# Lecture 4 Multivariate Distributions

## **Chao Song**

College of Ecology Lanzhou University

September 29, 2025

## **Multivariate distribution**

In many practical cases, it is possible, and often desirable, to take more than one measurement of a random observation. Moreover, we sometimes want to use these measurements to predict a third one. For example, we measure the GPA and extracurriculum activities of a student, and we give each of them a comprehensive evaluation score.

**Definition**: Let X and Y be two discrete random variables. Let S denote the two-dimensional space of X and Y. The probability that X = x and Y = y is denoted by f(x, y) = P(X = x, Y = y). The function f(x, y) is called the joint probability mass function.

# Joint probability mass function

**Example:** Roll a pair of fair dice. For each of the 36 sampling points with probability 1/36, let X denote the smaller and Y the larger outcome on the dice. For example, if the outcome is (3,2), then the observed values are X=2, Y=3. What is the joint PMF of X and Y?

The event X=2, Y=3 can happen in one of two ways (2,3) or (3,2). So its probability is 2/36. However, for event such as X=2, Y=2, it can only happen in one way. Thus, in general, the joint probability mass function is

$$f(x,y) = \begin{cases} \frac{1}{36} & x = y \\ \frac{1}{18} & x \neq y \end{cases}$$

#### **Multinomial distribution**

Suppose we have three mutually exclusive and exhaustive ways for an experiment to end: perfect, seconds, and defective. We repeat the experiment n independent times and the probability  $p_X$ ,  $p_Y$ ,  $1-p_X-p_Y$  of the three type of results. Let X and Y be the number of perfect and seconds. What is the joint probability mass function of X and Y?

The probability of having x perfects, y seconds, and n - x - y defective is

$$p_X^x p_Y^y (1 - p_X - p_Y)^{n-x-y}$$

And it can be achieved in

$$\mathbf{C}_{n}^{x}\mathbf{C}_{n-x}^{y} = \frac{n!}{x!(n-x)!} \frac{(n-x)!}{y!(n-x-y)!} = \frac{n!}{x!y!(n-x-y)!}$$

Thus, the joint PMF is

$$f(x,y) = \frac{n!}{x!y!(n-x-y)!} p_X^x p_Y^y (1 - p_X - p_Y)^{n-x-y}$$

# Marginal probability mass function

Let X and Y have the joint probability mass function f(x, y) with space S. The probability mass function of X alone is called the marginal probability mass function of X and is defined by

$$f_X(x) = \sum_y f(x, y) \ x \in S_X$$

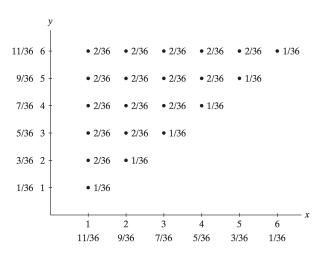
The random variables X and Y are independent if and only if, for every  $x \in S_X$  and  $y \in S_Y$ ,

$$f(x,y)=f_X(x)f_Y(y)$$

Otherwise, *X* ad *Y* are said to be dependent.

## Marginal probability mass function

**Example**: In the dice rolling example mentioned above, what is the marginal probability mass function of *X* and *Y*? Are *X* and *Y* independent?



# Marginal probability mass function

If X and Y has a multinomial distribution, are they independent?

It is easy to see by logic that X and Y both have a binomial distribution.

$$f_X(x) = \mathbf{C}_n^x p_X^x (1 - p_X)^{n-x}$$

$$f_Y(y) = \mathbf{C}_n^y p_Y^y (1 - p_Y)^{n-y}$$

Therefore,

$$f_X(x)f_Y(y) = \mathbf{C}_n^x \mathbf{C}_n^y p_X^x (1 - p_X)^{n-x} p_Y^y (1 - p_Y)^{n-y} \neq f(xy)$$

Thus, X and Y are not indepenent.

