

Lecture 6: Probability and Distributions

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Mathematics for Machine Learning

<https://yung-web.github.io/home/courses/mathml.html>
KAIST EE

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Roadmap

- (1) Construction of a Probability Space
- (2) Discrete and Continuous Probabilities
- (3) Sum Rule, Product Rule, and Bayes' Theorem
- (4) Summary Statistics and Independence
- (5) Gaussian Distribution
- (6) Conjugacy and the Exponential Family
- (7) Change of Variables/Inverse Transform

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What Do We Want?

Modeling: Approximate reality with a simple (mathematical) model

- Experiment
 - Flip two coins
- Observation: a random outcome
 - for example, (H, H)
- All outcomes
 - $\{(H, H), (H, T), (T, H), (T, T)\}$

-
- **Our goal:** Build up a probabilistic model for an experiment with random outcomes
 - **Probabilistic model?**
 - Assign a number to each outcome or a set of outcomes
 - Mathematical description of an uncertain situation
 - Which model is good or bad?

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Goal: Build up a probabilistic model. Hmm... How?

The first thing: What are the *elements* of a probabilistic model?

Elements of Probabilistic Model

1. All outcomes of my interest: Sample Space Ω
2. Assigned numbers to each outcome of Ω : Probability Law $\mathbb{P}(\cdot)$

Question: What are the conditions of Ω and $\mathbb{P}(\cdot)$ under which their induced probability model becomes "legitimate"?

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Sample Space Ω

The set of all outcomes of my interest

1. Mutually exclusive
2. Collectively exhaustive
3. At the right granularity (not too concrete, not too abstract)

1. Toss a coin. What about this?
 $\Omega = \{H, T, HT\}$
2. Toss a coin. What about this? $\Omega = \{H\}$
3. (a) Just figuring out prob. of H or T.
 $\implies \Omega = \{H, T\}$

 (b) The impact of the weather (rain or no rain) on the coin's behavior.

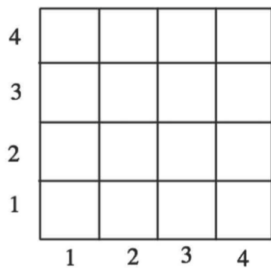
 $\implies \Omega = \{(H, R), (T, R), (H, NR), (T, NR)\}$,
 where R(Rain), NR(No Rain).

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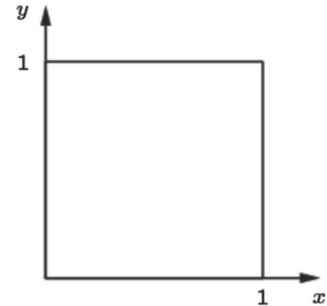
- **Discrete case:** Two rolls of a tetrahedral die

$$\Omega = \{(1, 1), (1, 2), \dots, (4, 4)\}$$



- **Continuous case:** Dropping a needle in a plain

$$\Omega = \{(x, y) \in \mathbb{R}^2 \mid 0 \leq x, y \leq 1\}$$



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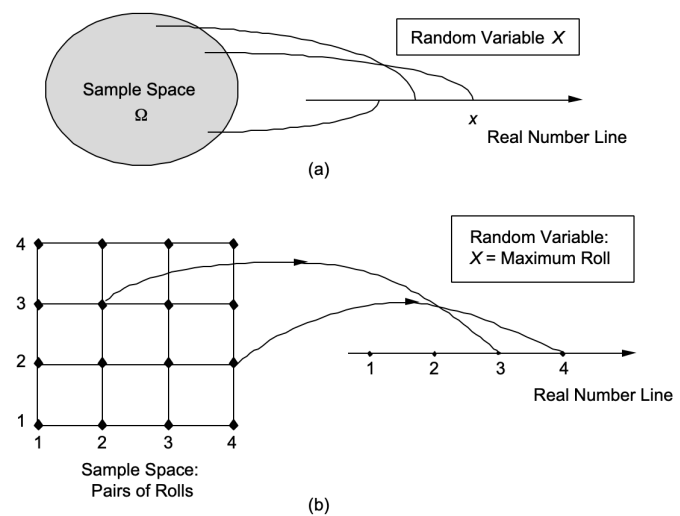
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- Assign numbers to what? Each outcome?
- What is the probability of dropping a needle at $(0.5, 0.5)$ over the 1×1 plane?
- Assign numbers to each **subset** of Ω : A subset of Ω : **an event**
- $\mathbb{P}(A)$: Probability of an event A .
 - This is where probability meets set theory.
 - Roll a dice. What is the probability of odd numbers?
$$\mathbb{P}(\{1, 3, 5\}), \text{ where } \{1, 3, 5\} \subset \Omega \text{ is an event.}$$
- **Event space \mathcal{A} :** The collection of subsets of Ω . For example, in the discrete case, the power set of Ω .
- **Probability Space $(\Omega, \mathcal{A}, \mathbb{P}(\cdot))$**

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- In reality, many outcomes are **numerical**, e.g., stock price.
- Even if not, very convenient if we map numerical values to random outcomes, e.g., '0' for male and '1' for female.



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Random Variable: More Formally

- Mathematically, a random variable X is a **function** which maps from Ω to \mathbb{R} .
- **Notation.** Random variable X , numerical value x .
- Different random variables X , Y , etc can be defined on the same sample space.
- For a fixed value x , we can associate an **event** that a random variable X has the value x , i.e., $\{\omega \in \Omega \mid X(\omega) = x\}$
- Generally,

$$\mathbb{P}_X(S) = \mathbb{P}(X \in S) = \mathbb{P}(X^{-1}(S)) = \mathbb{P}(\{\omega \in \Omega : X(\omega) \in S\})$$

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- Pick a person a at random
 - event A : a 's age ≤ 20
 - event B : a is married
- (Q1) What is the probability of A ?
- (Q2) What is the probability of A , given that B is true?
- Clearly the above two should be different.
- **Question.** How should I change my belief, given some additional information?
- Need to build up a new theory, which we call **conditional probability**.

