Lecture 9: Introduction to Statistical Inference

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What is Statistical Inference?

- Examples
  - Take 1000 voters uniformly at random, and count the popularity of each candidate to infer the true popularity.
  - COVID-19 has spread over a collection of people, and we collect a sample of COVID-19 infectees to infer the true source of infection.
  - When an original signal S is transmitted over the KAIST Wi-Fi connection, the received signal X becomes $X = aS + W$, where $0 < a < 1$ and $W \sim \mathcal{N}(0,1)$. If we have 10 samples of (S, X) values, what is the inferred value of a?
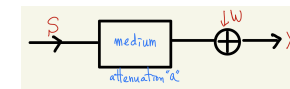

- Process of extracting information about an unknown variable or an unknown model from noisy available data

Statistical Inference: Three Main Ideas

1. Samples are likely to be a good represetnation of the unknown

2. There exists uncertainty (i.e., noise) as to how well the sample represents the unknown

3. How to obtain samples has impact on inference (e.g., when we need to pay for online surveys)

Inference, Real World, Probability Theory
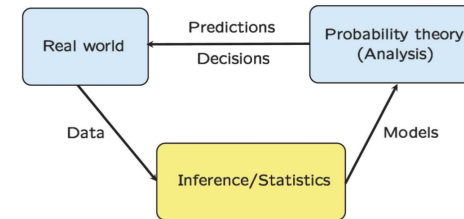
Source: Introduction to Probability course by MIT

- Inference
  - Using data, probabilistic models or parameters for models are determined.
- Why building up models?
  - Analysis is possible, so that predictions and decisions are made.
- Recently, deep learning
  - Connecting big data and big model building

What to Infer?: Unknown Model vs. Unknown Variable
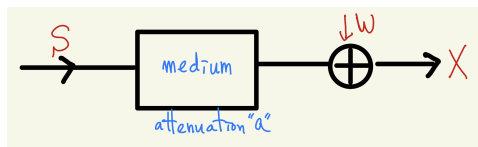
- $X = aS + W$
- Model building
  - know the original signal S, observe X
  - infer the model parameter a
- Variable estimation
  - know a, observe X
  - infer the original signal S
- Same mathematical structure, because the parameters in models are variables in many cases

What Kind?: Hypothesis Testing vs. Estimation

- Hypothesis testing
  - Unknown: a few possible ones
  - Goal: small probability of incorrect decision
  - (Ex) Something detected on the radar. Is it a bird or an airplane?

- Estimation
  - Unknown: a value included in an infinite, typically continuous set
  - Goal: Finding the value close to the true value
  - (Ex) Biased coin with unknown probability of head $\theta \in [0, 1]$. Data of heads and tails. What is θ?
  - (Note) If you have the candidate values of $\theta = \{1/4, 1/2, 3/4\}$, then it's a hypothesis testing problem

- Biased coin with parameter θ (probability of head). Assume that $\theta \in \{1/4, 3/4\}$.

- Throw the coin 3 times and get (H, H, H). Goal: infer θ, 1/4 or 3/4?

- Distribution of θ (prior) e.g.,

$$\mathbb{P}\left(\theta = \frac{3}{4}\right) = 1/2, \quad \mathbb{P}\left(\theta = \frac{1}{4}\right) = 1/2$$

- Use Bayes' rule and find the posterior:

$$\mathbb{P}\left[\theta = \frac{3}{4}\Big|(HHH)\right] = \frac{27}{28}, \ \mathbb{P}\left[\theta = \frac{1}{4}\Big|(HHH)\right] = \frac{1}{28}$$

- Choose θ with larger posterior probability.
- *Bayesian approach* (Chapter 8)

- Find the probability of (H, H, H), if $\theta = \frac{1}{4}$ or $\frac{3}{4}$ (likelihood)

$$\mathbb{P}\left[(HHH)|\theta = \frac{3}{4}\right] = \left(\frac{3}{4}\right)^3$$

$$\mathbb{P}\left[(HHH)|\theta = \frac{1}{4}\right] = \left(\frac{1}{4}\right)^3$$

- Choose θ with a larger likelihood.
- *Classical approach* (Chapter 9)

(Note) There are other inference methods, and here we just show examples.

Bayesian approach
- Unknown: random variable with some distribution (prior)

- Unknown model as chosen randomly from a give model class

- Observed data x gives:
  - posterior distribution $p_{\Theta|X}(\theta|x)$

- Choose θ with larger posterior probability (other methods exist)

Classical approach
- Unknown: deterministic value

- Unknown model as one of multiple probabilistic models

- Observed data x gives:
  - likelihood $p(X; \theta)$

- Choose θ with larger likelihood (other methods exist)

- Fundamental difference about the nature of unknown models or variables

- Random variable or deterministic quantity

- Who is the winner? A century-long debate

- Example of debate: mass of the electron by noisy measurement
  ∘ Classical. while unknown, it is a constant and there is no justification for modeling it as a random variable.

  ∘ Bayesian. Prior distribution reflects our state of knowledge, e.g., some range of candidate values from our previous noisy measurements.

- Particular prior? too arbitrary vs. every statistical procedure's hidden choices

- Pratical issues: Bayesian approach is often computationally intractable (multi-dimensional integrals)
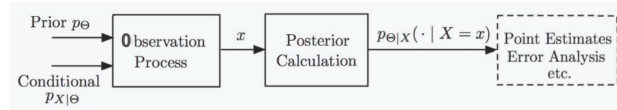
- Unknown Θ
  - physical quantity or model parameter
  - random variable
  - prior distribution p_Θ and f_Θ
- Observations or measurements X
  - observation model $p_{X|\Theta}$ and $f_{X|\Theta}$
- That is, the joint distribution of X and Θ ($p_{X,\Theta}(x,\theta)$ and $f_{X,\Theta}(x,\theta)$) is given
- Find the posterior distribution $p_{\Theta|X}$ and $f_{\Theta|X}$, using Bayes' rule.

