}^n \left(\frac{1}{\sqrt{2\pi}} e^{-\frac{(x_i - \theta)^2}{2}} \right)$ $(x_i - \theta)^2$ $\ln 2\pi$ $\ln \mathcal{L}(x_1, \dots, x_n | \theta) = -n$ 30

Example – Gaussian Parameters

Goal: estimate θ = expectation

n

Normal outcomes $x_1, ..., x_n$, known variance $\sigma^2 = 1$

$$\ln \mathcal{L}(x_1, \dots, x_n | \theta) = -n \frac{\ln 2\pi}{2} - \sum_{i=1}^{n} \frac{(x_i - \theta)^2}{2}$$
Note: $\frac{\partial}{\partial \theta} \frac{(x_i - \theta)^2}{2} = \frac{1}{2} \cdot 2 \cdot (x_i - \theta) \cdot (-1) = \theta - x_i$

$$\frac{d}{d \theta} \frac{LL}{2} = \sum_{i=1}^{n} \sum_{i=1}^{n} (x_i - \theta) \cdot (-1) = \theta - x_i$$

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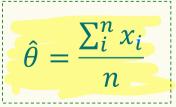
Example – Gaussian Parameters

Goal: estimate θ = expectation

Normal outcomes $x_1, ..., x_n$, known variance $\sigma^2 = 1$

$$\ln \mathcal{L}(x_1, \dots, x_n | \theta) = -n \frac{\ln 2\pi}{2} - \sum_{i=1}^n \frac{(x_i - \theta)^2}{2}$$

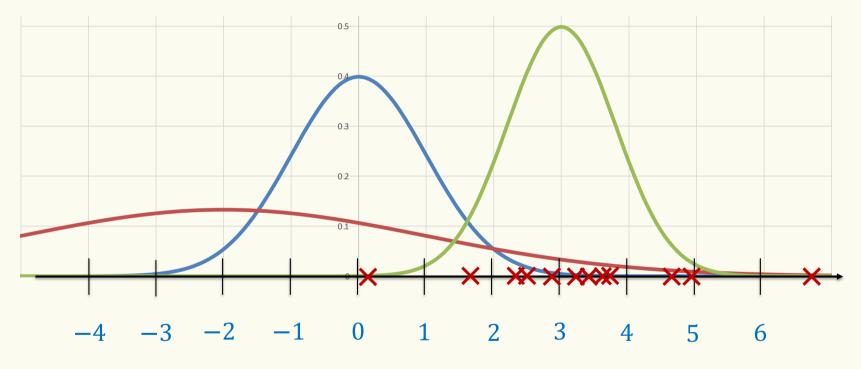
Note: $\frac{\partial}{\partial \theta} \frac{(x_i - \theta)^2}{2} = \frac{1}{2} \cdot 2 \cdot (x_i - \theta) \cdot (-1) = \theta - x_i$
 $\frac{\partial}{\partial \theta} \ln \mathcal{L}(x_1, \dots, x_n | \theta) = \sum_{i=1}^n (x_i - \theta) = \sum_{i=1}^n x_i - n\theta$
So... solve $\sum_{i=1}^n x_i - n\hat{\theta} = 0$ for $\hat{\theta}$



In other words, MLE is the sample mean of the data.

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Next: *n* samples $x_1, ..., x_n \in \mathbb{R}$ from Gaussian $\mathcal{N}(\mu, \sigma^2)$. <u>Most likely</u> μ and σ^2 ?



$$\mathcal{L} = \prod_{i=1}^{n} f(x_i; \theta_i, \theta_i)$$

$$\lim_{\substack{n(ab) = \ln(a) + \ln(b) \\ \ln(ab) = \ln(a) - \ln(b) \\ \ln(a^b) = b \cdot \ln(a)}$$
Normal outcomes x_1, \dots, x_n
Goal: estimate $\theta_1 = \mu$ = expectation and $\theta_2 = \sigma^2$ = variance
$$\int_{\substack{n(a^b) = b \cdot \ln(a)}} \mathcal{L}(x_1, \dots, x_n | \theta_1, \theta_2) = \left(\frac{1}{\sqrt{2\pi\theta_2}} \right)^n \prod_{i=1}^n e^{\frac{(x_i - \theta_1)^2}{2\theta_2}}$$

$$\ln \mathcal{L}(x_1, \dots, x_n | \theta_1, \theta_2) = \left(\frac{1}{\sqrt{2\pi\theta_2}} \right)^n \prod_{i=1}^n e^{\frac{(x_i - \theta_1)^2}{2\theta_2}}$$

Two-parameter estimation

$$\ln \mathcal{L}(x_1, \dots, x_n | \theta_1, \theta_2) = -\frac{\ln(2\pi \theta_2)}{2} - \sum_{i=1}^n \frac{(x_i - \theta_1)^2}{2\theta_2}$$