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- $\mathbb{P}(A \mid B)$: $\mathbb{P}(\cdot \mid B)$ should be a new **probability law**.
- **Definition.**
$$\mathbb{P}(A \mid B) := \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}, \quad \text{for } \mathbb{P}(B) > 0.$$
 - Note that this is a **definition**, not a **theorem**.
- All other properties of the law $\mathbb{P}(\cdot)$ is applied to the conditional law $\mathbb{P}(\cdot \mid B)$.
- For example, for two disjoint events A and C ,

$$\mathbb{P}(A \cup C \mid B) = \mathbb{P}(A \mid B) + \mathbb{P}(C \mid B)$$

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- The values that a random variable X takes is discrete (i.e., finite or countably infinite).
- Then, $p_X(x) := \mathbb{P}(X = x) := \mathbb{P}(\{\omega \in \Omega \mid X(\omega) = x\})$, which we call **probability mass function** (PMF).
- Examples: Bernoulli, Uniform, Binomial, Poisson, Geometric

- Only **binary** values

$$X = \begin{cases} 0, & \text{w.p.}^1 \ 1 - p, \\ 1, & \text{w.p.} \ p \end{cases}$$

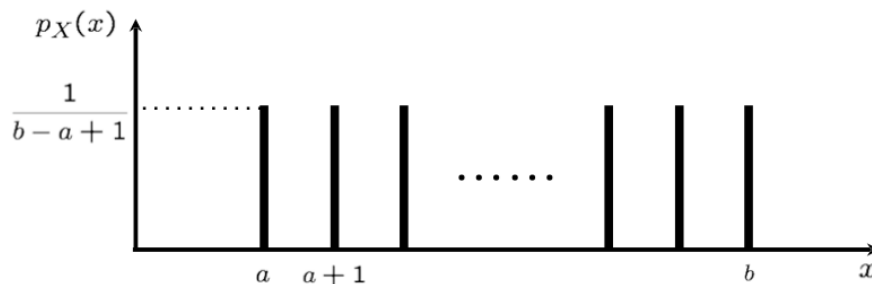
In other words, $p_X(0) = 1 - p$ and $p_X(1) = p$ from our PMF notation.

- Models a trial that results in binary results, e.g., success/failure, head/tail
- Very useful for an **indicator rv** of an event A . Define a rv 1_A as:

$$1_A = \begin{cases} 1, & \text{if } A \text{ occurs,} \\ 0, & \text{otherwise} \end{cases}$$

¹with probability
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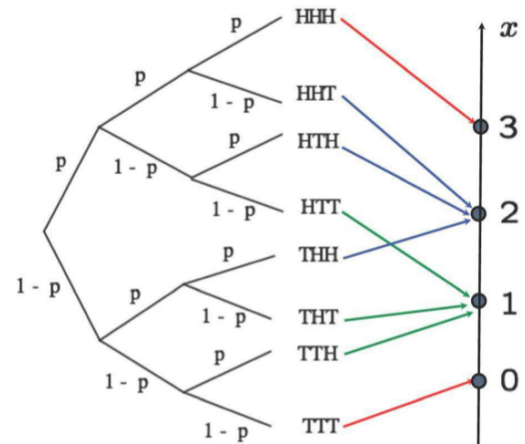
- integers a, b , where $a \leq b$
- Choose a number of $\Omega = \{a, a + 1, \dots, b\}$ uniformly at random.
- $p_X(i) = \frac{1}{b-a+1}$, $i \in \Omega$.



- Models complete ignorance (I don't know anything about X)

- Models the number of successes in a given number of independent trials
- n independent trials, where one trial has the success probability p .

$$p_X(k) = \binom{n}{k} p^k (1-p)^{n-k}$$



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- Binomial*(n, p): Models the number of successes in a given number of independent trials with success probability p .
- Very large n and very small p , such that $np = \lambda$

$$p_X(k) = e^{-\lambda} \frac{\lambda^k}{k!}, \quad k = 0, 1, \dots$$

- Is this a legitimate PMF?

$$\sum_{k=0}^{\infty} e^{-\lambda} \frac{\lambda^k}{k!} = e^{-\lambda} \left(1 + \lambda + \frac{\lambda^2}{2!} + \frac{\lambda^3}{3!} \dots \right) = e^{-\lambda} e^{\lambda} = 1$$

- Prove this:

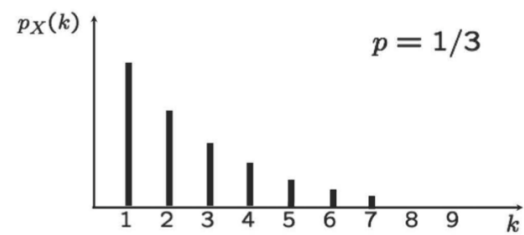
$$\lim_{n \rightarrow \infty} p_X(k) = \binom{n}{k} (1/n)^k (1 - 1/n)^{n-k} = e^{-\lambda} \frac{\lambda^k}{k!}$$

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- Experiment: infinitely many independent Bernoulli trials, where each trial has success probability p
- Random variable: number of trials until the **first success**.
- Models waiting times until something happens.

$$p_X(k) = (1 - p)^{k-1} p$$



Joint PMF

- **Joint PMF.** For two random variables X, Y , consider two events $\{X = x\}$ and $\{Y = y\}$, and

$$p_{X,Y}(x,y) := \mathbb{P}(\{X=x\} \cap \{Y=y\})$$

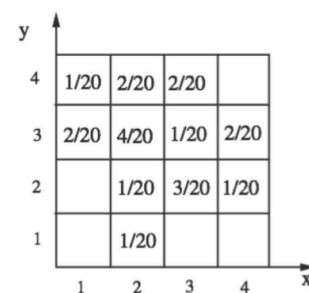
- $\sum_x \sum_y p_{X,Y}(x,y) = 1$

- Marginal PMF.

$$p_X(x) = \sum_y p_{X,Y}(x, y),$$

$$p_Y(y) = \sum_x p_{X,Y}(x,y)$$

Example.



$$p_{X,Y}(1,3) = 2/20$$

$$p_X(4) = 2/20 + 1/20 = 3/20$$

$$\mathbb{P}(X = Y) = 1/20 + 4/20 + 3/20 = 8/20$$

- Conditional PMF

$$p_{X|Y}(x|y) := \mathbb{P}(X = x|Y = y) = \frac{p_{X,Y}(x,y)}{p_Y(y)}$$

for y such that $p_Y(y) > 0$.

- $\sum_x p_{X|Y}(x|y) = 1$

- Multiplication rule.

$$\begin{aligned} p_{X,Y}(x,y) &= p_Y(y)p_{X|Y}(x|y) \\ &= p_X(x)p_{Y|X}(y|x) \end{aligned}$$

- $p_{X,Y,Z}(x,y,z) = p_X(x)p_{Y|X}(y|x)p_{Z|X,Y}(z|x,y)$

y				
4	1/20	2/20	2/20	
3	2/20	4/20	1/20	2/20
2		1/20	3/20	1/20
1		1/20		
	1	2	3	4
	x			

$$p_{X|Y}(2|2) = \frac{1}{1+3+1}$$

$$p_{X|Y}(3|2) = \frac{3}{1+3+1}$$

$$\mathbb{E}[X|Y = 3] = 1(2/9) + 2(4/9) + 3(1/9) + 4(2/9)$$

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Continuous RV and Probability Density Function (PDF)

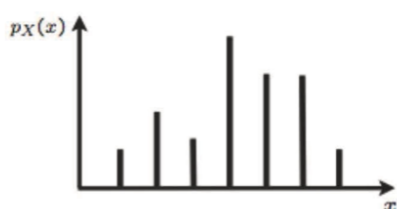
- Many cases when random variable have "continuous values", e.g., velocity of a car

Continuous Random Variable

A rv X is **continuous** if \exists a function f_X , called **probability density function (PDF)**, s.t.