## **Mathematical expectation**

Let  $X_1$  and  $X_2$  be random variables of the discrete type with the joint PMF  $f(x_1, x_2)$  on the space S. If  $u(X_1, X_2)$  is a function of these two random variables, then

$$E[u(X_1, X_2)] = \sum_{(x_1, x_2) \in S} u(x_1, x_2) f(x_1, x_2)$$

if it exists, is called the mathematical expectation of  $u(X_1, X_2)$ .

If 
$$u(X_1, X_2) = X_i$$
, then  $E[u(X_1, X_2)] = E(X_i) = \mu_i$ ; if  $u(X_1, X_2) = (X_i - \mu_i)^2$ , then  $E[u(X_1, X_2)] = E[(X_i - \mu_i)^2] = Var(X_i)$ 

## **Mathematical expectation**

**Example**: There are eight chips in a bow: three marked (0,0), two marked (1,0), two marked (0,1), and one marked (1,1). A player selects a chip at random and is given the sum of the two coordinates in dollars as a prize. What is the expected prize money a play can get?

Let  $X_1$  and  $X_2$  denote the two coordinates. Their joint PMF is

$$f(x,y) = \frac{3 - x_1 - x_2}{8}, x_1 = 0, 1 \text{ and } x_2 = 0, 1$$

Thus,

$$E(X_1 + X_2) = \sum_{x_2=0}^{1} \sum_{x_1=0}^{1} (x_1 + x_2) \frac{3 - x_1 - x_2}{8}$$
$$= (0)(\frac{3}{8}) + (1)(\frac{2}{8}) + (1)(\frac{2}{8}) + (2)(\frac{1}{8}) = \frac{3}{4}$$

Let  $u(X, Y) = (X - \mu_X)(Y - \mu_Y)$ , then

$$E[u(X,Y)] = E[(X - \mu_X)(Y - \mu_Y)] = Cov(X,Y) = \sigma_{XY}$$

is called the covariance of *X* and *Y*.

$$\rho = \frac{Cov(X, Y)}{\sigma_X \sigma_Y} = \frac{\sigma_{XY}}{\sigma_X \sigma_Y}$$

is called the correlation coefficient of *X* and *Y*.

A commonly used formula to calculate covariance:

$$Cov(X, Y) = E[(X - \mu_X)(Y - \mu_Y)]$$

$$= E(XY - \mu_X Y - \mu_Y X + \mu_X \mu_Y)$$

$$= E(XY) - \mu_X E(Y) - \mu_Y E(X) + \mu_X \mu_Y$$

$$= E(XY) - \mu_X \mu_Y$$

**Example**: Let *X* and *Y* have the joint PMF

$$f(x,y) = \frac{x+2y}{18}$$
,  $x = 1,2$  and  $y = 1,2$ 

What is the correlation coefficient of *X* and *Y*?

The marginal PMF are respectively

$$f_X(x) = \sum_{y=1}^{2} \frac{x+2y}{18} = \frac{x+3}{9}$$
$$f_Y(y) = \sum_{y=1}^{2} \frac{x+2y}{18} = \frac{3+4y}{18}$$

The mean and variance of X are

$$\mu_X = \sum_{x=1}^2 x \frac{x+3}{9} = (1)\frac{4}{9} + (2)\frac{5}{9} = \frac{14}{9}$$

$$\sigma_X^2 = E(X^2) - \mu_X^2 = \sum_{x=1}^2 x^2 \frac{x+3}{9} - \left(\frac{14}{9}\right)^2 = \frac{20}{81}$$

