

# ML&MEA (2024)

## Lecture 3 - Frequentist vs Bayesian

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# Content

- 1 Recap
- 2 Review Probability Theory
- 3 Frequentist vs Bayesian
- 4 Rethink linear regression
- 5 Summary

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# Recap Lecture 2 - Linear regression

## Simple linear regression

- ① Data:  $\{(x^{(i)}, y^{(i)})\}_{i=1}^n, x^{(i)} \in \mathbb{R}^1, y^{(i)} \in \mathbb{R}^1$

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- 2 Model:  $y = \beta x$  with single parameter  $\beta$ ;  
Loss function  $\mathcal{L}(\beta) = \frac{1}{n} \sum_{i=1}^n (y^{(i)} - \beta x^{(i)})^2$

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- 3 Optimization algorithms

$$\text{Gradient: } \nabla \mathcal{L} = \frac{d\mathcal{L}(\beta)}{d\beta} = -\frac{2}{n} \sum_i x_i (y^{(i)} - \beta x^{(i)})$$

$$\text{Analytical solution: } \hat{\beta} = \frac{\sum_{i=1}^n x^{(i)} y^{(i)}}{\sum_{i=1}^n (x^{(i)})^2} = \frac{\mathbf{X}^T \mathbf{Y}}{\mathbf{X}^T \mathbf{X}}$$

$$\text{Gradient descent: } \beta^{(j+1)} \leftarrow \beta^{(j)} - \eta \nabla \mathcal{L}$$

# Recap Lecture 2 - Linear regression

## Multiple linear regression

① Data:  $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^n$ ,  $\mathbf{x}^{(i)} = [x_1 \ x_2 \ \dots \ x_p]^T$

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$$\text{Gradient descent: } \beta^{(j+1)} \leftarrow \beta^{(j)} - \eta \nabla \mathcal{L}$$

## Recap Lecture 2 - Linear regression

**Derive the gradient of loss function using matrix calculus:**

$$\begin{aligned}\mathcal{L}(\beta) &= \frac{1}{n} (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \\ &= \frac{1}{n} (\mathbf{y}^T - (\mathbf{X}\beta)^T) (\mathbf{y} - \mathbf{X}\beta) \\ &= \frac{1}{n} \left( \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\beta - \beta^T \mathbf{X}^T \mathbf{y} + \beta^T \mathbf{X}^T \mathbf{X}\beta \right)\end{aligned}$$

From Eq(69) in the *Matrix Cookbook* :  $\frac{\partial(\beta^T \mathbf{a})}{\partial \beta} = \frac{\partial(\mathbf{a}^T \beta)}{\partial \beta} = \mathbf{a}$

$$\begin{aligned}\text{Gradient: } \nabla \mathcal{L} &= \frac{1}{n} \left( -(\mathbf{y}^T \mathbf{X})^T - (\mathbf{X}^T \mathbf{y}) + \mathbf{X}^T \mathbf{X}\beta + (\beta^T \mathbf{X}^T \mathbf{X})^T \right) \\ &= -\frac{2}{n} \mathbf{X}^T (\mathbf{y} - \mathbf{X}\beta)\end{aligned}$$

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# Basics of probability

- **Definition of *probability*:**

With each event  $X$ , one associates a number denoted by  $P(X)$  and called the “probability of  $X$ ”.

This number measures the likelihood of the event  $X$  to be realized a priori, before performing the experiment. It is chosen between 0 and 1, and the more likely the event is, the closer to 1 this number is. [Probability Essential, by Jean Jacod and Philip Protter]

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- **Rules of probability:**

$$0 \leq P(X) \leq 1$$

$P(\Omega) = 1$ , where  $\Omega$  is the full set of all possible events

$$P(A \cup B) = P(A) + P(B), \text{ if } A \cap B = \emptyset$$

# Random variable

- A *random variable*  $x$  is a quantity that is **uncertain**.  
It may be the result of experiment (e.g., , draw a dice) or real-world measurement (e.g., , measuring temperature).

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If  $x$  is discrete, then  $p(x)$  is probability mass function (PMF) with  $\sum_x p(x) = 1$

If  $x$  is continuous, then  $p(x)$  is probability density function (PDF) with  $\int_x p(x) dx = 1$



# PMF of discrete random variable

- A discrete random variable  $x$  can be fully described by a probability mass function (PMF).

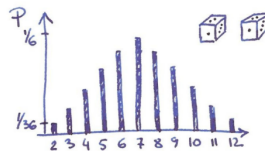
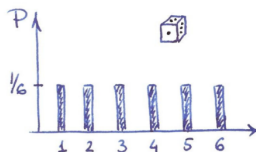


图 1: Two examples of PMF: (left)  $p(x)$  where  $x \in \{1, 2, \dots, 6\}$ . (right)  $p(x)$  where  $x \in \{1, 2, \dots, 12\}$ .