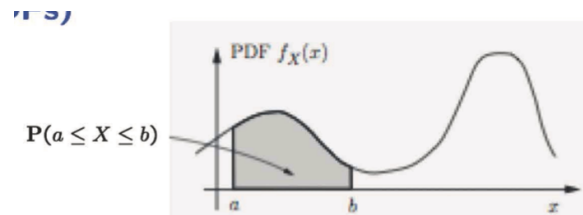
$$\mathbb{P}(X \in B) = \int_B f_X(x) dx$$

- All of the concepts and methods (expectation, PMFs, and conditioning) for discrete rvs have continuous counterparts



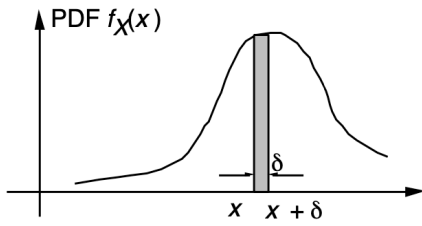
- $\mathbb{P}(a \leq X \leq b) = \sum_{x: a \leq x \leq b} p_X(x)$
- $p_X(x) \geq 0, \sum_x p_X(x) = 1$

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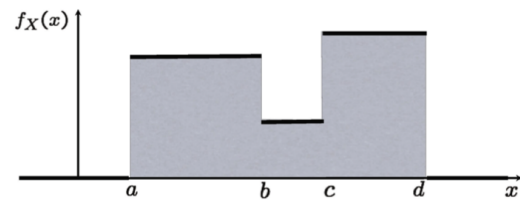
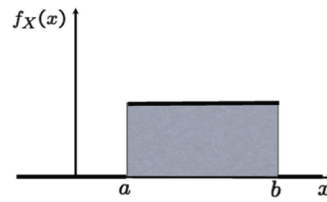
- $\mathbb{P}(a \leq X \leq b) = \int_a^b f_X(x) dx$
- $f_X(x) \geq 0, \int_{-\infty}^{\infty} f_X(x) dx = 1$

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- $\mathbb{P}(a \leq X \leq a + \delta) \approx f_X(a) \cdot \delta$
- $\mathbb{P}(X = a) = 0$

Examples

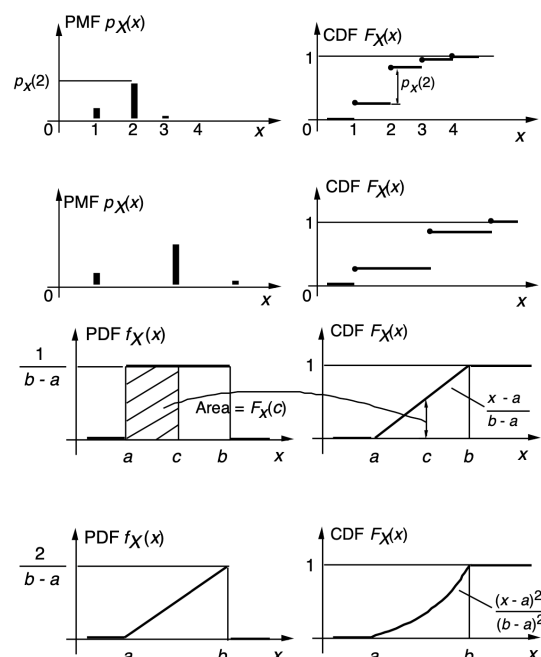


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Cumulative Distribution Function (CDF)

- Discrete: PMF, Continuous: PDF
 - Can we describe all rvs with a single mathematical concept?
- $$F_X(x) = \mathbb{P}(X \leq x) = \begin{cases} \sum_{k \leq x} p_X(k), & \text{discrete} \\ \int_{-\infty}^x f_X(t) dt, & \text{continuous} \end{cases}$$
- always well defined, because we can always compute the probability for the event $\{X \leq x\}$
 - CCDF (Complementary CDF): $\mathbb{P}(X > x)$



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- Non-decreasing
- $F_X(x)$ tends to 1, as $x \rightarrow \infty$
- $F_X(x)$ tends to 0, as $x \rightarrow -\infty$

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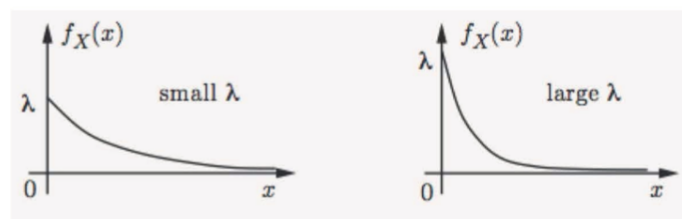
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Exponential RV with parameter $\lambda > 0$: $\exp(\lambda)$

- A rv X is called **exponential with λ** , if

$$f_X(x) = \begin{cases} \lambda e^{-\lambda x}, & x \geq 0 \\ 0, & x < 0 \end{cases} \quad \text{or} \quad F_X(x) = 1 - e^{-\lambda x}$$

- Models a waiting time
- CCDF $\mathbb{P}(X \geq x) = e^{-\lambda x}$ (waiting time decays exponentially)
- $\mathbb{E}[X] = 1/\lambda$, $\mathbb{E}[X^2] = 2/\lambda^2$, $\text{var}[X] = 1/\lambda^2$
- (Q) What is the discrete rv which models a waiting time?