- The posterior distribution is the complete answer of the Bayesian inference.
- However, one may use it for further processing, depending on what he/she wants, e.g., point estimation.
- Multiple observations and multiple parameters are possible
  - $X = (X_1, \ldots, X_n)$
  - $\Theta = (\Theta_1, \ldots, \Theta_n)$

Remind: Bayes' Rule: 4 Versions

- Θ: discrete, X: discrete
$$p_{\Theta|X}(\theta|x) = \frac{p_\Theta(\theta)p_{X|\Theta}(x|\theta)}{p_X(x)}$$
$$p_X(x) = \sum_{\theta'} p_\Theta(\theta')p_{X|\Theta}(x|\theta')$$

- Θ: continuous, X: continuous
$$f_{\Theta|X}(\theta|x) = \frac{f_\Theta(\theta)f_{X|\Theta}(x|\theta)}{f_X(x)}$$
$$f_X(x) = \int f_\Theta(\theta')f_{X|\Theta}(x|\theta')d\theta'$$

- Θ: discrete, X: continuous
$$p_{\Theta|X}(\theta|x) = \frac{p_\Theta(\theta)f_{X|\Theta}(x|\theta)}{f_X(x)}$$
$$f_X(x) = \sum_{\theta'} p_\Theta(\theta')f_{X|\Theta}(x|\theta')$$

- Θ: continuous, X: discrete
$$f_{\Theta|X}(\theta|x) = \frac{f_\Theta(\theta)p_{X|\Theta}(x|\theta)}{p_X(x)}$$
$$p_X(x) = \int f_\Theta(\theta')p_{X|\Theta}(x|\theta')d\theta'$$

Roadmap

Example: Romeo and Juliet, Single Observation

- Romeo and Juliet start dating, where Romeo is late by $X \sim \mathcal{U}[0,\theta]$.
- Unknown: θ modeled by a rv $\Theta \sim \mathcal{U}[0,1]$.
- Observation: Romeo was late by x.
- Prior and observation model (likelihood)
$$f_\Theta(\theta) = \begin{cases} 1, & 0 \le \theta \le 1 \\ 0, & \text{otherwise} \end{cases}, \qquad f_{X|\Theta}(x|\theta) = \begin{cases} \frac{1}{\theta}, & 0 \le x \le \theta \\ 0, & \text{otherwise} \end{cases}$$
- Posterior
$$f_{\Theta|X}(\theta|x) = \frac{f_\Theta(\theta)f_{X|\Theta}(x|\theta)}{\int_0^1 f_\Theta(\theta')f_{X|\Theta}(x|\theta')d\theta'} = \begin{cases} \frac{1/\theta}{\int_x^1 \frac{1}{\theta'}d\theta'} = \frac{1}{\theta|\log x|}, & x \le \theta \le 1, \\ 0, & \theta < x \text{ or } \theta > 1 \end{cases}$$

○ What happens if we have more observation samples?

- Romeo was late n times by $\boldsymbol{X} = (X_1, X_2, \ldots, X_n)$, $X_i \sim \mathcal{U}[0, \theta]$.

- $X_1, \ldots, X_n$ are conditionally independent, given $\Theta = \theta$.

- Unknown: θ modeled by a rv $\Theta \sim \mathcal{U}[0, 1]$.

- Observation: Romeo was late n times by $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$

- See Example 8.2 at pp. 414 for more detailed treatment.

- E-mail: spam (1) or legitimate (2), $\Theta \in \{1, 2\}$, with prior $p_\Theta(1)$ and $p_\Theta(2)$.

- $\{w_1, w_2, \ldots, w_n\}$: a collection of words which suggest "spam".

- For each i, a Bernoulli $X_i = 1$ if w_i appears and 0 otherwise.

- Observation model $p_{X_i|\Theta(x_i|1)}$ and $p_{X_i|\Theta(x_i|2)}$ are known.

- Assumption: Conditioned on Θ, X_i are independent.

- Posterior PMF

$$\mathbb{P}\Big[\Theta = m | (x_1, \ldots, x_n)\Big] = \frac{p_\Theta(m) \prod_{i=1}^n p_{X_i|\Theta}(x_i|m)}{\sum_{j=1,2} p_\Theta(j) \prod_{i=1}^n p_{X_i|\Theta}(x_i|j)}, \quad m = 1, 2$$

- Biased coin with probability of head θ

- Unknown θ: modeled by Θ with some prior $f_\Theta(\theta)$

- Observation X: number of heads out of n tosses

- Question. Suppose that you have freedom to choose the form of the prior distribution. What prior will you choose? Requirement of "good" priors?

- We will look at the prior whose distribution is something called the Beta distribution.

Beta distribution

A continuous rv Θ follows a beta distribution with integer parameters $\alpha, \beta > 0$, if

$$f_\Theta(\theta) = \begin{cases} \frac{1}{B(\alpha,\beta)} \theta^{\alpha-1}(1-\theta)^{\beta-1}, & 0 < \theta < 1, \\ 0, & \text{otherwise,} \end{cases}$$

where $B(\alpha, \beta)$, called Beta function, is a normalizing constant, given by

$$B(\alpha, \beta) = \int_0^1 \theta^{\alpha-1}(1-\theta)^{\beta-1} d\theta = \frac{(\alpha-1)!(\beta-1)!}{(\alpha+\beta-1)!}$$

- See https://youtu.be/8yaRt24qA1M for the integration in the Beta function formula.

- A special case of Beta(1, 1) is $\mathcal{U}[0, 1]$

- If $\Theta \sim \text{Beta}(\alpha, \beta)$, then $\Theta|\{X = k\} \sim \text{Beta}(k + \alpha, n - k + \beta)$

- In other words, Beta prior $\implies$ Beta posterior (why useful?)

Proof.

(a) First, the posterior pdf is given by:

$$f_{\Theta|X}(\theta|k) = c f_\Theta(\theta) p_{X|\Theta}(k|\theta) = c \binom{n}{k} f_\Theta(\theta) \theta^k (1-\theta)^{n-k}, \ c \text{ the normalizing constant}$$

(b) Next, for $\text{Beta}(\alpha, \beta)$ prior, $f_\Theta(\theta) = \dfrac{1}{B(\alpha, \beta)} \theta^{\alpha-1}(1-\theta)^{\beta-1}$.

(c) Then, $f_{\Theta|X}(\theta|k) = c \binom{n}{k} f_\Theta(\theta) \theta^k (1-\theta)^{n-k} = \dfrac{d}{B(\alpha, \beta)} \cdot \theta^{\alpha+k-1}(1-\theta)^{\beta+n-k-1}$,

where $d = c \binom{n}{k}$.

○ Inference of a parameter θ

- Single observation

- X: noisy observation of θ, modeled as:
  $X = \theta + W$, where $W \sim \mathcal{N}(0, \sigma^2)$

- Model θ with a rv $\Theta \sim \mathcal{N}(x_0, \sigma_0^2)$ (normal prior)

- Θ and W are indendent

- Question. Given an observation x, what is the posterior $f_{\Theta|X}(\theta|x)$?

