



#### Lecture 6: Probability and Distributions

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Mathematics for Machine Learning KAIST EE

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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

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#### Roadmap

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#### What Do We Want?



- (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
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Modeling: Approximate reality with a simple (mathematical) model

Experiment

- Flip two coins
- Observation: a random outcome
- o for example, (H, H)

All outcomes

- $\circ \{(H,H),(H,T),(T,H),(T,T)\}$
- 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?

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  $\Omega$
- 2. Assigned numbers to each outcome of  $\Omega$ : Probability Law  $\mathbb{P}(\cdot)$

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

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.

$$\Longrightarrow \Omega = \{(H, R), (T, R), (H, NR), (T, NR)t\},\$$

where R(Rain), NR(No Rain).

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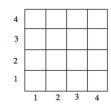
### Examples: Sample Space $\Omega$

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### Probability Law

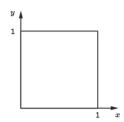


- *Discrete case:* Two rolls of a tetrahedral die
- $\Omega = \{(1,1), (1,2), \dots, (4,4)\}$



• Continuous case: Dropping a needle in a plain

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



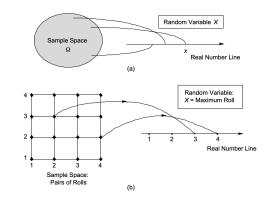
- Assign numbers to what? Each outcome?
- What is the probability of dropping a needle at (0.5, 0.5) over the  $1 \times 1$  plane?
- Assign numbers to each subset of  $\Omega$ : A subset of  $\Omega$ : an event
- $\mathbb{P}(A)$ : Probability of an event A.
  - This is where probability meets set theory.
  - Roll a dice. What is the probability of odd numbers?

 $\mathbb{P}(\{1,3,5\})$ , where  $\{1,3,5\}\subset\Omega$  is an event.

- Event space A: The collection of subsets of  $\Omega$ . For example, in the discrete case, the power set of  $\Omega$ .
- Probability Space  $(\Omega, \mathcal{A}, \mathbb{P}(\cdot))$



- 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.



- Mathematically, a random variable X is a function which maps from  $\Omega$  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.,  $\{\omega \in \Omega \mid X(w) = x\}$
- Generally,

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

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### Conditioning: Motivating Example



Conditional Probability



- Pick a person a at random
  - event A: a's age  $\leq 20$
- 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.

- $\mathbb{P}(A \mid B)$ :  $\mathbb{P}(\cdot \mid B)$  should be a new probability law.
- Definition.

$$\mathbb{P}(A \mid B) := \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}, \quad \textit{for} \quad \mathbb{P}(B) > 0.$$

- Note that this is a definition, not a theorem.
- All other properties of the law  $\mathbb{P}(\cdot)$  is applied to the conditional law  $\mathbb{P}(\cdot|B)$ .
- 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,  $p_X(x) := \mathbb{P}(X = x) := \mathbb{P}\Big(\{\omega \in \Omega \mid X(w) = x\}\Big)$ , which we call probability mass function (PMF).
- Examples: Bernoulli, Uniform, Binomial, Poisson, Geometric

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### Bernoulli X with parameter $p \in [0, 1]$



Uniform X with parameter a, b



Only binary values

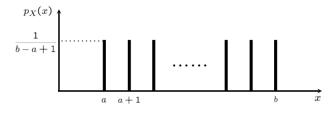
$$X = \begin{cases} 0, & \text{w.p.}^1 \quad 1 - p, \\ 1, & \text{w.p.} \quad p \end{cases}$$

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:

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

- 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)

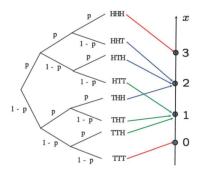
<sup>•</sup> integers a, b, where  $a \le b$ 

 $<sup>^{1}</sup>$ with probability



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

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



- 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:

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

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### Geometric X with parameter p

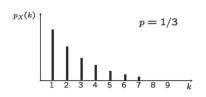
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#### Joint PMF



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

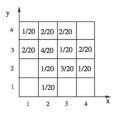
$$p_{X,Y}(x,y) := \mathbb{P}(\lbrace X=x \rbrace \cap \lbrace Y=y \rbrace)$$

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

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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

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

Conditional PMF

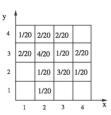
$$p_{X|Y}(x|y) := \mathbb{P}(X = x|Y = y) = \frac{p_{X,Y}(x,y)}{p_{Y}(y)}$$

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

- $\sum_{x} p_{X|Y}(x|y) = 1$
- Multiplication rule.