Find pair $\hat{\theta}_1, \hat{\theta}_2$ that maximizes $\ln \mathcal{L}(x_1, \dots, x_n | \theta_1, \theta_2)$

$$\frac{\partial}{\partial \Theta_{1}} LL = 0$$

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Two-parameter estimation

$$\ln \mathcal{L}(x_1, \dots, x_n \mid \theta_1, \theta_2) = -\frac{\ln(2\pi \theta_2)}{2} - \sum_{i=1}^n \frac{(x_i - \theta_1)^2}{2\theta_2}$$

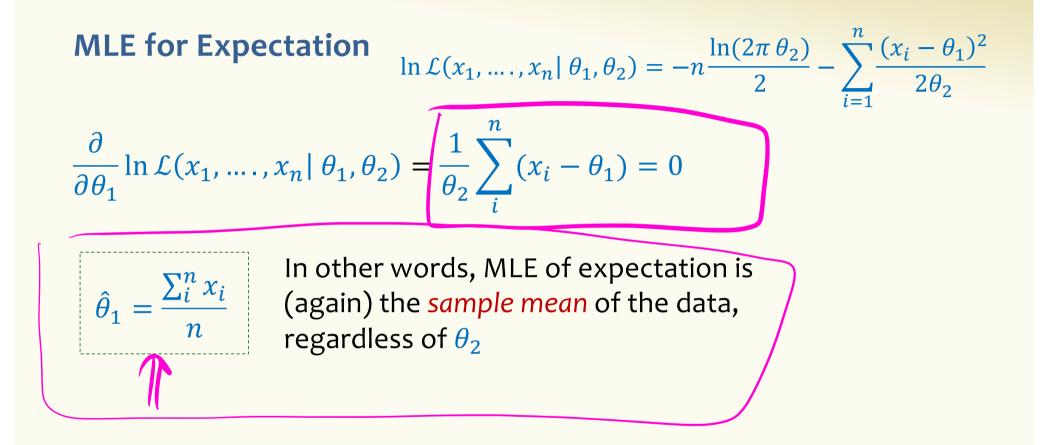
We need to find a solution $\hat{\theta}_1$, $\hat{\theta}_2$ to

$$\frac{\partial}{\partial \theta_1} \ln \mathcal{L}(x_1, \dots, x_n | \theta_1, \theta_2) = 0$$
$$\frac{\partial}{\partial \theta_2} \ln \mathcal{L}(x_1, \dots, x_n | \theta_1, \theta_2) = 0$$

MLE for Expectation

$$\ln \mathcal{L}(x_1, \dots, x_n | \theta_1, \theta_2) = -n \frac{\ln(2\pi \theta_2)}{2} - \sum_{i=1}^n \frac{(x_i - \theta_1)^2}{2\theta_2}$$

$$\frac{\partial}{\partial \theta_1} \ln \mathcal{L}(x_1, \dots, x_n | \theta_1, \theta_2) =$$



What about the variance?

Xn

MLE for Variance

$$\ln \mathcal{L}(x_{1}, \dots, x_{n} \mid \hat{\theta}_{1}, \theta_{2}) = -n \frac{\ln(2\pi \theta_{2})}{2} - \sum_{i=1}^{n} \frac{(x_{i} - \hat{\theta}_{1})^{2}}{2\theta_{2}} \mathbf{1}$$
$$= -n \frac{\ln 2\pi}{2} - n \frac{\ln \theta_{2}}{2} - \frac{1}{2\theta_{2}} \sum_{i=1}^{n} (x_{i} - \hat{\theta}_{1})^{2}$$
$$\frac{\partial}{\partial \theta_{2}} \ln \mathcal{L}(x_{1}, \dots, x_{n} \mid \hat{\theta}_{1}, \theta_{2}) = -\frac{n}{2\theta_{2}} + \frac{1}{2\theta_{2}^{2}} \sum_{i=1}^{n} (x_{i} - \hat{\theta}_{1})^{2} = 0$$

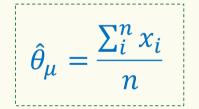
$$\hat{\theta}_2 = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\theta}_1)^2$$

In other words, MLE of variance is the population variance of the data. (Note that this is not called sample variance!)