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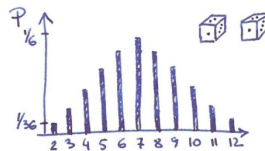
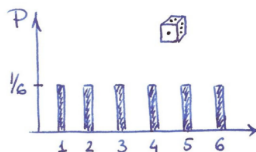


图 1: Two examples of PMF: (left)  $p(x)$  where  $x \in \{1, 2, \dots, 6\}$ . (right)  $p(x)$  where  $x \in \{1, 2, \dots, 12\}$ .

- We do an experiment (e.g., draw a dice once), and then observe an event  $X$ , which means **sampling** from  $p(x)$ .

# PDF of continuous random variable

- A continuous random variable  $x$  can be fully described by its probability density function (PDF).

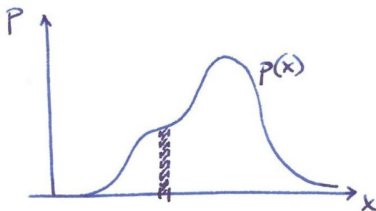


图 2: An example of PDF.  $p(x)$  is the probability of an event  $X$  falling into the shadowed zone.

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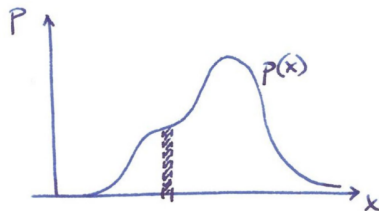


图 2: An example of PDF.  $p(x)$  is the probability of an event  $X$  falling into the shadowed zone.

- Two properties of a PDF:

$$p(x) \geq 0, \quad \int_x p(x) dx = 1$$

# Gaussian Distribution (or Normal Distribution)

- Gaussian Distribution is the most well-known and widely-used PDF, a special function with two parameters (mean  $\mu$ , and variance  $\sigma^2$ ),

$$p(x|\mu, \sigma^2) = \mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x - \mu)^2}{2\sigma^2}\right] \quad (1)$$

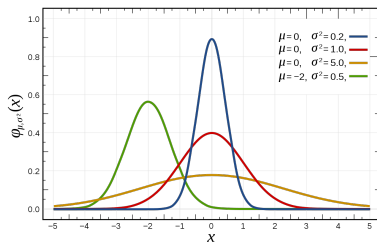


图 3: Four examples of Gaussian distribution.

# Multivariate Gaussian Distribution

- To describe one random variable (1-dimension), we use the univariate Gaussian distribution:

$$p(x|\mu, \sigma^2) = \mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x - \mu)^2}{2\sigma^2}\right] \quad (2)$$

# Multivariate Gaussian Distribution

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- To describe high-dimensional random variables  $\mathbf{x} \in \mathbb{R}^p$ , we have to use multivariate Gaussian distribution.
- $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \in \mathbb{R}^p$  with the mean  $\boldsymbol{\mu} \in \mathbb{R}^p$  and the covariance matrix  $\boldsymbol{\Sigma} \in \mathbb{R}^{p \times p}$  (协方差矩阵)

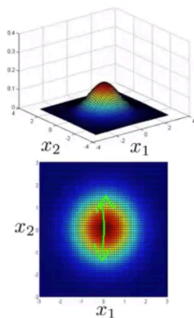
$$\begin{aligned} P(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) &= \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \\ &= \frac{1}{\sqrt{(2\pi)^p \det(\boldsymbol{\Sigma})}} \exp\left[-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right] \end{aligned}$$



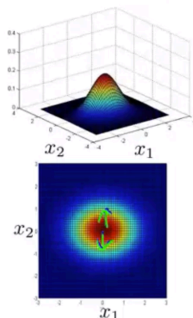
# Visualize Multivariate Gaussian Distribution

## Multivariate Gaussian (Normal) examples

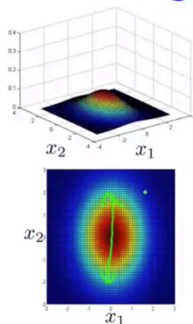
$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 0.6 \end{bmatrix}$$



$$\mu = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$



Andrew Ng

图 4: Three examples of Multivariate Gaussian Distribution.