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

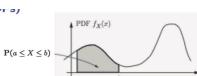
•  $p_{X,Y,Z}(x,y,z) =$  $p_X(x)p_{Y|X}(y|x)p_{Z|X,Y}(z|x,y)$ 



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

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

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



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

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•  $\mathbb{P}(a \le X \le b) = \sum_{x:a \le x \le b} p_X(x)$ •  $p_X(x) \ge 0$ ,  $\sum_x p_X(x) = 1$ 

continuous counterparts

 $p_X(x)$ 

Continuous Random Variable

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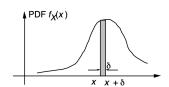
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# PDF and Examples

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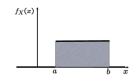
### Cumulative Distribution Function (CDF)

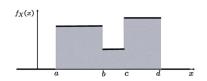
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- $\mathbb{P}(a \leq X \leq a + \delta) \approx |f_X(a) \cdot \delta|$
- $\mathbb{P}(X = a) = 0$

#### Examples

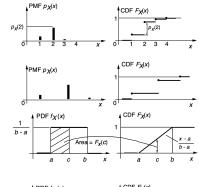


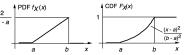


- Discrete: PMF, Continuous: PDF
- Can we describe all rvs with a single mathematical concept?

$$F_X(x) = \mathbb{P}(X \le x) =$$
 
$$\begin{cases} \sum_{k \le x} p_X(k), & \text{discrete} \\ \int_{-\infty}^x f_X(t) dt, & \text{continuous} \end{cases}$$

- always well defined, because we can always compute the probability for the event  $\{X < x\}$
- CCDF (Complementary CDF):  $\mathbb{P}(X > x)$





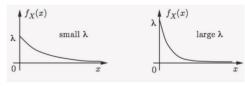


- Non-decreasing
- $F_X(x)$  tends to 1, as  $x \to \infty$
- $F_X(x)$  tends to 0, as  $x \to -\infty$

• A rv X is called exponential with  $\lambda$ , if

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

- Models a waiting time
- CCDF  $\mathbb{P}(X \ge x) = e^{-\lambda x}$  (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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### Continuous: Joint PDF and CDF (1)

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Continuous: Joint PDF and CDF (2)



### 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,

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

1. The joint PDF is used to calculate probabilities

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

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

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  $F_{X,Y}(x,y) = \mathbb{P}(X \le x, Y \le y)$ , 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

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



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

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

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• 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  $X = (X_1, X_2, \dots, X_D)$ ,

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

- 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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#### Bayes Rule

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Bayes Rule for Mixed Case



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

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

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

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

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

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

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

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

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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Occurrence of A provides no new information about B. Thus, knowledge about A
does no 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 ⇒ A ⊥ 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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 $A \perp \!\!\!\perp B \rightarrow A \perp \!\!\!\perp B | C?$ 



## Conditional Independence

- 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  $\mathbb{P}(\cdot|B)$ .
- ullet 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,  $A \perp \!\!\!\perp B \mid C$ 

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

- 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  $A \perp \!\!\!\perp B \mid C$ ,  $A \perp \!\!\!\perp B$ ?

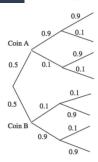
- Two independent coin tosses
  - $\circ$   $H_1$ : 1st toss is a head
  - $H_2$ : 2nd toss is a head
  - D: two tosses have different results.
- $\mathbb{P}(H_1|D) = 1/2, \, \mathbb{P}(H_2|D) = 1/2$
- $\mathbb{P}(H_1 \cap H_2|D) = 0$ ,
- No.