Similarly, we get the mean and variance of Y

$$\mu_{Y} = \frac{29}{18} \ \sigma_{Y}^{2} = \frac{77}{324}$$

The covariance of X and Y

$$Cov(X, Y) = \sum_{x=1}^{2} \sum_{y=1}^{2} xy \frac{x+2y}{18} - \frac{14}{9} \frac{29}{18}$$

$$= (1)(1) \frac{3}{18} + (2)(1) \frac{4}{18} + (1)(2) \frac{5}{18} + (2)(2) \frac{6}{18} - \frac{14}{9} \frac{29}{18}$$

$$= -\frac{1}{162}$$

$$\rho = \frac{Cov(X, Y)}{\sigma_X \sigma_Y} = -0.025$$

**Proposition**: If *X* and *Y* are independent, Cov(X, Y) = 0.

$$E(XY) = \sum_{S_X} \sum_{S_Y} xyf(x, y)$$

$$= \sum_{S_X} \sum_{S_Y} xyf_X(x)f_Y(y)$$

$$= \sum_{S_X} xf_X(x) \sum_{S_Y} yf_Y(y)$$

$$= \mu_X \mu_Y$$

Thus, we have

$$Cov(X, Y) = E(XY) - \mu_X \mu_Y = 0$$

If Cov(X, Y) = 0, are X and Y necessarily independent?

**Example**: Let *X* and *Y* have the joint PMF

$$f(x,y) = \frac{1}{3}, \quad (x,y) = (0,1), (1,0), (2,1).$$

It is easy to get the marginal PMF of X and Y:

$$f_X(x) = \frac{1}{3}, \ x = 0, 1, 2; \quad f_Y(y) = \begin{cases} \frac{1}{3}, \ y = 0 \\ \frac{2}{3}, \ y = 1 \end{cases}$$

Thus,  $\mu_X = 1$  amd  $\mu_Y = 2/3$ . Then

$$Cov(X, Y) = E(XY) - \mu_X \mu_Y$$

$$= (0)(1)\frac{1}{3} + (1)(0)\frac{1}{3} + (2)(1)\frac{1}{3} - (1)\frac{2}{3}$$

$$= 0$$

It is obvious that  $f(x, y) \neq f_X(x)f_Y(y)$ . Thus, X and Y are dependent.

## **Conditional distributions**

Let X and Y have a joint discrete distribution with PMF f(x, y) on space S.

Say the marginal PMF are  $f_X(x)$  and  $f_Y(y)$  respectively. Let event

$$A = \{X = x\}$$
 and event  $B = \{Y = y\}$ . Thus  $A \cap B = \{X = x, Y = y\}$ .

Because  $P(A \cap B) = P(X = x, Y = y) = f(x, y)$  and

 $P(B) = P(Y = y) = f_Y(y)$ , the conditional probability of A given B is

$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{f(x,y)}{f_Y(y)}$$

**Definition**: The conditional probability mass function of X, given that Y = y, is defined by

$$g(x|y) = \frac{f(x,y)}{f_Y(y)}$$

provided that  $f_Y(y) > 0$ 

## **Conditional distributions**

**Example**: Let *X* and *Y* have the joint PMF

$$f(x,y) = \frac{x+y}{21}, \quad x = 1,2,3, \quad y = 1,2.$$

Find the conditional distribution g(x|y).

We first calculate marginal PMF of y:

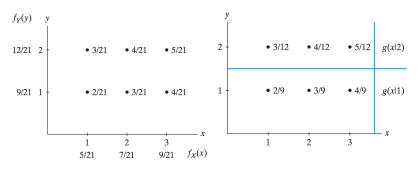
$$f_Y(y) = \sum_{x=1}^3 \frac{x+y}{21} = \frac{y+2}{7}, \quad y = 1, 2$$

Thus, the conditional PMF of X given Y is

$$g(x|y) = \frac{f(x,y)}{f_Y(y)} = \frac{(x+y)/21}{(y+2)/7} = \frac{x+y}{3y+6}$$

## **Conditional distribution**

Similar to conditional probability, we can visualize the joint, marginal, and conditional PMF.



(Graphic illustration of joint, marginal and conditional PMF.)