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Jointly Continuous

Two continuous rvs are **jointly continuous** if a non-negative function $f_{X,Y}(x,y)$ (called joint PDF) satisfies: for **every** subset B of the two dimensional plane,

$$\mathbb{P}((X, Y) \in B) = \iint_{(x,y) \in B} f_{X,Y}(x,y) dx dy$$

1. The joint PDF is used to calculate probabilities

$$\mathbb{P}((X, Y) \in B) = \iint_{(x,y) \in B} f_{X,Y}(x,y) dx dy$$

Our particular interest: $B = \{(x, y) \mid a \leq x \leq b, c \leq y \leq d\}$

2. The marginal PDFs of X and Y are from the joint PDF as:

$$f_X(x) = \int_{-\infty}^{\infty} f_{X,Y}(x,y) dy, \quad f_Y(y) = \int_{-\infty}^{\infty} f_{X,Y}(x,y) dx$$

3. The joint CDF is defined by $F_{X,Y}(x,y) = \mathbb{P}(X \leq x, Y \leq y)$, and determines the joint PDF as:

$$f_{X,Y}(x,y) = \frac{\partial^2 F_{X,Y}}{\partial x \partial y}(x,y)$$

4. A function $g(X, Y)$ of X and Y defines a new random variable, and

$$\mathbb{E}[g(X, Y)] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x,y) f_{X,Y}(x,y) dx dy$$

- $p_{X|Y}(x|y) = \frac{p_{X,Y}(x,y)}{p_Y(y)}$

- Similarly, for $f_Y(y) > 0$,

$$f_{X|Y}(x|y) = \frac{f_{X,Y}(x,y)}{f_Y(y)}$$

- Remember: For a fixed event A , $\mathbb{P}(\cdot|A)$ is a legitimate probability law.

- Similarly, For a fixed y , $f_{X|Y}(x|y)$ is a legitimate PDF, since

$$\int_{-\infty}^{\infty} f_{X|Y}(x|y) dx = \frac{\int_{-\infty}^{\infty} f_{X,Y}(x,y) dx}{f_Y(y)} = 1$$

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Sum Rule and Product Rule

- Sum Rule

$$p_X(x) = \begin{cases} \sum_{y \in \mathcal{Y}} p_{X,Y}(x,y) & \text{if discrete} \\ \int_{y \in \mathcal{Y}} f_{X,Y}(x,y) dy & \text{if continuous} \end{cases}$$

- Generally, for $X = (X_1, X_2, \dots, X_D)$,

$$p_{X_i}(x_i) = \int p_X(x_1, \dots, x_i, \dots, x_D) d\mathbf{x}_{-i}$$

- Computationally challenging, because of high-dimensional sums or integrals

- Product Rule

$$p_{X,Y}(x,y) = p_X(x) \cdot p_{Y|X}(y|x)$$

joint dist. = **marginal** of the first \times **conditional** dist. of the second given the first

- Same as $p_Y(y) \cdot p_{X|Y}(x|y)$

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- X : state/cause/original value $\rightarrow Y$: result/resulting action/noisy measurement
- Model: $\mathbb{P}(X)$ (prior) and $\mathbb{P}(Y|X)$ (cause \rightarrow result)
- Inference: $\mathbb{P}(X|Y)$?

$$p_{X,Y}(x,y) = p_X(x)p_{Y|X}(y|x)$$

$$= p_Y(y)p_{X|Y}(x|y)$$

$$p_{X|Y}(x|y) = \frac{p_X(x)p_{Y|X}(y|x)}{p_Y(y)}$$

$$p_Y(y) = \sum_{x'} p_X(x')p_{Y|X}(y|x')$$

$$f_{X,Y}(x,y) = f_X(x)f_{Y|X}(y|x)$$

$$= f_Y(y)f_{X|Y}(x|y)$$

$$f_{X|Y}(x|y) = \frac{f_X(x)f_{Y|X}(y|x)}{f_Y(y)}$$

$$f_Y(y) = \int f_X(x')f_{Y|X}(y|x')dx'$$

$$\underbrace{p_{X|Y}(x|y)}_{\text{posterior}} = \frac{\overbrace{p_{Y|X}(y|x)}^{\text{likelihood}} \overbrace{p_X(x)}^{\text{prior}}}{\underbrace{p_Y(y)}_{\text{evidence}}}$$

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K : discrete, Y : continuous

- Inference of K given Y

$$p_{K|Y}(k|y) = \frac{p_K(k)f_{Y|K}(y|k)}{f_Y(y)}$$

$$f_Y(y) = \sum_{k'} p_K(k')f_{Y|K}(y|k')$$

- Inference of Y given K

$$f_{Y|K}(y|k) = \frac{f_Y(y)p_{K|Y}(k|y)}{p_K(k)}$$

$$p_K(k) = \int f_Y(y')p_{K|Y}(k|y')dy'$$

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Independence

- Occurrence of A provides no new information about B . Thus, knowledge about A does not change my belief about B .

$$\mathbb{P}(B|A) = \mathbb{P}(B)$$

- Using $\mathbb{P}(B|A) = \mathbb{P}(B \cap A)/\mathbb{P}(A)$,

Independence of A and B , $A \perp\!\!\!\perp B$

$$\mathbb{P}(A \cap B) = \mathbb{P}(A) \times \mathbb{P}(B)$$

- Q1.** A and B disjoint $\implies A \perp\!\!\!\perp B$?
No. Actually, really dependent, because if you know that A occurred, then, we know that B did not occur.
- Q2.** If $A \perp\!\!\!\perp B$, then $A \perp\!\!\!\perp B^c$? Yes.

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- Remember: for a probability law $\mathbb{P}(\cdot)$, given, say B , $\mathbb{P}(\cdot|B)$ is a new probability law.
- Thus, we can talk about independence under $\mathbb{P}(\cdot|B)$.
- Given that C occurs, occurrence of A provides no new information about B .

$$\mathbb{P}(B|A \cap C) = \mathbb{P}(B|C)$$

Conditional Independence of A and B given C , $A \perp\!\!\!\perp B|C$

$$\mathbb{P}(A \cap B|C) = \mathbb{P}(A|C) \times \mathbb{P}(B|C)$$

- Q1. If $A \perp\!\!\!\perp B$, then $A \perp\!\!\!\perp B|C$? Suppose that A and B are independent. If you heard that C occurred, A and B are still independent?
- Q2. If $A \perp\!\!\!\perp B|C$, $A \perp\!\!\!\perp B$?

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$A \perp\!\!\!\perp B \rightarrow A \perp\!\!\!\perp B|C?$

- Two independent coin tosses
 - H_1 : 1st toss is a head
 - H_2 : 2nd toss is a head
 - D : two tosses have different results.
- $\mathbb{P}(H_1|D) = 1/2$, $\mathbb{P}(H_2|D) = 1/2$
- $\mathbb{P}(H_1 \cap H_2|D) = 0$,
- No.