# Motivation of Bayes' Theorem

- Sometime we have some prior information/knowledge about parameter  $\theta$ . We want to **incorporate our prior knowledge of  $\theta$  into the model**, such as the mean/variance/range of  $\theta$ .
- For example, Let's denote the random variable  $x$  as Shenzhen's temperature.  
A simple model of  $x$  is  $x \sim \mathcal{N}(\mu, \sigma^2)$ .
- Our prior experiences tell us  $\mu$  is close to  $25^\circ\text{C}$ . We can assign a prior distribution to  $\mu$  as  $\mu \sim \mathcal{N}(25, 5^2)$ .  
We just observed 5 days of temperature in Shenzhen is  $\mathbf{X} = (12, 15, 13, 16, 17)^T$ .
- Now our belief in  $\mu$  is not  $\mathcal{N}(25, 5^2)$  any more. We should update our belief in  $\mu$ . How to update it based on our **prior knowledge** and our **current observations**?

# Bayes' Theorem

**Posterior** is proportional to **likelihood** times **prior**.

$$P(\theta|\mathbf{X}) = \frac{P(\mathbf{X}|\theta)P(\theta)}{P(\mathbf{X})} = \frac{P(\mathbf{X}|\theta)P(\theta)}{\int_{\theta} P(\mathbf{X}|\theta)P(\theta)d\theta} \propto P(\mathbf{X}|\theta)P(\theta)$$

- **4 core components**

- ① **Prior:**  $P(\theta)$  – what we know about  $\theta$  BEFORE collecting any data  $\mathbf{X}$
- ② **Likelihood:**  $P(\mathbf{X}|\theta)$  – likelihood for observing a certain value of  $\mathbf{X}$  given a certain value of  $\theta$
- ③ **Posterior:**  $P(\theta|\mathbf{X})$  – what we know about  $\theta$  AFTER observing  $\mathbf{X}$  just happened.
- ④ **Evidence:**  $P(\mathbf{X})$  – a constant, to ensure that the left hand side is a valid distribution

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# Differences between Frequentist & Bayesian

- The fundamental difference between frequentist and Bayesian approaches lies in how they interpret probability and handle uncertainty, especially in the context of statistical inference and parameter estimation. Let's explore these differences and illustrate them with the example of estimating the mean temperature  $\mu$  in Shenzhen based on observed temperatures.

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- **Interpretation of Probability:** In the frequentist view, probability is interpreted as the long-run frequency of events. It does not assign probabilities to hypotheses or fixed parameters. Thus, the true mean temperature  $\mu$  is considered a fixed but unknown value.  
Bayesian probability is a measure of belief or certainty about events, including hypotheses or parameter values. It allows for the incorporation of prior knowledge and evidence to update beliefs.

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Bayesian probability is a measure of belief or certainty about events, including hypotheses or parameter values. It allows for the incorporation of prior knowledge and evidence to update beliefs.
- **Parameter Estimation:** Frequentist methods use data to calculate a point estimate (e.g., the sample mean) or interval estimates (e.g., confidence intervals) for parameters without incorporating prior knowledge. Uncertainty in parameter estimates is expressed through confidence intervals and p-values. Bayesian methods combine prior beliefs about parameters (prior distributions) with observed data (likelihood) to update beliefs (posterior distributions). The result is a full probability distribution over the parameter, reflecting all known information.

## Probabilistic model

- So far in this course, a *model* is referred to a parametric family of functions  $f(x, \theta)$ , where  $\theta$  is the vector of parameters. For example, the simplest linear regression model,  $f(x) = \beta x$ .



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- Now we will discuss *probabilistic models*, such as

$$f(x) = \beta x + \epsilon$$
$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

where  $\mathcal{N}(0, \sigma^2)$  denotes a Gaussian distribution with mean 0 and variance  $\sigma^2$ , referring to the distribution of error.

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- Probabilistic models can be considered as *generative models*, where each data  $\mathbf{x}$  is generated by sampling from the distribution  $P(\mathbf{x}|\theta)$ .

Notice: Since  $\mathbf{x} \in \mathbb{R}^{p \times 1}$ ,  $P(\mathbf{x}|\theta)$  has  $p$  dimensions as well.

# *iid* assumption

All data are independent and identically distributed (iid).

$$\mathbf{x}^{(i)} \overset{iid}{\sim} P(\mathbf{x}|\theta), \quad i \in \{1, 2, \dots, N\}$$

- Can you take some examples?

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The probability the event 'head' happens is  $1/2$  in each time.

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  - 3 Scores of students in our course are iid,  $x \stackrel{iid}{\sim} \mathcal{N}(90, 5^2)$ .