# **Conditional expectation**

Because conditional PMF is a PMF, we thus can define conditional expectation the same way we define mathematical expectation:

$$E[u(Y)|X=x] = \sum_{y} u(y)g(y|x)$$

Conditional mean and conditional variance are defined by

$$\mu_{Y|X} = E(Y|X) = \sum_{y} yg(y|X)$$
 $\sigma_{Y|X}^2 = E[(Y - \mu_{Y|X})^2|X] = \sum_{y} (y - \mu_{Y|X})^2 g(y|X)$ 

# **Conditional expectation**

**Example**: Let X and Y have a multinomial PMF with parameters n,  $p_X$ , and  $p_Y$ . That is,

$$f(x,y) = \frac{n!}{x!y!(n-x-y)!} p_X^x p_Y^y (1 - p_X - p_Y)^{n-x-y}$$

What is the conditional mean of X given Y?

We know that the marginal distribution of Y is binomial,. i.e.,

$$f_Y(y) = \frac{n!}{y!(n-y)!}p_Y^y(1-p_Y)^{n-y}$$

Thus, the conditional PMF of X given Y is

$$g(x|y) = \frac{f(x,y)}{f_Y(y)} = \frac{(n-y)!}{x!(n-y-x)!} (\frac{p_X}{1-p_Y})^x (1-\frac{p_X}{1-p_Y})^{n-y-x}$$

This is a binomial distribution with parameters n-y and  $\frac{\rho_X}{1-\rho_Y}$ . Thus, the conditional mean is  $(n-y)\frac{\rho_X}{1-\rho_Y}$ .

The idea of joint distributions of discrete random variables can be extended to that of continuous random variables. The **joint probability density function** of two continuous random variables is an integrable function f(x, y) such that

- $f(x,y) \ge 0$ , where f(x,y) = 0 when (x,y) is not in the space of X and Y;
- $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y) dx dy = 1;$
- $P(X, Y) \in A = \int \int_A f(x, y) dx dy$

The marginal probability density function of X and Y are given by

$$f_X(x) = \int_{-\infty}^{\infty} f(x, y) dy, \quad x \in S_X;$$
  
 $f_Y(y) = \int_{-\infty}^{\infty} f(x, y) dx, \quad y \in S_Y;$ 

X and Y are **independent** if and only if  $f(x, y) = f_X(x)f_Y(y)$ 

The correlation coefficient of two continuous random variables X and Y is defined in the same way as the discrete random variables as

$$\rho = \frac{Cov(X, Y)}{\sigma_X \sigma_Y} = \frac{\sigma_{XY}}{\sigma_X \sigma_Y}$$

The Conditional probability density function of X, given that Y = y, is

$$f(x|y) = \frac{f(x,y)}{f_Y(y)},$$

provided that  $f_Y(y) > 0$ .

**Example**: Let X and Y have the joint PDF

$$f(x,y) = 1$$
,  $x \leqslant y \leqslant x + 1$ ,  $0 \leqslant x \leqslant 1$ .

Find the marginal PDF and the correlation coefficient of X and Y.

The marginal PDFs of X and Y are

$$f_X(x) = \int_x^{x+1} 1 \, dy = 1, \quad 0 \leqslant x \leqslant 1$$

$$f_Y(y) = \begin{cases} \int_0^y 1 \, dx = y, \quad 0 \leqslant y \leqslant 1, \\ \int_{y-1}^1 1 \, dx = 2 - y, \quad 1 \leqslant y \leqslant 2. \end{cases}$$