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$A \perp\!\!\!\perp B|C \rightarrow A \perp\!\!\!\perp B?$

- Two coins: **Blue** and **Red**. Choose one uniformly at random, and proceed with two independent tosses.
- $\mathbb{P}(\text{head of blue}) = 0.9$ and $\mathbb{P}(\text{head of red}) = 0.1$
 H_i : i -th toss is head, and B : blue is selected.
- $H_1 \perp\!\!\!\perp H_2|B$? Yes

$$\mathbb{P}(H_1 \cap H_2|B) = 0.9 \times 0.9, \quad \mathbb{P}(H_1|B)\mathbb{P}(H_2|B) = 0.9 \times 0.9$$

- $H_1 \perp\!\!\!\perp H_2$? No

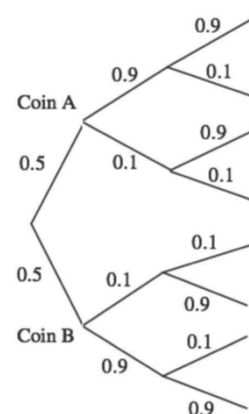
$$\mathbb{P}(H_1) = \mathbb{P}(B)\mathbb{P}(H_1|B) + \mathbb{P}(B^c)\mathbb{P}(H_1|B^c)$$

$$= \frac{1}{2}0.9 + \frac{1}{2}0.1 = \frac{1}{2}$$

$$\mathbb{P}(H_2) = \mathbb{P}(H_2) \quad (\text{because of symmetry})$$

$$\mathbb{P}(H_1 \cap H_2) = \mathbb{P}(B)\mathbb{P}(H_1 \cap H_2|B) + \mathbb{P}(B^c)\mathbb{P}(H_1 \cap H_2|B^c)$$

$$= \frac{1}{2}(0.9 \times 0.9) + \frac{1}{2}(0.1 \times 0.1) \neq \frac{1}{2}$$



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Independence for Random Variables

- Two rvs

$$\mathbb{P}(\{X = x\} \cap \{Y = y\}) = \mathbb{P}(X = x) \cdot \mathbb{P}(Y = y), \quad \text{for all } x, y$$

$$p_{X,Y}(x, y) = p_X(x) \cdot p_Y(y)$$

$$\mathbb{P}(\{X = x\} \cap \{Y = y\} | C) = \mathbb{P}(X = x | C) \cdot \mathbb{P}(Y = y | C), \quad \text{for all } x, y$$

$$p_{X,Y|C}(x, y) = p_{X|C}(x) \cdot p_{Y|C}(y)$$

- Notation: $X \perp\!\!\!\perp Y$ (independence), $X \perp\!\!\!\perp Y|Z$ (conditional independence)

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- Expectation

$$\mathbb{E}[X] = \sum_x x p_X(x), \quad \mathbb{E}[X] = \int_x x f_X(x) dx$$

- Variance, Standard deviation

- Measures how much the spread of PMF/PDF is

$$\text{var}[X] = \mathbb{E}[(X - \mu)^2]$$

$$\sigma_X = \sqrt{\text{var}[X]}$$

Properties

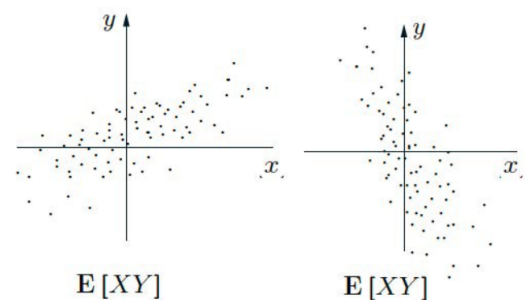
- $\mathbb{E}[aX + bY + c] = a\mathbb{E}[X] + b\mathbb{E}[Y] + c$
- $\text{var}[aX + b] = a^2 \text{var}[X]$
- $\text{var}[X + Y] = \text{var}[X] + \text{var}[Y]$ if $X \perp\!\!\!\perp Y$ (generally not equal)

L6(4)

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Covariance

- Goal: Given two rvs X and Y , quantify the degree of their dependence
 - Dependent: Positive (If $X \uparrow$, $Y \uparrow$) or Negative (If $X \uparrow$, $Y \downarrow$)
 - Simple case: $\mathbb{E}[X] = \mu_X = 0$ and $\mathbb{E}[Y] = \mu_Y = 0$
- What about $\mathbb{E}[XY]$? Seems good.
- $\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y] = 0$ when $X \perp\!\!\!\perp Y$
- More data points (thus increases) when $xy > 0$ (both positive or negative)



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- Solution: Centering. $X \rightarrow X - \mu_X$ and $Y \rightarrow Y - \mu_Y$

Covariance

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

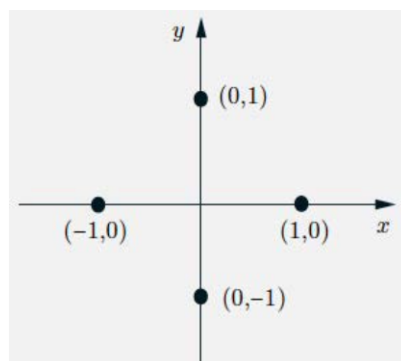
- After some algebra, $\text{cov}(X, Y) = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$
- $X \perp\!\!\!\perp Y \implies \text{cov}(X, Y) = 0$
- $\text{cov}(X, Y) = 0 \implies X \perp\!\!\!\perp Y$? NO.
- When $\text{cov}(X, Y) = 0$, we say that X and Y are uncorrelated.

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Example: $\text{cov}(X, Y) = 0$, but not independent

- $p_{X,Y}(1, 0) = p_{X,Y}(0, 1) = p_{X,Y}(-1, 0) = p_{X,Y}(0, -1) = 1/4$.
- $\mathbb{E}[X] = \mathbb{E}[Y] = 0$, and $\mathbb{E}[XY] = 0$. So, $\text{cov}(X, Y) = 0$
- Are they independent? No, because if $X = 1$, then we should have $Y = 0$.



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$$\text{cov}(X, X) = 0$$

$$\text{cov}(aX + b, Y) = \mathbb{E}[(aX + b)Y] - \mathbb{E}[aX + b]\mathbb{E}[Y] = a \cdot \text{cov}(X, Y)$$

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

$$\text{var}[X + Y] = \mathbb{E}[(X + Y)^2] - (\mathbb{E}[X + Y])^2 = \text{var}[X] + \text{var}[Y] - 2\text{cov}(X, Y)$$

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Correlation Coefficient: Bounded Dimensionless Metric

- Always bounded by some numbers, e.g., $[-1, 1]$
- Dimensionless metric. How? Normalization, but by what?