- Multiple n observations

- n observations of θ: $W_i \sim \mathcal{N}(0, \sigma_i^2)$

  $X_1 = \theta + W_1, \quad W_1 \sim \mathcal{N}(0, \sigma_1^2)$

  $\vdots$

  $X_n = \theta + W_n, \quad W_n \sim \mathcal{N}(0, \sigma_n^2)$

- Model θ with $\Theta \sim \mathcal{N}(x_0, \sigma_0^2)$

- $\Theta, W_1, \ldots, W_n$ are indendent

- Question. Given an observation x, what is the posterior $f_{\Theta|X}(\theta|x)$?
  ○ $X = (X_1, \ldots, X_n)$ and $x = (x_1, \ldots, x_n)$,

Lemma. Up to recaling, the pdf of the form $e^{-\frac{1}{2}(ax^2 - 2bx + c)}$ is $\mathcal{N}(\frac{b}{a}, \frac{1}{a})$.

- (Rough) Proof. Note that the pdf of $\mathcal{N}(\mu, \sigma^2)$: $f_X(x) = e^{-(x-\mu)^2/2\sigma^2}$ up to rescaling. Then,

  ○ $-\dfrac{1}{2\sigma^2}(x^2 - 2\mu x + \mu^2) = -\dfrac{1}{2}(ax^2 - 2bx + c)$

  ○ Thus, $\sigma^2 = \dfrac{1}{a}$ and $\dfrac{\mu}{\sigma^2} = b \implies \mu = b\sigma^2 = \dfrac{b}{a}$

Theorem. The product of two Gaussian pdfs $\mathcal{N}(\mu_0, \nu_0)$ and $\mathcal{N}(\mu_1, \nu_1)$ is
$$\mathcal{N}\left(\frac{\nu_1 \mu_0 + \nu_0 \mu_1}{\nu_0 + \nu_1}, \frac{\nu_0 \nu_1}{\nu_0 + \nu_1}\right).$$

Proof. Using the Lemma in the previous slide, i.e., up to recaling, the pdf of the form $e^{-\frac{1}{2}(ax^2 - 2bx + c)}$ is $\mathcal{N}(\frac{b}{a}, \frac{1}{a})$,

$$\exp\left(-(x-\mu_0)^2/2\nu_0\right) \times \exp\left(-(x-\mu_1)^2/2\nu_1\right)$$

$$= \exp\left[-\frac{1}{2}\left(\left(\frac{1}{\nu_0} + \frac{1}{\nu_1}\right)x^2 - 2\left(\frac{\mu_0}{\nu_0} + \frac{\mu_1}{\nu_1}\right)x + c\right)\right]$$

$$\implies \mathcal{N}\left(\nu\left(\frac{\mu_0}{\nu_0} + \frac{\mu_1}{\nu_1}\right), \overbrace{\frac{1}{\nu_0^{-1} + \nu_1^{-1}}}^{=\nu}\right) = \mathcal{N}\left(\frac{\nu_1 \mu_0 + \nu_0 \mu_1}{\nu_0 + \nu_1}, \frac{\nu_0 \nu_1}{\nu_0 + \nu_1}\right)$$

Background: Product of $n+1$ Gaussian Densities

> **Theorem.** The product of $n+1$ Gaussian pdfs $\mathcal{N}(\mu_0, \nu_0)$, $\mathcal{N}(\mu_1, \nu_1), \ldots,$ $\mathcal{N}(\mu_n, \nu_n)$, is $\mathcal{N}(\mu, \nu)$, where
> $$\mu = \frac{\sum_{i=0}^{n} \frac{\mu_i}{\nu_i}}{\sum_{i=0}^{n} \frac{1}{\nu_i}}, \qquad \nu = \frac{1}{\sum_{i=0}^{n} \frac{1}{\nu_i^2}}$$

Example: Parameter Inference with Normal Prior (2)

- n observations of θ: $W_i \sim \mathcal{N}(0, \sigma_i^2)$, and θ with the normal prior $\Theta \sim \mathcal{N}(x_0, \sigma_0^2)$

> $$X_i = \theta + W_i, \quad W_i \sim \mathcal{N}(0, \sigma_i^2), \quad i = 1, \ldots, n$$

- $\Theta, W_1, \ldots, W_n$ are indendent and let $X = (X_1, \ldots, X_n)$, $x = (x_1, \ldots, x_n)$.
- Our interest. The poterior pdf $f_{\Theta|X}(\theta|x)$.

- Prior. $f_\Theta(\theta) = c_1 \cdot \exp\left\{-\frac{(\theta - x_0)^2}{2\sigma_0^2}\right\}$
- Observation model. Noting that $X_1, X_2, \ldots, X_n$ are indpendent,
$$f_{X|\Theta}(x|\theta) = c_2 \cdot \exp\left\{-\frac{(\theta - x_1)^2}{2\sigma_1^2}\right\} \cdots \exp\left\{-\frac{(\theta - x_n)^2}{2\sigma_n^2}\right\}$$

Example: Parameter Inference with Normal Prior (3)

- Numerator: $f_\Theta(\theta) f_{X|\Theta}(x|\theta) = c_1 c_2 \cdot \exp\left\{-\sum_{i=0}^{n} \frac{(x_i - \theta)^2}{2\sigma_i^2}\right\}$, which can be reexpressed as the following, using the product of $n+1$ Gaussians:

$$c_1 c_2 \cdot \exp\left\{-\sum_{i=0}^{n} \frac{(x_i - \theta)^2}{2\sigma_i^2}\right\} = d \cdot \exp\left\{-\frac{(\theta - m)^2}{2v}\right\},$$

where $m = \dfrac{\sum_{i=0}^{n} \frac{x_i}{\sigma_i^2}}{\sum_{i=0}^{n} \frac{1}{\sigma_i^2}}, \qquad v = \dfrac{1}{\sum_{i=0}^{n} \frac{1}{\sigma_i^2}}$

- Denominator: just a constant, not a function of θ

> $$f_{\Theta|X}(\theta|x) = \frac{f_\Theta(\theta) f_{X|\Theta}(x|\theta)}{\int f_\Theta(\theta') f_{X|\Theta}(x|\theta') d\theta'}$$

Example: Parameter Inference with Normal Prior (4)

- Thus, the posterior pdf $f_{\Theta|X}(\theta|x) = a \cdot \exp\left\{-\frac{(\theta - m)^2}{2v}\right\}$, where
$$m = \frac{\sum_{i=0}^{n} \frac{x_i}{\sigma_i^2}}{\sum_{i=0}^{n} \frac{1}{\sigma_i^2}}, \qquad v = \frac{1}{\sum_{i=0}^{n} \frac{1}{\sigma_i^2}}$$

- Prior: Normal, Posterior: Normal
- Special case when $\sigma^2 = \sigma_0^2 = \sigma_1^2 = \cdots = \sigma_n^2$. Then,
$$m = \frac{x_0 + x_1 + \ldots x_n}{n+1}, \qquad v = \frac{\sigma^2}{n+1}$$

  ○ the prior mean x_0 acts just as another observation.
  ○ the standard deviation of the posterior goes to 0, at the rough rate of $1/\sqrt{n}$.