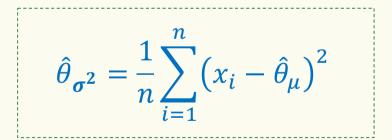
Likelihood – Continuous Case

Definition. The **likelihood** of independent observations x_1, \dots, x_n is $\mathcal{L}(x_1, \dots, x_n \mid \theta) = \prod_{i=1}^n f(x_i \mid \theta)$

Normal outcomes x_1, \ldots, x_n



MLE estimator for expectation



MLE estimator for **variance**

General Recipe

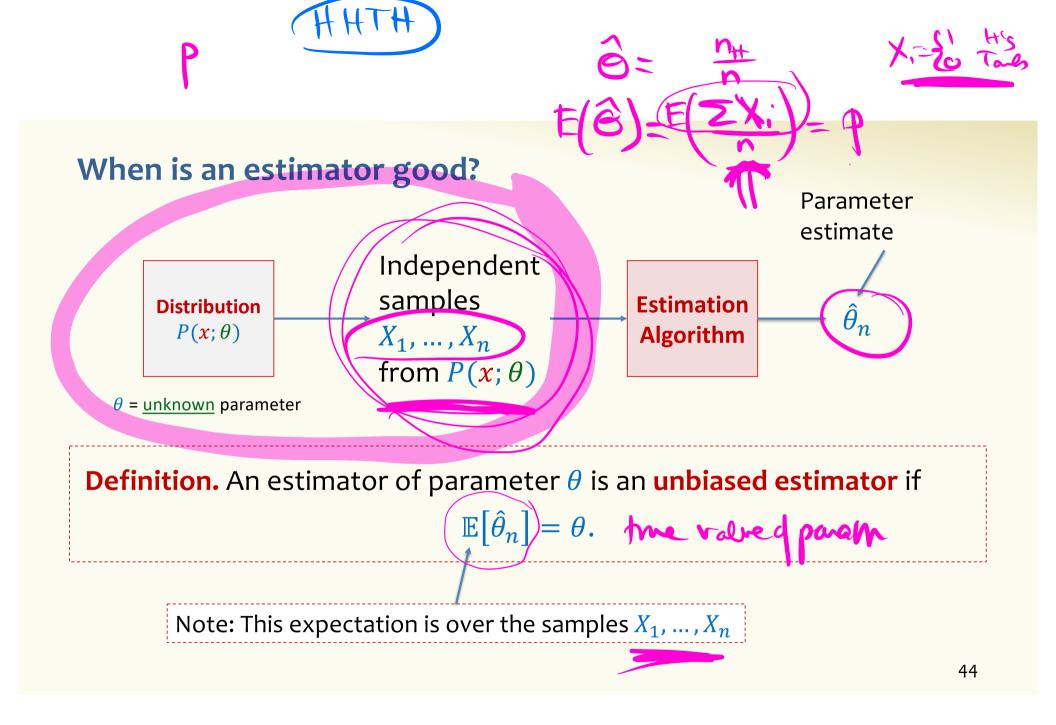
- 1. Input Given *n* i.i.d. samples $x_1, ..., x_n$ from parametric model with parameter θ .
- 2. Likelihood Define your likelihood $\mathcal{L}(x_1, \dots, x_n | \vec{\theta})$.
 - For discrete $\mathcal{L}(x_1, \dots, x_n | \theta) = \prod_{i=1}^n P(x_i; \theta)$
 - For continuous $\mathcal{L}(x_1, \dots, x_n | \theta) = \prod_{i=1}^n f(x_i; \overline{\theta})$
- 3. Log Compute $\ln \mathcal{L}(x_1, \dots, x_n | \vec{\theta})$
- 4. Differentiate Compute $\frac{\partial}{\partial \theta} \ln \mathcal{L}(x_1, \dots, x_n | \theta)$
- 5. Solve for $\hat{\theta}$ by setting derivative to 0 and solving for max.

Generally, you need to do a second derivative test to verify it is a maximum, but we won't ask you to do that in CSE 312.



Agenda

- MLE for Normal Distribution
- Unbiased and Consistent Estimators
- Intuition and Bigger Picture