Correlation Coefficient

$$\rho(X, Y) = \mathbb{E} \left[\frac{(X - \mu_X)}{\sigma_X} \cdot \frac{Y - \mu_Y}{\sigma_Y} \right] = \frac{\text{cov}(X, Y)}{\sqrt{\text{var}[X]\text{var}[Y]}}$$

- $-1 \leq \rho \leq 1$
- $|\rho| = 1 \implies X - \mu_X = c(Y - \mu_Y)$ (linear relation, VERY related)

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Extension to Random Vectors $\mathbf{X} = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix}$

Expectation, Covariance, Variance

- $\mathbb{E}(\mathbf{X}) := \begin{pmatrix} \mathbb{E}(X_1) \\ \vdots \\ \mathbb{E}(X_n) \end{pmatrix}$
- Covariance of $\mathbf{X} \in \mathbb{R}^n$ and $\mathbf{Y} \in \mathbb{R}^m$

$$\text{cov}(\mathbf{X}, \mathbf{Y}) = \mathbb{E}(\mathbf{X}\mathbf{Y}^T) - \mathbb{E}(\mathbf{X})\mathbb{E}(\mathbf{Y})^T \in \mathbb{R}^{n \times m}$$
- Variance of \mathbf{X} : $\text{var}(\mathbf{X}) = \text{cov}(\mathbf{X}, \mathbf{X}) \in \mathbb{R}^{n \times n}$, often denoted by $\Sigma_{\mathbf{X}}$ (or simply Σ):

$$\Sigma_{\mathbf{X}} := \text{var}[\mathbf{X}] = \begin{pmatrix} \text{cov}(X_1, X_1) & \text{cov}(X_1, X_2) & \cdots & \text{cov}(X_1, X_n) \\ \vdots & \vdots & & \vdots \\ \text{cov}(X_n, X_1) & \text{cov}(X_n, X_2) & \cdots & \text{cov}(X_n, X_n) \end{pmatrix}$$
 - We call $\Sigma_{\mathbf{X}}$ **covariance matrix** of \mathbf{X} .

뒤에 나올 data covariance matrix를 여기서 한번 보여준다.

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Properties

For two random vectors $\mathbf{X}, \mathbf{Y} \in \mathbb{R}^n$,

- $\mathbb{E}(\mathbf{X} + \mathbf{Y}) = \mathbb{E}(\mathbf{X}) + \mathbb{E}(\mathbf{Y}) \in \mathbb{R}^n$
- $\text{var}(\mathbf{X} + \mathbf{Y}) = \text{var}(\mathbf{X}) + \text{var}(\mathbf{Y}) \in \mathbb{R}^{n \times n}$
- Assume $\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{b}$.
 - $\mathbb{E}(\mathbf{Y}) = \mathbf{A}\mathbb{E}(\mathbf{X}) + \mathbf{b}$
 - $\text{var}(\mathbf{Y}) = \text{var}(\mathbf{A}\mathbf{X}) = \mathbf{A} \text{var}(\mathbf{X}) \mathbf{A}^T$
 - $\text{cov}(\mathbf{X}, \mathbf{Y}) = \Sigma_{\mathbf{X}} \mathbf{A}^T$ (Please prove)

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- (1) Construction of a Probability Space
- (2) Discrete and Continuous Probabilities
- (3) Sum Rule, Product Rule, and Bayes' Theorem
- (4) Summary Statistics and Independence
- (5) **Gaussian Distribution**
- (6) Conjugacy and the Exponential Family
- (7) Change of Variables/Inverse Transform

L6(5)

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Normal (also called Gaussian) Random Variable

- Why important?
 - Central limit theorem (중심극한정리)
 - One of the most remarkable findings in the probability theory
 - Convenient analytical properties
 - Modeling aggregate noise with many small, independent noise terms

- Standard Normal $\mathcal{N}(0, 1)$

$$f_X(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

- $\mathbb{E}[X] = 0$
- $\text{var}[X] = 1$

- General Normal $\mathcal{N}(\mu, \sigma^2)$

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}$$

- $\mathbb{E}[X] = \mu$
- $\text{var}[X] = \sigma^2$

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- $\mathbf{X} = (X_1, X_2, \dots, X_n)^\top$ with the mean vector $\boldsymbol{\mu} = \begin{pmatrix} \mathbb{E}(X_1) \\ \vdots \\ \mathbb{E}(X_n) \end{pmatrix}$ and the covariance matrix $\boldsymbol{\Sigma}$.

- A Gaussian random vector $\mathbf{X} = (X_1, X_2, \dots, X_n)^\top$ has a joint pdf of the form:

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n |\boldsymbol{\Sigma}|}} \exp \left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right),$$

where $\boldsymbol{\Sigma}$ is symmetric and positive definite.

- We write $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, or $p_{\mathbf{X}}(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$.

- Marginals of Gaussians are Gaussians
- Conditionals of Gaussians are Gaussians
- Products of Gaussian Densities are Gaussians.
- A sum of two Gaussians is Gaussian if they are independent
- Any linear/affine transformation of a Gaussian is Gaussian.

- \mathbf{X} and \mathbf{Y} are Gaussians with mean vectors $\mu_{\mathbf{X}}$ and $\mu_{\mathbf{Y}}$, respectively.
- Gaussian random vector $\mathbf{Z} = \begin{pmatrix} \mathbf{X} \\ \mathbf{Y} \end{pmatrix}$ with $\mu = \begin{pmatrix} \mu_{\mathbf{X}} \\ \mu_{\mathbf{Y}} \end{pmatrix}$ and the covariance matrix

$$\Sigma_{\mathbf{Z}} = \begin{pmatrix} \Sigma_{\mathbf{X}} & \Sigma_{\mathbf{XY}} \\ \Sigma_{\mathbf{YX}} & \Sigma_{\mathbf{Y}} \end{pmatrix}, \text{ where } \Sigma_{\mathbf{XY}} = \text{cov}(\mathbf{X}, \mathbf{Y}).$$

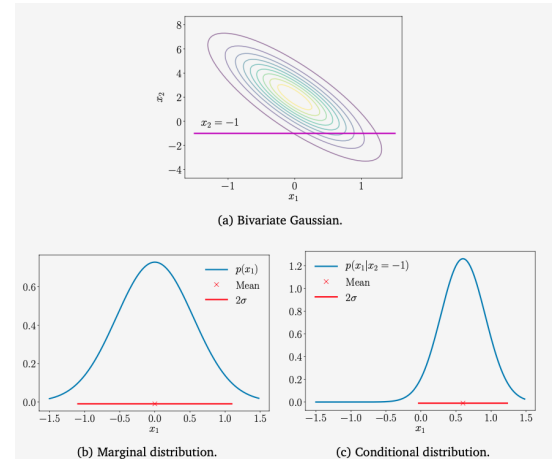
- Marginal.

$$f_{\mathbf{X}}(\mathbf{x}) = \int f_{\mathbf{X},\mathbf{Y}}(\mathbf{x}, \mathbf{y}) d\mathbf{y} \sim \mathcal{N}(\mu_{\mathbf{X}}, \Sigma_{\mathbf{X}})$$