- Recursive inference is possible.

- Suppose that after $X_1, \ldots, X_n$ are observed, an additional observation X_{n+1} is observed.

- Instead of solving the inference problem from scratch, we can view $f_{\Theta|X_1,\ldots,X_n}$ as our prior, use the new observation to obtain the new posterior $f_{\Theta|X_1,\ldots,X_n,X_{n+1}}$

- In the example of parameter inference with the Normal prior, with the new observation $x_{n+1} \sim \mathcal{N}(x_{n+1}, \sigma_{n+1}^2)$, the posterior pdf is nothing but the Normal pdf of:

$$\text{mean} = \frac{(m/v) + (x_{n+1}/\sigma_{n+1}^2)}{(1/v) + (1/\sigma_{n+1}^2)}, \qquad \text{variance} = \frac{1}{(1/v) + (1/\sigma_{n+1}^2)}$$
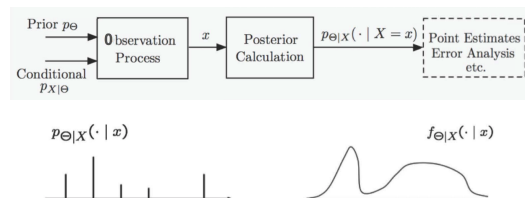

- Point Estimate
  - Given observation x, which single value θ are you going to choose as your inference result? People often want just the summary and a simple answer.
  - Very often, θ, our inference target, is by nature a single value, i.e., mass of the electron.

M1. Choose the largest: Maximum a posteriori probability (MAP) rule

$$\hat{\theta}_{\text{MAP}} = \arg\max_\theta p_{\Theta|X}(\theta|x), \quad \hat{\theta}_{\text{MAP}} = \arg\max_\theta f_{\Theta|X}(\theta|x)$$

M2. Choose the mean: Conditional expectation, aka LMS (Least Mean Square)

$$\hat{\theta}_{\text{LMS}} = \mathbb{E}[\Theta|X = x]$$

- Why MAP and LMS are good? Not mathematically clear yet (We will discuss later)
- Notation: The community uses $\hat{\theta}$ to mean the estiamted value, i.e., hat for estimated value.

Estimator as a Function

- Random observation: X

- Observation instance: x

- Estimate as a mapping from x to a number
$$\hat{\theta} = g(x), \quad \hat{\theta}_{\text{MAP}} = g_{\text{MAP}}(x), \quad \hat{\theta}_{\text{LMS}} = g_{\text{LMS}}(x)$$

- Estimator as a mapping from X to a random variable
$$\hat{\Theta} = g(X), \quad \hat{\Theta}_{\text{MAP}} = g_{\text{MAP}}(X), \quad \hat{\Theta}_{\text{LMS}} = g_{\text{LMS}}(X)$$

From now on we focus on the MAP estimate, mainly based on the examples that we've discussed in the previous section.

Example: Romeo and Juliet

- Romeo and Juliet start dating, where Romeo is late by $X \sim \mathcal{U}[0, \theta]$.
- Unknown: θ modeled by a rv $\Theta \sim \mathcal{U}[0, 1]$.
- Observation: Romeo was late by x.
- **Question.** Given the observation sample x, what is $\hat{\theta}_{\text{MAP}}$?
- **Intuition.** As x grows, $\hat{\theta}_{\text{MAP}}$ decreases or increases? Increases. Why?
- Posterior: $f_{\Theta|X}(\theta|x) = \begin{cases} \frac{1}{\theta |\log x|}, & x \le \theta \le 1, \\ 0, & \theta < x \text{ or } \theta > 1 \end{cases}$
- Given x, $f_{\Theta|X}(\theta|x)$ is decreasing in θ over $[x, 1]$. $\implies \hat{\theta}_{\text{MAP}} = x$.

Example: Spam Filtering

- E-mail: spam (1) or legitimate (2), $\Theta \in \{1, 2\}$, with prior $p_\Theta(1)$ and $p_\Theta(2)$.
- $\{w_1, w_2, \ldots, w_n\}$: a collection of words which suggest "spam".
- For each i, a Bernoulli $X_i = 1$ if w_i appears and 0 otherwise.
- Assumption: Conditioned on Θ, X_i are independent.
- Posterior PMF
$$\mathbb{P}\Big[\Theta = m | (x_1, \ldots, x_n)\Big] = \frac{p_\Theta(m) \prod_{i=1}^{n} p_{X_i|\Theta}(x_i|m)}{\sum_{j=1,2} p_\Theta(j) \prod_{i=1}^{n} p_{X_i|\Theta}(x_i|j)}, \quad m = 1, 2$$
- MAP rule for this hypothesis testing problem. Decided that the message is spam if
$$p_\Theta(1) \prod_{i=1}^{n} p_{X_i|\Theta}(x_i|1) > p_\Theta(2) \prod_{i=1}^{n} p_{X_i|\Theta}(x_i|2)$$

Slide 21 for more details

- Biased coin with probability of head θ
- Unknown θ: modeled by Θ with some prior $f_\Theta(\theta)$
- Observation X: number of heads out of n tosses

  ○ If $\Theta \sim \text{Beta}(\alpha, \beta)$, then $\Theta|\{X = k\} \sim \text{Beta}(k + \alpha, n - k + \beta)$
  ○ $f_{\Theta|X}(\theta|k) \propto \theta^{\alpha+k-1}(1-\theta)^{\beta+n-k-1}$

- MAP estimate: Taking the logarithm,

$$\hat{\theta}_{\text{MAP}} = \arg\max_\theta \Big[(\alpha + k - 1)\log\theta + (\beta + n - k + 1)\log(1-\theta)\Big] = \frac{\alpha + k - 1}{\alpha + \beta - 2 + n}$$

- When $\alpha = \beta = 1$ (i.e., $\mathcal{U}[0,1]$ prior), $\hat{\theta}_{\text{MAP}} = \frac{k}{n}$

Slide 27 for more details

- The posterior pdf $f_{\Theta|X}(\theta|x) = a \cdot \exp\left\{-\frac{(\theta - m)^2}{2v}\right\}$, where

$$m = \frac{\sum_{i=0}^{n} \frac{x_i}{\sigma_i^2}}{\sum_{i=0}^{n} \frac{1}{\sigma_i^2}}, \qquad v = \frac{1}{\sum_{i=0}^{n} \frac{1}{\sigma_i^2}}$$
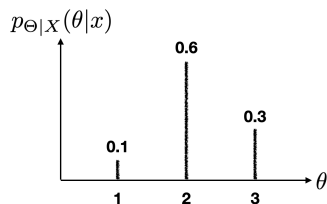
- The pdf is normal, so it is maximized when $\theta = $ mean.
- Thus, $\hat{\theta}_{\text{MAP}} = m$.