The mean and variance of X and Y are

$$\mu_X = \int_0^1 x \cdot 1 dx = \frac{1}{2}$$

$$\mu_Y = \int_0^1 y \cdot y dy + \int_1^2 y \cdot (2 - y) dy = \frac{1}{3} + \frac{2}{3} = 1$$

$$E(X^2) = \int_0^1 x^2 \cdot 1 dx = \frac{1}{3}$$

$$E(Y^2) = \int_0^1 y^2 \cdot y dy + \int_1^2 y^2 \cdot (2 - y) dy = \frac{7}{6}$$

$$E(XY) = \int_0^1 \int_x^{x+1} xy \cdot 1 dy dx = \int_0^1 \frac{1}{2} x(2x+1) dx = \frac{7}{12}$$

$$\sigma_X^2 = \frac{1}{3} - \left(\frac{1}{2}\right)^2 = \frac{1}{12}$$

$$\sigma_Y^2 = \frac{7}{6} - 1^2 = \frac{1}{6}$$

$$\sigma_{XY} = \frac{7}{12} - \left(\frac{1}{2}\right)(1) = \frac{1}{12}$$

Therefore, the correlation coefficient is

$$\rho = \frac{\sigma_{XY}}{\sigma_X \sigma_Y} = \frac{1/12}{\sqrt{(1/12)(1/6)}} = \frac{\sqrt{2}}{2}$$

A very commonly used multivariate distribution is the multivariate normal distribution. Random variables *X* and *Y* have a bivariate normal distribution if its joint PDF is

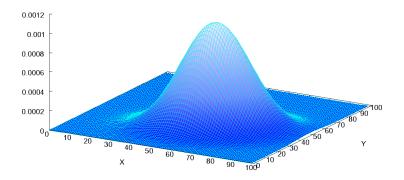
$$f(x,y) = \frac{1}{2\pi\sigma_X\sigma_Y\sqrt{1-\rho^2}}\exp\Big[-\frac{q(x,y)}{2}\Big],$$

where

$$q(x,y) = \frac{1}{1-\rho^2} \left[ \left( \frac{x-\mu_X}{\sigma_X} \right)^2 - 2\rho \left( \frac{x-\mu_X}{\sigma_X} \right) \left( \frac{y-\mu_Y}{\sigma_Y} \right) + \left( \frac{y-\mu_Y}{\sigma_Y} \right)^2 \right]$$

Here,  $\mu_X$  and  $\mu_Y$  are the mean of X and Y,  $\sigma_X$  and  $\sigma_Y$  are the standard deviation of X and Y, and  $\rho$  is the correlation coefficient.

A bivariate normal distribution has a typical PDF figure as follows.



If random variables X and Y have a bivariate normal distribution, then the marginal distribution of X and Y are both normal.

$$q(x,y) = \frac{1}{1-\rho^2} \left[ \left( \frac{x-\mu_X}{\sigma_X} \right)^2 - 2\rho \left( \frac{x-\mu_X}{\sigma_X} \right) \left( \frac{y-\mu_Y}{\sigma_Y} \right) + \left( \frac{y-\mu_Y}{\sigma_Y} \right)^2 \right]$$

$$= \frac{1}{1-\rho^2} \left[ \left( \frac{x-\mu_X}{\sigma_X} - \rho \frac{y-\mu_Y}{\sigma_Y} \right)^2 + (1-\rho^2) \left( \frac{y-\mu_Y}{\sigma_Y} \right)^2 \right]$$

$$= \frac{1}{\sigma_X^2 (1-\rho^2)} \left( x - \mu_X - \rho \frac{\sigma_X}{\sigma_Y} (y-\mu_Y) \right)^2 + \left( \frac{y-\mu_Y}{\sigma_Y} \right)^2$$