- Conditional. $\mathbf{X} | \mathbf{Y} \sim \mathcal{N}(\mu_{\mathbf{X}|\mathbf{Y}}, \Sigma_{\mathbf{X}|\mathbf{Y}})$,

$$\mu_{\mathbf{X}|\mathbf{Y}} = \mu_{\mathbf{X}} + \Sigma_{\mathbf{XY}} \Sigma_{\mathbf{Y}}^{-1} (\mathbf{Y} - \mu_{\mathbf{Y}})$$

$$\Sigma_{\mathbf{X}|\mathbf{Y}} = \Sigma_{\mathbf{X}} - \Sigma_{\mathbf{XY}} \Sigma_{\mathbf{Y}}^{-1} \Sigma_{\mathbf{YX}}$$



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Product of Two Gaussian Densities

- **Lemma.** Up to recaling, the pdf of the form $\exp(-\frac{1}{2}ax^2 - 2bx + c)$ is $\mathcal{N}(\frac{b}{a}, \frac{1}{a})$.
- Using the above Lemma, the product of two Gaussians $\mathcal{N}(\mu_0, \nu_0)$ and $\mathcal{N}(\mu_1, \nu_1)$ is Gaussian up to rescaling.

Proof.

$$\begin{aligned} & \exp(-(x - \mu_0)^2/2\nu_0) \times \exp(-(x - \mu_1)^2/2\nu_1) \\ &= \exp \left[-\frac{1}{2} \left(\left(\frac{1}{\nu_0} + \frac{1}{\nu_1} \right) x^2 - 2 \left(\frac{\mu_0}{\nu_0} + \frac{\mu_1}{\nu_1} \right) x + c \right) \right] \\ &\Rightarrow \mathcal{N} \left(\overbrace{\frac{1}{\nu_0^{-1} + \nu_1^{-1}}}^{\nu}, \left(\frac{\mu_0}{\nu_0} + \frac{\mu_1}{\nu_1} \right) \right) = \mathcal{N} \left(\frac{\nu_1 \mu_0 + \nu_0 \mu_1}{\nu_0 + \nu_1}, \frac{\nu_0 \nu_1}{\nu_0 + \nu_1} \right) \end{aligned}$$

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- Similar results for the matrix version.
- The product of the densities of two Gaussian vectors $\mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ and $\mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$ is Gaussian up to rescaling.
- The resulting Gaussian is given by:

$$\mathcal{N}\left(\boldsymbol{\Sigma}_1(\boldsymbol{\Sigma}_0 + \boldsymbol{\Sigma}_1)^{-1}\boldsymbol{\mu}_0 + \boldsymbol{\Sigma}_0(\boldsymbol{\Sigma}_0 + \boldsymbol{\Sigma}_1)^{-1}\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1(\boldsymbol{\Sigma}_0 + \boldsymbol{\Sigma}_1)^{-1}\boldsymbol{\Sigma}_0\right)$$

Compare the above to this:

$$\mathcal{N}\left(\frac{\nu_1\mu_0 + \nu_0\mu_1}{\nu_0 + \nu_1}, \frac{\nu_0\nu_1}{\nu_0 + \nu_1}\right)$$

Bishop책에서 공식을 찾아서, 여기에 한 페이지로 정리해 놓는다

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- $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}_X, \boldsymbol{\Sigma}_X)$ and $\mathbf{Y} \sim \mathcal{N}(\boldsymbol{\mu}_Y, \boldsymbol{\Sigma}_Y)$

$$\Rightarrow a\mathbf{X} + b\mathbf{Y} \sim \mathcal{N}(a\boldsymbol{\mu}_X + b\boldsymbol{\mu}_Y, a^2\boldsymbol{\Sigma}_X + b^2\boldsymbol{\Sigma}_Y)$$

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Mixture of Two Gaussian Densities

- $f_1(x)$ is the density of $\mathcal{N}(\mu_1, \sigma_1^2)$ and $f_2(x)$ is the density of $\mathcal{N}(\mu_2, \sigma_2^2)$
- **Question.** What are the mean and the variance of the random variable Z which has the following density $f(x)$?

$$f(x) = \alpha f_1(x) + (1 - \alpha) f_2(x)$$

Answer:

$$\mathbb{E}(Z) = \alpha\mu_1 + (1 - \alpha)\mu_2$$

$$\text{var}(Z) = \left(\alpha\sigma_1^2 + (1 - \alpha)\sigma_2^2 \right) + \left([\alpha\mu_1^2 + (1 - \alpha)\mu_2^2] - [\alpha\mu_1 + (1 - \alpha)\mu_2]^2 \right)$$

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- Linear transformation² preserves normality

Linear transformation of Normal

If $X \sim \mathcal{N}(\mu, \sigma^2)$, then for $a \neq 0$ and b , $Y = aX + b \sim \mathcal{N}(a\mu + b, a^2\sigma^2)$.

- Thus, every normal rv can be **standardized**:

If $X \sim \mathcal{N}(\mu, \sigma^2)$, then $Y = \frac{X - \mu}{\sigma} \sim \mathcal{N}(0, 1)$

- Thus, we can make the **table** which records the following CDF values:

$$\Phi(y) = \mathbb{P}(Y \leq y) = \mathbb{P}(Y < y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^y e^{-t^2/2} dt$$

²Strictly speaking, this is affine transformation.

Linear Transformation for Random Vectors

- $\mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- $\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{b}$, where $\mathbf{X} \in \mathbb{R}^n$, $\mathbf{Y}, \mathbf{b} \in \mathbb{R}^m$, and $\mathbf{A} = \mathbb{R}^{m \times n}$

$$\Rightarrow \mathbf{Y} \sim \mathcal{N}(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$$

- (1) Construction of a Probability Space
- (2) Discrete and Continuous Probabilities
- (3) Sum Rule, Product Rule, and Bayes' Theorem
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- (6) Conjugacy and the Exponential Family
- (7) Change of Variables/Inverse Transform

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Conjugate Prior: Motivation

- Bayesian Inference

$$\underbrace{p(\theta | D)}_{\text{posterior}} = \frac{\overbrace{p(D | \theta)}^{\text{likelihood}} \overbrace{p(\theta)}^{\text{prior}}}{\underbrace{p(D)}_{\text{evidence}}}$$

- The forms of likelihood and prior come from a model.
- **Question.** Given a form of likelihood, how can I choose a prior such that the resulting posterior has the same form as the prior?
 - Such prior is called **conjugate prior** (to the given likelihood)
 - **Pros:** Algebraic calculation of posterior and even analytical description is often possible.
 - **Cons:** A restricted form of prior, which may lead to distorted understanding about data interpretation.