Why MAP Is Good? (1) **KAIST EE**

- MAP estimate is intuitive, but we need more mathematical evidence for its performance guarantee. We would trust its quality if it is optimal in some sense.

$p_{\Theta|X}(\theta|x)$

○ MAP: $\hat{\theta}_{\text{MAP}} = 2$

○ Given $X = x$, θ that minimizes the probability of incorrect decision?

$$\hat{\theta}_{\text{MAP}} = \arg\min_{\hat{\theta}=1,2,3} \mathbb{P}(\hat{\theta} \neq \Theta | X = x)$$

○ Average probability of incorrect decision

$$\mathbb{P}(\hat{\Theta} \neq \Theta) = \sum_x \mathbb{P}(\hat{\Theta} \neq \Theta | X = x) p_X(x)$$
$$= \sum_x \mathbb{P}(\hat{\theta} \neq \Theta | X = x) p_X(x)$$
$$\geq \sum_x \mathbb{P}(\hat{\theta}_{\text{MAP}} \neq \Theta | X = x) p_X(x)$$

Why MAP Is Good? (2) **KAIST EE**

- Claim 1. For a given x, the MAP rule minimizes the probability of an incorrect decision.
- Claim 2. The MAP rule minimizes the overall probability of an incorrect decision, averaged over x.

- Proof. Let I and I_{MAP} be the indicator rv, representing the correct decision by any general estimator and the MAP estimator, respectively.

$$\mathbb{E}[I|X = x] = \mathbb{P}\Big[g(X) = \Theta | X = x\Big] \leq \mathbb{P}\Big[g_{\text{MAP}}(X) = \Theta | X = x\Big] = \mathbb{E}[I_{\text{MAP}}|X = x]$$

Thus, Claim 1 holds. We now take the expectation of the above equations, the law of iterated expectations leads to Claim 2.

(1) Overview on Statistical Inference

(2) Bayesian Inference: Framework

(3) Examples

(4) MAP (Maximum A Posteriori) Estimator

(5) LMS (Least Mean Squares) Estimator

(6) LLMS (Linear LMS) Estimator

(7) Classical Inference: ML Estimator

- MAP: the estimate which maximizes the posterior pdf, which solves the following optimization problem (minimizing the prob. of incorrect decision):

$$\min_{\hat{\theta}} \mathbb{P}\left[\Theta \neq \hat{\theta} | X = x\right]$$

- What about applying other objective function? Like the following one (mean squared error)?

$$\min_{\hat{\theta}} \mathbb{E}\left[(\Theta - \hat{\theta})^2 | X = x\right]$$

  ○ Least Mean Square (LMS) Estimate

What's the Form?: LMS Estimator (1)

- Unknown: θ modeled by Θ with prior $f_\Theta(\cdot)$. Assume $\Theta \sim \mathcal{U}[4, 10]$.

- Assume that no observations available

- MAP estimate
  - Any value $\hat{\theta}_{\text{MAP}} \in [4, 10]$ (why? posterior = prior), not very useful

- What is the other choice?
  - Expectation: $\hat{\theta} = \mathbb{E}[\Theta] = 7$
  - looks reasonable, but why?

- First, it makes sense, but, second, it also minimizes the mean squared error (MSE)

$$\min_{\hat{\theta}} \mathbb{E}\left[(\Theta - \hat{\theta})^2\right] = \min_{\hat{\theta}} \left(\text{var}(\Theta - \hat{\theta}) + \left(\mathbb{E}[\Theta - \hat{\theta}]\right)^2\right) = \min_{\hat{\theta}} \left(\text{var}(\Theta) + \left(\mathbb{E}[\Theta - \hat{\theta}]\right)^2\right)$$

  - minimized when $\hat{\theta} = \mathbb{E}[\Theta]$.

What's the Form?: LMS Estimator (2)

- Unknown: θ modeled by Θ with prior $f_\Theta(\cdot)$.

- Observation $X = x$ with model $f_{X|\Theta}(x|\theta)$

- Minimizing conditional mean squared error

$$\min_{\hat{\theta}} \mathbb{E}\left[(\Theta - \hat{\theta})^2 | X = x\right]$$

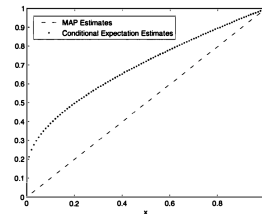 ○ minimized when $\hat{\theta} = \mathbb{E}[\Theta | X = x]$.

  ○ LMS estimator $\hat{\Theta} = \mathbb{E}[\Theta | X]$

- What is the mean squared error of the LMS estimate?
  ○ When $X = x$, $\mathbb{E}\left[(\Theta - \mathbb{E}[\Theta | X = x])^2 | X = x\right] = \text{var}\left(\Theta | X = x\right)$

  ○ Averaged over X: $\mathbb{E}\left[(\Theta - \mathbb{E}[\Theta | X])^2\right] = \mathbb{E}\left[\text{var}(\Theta | X)\right]$

Example: Romeo and Juliet

- Romeo and Juliet start dating, where Romeo is late by $X \sim \mathcal{U}[0, \theta]$.
- Unknown: θ modeled by a rv $\Theta \sim \mathcal{U}[0, 1]$.
- Observation: Romeo was late by x.
- Posterior: $f_{\Theta|X}(\theta|x) = \begin{cases} \frac{1}{\theta |\log x|}, & x \le \theta \le 1, \\ 0, & \theta < x \text{ or } \theta > 1 \end{cases}$

  ◦ $\hat{\theta}_{\text{MAP}} = x$.