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- **Why iid assumption is important?**

For a set of  $N$  observed samples,  $\mathbf{X} = [\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N)}]^T$ , the probability that the event  $\mathbf{X}$  happens is

$$P(\mathbf{X}|\theta) = \prod_{i=1}^N P(\mathbf{x}^{(i)}|\theta).$$

# Frequentist vs Bayesian

## Frequentist:

- **Core idea:** The parameters  $\theta$  are constant.



# Frequentist vs Bayesian

## Frequentist:

- **Core idea:** The parameters  $\theta$  are constant.
- Maximum log-likelihood estimation (i.e., MLE) to estimate parameters  $\theta$ :

$$\theta_{MLE} = \arg \max_{\theta} \log P(\mathbf{X}|\theta) \quad (3)$$

$$= \arg \max_{\theta} \log \prod_{i=1}^N P(\mathbf{x}^{(i)}|\theta) \quad (4)$$

$$= \arg \max_{\theta} \sum_{i=1}^N \log P(\mathbf{x}^{(i)}|\theta) \quad (5)$$

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- Recall Bayes' theorem:

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## Bayesian:

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- Maximum a posterior (i.e., MAP) to estimate parameters  $\theta$ :

$$\theta_{MAP} = \arg \max_{\theta} \log P(\theta|\mathbf{X}) \quad (6)$$

$$= \arg \max_{\theta} \sum_{i=1}^N [\log P(\mathbf{x}^{(i)}|\theta) + \log P(\theta)] \quad (7)$$

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# Rethink linear regression as a Probabilistic model

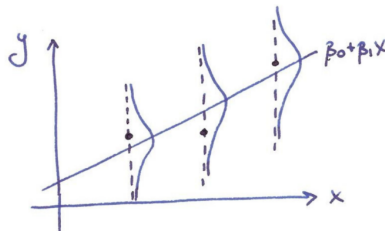
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 5: The error from each sample is assumed as iid Gaussian distribution.

# Likelihood

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- For a given  $\beta$  and given  $\mathbf{x}^{(i)}$ , the likelihood  $P(y|\mathbf{x}^{(i)}, \beta)$  is as follows,

$$y^{(i)} \sim \mathcal{N}(\beta^T \mathbf{x}^{(i)}, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp \left[ -\frac{(y - \beta^T \mathbf{x}^{(i)})^2}{2\sigma^2} \right] \quad (8)$$

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- For the entire training set  $(\mathbf{X}, \mathbf{y}) = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ ,

$$P(\mathbf{y}|\mathbf{X}, \beta) = \prod_{i=1}^N \frac{1}{\sigma\sqrt{2\pi}} \exp \left[ -\frac{(y^{(i)} - \beta^T \mathbf{x}^{(i)})^2}{2\sigma^2} \right] \quad (9)$$

# Linear regression in frequentist view

- For the entire training set  $(\mathbf{X}, \mathbf{y}) = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^N$ ,

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- MLE to estimate the parameter  $\beta$

$$\begin{aligned} \beta_{MLE} &= \arg \max_{\beta} \log P(\mathbf{y}|\mathbf{X}, \beta) \\ &= \arg \max_{\beta} \sum_{i=1}^N \log \left( \frac{1}{\sigma\sqrt{2\pi}} \exp \left[ -\frac{(y^{(i)} - \beta^T \mathbf{x}^{(i)})^2}{2\sigma^2} \right] \right) \\ &= - \arg \max_{\beta} \sum_{i=1}^N \left( y^{(i)} - \beta^T \mathbf{x}^{(i)} \right)^2 \end{aligned}$$

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- Big surprise! It is the same as the mean-squared-error (MSE) loss in Lecture 2.

Here, MLE is the same as minimizing MSE loss.

- 1 Recap
- 2 Review Probability Theory
- 3 Frequentist vs Bayesian
- 4 Rethink linear regression
- 5 Summary



# Summary of Lecture 4

- **Probability theory:** random variable, PMF, PDF  
Gaussian distribution, Multivariate Gaussian distribution
- **Frequentist vs Bayesian:**

- ① Frequentist: The parameters  $\theta$  are constant.  
Maximum (log-)likelihood estimation (MLE) to estimate  $\theta$ :

$$\theta_{MLE} = \arg \max_{\theta} \log P(\mathbf{X}|\theta)$$

- ② Bayesian: The parameters  $\theta$  are not constant. We have some prior information of  $\theta$ .  
Maximum a posterior (MAP) to estimate  $\theta$ :

$$\theta_{MAP} = \arg \max_{\theta} \log P(\theta|\mathbf{X}) = \arg \max_{\theta} \log P(\mathbf{X}|\theta) + \log P(\theta)$$

- **Linear regression in frequentist view:**  
MLE = minimizing *negative log-likelihood* = minimizing MSE