- 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*<sub>1</sub> ⊥⊥ *H*<sub>2</sub>|*B*? Yes

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

$$\begin{split} \bullet \ \, H_1 \perp \!\!\! \perp H_2? \ \, \text{No} \\ \mathbb{P}(H_1) &= \mathbb{P}(B)\mathbb{P}(H_1|B) + \mathbb{P}(B^c)\mathbb{P}(H_1|B^c) \\ &= \frac{1}{2}0.9 + \frac{1}{2}0.1 = \frac{1}{2} \\ \mathbb{P}(H_2) &= \mathbb{P}(H_2) \quad \text{(because of symmetry)} \\ \mathbb{P}(H_1 \cap H_2) &= \mathbb{P}(B)\mathbb{P}(H_1 \cap H_2|B) + \mathbb{P}(B^c)\mathbb{P}(H_1 \cap H_2|B^c) \\ &= \frac{1}{2}(0.9 \times 0.9) + \frac{1}{2}(0.1 \times 0.1) \neq \frac{1}{2} \end{split}$$



Two rvs

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

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

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

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### Expectation/Variance

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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  $\ensuremath{\mathsf{PMF/PDF}}$  is

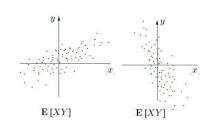
$$var[X] = \mathbb{E}[(X - \mu)^2]$$

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

#### Properties

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

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





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

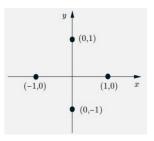
#### Covariance

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

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

•  $p_{XY}(1,0) = p_{XY}(0,1) = p_{XY}(-1,0) = p_{XY}(0,-1) = 1/4$ .

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



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#### **Properties**



#### Correlation Coefficient: Bounded Dimensionless Metric



cov(X,X)=0

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

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

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

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

#### Correlation Coefficient

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

- $-1 \le \rho \le 1$
- $|
  ho|=1\Longrightarrow X-\mu_X=c(Y-\mu_Y)$  (linear relation, VERY related)

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

• 
$$\mathbb{E}(oldsymbol{X}) := egin{pmatrix} \mathbb{E}(X_1) \\ \vdots \\ \mathbb{E}(X_n) \end{pmatrix}$$

• Covariance of  $\boldsymbol{X} \in \mathbb{R}^n$  and  $\boldsymbol{Y} \in \mathbb{R}^m$ 

$$\operatorname{\mathsf{cov}}(oldsymbol{X},oldsymbol{Y}) = \mathbb{E}(oldsymbol{X}oldsymbol{Y}^\mathsf{T}) - \mathbb{E}(oldsymbol{X})\mathbb{E}(oldsymbol{Y})^\mathsf{T} \in \mathbb{R}^{n imes m}$$

• Variance of X:  $var(X) = cov(X, X) \in \mathbb{R}^{n \times n}$ , often denoted by  $\Sigma_X$  (or simply  $\Sigma$ ):

$$oldsymbol{\Sigma}_{oldsymbol{X}} := \mathsf{var}[oldsymbol{X}] = egin{pmatrix} \mathsf{cov}(X_1, X_1) & \mathsf{cov}(X_1, X_2) & \cdots \mathsf{cov}(X_1, X_n) \\ dots & dots & dots \\ \mathsf{cov}(X_n, X_1) & \mathsf{cov}(X_n, X_2) & \cdots \mathsf{cov}(X_n, X_n) \end{pmatrix}$$

 $\circ$  We call  $\Sigma_{\pmb{X}}$  covariance matrix of  $\pmb{X}$ .

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Data Covariance Matrix



**Properties** 



뒤에 나올 data covariance matrix를 여기서 한번 보여준다.

•

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

• 
$$\mathbb{E}(\boldsymbol{X} + \boldsymbol{Y}) = \mathbb{E}(\boldsymbol{X}) + \mathbb{E}(\boldsymbol{Y}) \in \mathbb{R}^n$$

• 
$$\operatorname{var}(\boldsymbol{X} + \boldsymbol{Y}) = \operatorname{var}(\boldsymbol{X}) + \operatorname{var}(\boldsymbol{Y}) \in \mathbb{R}^{n \times n}$$

• Assume 
$$\mathbf{Y} = \mathbf{A}\mathbf{X} + \mathbf{b}$$
.