  ◦ LMS estimator:

  $\hat{\theta}_{\text{LMS}} = \mathbb{E}[\theta|X = x] = \int_x^1 \theta \frac{1}{\theta |\log x|} d\theta =$

  $(1 - x)/|\log x|$

Example: Biased Coin with Beta Prior

- Biased coin with prob. of head θ. Unknown θ modeled by Θ with prior $f_\Theta(\theta)$.
- Observation X: number of heads out of n tosses
- If $\Theta \sim \text{Beta}(\alpha, \beta)$, then $\Theta|\{X = k\} \sim \text{Beta}(k + \alpha, n - k + \beta)$

◦ MAP estimate

$\hat{\theta}_{\text{MAP}} = \dfrac{\alpha + k - 1}{\alpha + \beta - 2 + n}$

◦ For $\alpha = \beta = 1$ ($\mathcal{U}[0, 1]$ prior),

$\hat{\theta}_{\text{MAP}} = \dfrac{k}{n}$

◦ Fact. If $\Theta \sim \text{Beta}(\alpha, \beta)$,

$\mathbb{E}[\Theta] = \dfrac{1}{B(\alpha, \beta)} \int_0^1 \theta \theta^{\alpha - 1}(1 - \theta)^{\beta - 1} d\theta = \dfrac{B(\alpha + 1, \beta)}{B(\alpha, \beta)} = \dfrac{\alpha}{\alpha + \beta}$

◦ LMS estimate:

$\mathbb{E}[\Theta|X = k] = \dfrac{k + \alpha}{k + \alpha + n - k + \beta} = \dfrac{k + \alpha}{\alpha + \beta + n}$

◦ For $\alpha = \beta = 1$ ($\mathcal{U}[0, 1]$ prior): $\mathbb{E}[\Theta|X = k] = \dfrac{k + 1}{n + 2}$

Example: Parameter Inference with Normal Prior

- The posterior pdf $f_{\Theta|X}(\theta|x) = a \cdot \exp\left\{-\dfrac{(\theta - m)^2}{2v}\right\}$, where

  $m = \dfrac{\sum_{i=0}^n \frac{x_i}{\sigma_i^2}}{\sum_{i=0}^n \frac{1}{\sigma_i^2}}, \qquad v = \dfrac{1}{\sum_{i=0}^n \frac{1}{\sigma_i^2}}$

- The pdf is normal, so it is maximized when $\theta = $ mean.
- Thus, $\hat{\theta}_{\text{MAP}} = m$.
- What is the LMS esitmate?

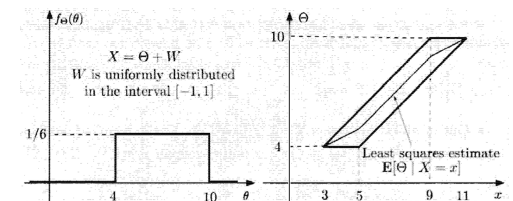 $\hat{\theta}_{\text{LMS}} = \mathbb{E}[\Theta|X = x] = m$

Example: Signal Recovery from Noisy Measurement (1)

- Send signal θ with the uniform noise $W \sim \mathcal{U}[-1, 1]$. Observe X
- $X = \Theta + W$, where model θ with $\Theta \sim \mathcal{U}[4, 10]$
- Given $\Theta = \theta$, $X = \theta + W \sim \mathcal{U}[\theta - 1, \theta + 1]$.

$f_{\Theta, X}(\theta, x) = f_\Theta(\theta) f_{X|\Theta}(x|\theta) = \begin{cases} \frac{1}{6} \cdot \frac{1}{2} = \frac{1}{12}, & \text{if } 4 \le \theta \le 10, \ \theta - 1 \le x \le \theta + 1, \\ 0, & \text{otherwise} \end{cases}$
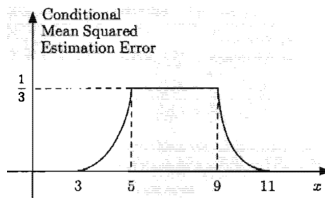
$\hat{\theta}_{\text{LMS}} = \mathbb{E}[\Theta|X = x]$: midpoint of the corresponding vertical section

KAIST EE

- What is conditional MSE? $\mathbb{E}\left[(\Theta - \mathbb{E}[\Theta|X = x])^2|X = x\right]$

- Given $X = 3$, it's the variance of $\mathcal{U}[4, 4] = 0$

- Given $X = 5$, it's the variance of $\mathcal{U}[4, 6] = (6 - 4)^2/12 = 1/3$

- The rising pattern between $X = 3$ and $X = 5$ is quadratic. This is because the expectation increases linearly, where the variance increases in a quadratic manner.

KAIST EE

$$f_{\Theta|X}(\theta|x) = \frac{f_\Theta(\theta)f_{X|\Theta}(x|\theta)}{f_X(x)}$$

$$f_X(x) = \int f_\Theta(\theta')f_{X|\Theta}(x|\theta')d\theta'$$

- Observation model $f_{X|\Theta}(x|\theta)$ may not be always available

- Finding the posterior distribution is hard for multi-dimensional Θ

- Θ is very often high-dimensional, especially in the era of big data and deep learning
  - AlexNet in image recognition: 61M parameters
  - GPT-3 in natural language processing: 175B parameters

- Any alternative to LMS estimator?

KAIST EE

KAIST EE

- Give up optimality, but choose a simple, but good one.

- General estimators $\hat{\Theta} = g(X)$, LMS estimator $\hat{\Theta}_{LMS} = \mathbb{E}[\Theta|X]$

- We consider a restricted class of $g(X)$
  - Estimator: $\hat{\Theta} = \boxed{aX + b}$.
  - Estimate: Given $X = x$, $\hat{\theta} = \boxed{ax + b}$.

- Our goal is to try our best within this restricted class:
$$\min_{a,b} \mathbb{E}\left[(\Theta - aX - b)^2|X = x\right], \qquad \min_{a,b} \mathbb{E}\left[(\Theta - aX - b)^2\right]$$

- Linear models are always the first choice for a simple design in engineering.

LLMS

$$\hat{\Theta}_L = \mathbb{E}(\Theta) + \frac{\text{cov}(\Theta, X)}{\text{var}(X)}\Big(X - \mathbb{E}(X)\Big) = \mathbb{E}(\Theta) + \rho\frac{\sigma_\Theta}{\sigma_X}\Big(X - \mathbb{E}(X)\Big),$$

where the correlation coefficient $\rho = \frac{\text{cov}(\Theta,X)}{\sigma_\Theta \sigma_X}$.