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- **Definition.** A prior is **conjugate** for the likelihood function if the posterior is of the same form/type as the prior.
- Representative conjugate priors

Likelihood	Prior	Posterior
Poisson	Gamma	Gamma
Bernoulli	Beta	Beta
Binomial	Beta	Beta
Normal	Normal/inverse Gamma	Normal/inverse Gamma
Normal	Normal/inverse Wishart	Normal/inverse Wishart
Exponential	Gamma	Gamma
Multinomial	Dirichlet	Dirichlet

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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

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

- Beta distribution models a continuous random variable over a finite interval $[0, 1]$.
- A special case of $Beta(1, 1)$ is $Uniform[0, 1]$

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- Assume that the parameter $\Theta \sim \text{Beta}(\alpha, \beta)$ (prior): $p(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$
- $\theta \sim \Theta$ and $X \sim \text{Bin}(N, \theta)$. Thus, $p(x | \theta) = \binom{N}{x} \theta^x (1-\theta)^{N-x}$ (likelihood)
- **Posterior** \propto (likelihood) \times (prior)

$$\begin{aligned} p(\theta | x = h) &\propto \binom{N}{h} \theta^h (1-\theta)^{N-h} \times \theta^{\alpha-1} (1-\theta)^{\beta-1} \\ &= \theta^{h+\alpha-1} (1-\theta)^{(N-h)+\beta-1} \\ &\sim \text{Beta}(h + \alpha, N - h + \beta) \end{aligned}$$

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Sufficient Statistics

- A **statistic** of a random variable \mathbf{X} is a deterministic function of \mathbf{X} .
- **Example.** For $\mathbf{X} = (X_1 \ X_2 \ \dots \ X_n)^\top$, the sample mean $T(\mathbf{X}) = \frac{1}{N}(X_1 + \dots + X_n)$ is a statistic.
- **Question.** Does a statistic contain all the information for the inference from data? (e.g., the parameter estimation of a distribution based on data)
- **Sufficient statistics:** carry all the information for the inference
- **Definition.** A statistic $T = T(\mathbf{X})$ is said to be **sufficient** for \mathbf{X} with its pdf or pmf $p_{\mathbf{X}}(\mathbf{x}; \theta)$,³ if the conditional distribution of \mathbf{X} given $T(\mathbf{X}) = t$ is **independent** of θ for all t .

³The parameter can be a vector, but we do not use θ for simplicity.

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- X_1, X_2 : independent Poisson variables with common parameter λ which is the expectation.

- **Claim.** $T(\mathbf{X}) = X_1 + X_2$ is a sufficient statistic for inference of λ .

- Joint distribution

$$\mathbb{P}(x_1, x_2) = \frac{\lambda^{x_1+x_2}}{x_1!x_2!} e^{-2\lambda}$$

- Conditional dist. of X_1 given $X_1 + X_2 = t$

$$\mathbb{P}(x_1 | X_1 + X_2 = t) = \frac{1}{x_1!(t-x_1)!} \left(\frac{1}{\sum_{y=0}^t \frac{1}{y!(t-y)!}} \right)^{-1}$$

- Independent of $\lambda \implies T$ is a sufficient statistic.

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Factorization Theorem

A necessary and sufficient condition for a statistic T to be sufficient for X with its pdf or pmf $p_{\mathbf{X}}(\mathbf{x}; \theta)$ is that there exist non-negative functions g_{θ} and h such that

$$p_{\mathbf{X}}(\mathbf{x}; \theta) = g_{\theta}(T(\mathbf{x}))h(\mathbf{x}).$$

- **Example.** Continuing the Poisson example, suppose that X_1, \dots, X_n are iid according to a Poisson distribution with parameter λ . Then, with $\mathbf{X} = (X_1, \dots, X_n)$,

$$\mathbb{P}_{\mathbf{X}}(x_1, \dots, x_n) = \lambda^{\sum x_i} e^{-n\lambda} / \prod (x_i!)$$

- $T(\mathbf{X}) = \sum X_i$ is a sufficient statistic.

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- Three levels of abstraction when we use a distribution to model a random phenomenon
- L1.** Fix a particular named distribution with fixed parameters
 - **Example.** Use a Gaussian with zero mean and unit variance, $\mathcal{N}(0, 1)$
- L2.** Use a parametric distribution and infer the parameters from data
 - **Example.** Use a Gaussian with unknown mean and variance, $\mathcal{N}(\mu, \sigma^2)$, and infer (μ, σ^2) from data
- L3.** Consider a family of distributions which satisfy “nice” properties
 - **Example.** Exponential family

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Exponential Family: Definition

Exponential Family

An exponential family is a family of probability distributions, parameterized by $\theta \in \mathbb{R}^D$, of the form

$$p_{\mathbf{X}}(\mathbf{x}; \theta) = h(\mathbf{x}) \exp \left(\langle \theta, T(\mathbf{x}) \rangle - A(\theta) \right),$$

where $\mathbf{X} \in \mathbb{R}^n$ and $T(\mathbf{x}) : \mathbb{R}^n \mapsto \mathbb{R}^D$ is a vector of sufficient statistics.

- Nothing but a particular form of $g_{\theta}(\cdot)$ in the F-N factorization theorem
- $\langle \theta, T(\mathbf{x}) \rangle$ is an inner product, e.g., the standard dot product.
- Essentially, it is of the form: $p_{\mathbf{X}}(\mathbf{x}; \theta) \propto \exp(\theta^T T(\theta))$
- $A(\theta)$: normalization constant, called **log-partition function**.
- Why Useful?
 - Parametric form of conjugate priors (see pp. 190 in the text), offering sufficient statistics, etc.

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- Gaussian as exponential family, a random variable $X \sim \mathcal{N}(\mu, \sigma^2)$.
 - Let $T(\mathbf{x}) = \begin{pmatrix} x \\ x^2 \end{pmatrix}$ and $\boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = \begin{pmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{pmatrix}$

$$p(\mathbf{x} \mid \boldsymbol{\theta}) \propto \exp(\boldsymbol{\theta}^T T(\mathbf{x})) = \exp\left(\frac{\mu x}{\sigma^2} - \frac{x^2}{2\sigma^2}\right) = \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right)$$

- (1) Construction of a Probability Space
- (2) Discrete and Continuous Probabilities
- (3) Sum Rule, Product Rule, and Bayes' Theorem
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- (5) Gaussian Distribution
- (6) Conjugacy and the Exponential Family
- (7) Change of Variables/Inverse Transform

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Questions?

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