$$\circ \ \mathbb{E}(\mathbf{Y}) = \mathbf{A}\mathbb{E}(\mathbf{X}) + \mathbf{b}$$

$$\circ$$
 var $(\mathbf{Y}) = \text{var}(\mathbf{AX}) = \mathbf{A} \text{var}(\mathbf{X})\mathbf{A}^{\mathsf{T}}$ 

$$\circ \operatorname{\mathsf{cov}}(oldsymbol{X},oldsymbol{Y}) = \Sigma_{oldsymbol{X}} oldsymbol{A}^\mathsf{T}$$
 (Please prove)



- (1) Construction of a Probability Space
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- (7) Change of Variables/Inverse Transform

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

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

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

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

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

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

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### Gaussian Random Vector



Power of Gaussian Random Vectors



- $m{X} = (X_1, X_2, \cdots, X_n)^\mathsf{T}$  with the mean vector  $m{\mu} = \begin{pmatrix} \mathbb{E}(X_1) \\ \vdots \\ \mathbb{E}(X_n) \end{pmatrix}$  and the covariance matrix  $m{\Sigma}$ .
- A Gaussian random vector  $\boldsymbol{X} = (X_1, X_2, \cdots, X_n)^T$  has a joint pdf of the form:

$$f_{m{X}}(m{x}) = rac{1}{\sqrt{(2\pi)^n |m{\Sigma}|}} \exp\left(-rac{1}{2}(m{x}-m{\mu})^\mathsf{T}m{\Sigma}^{-1}(m{x}-m{\mu})
ight),$$

where  $\Sigma$  is symmetric and positive definite.

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

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



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

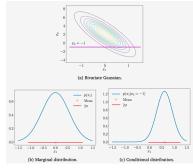
$$oldsymbol{\Sigma}_{oldsymbol{Z}} = egin{pmatrix} oldsymbol{\Sigma}_{oldsymbol{X}} & oldsymbol{\Sigma}_{oldsymbol{X}oldsymbol{Y}} \\ oldsymbol{\Sigma}_{oldsymbol{Y}oldsymbol{X}} & oldsymbol{\Sigma}_{oldsymbol{Y}} \end{pmatrix}, ext{ where } oldsymbol{\Sigma}_{oldsymbol{X}oldsymbol{Y}} = ext{cov}(oldsymbol{X}, oldsymbol{Y}).$$

- Marginal

$$f_{m{X}}(m{x}) = \int f_{m{X},m{Y}}(m{x},m{y}) dm{y} \sim \mathcal{N}(m{\mu}_{m{x}},m{\Sigma}_{m{X}})$$

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

$$\mu_{X|Y} = \mu_X + \Sigma_{XY}\Sigma_Y^{-1}(Y - \mu_Y)$$
  
 $\Sigma_{X|Y} = \Sigma_X - \Sigma_{XY}\Sigma_Y^{-1}\Sigma_{YX}$ 



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

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

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### Product of Two Gaussian Densities for Random Vectors



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Formula: Conditional and Marginal Gaussians



- Similar results for the matrix version.
- The product of the densities of two Gaussian vectors  $\mathcal{N}(\mu_0, \Sigma_0)$  and  $\mathcal{N}(\mu_1, \Sigma_1)$  is Gaussian up to rescaling.
- The resulting Gaussian is given by:

$$\mathcal{N}\Bigg(\Sigma_1(\Sigma_0+\Sigma_1)^{-1}\mu_0+\Sigma_0(\Sigma_0+\Sigma_1)^{-1}\mu_1,\Sigma_1(\Sigma_0+\Sigma_1)^{-1}\Sigma_0\Bigg)$$

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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- ullet  $oldsymbol{X} \sim \mathcal{N}(oldsymbol{\mu_X}, oldsymbol{\Sigma_X})$  and  $oldsymbol{Y} \sim \mathcal{N}(oldsymbol{\mu_Y}, oldsymbol{\Sigma_Y})$
- $\implies a\mathbf{X} + b\mathbf{Y} \sim \mathcal{N}(a\mu_{\mathbf{X}} + b\mu_{\mathbf{Y}}, a^2\Sigma_{\mathbf{X}} + b^2\Sigma_{\mathbf{Y}})$

- $f_1(x)$  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:

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

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

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#### Linear Transformation



Linear Transformation for Random Vectors



• Linear transformation<sup>2</sup> 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:

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

• 
$$m{X} \sim \mathcal{N}(m{\mu}, m{\Sigma})$$

• 
$$\mathbf{Y} = \mathbf{AX} + \mathbf{b}$$
, where  $\mathbf{X} \in \mathbb{R}^n$ ,  $\mathbf{Y}, \mathbf{b} \in \mathbb{R}^m$ , and  $\mathbf{A} = \mathbb{R}^{m \times n}$ 

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

<sup>&</sup>lt;sup>2</sup>Strictly speaking, this is affine transformation.