- No need of distributions on Θ and X: only means, variances, and covariances

○ If $\rho > 0$:
  - Baseline ($\mathbb{E}[\Theta]$) + correction term
  - If $X > \mathbb{E}[X] \Longrightarrow \hat{\Theta}_L > \mathbb{E}[\Theta]$
  - If $X < \mathbb{E}[X] \Longrightarrow \hat{\Theta}_L < \mathbb{E}[\Theta]$

○ If $\rho = 0$ (uncorrelated):
  - Just baseline ($\mathbb{E}[\Theta]$)
  - $\hat{\Theta}_L = \mathbb{E}[\Theta]$
  - No use of data X

- MSE $\mathbb{E}[(\hat{\Theta}_L - \Theta)^2]$?
  ○ Assume $\mathbb{E}[\Theta] = \mathbb{E}[X] = 0$ (for simplicity). Then, MSE $= \mathbb{E}\Big[(\Theta - \rho\frac{\sigma_\Theta}{\sigma_X}X)^2\Big]$
  ○ Note that $\text{var}[\Theta] = \sigma_\Theta^2 = \mathbb{E}(\Theta^2)$ and $\text{var}[X] = \sigma_X^2 = \mathbb{E}(X^2)$

$$\mathbb{E}\Big[(\Theta - \rho\frac{\sigma_\Theta}{\sigma_X}X)^2\Big] = \text{var}(\Theta - \rho\frac{\sigma_\Theta}{\sigma_X}X)$$

$$= \text{var}(\Theta) + \Big(\rho\frac{\sigma_\Theta}{\sigma_X}\Big)^2\text{var}(X) - 2\Big(\rho\frac{\sigma_\Theta}{\sigma_X}\Big)\text{cov}(\Theta, X) = (1 - \rho^2)\text{var}[\Theta]$$

- Uncertainty about Θ after observation decreases by the factor of $1 - \rho^2$
- What happens if $|\rho| = 1$ or $\rho = 0$?

$$\boxed{\hat{\Theta}_L = \mathbb{E}(\Theta) + \rho\frac{\sigma_\Theta}{\sigma_X}\Big(X - \mathbb{E}(X)\Big)}$$

$$\hat{\Theta}_L = \mathbb{E}(\Theta) + \frac{\text{cov}(\Theta, X)}{\text{var}(X)}\Big(X - \mathbb{E}(X)\Big) \qquad (1)$$

$$= \mathbb{E}(\Theta) + \rho\frac{\sigma_\Theta}{\sigma_X}\Big(X - \mathbb{E}(X)\Big) \qquad (2)$$

$$\min_{a,b} \text{ERR}(a, b) = \min_{a,b} \mathbb{E}\Big[(\Theta - aX - b)^2\Big]$$

- Assume a was found.

$$\mathbb{E}\Big[(Y - b)^2\Big], \quad Y = \Theta - aX$$

- Minimized when $b = \mathbb{E}(Y) = \mathbb{E}(\Theta) - a\mathbb{E}(X)$.
<mark>Slide pp. 43</mark>

$$\text{ERR}(a, b) = \mathbb{E}[(Y - \mathbb{E}[Y])^2] = \text{var}(Y)$$
$$= \text{var}[\Theta] + a^2\text{var}[X] - 2a\,\text{cov}(\Theta, X) \qquad (3)$$

- (3) is minimized when $a = \frac{\text{cov}(\Theta,X)}{\text{var}[X]}$. Then,

$$\hat{\Theta}_L = aX + b = aX + \mathbb{E}(\Theta) - a\mathbb{E}(X)$$
$$= \mathbb{E}(\Theta) + a(X - \mathbb{E}(X)) = (1)$$

- Using $\rho = \frac{\text{cov}(\Theta,X)}{\sigma_\Theta \sigma_X}$, we get:

$$a = \frac{\rho\sigma_\Theta\sigma_X}{\sigma_X^2} = \frac{\rho\sigma_\Theta}{\sigma_X}$$

- Then, we have (2).

<mark>Slides 17, 35, and 45 for more details</mark>

- Romeo and Juliet start dating, where Romeo is late by $X \sim \mathcal{U}[0, \theta]$.
- Unknown: θ modeled by a rv $\Theta \sim \mathcal{U}[0, 1]$.
- Random observation: X
- $\hat{\Theta}_{\text{MAP}} = X$, and $\hat{\Theta}_{\text{LMS}} = (1 - X)/|\log X$.
- Question. What is the LLMS estimator $\hat{\Theta}_L$?

$$\hat{\Theta}_L = \mathbb{E}(\Theta) + \frac{\text{cov}(\Theta, X)}{\text{var}(X)}\left(X - \mathbb{E}(X)\right)$$

- $\mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X|\Theta]] = \mathbb{E}[\Theta/2] = 1/4$
- Using $\mathbb{E}[\Theta] = 1/2$ and $\mathbb{E}[\Theta^2] = 1/3$,

$$\text{var}[X] = \mathbb{E}[\text{var}[X|\Theta]] + \text{var}[\mathbb{E}[X|\Theta]]$$
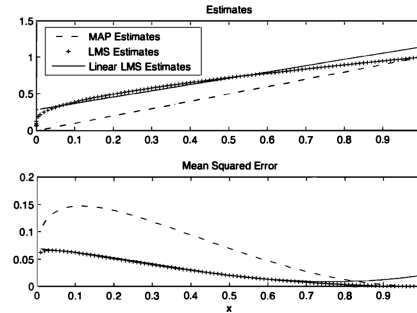$$= \frac{1}{12}\mathbb{E}[\Theta^2] + \frac{1}{4}\text{var}[\Theta] = \frac{7}{144}$$

- $\text{cov}(\Theta, X) = \mathbb{E}[\Theta X] - \mathbb{E}[\Theta]\mathbb{E}[X]$

$$\mathbb{E}[\Theta X] = \mathbb{E}[\mathbb{E}[\Theta X|\Theta]] = \mathbb{E}[\Theta\mathbb{E}[X|\Theta]]$$
$$= \mathbb{E}[\Theta^2/2] = 1/6$$

$$\text{cov}(\Theta, X) = 1/6 - 1/2 \cdot 1/4 = 1/24$$

- $\hat{\Theta}_L = \frac{1}{2} + \frac{1/24}{7/144}(X - \frac{1}{4}) = \frac{6}{7}X + \frac{2}{7}$