Three samples from $U(0, \theta)$

Example – Coin Flips

Recall:
$$\hat{\theta}_{\mu} = \frac{n_H}{n}$$

Coin-flip outcomes $x_1, ..., x_n$, with n_H heads, n_T tails

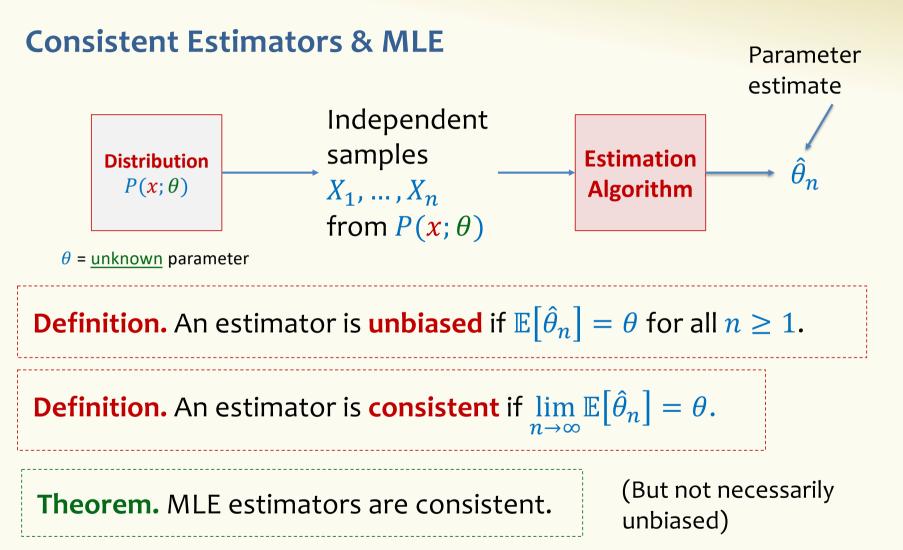
-[\$]

Fact. $\hat{\theta}_{\mu}$ is unbiased

i.e., $\mathbb{E}[\hat{\theta}_{\mu}] = p$, where p is the probability that the coin turns out head.

Why?

Because $\mathbb{E}[n_H] = np$ when p is the true probability of heads.



Example – Consistency

Normal outcomes $X_1, ..., X_n$ i.i.d. according to $\mathcal{N}(\mu, \sigma^2)$ Assume: $\sigma^2 > 0$

$$\widehat{\Theta}_{\sigma^2} = \frac{1}{n} \sum_{i=1}^n (X_i - \widehat{\Theta}_{\mu})^2$$

Population variance – Biased!

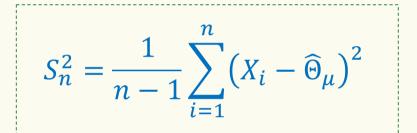
 $\widehat{\Theta}_{\sigma^2}$ is "consistent"

Example – Consistency

Normal outcomes $X_1, ..., X_n$ i.i.d. according to $\mathcal{N}(\mu, \sigma^2)$ Assume: $\sigma^2 > 0$

$$\widehat{\Theta}_{\sigma^2} = \frac{1}{n} \sum_{i=1}^n (X_i - \widehat{\Theta}_{\mu})^2$$

Population variance – Biased!



Sample variance – Unbiased!

 $\widehat{\Theta}_{\sigma^2}$ converges to same value as S_n^2 , i.e., σ^2 , as $n \to \infty$. $\widehat{\Theta}_{\sigma^2}$ is "consistent"

Why does it matter?

- When statisticians are estimating a variance from a sample, they usually divide by n-1 instead of n.
- They and we not only want good estimators (unbiased, consistent)
 - They/we also want confidence bounds
 - Upper bounds on the probability that these estimators are far the truth about the underlying distributions
 - Confidence bounds are just like what we wanted for our polling problems, but CLT is usually not the best thing to use to get them (unless the variance is known)

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Another approach to parameter estimation

Assume we have prior distribution over what values of θ are likely. In other words...

assume that we know $P(\theta) = \text{probability } \theta$ is used, for every θ .

Maximum a-posteriori probability estimation (MAP)

$$\hat{\theta}_{MAP} = \operatorname{argmax}_{\theta} \frac{\mathcal{L}(x_1, \dots, x_n | \theta) \cdot P(\theta)}{\sum_{\theta} \mathcal{L}(x_1, \dots, x_n | \theta) \cdot P(\theta)}$$
$$= \operatorname{argmax}_{\theta} \mathcal{L}(x_1, \dots, x_n | \theta) \cdot P(\theta)$$

Note when prior is constant, you get MLE!

MLE and MAP in AI and Machine Learning

- MLE and MAP can be defined over distributions that are not the nice well-defined families as we have been considering here
 - e.g. $\vec{\theta}$ might be the vector of parameters in some Neural Net or unknown entries in some Bayes Net.
 - A variety of optimization methods and heuristic methods are used to compute/approximate them.

General Recipe

1. Input Given *n* i.i.d. samples $x_1, ..., x_n$ from parametric model with parameter θ .

- 2. Likelihood Define your likelihood $\mathcal{L}(x_1, \dots, x_n | \theta)$.
 - For discrete $\mathcal{L}(x_1, \dots, x_n | \theta) = \prod_{i=1}^n P(x_i; \theta)$
 - For continuous $\mathcal{L}(x_1, \dots, x_n | \theta) = \prod_{i=1}^n f(x_i; \theta)$
- 3. **Log** Compute $\ln \mathcal{L}(x_1, \dots, x_n | \theta)$
- 4. **Differentiate** Compute $\frac{\partial}{\partial \theta} \ln \mathcal{L}(x_1, \dots, x_n | \theta)$
- 5. Solve for $\hat{\theta}$ by setting derivative to 0 and solving for max.

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