Thus, the marginal distribution of Y is

$$f_{Y}(y) = \int_{-\infty}^{\infty} f(x,y) dx = \int_{-\infty}^{\infty} \frac{1}{2\pi\sigma_{X}\sigma_{Y}\sqrt{1-\rho^{2}}} \exp\left[-\frac{q(x,y)}{2}\right] dx$$

$$= \frac{1}{2\pi\sigma_{X}\sigma_{Y}\sqrt{1-\rho^{2}}} \exp\left[-\frac{(y-\mu_{Y})^{2}}{2\sigma_{Y}^{2}}\right]$$

$$\int_{-\infty}^{\infty} \exp\left[-\frac{1}{2\sigma_{X}^{2}(1-\rho^{2})}\left(x-\mu_{X}-\rho\frac{\sigma_{X}}{\sigma_{Y}}(y-\mu_{Y})\right)^{2}\right] dx$$

$$= \frac{1}{2\pi\sigma_{X}\sigma_{Y}\sqrt{1-\rho^{2}}} \exp\left[-\frac{(y-\mu_{Y})^{2}}{2\sigma_{Y}^{2}}\right] (\sigma_{X}\sqrt{2\pi}\sqrt{1-\rho^{2}})$$

$$= \frac{1}{\sigma_{Y}\sqrt{2\pi}} \exp\left[-\frac{(y-\mu_{Y})^{2}}{2\sigma_{Y}^{2}}\right]$$

Thus, the marginal distribution of Y is  $N(\mu_Y, \sigma_Y^2)$ . Using the procedure, it is obvious that  $X \sim N(\mu_X, \sigma_X^2)$ .

If If random variables X and Y have a bivariate normal distribution, then the conditional distribution of X given Y is normal.

The joint PDF is

$$f(x,y) = \frac{1}{2\pi\sigma_X\sigma_Y\sqrt{1-\rho^2}}\exp\Big[-\frac{q(x,y)}{2}\Big],$$

where

$$q(x,y) = \frac{1}{\sigma_X^2(1-\rho^2)} \left(x - \mu_X - \rho \frac{\sigma_X}{\sigma_Y}(y - \mu_Y)\right)^2 + \left(\frac{y - \mu_Y}{\sigma_Y}\right)^2$$

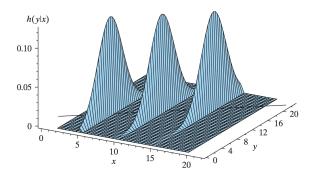
The marginal PDF of Y is

$$f_Y(y) = \frac{1}{\sigma_Y \sqrt{2\pi}} \exp\left[-\frac{(y - \mu_Y)^2}{2\sigma_Y^2}\right]$$

The conditional distribution of X given Y is thus

$$g(x|y) = \frac{f(x,y)}{f_Y(y)} = \frac{1}{\sigma_X \sqrt{2\pi} \sqrt{1 - \rho^2}} \exp\left[-\frac{[x - \mu_X - \rho(\sigma_X/\sigma_Y)(y - \mu_Y)]^2}{2\sigma_X^2(1 - \rho^2)}\right]$$

Thus, g(x|y) is  $N(\mu_X + \rho \frac{\sigma_X}{\sigma_Y}(y - \mu_Y), (1 - \rho^2)\sigma_X^2)$ .



(Illustration of conditional distribution of a bivariate normal distribution)

We can extend the case of bivariate normal distribution to more than two variables. For more k variables, we write the PDF of a multivariate normal distribution in matrix notation:

$$f(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^k |\Sigma|}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu)^T \Sigma^{-1}(\mathbf{x} - \mu)\right)$$

where  ${\bf x}$  and  ${\bf \mu}$  are column vectors of the variables and its means,  ${\bf \Sigma}$  is the  $k \times k$  variance covariance matrix, i.e.,

$$\mathbf{X} = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_k \end{bmatrix}; \quad \boldsymbol{\mu} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_k \end{bmatrix}; \quad \boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{X_1}^2 & \sigma_{X_1 X_2} & \cdots & \sigma_{X_1 X_k} \\ \sigma_{X_1 X_1} & \sigma_{X_2}^2 & \cdots & \sigma_{X_2 X_k} \\ \vdots & \vdots & & \vdots \\ \sigma_{X_k X_1} & \sigma_{X_k X_2}^2 & \cdots & \sigma_{X_k}^2 \end{bmatrix}$$