Estimates
- - - MAP Estimates
+ LMS Estimates
— Linear LMS Estimates

Mean Squared Error

x

- Biased coin with probability of head θ
- Unknown $\Theta \sim \mathcal{U}[0,1]$,
  - $\mathbb{E}[\Theta] = 1/2$, $\text{var}[\Theta] = 1/12$
- n tosses, X: number of heads.
- $p_{X|\Theta}(k|\theta) \sim \text{Binomial}(n, \theta)$
- $\mathbb{E}[X] = \mathbb{E}[\mathbb{E}[X|\Theta]] = \mathbb{E}[n\Theta] = n/2$

$$\text{var}(X) = \mathbb{E}[\text{var}(X|\Theta)] + \text{var}(\mathbb{E}[X|\Theta])$$
$$= \mathbb{E}[n\Theta(1-\Theta)] + \text{var}[n\Theta]$$
$$= \frac{n}{2} - \frac{n}{3} + \frac{n^2}{12} = \frac{n(n+2)}{12}$$

$$\text{cov}(\Theta, X) = \mathbb{E}[\Theta X] - \mathbb{E}[\Theta]\mathbb{E}[X] = \mathbb{E}[\Theta X] - n/4$$

$$\mathbb{E}[\Theta X] = \mathbb{E}[\mathbb{E}[\Theta X|\Theta]] = \mathbb{E}[\Theta\mathbb{E}[X|\Theta]]$$
$$= \mathbb{E}[n\Theta^2] = n/3$$

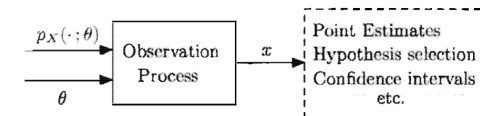$$\text{cov}(\Theta, X) = \frac{n}{3} - \frac{n}{4} = \frac{12}{n}$$

$$\hat{\Theta}_L = \frac{1}{2} + \frac{n/12}{n(n+2)/12}(X - \frac{n}{2}) = \frac{X+1}{n+2}$$

- $\hat{\Theta}_{MAP} = \frac{X}{n}$
- $\hat{\Theta}_{LMS} = \frac{X+1}{n+2}$
- $\hat{\Theta}_L = \hat{\Theta}_{LMS}$! Intuitive?
- Yes, because the LMS esitmator was linear.

$p_X(\cdot; \theta)$ → Observation Process → x → Point Estimates / Hypothesis selection / Confidence intervals / etc.

θ

- Unknown θ
  - deterministic (not random) quantity (thus, no prior distribution)
  - No prior, No posterior probabilities
- Observations or measurements X
  - Random observation X's distribution just depends on θ
  - Notation: $p_X(x; \theta)$ and $f_X(x; \theta)$, θ-parameterized distribution of observations
- Choosing one among multiple probabilistic models
  - Each θ corresponds to a probabilistic model

- Problem types
  - Estimation
  - Hypothesis testing
  - Significance testing

- Key inference methods
  - ML (Maximum Likelihood) estimation
  - Linear regression
  - Likelihood ratio test
  - Significant testing

- Just a taste in this course.

- Random observation $x = (x_1, x_2, \ldots, x_n)$ of $X = (X_1, X_2, \ldots, X_n)$
  - Assume a scalar θ and a vector of observations in this lecture.

- Likelihood $p_X(x_1, x_2, \ldots, x_n; \theta)$

  - $p_X(x_1, x_2, \ldots, x_n; \theta)$
    - The probability that the observed value x arises when the parameter is θ.
    - NOT the probability that the unknown parameter is equal to θ.

  - ML (Maximum Likelihood) estimation

    $$\hat{\theta}_{\mathsf{ML}} = \arg\max_\theta p_X(x_1, x_2, \ldots, x_n; \theta)$$

- Very often, X_is are independent. Then, ML equals to maximizing the log-likelihood:

$$\log p_X(x_1, x_2, \ldots, x_n; \theta) = \log \prod_{i=1}^n p_{X_i}(x_i; \theta) = \sum_{i=1}^n \log p_{X_i}(x_i; \theta)$$

- ML and MAP: How are they related?

- MAP in the Bayesian inference

$$\hat{\theta}_{\mathsf{MAP}} = \arg\max_\theta p_{\Theta|X}(\theta|x) = \arg\max_\theta \frac{p_{X|\Theta}(x|\theta)p_\Theta(\theta)}{p_X(x)} = \frac{1}{p_X(x)}\arg\max_\theta p_{X|\Theta}(x|\theta)p_\Theta(\theta)$$

- ML in the classical inference

$$\hat{\theta}_{\mathsf{ML}} = \arg\max_\theta p_X(x; \theta)$$

- $p_{X|\Theta}(x|\theta)$ in the Bayesian setting corresponds to $p_X(x; \theta)$ in the classical setting.

- Thus, when Θ is uniform (complete ignorance of Θ) in MAP, MAP == ML

- Romeo and Juliet start dating. Romeo: late by $X \sim U[0, \theta]$.

- Unknown: θ modeled by a rv $\Theta \sim U[0, 1]$.

- MAP: $\hat{\theta}_{\mathsf{MAP}} = x$

- LMS: $\hat{\theta}_{\mathsf{LMS}} = (1 - x)/|\log x|$

- LLMS: $\hat{\theta}_{\mathsf{L}} = \frac{6}{7}x + \frac{2}{7}$

- ML: $\hat{\theta}_{\mathsf{ML}} = \hat{\theta}_{\mathsf{MAP}} = x$

Example: Estimation of Parameter of Exponential rv **KAIST EE**

- n identical, independent exponential rvs, $X_1, X_2, \ldots, X_n$ with parameter θ.

- Observation $x_1, x_2, \ldots, x_n$

- What is the ML estimate of θ?

- Reminder. $X \sim \exp(\lambda)$

$$f_X(x) = \begin{cases} \lambda e^{-\lambda x}, & x \geq 0 \\ 0, & x < 0 \end{cases} \quad \mathbb{E}[X] = 1/\lambda$$

- Any guess? $\hat{\theta}_{ML} = \frac{n}{x_1 + x_2 \ldots x_n}$

$$\arg\max_\theta f_X(x; \theta) = \arg\max_\theta \prod_{i=1}^{n} \theta e^{-\theta x_i} = \arg\max_\theta \left(n \log \theta - \theta \sum_{i=1}^{n} x_i \right)$$

Questions?

Review Questions **KAIST EE**

1) What is statistical inference?

2) Draw the building blocks of Bayesian inference and explain how it works.

3) What are MAP and LMS estimators and their underlying philosophies?

4) What is LLMS estimator and why is it useful?

5) Compare the classical and Bayesian inference.

6) What is the ML estimator and how is it related to the MAP estimator?