- (1) Construction of a Probability Space
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• Bayesian Inference

$$\underbrace{p(\theta \mid D)}_{\text{posterior}} = \underbrace{\frac{p(D \mid \theta)}{p(D)}}_{\substack{p(D) \\ \text{ovidence}}}$$

- 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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#### Conjugate Priors: Definition and Examples



Beta Distribution



- 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	Dirchlet

#### Beta distribution

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

$$f_{\Theta}(\theta) = egin{cases} rac{1}{B(lpha,eta)} heta^{lpha-1} (1- heta)^{eta-1}, & 0 < heta < 1, \ 0, & ext{otherwise,} \end{cases}$$

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,  $p(x \mid \theta) = \binom{N}{x} \theta^x (1 \theta)^{N-x}$  (likelihood)
- Posterior ∝ (likelihood) × (prior)

$$\rho(\theta \mid x = h) \propto \binom{N}{h} \theta^{h} (1 - \theta)^{N - h} \times \theta^{\alpha - 1} (1 - \theta)^{\beta - 1} \\
= \theta^{h + \alpha - 1} (1 - \theta)^{(N - h) + \beta - 1} \\
\sim \text{Beta}(h + \alpha, N - h + \beta)$$

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- A statistic of a random variable **X** is a deterministic function of **X**.
- Example. For  $\mathbf{X} = \begin{pmatrix} X_1 & X_2 & \dots & X_n \end{pmatrix}^\mathsf{T}$ , 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  $p_{\mathbf{X}}(\mathbf{x};\theta)$ , if the conditional distribution of  $\mathbf{X}$  given  $T(\mathbf{X}) = t$  is independent of  $\theta$  for all t.

#### Poisson Example



Fisher-Neyman Factorization Theorem



- $X_1, X_2$ : independent Poisson variables with common parameter  $\lambda$  which is the expectation.
- Claim.  $T(X) = X_1 + X_2$  is a sufficient statistic for inference of  $\lambda$ .
- Joint distribution

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

ullet 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.

#### Factorization Theorem

A necessary and sufficient condition for a statistic T to be sufficient for X with its pdf or pmf  $p_X(x;\theta)$  is that there exist non-negative functions  $g_\theta$  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  $X_1, \ldots, X_n$  are iid according to a Poisson distribution with parameter  $\lambda$ . Then, with  $\mathbf{X} = (X_1, \ldots, X_n)$ ,

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

•  $T(X) = \sum X_i$  is a sufficient statistic.

<sup>&</sup>lt;sup>3</sup>The parameter can be a vector, but we do not use  $\theta$  for simplicity.

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### Exponential Family: Definition



- Three levels of abstraction when we use a distribution to model a random phenomenon
- L1. Fix a particular named distribution with fixed parameters
  - $\circ$  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  $(\mu, \sigma^2)$  from data
- L3. Consider a family of distributions which satisfy "nice" properties
  - Example. Exponential family

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#### **Exponential Family**

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

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

where  $\mathbf{X} \in \mathbb{R}^n$  and  $T(\mathbf{x}) : \mathbb{R}^n \mapsto \mathbb{R}^D$  isavectorofsufficientstatistics.

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

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 Parametric form of conjugate priors (see pp. 190 in the text), offering sufficient statistics, etc.

Example



Roadmap



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• Gaussian as exponential family, a random variable  $X \sim \mathcal{N}(\mu, \sigma^2)$ .

• Let 
$$T(\mathbf{x}) = \begin{pmatrix} \mathbf{x} \\ \mathbf{x}^2 \end{pmatrix}$$
 and  $\boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = \begin{pmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{pmatrix}$ 

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

- (1) Construction of a Probability Space
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Figuring Out Distributions: Change of Variables

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Questions?



1)

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